



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:43 PM GMT

PDB ID : 4J2O  
Title : Crystal structure of NADP-bound WbjB from *A. baumannii* community strain D1279779  
Authors : Shah, B.S.; Harrop, S.J.; Paulsen, I.T.; Mabbutt, B.C.  
Deposited on : 2013-02-05  
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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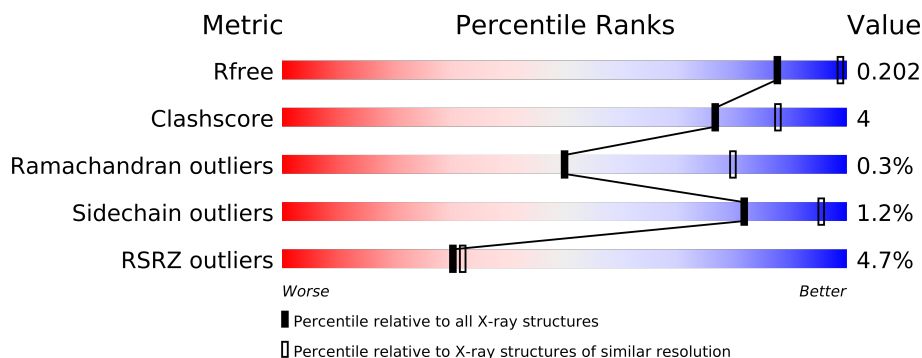
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 2.65 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))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	

## 2 Entry composition i

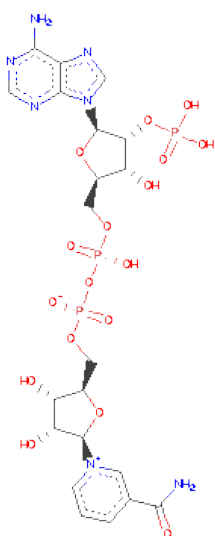
There are 3 unique types of molecules in this entry. The entry contains 15097 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UDP-N-acetylglucosamine4,6-dehydratase/5-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	Se	0	0	0
			2480	1570	431	462	3	14			
1	B	313	Total	C	N	O	S	Se	0	0	0
			2468	1565	425	462	3	13			
1	C	316	Total	C	N	O	S	Se	0	0	0
			2491	1576	434	464	3	14			
1	D	312	Total	C	N	O	S	Se	0	0	0
			2457	1556	428	456	3	14			
1	E	303	Total	C	N	O	S	Se	0	0	0
			2389	1516	413	444	3	13			
1	F	300	Total	C	N	O	S	Se	0	0	0
			2364	1501	408	439	3	13			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

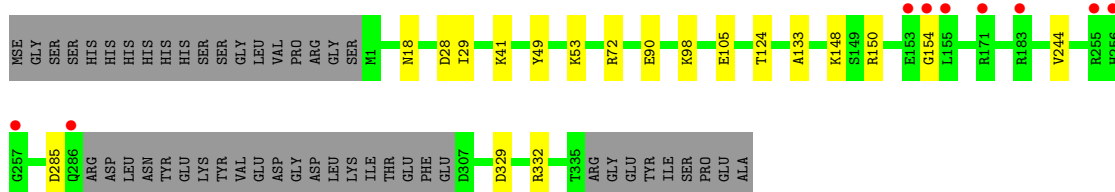
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	38	Total	O	0	0
			38	38		
3	C	25	Total	O	0	0
			25	25		
3	D	22	Total	O	0	0
			22	22		
3	E	22	Total	O	0	0
			22	22		
3	F	15	Total	O	0	0
			15	15		

### 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.

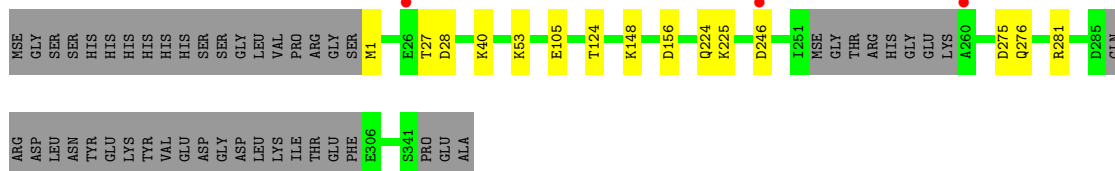
- Molecule 1: UDP-N-acetylglucosamine4,6-dehydratase/5-epimerase

Chain A: 



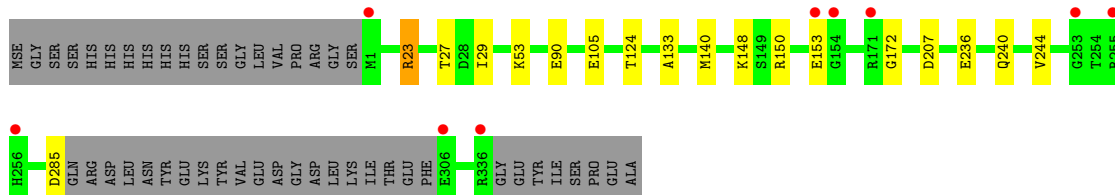
- Molecule 1: UDP-N-acetylglucosamine4,6-dehydratase/5-epimerase

Chain B: 



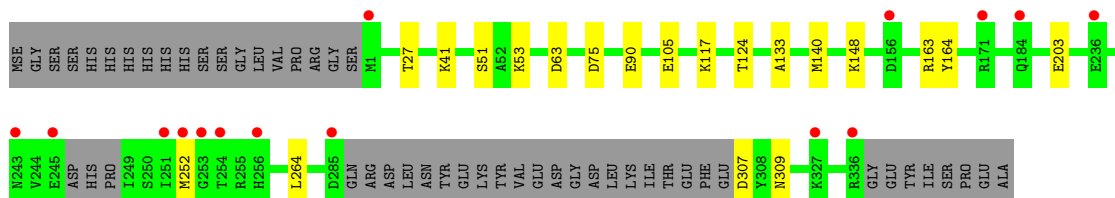
- Molecule 1: UDP-N-acetylglucosamine4,6-dehydratase/5-epimerase

Chain C: 



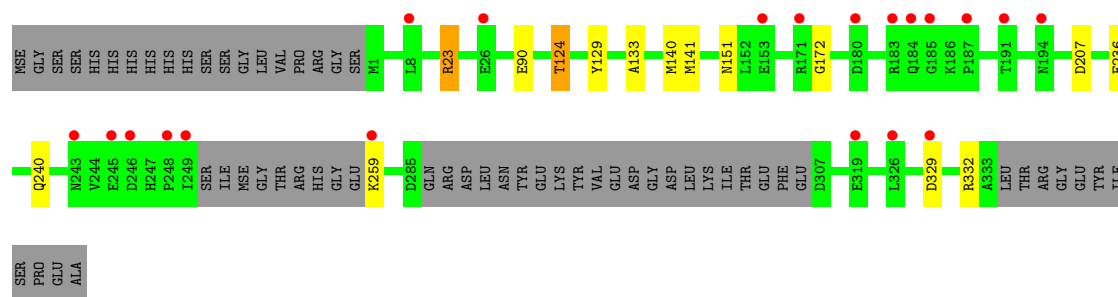
- Molecule 1: UDP-N-acetylglucosamine4,6-dehydratase/5-epimerase

Chain D: 



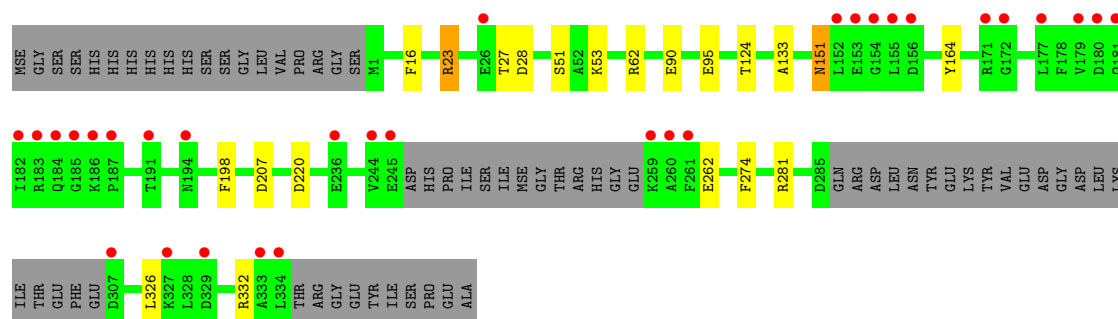
• Molecule 1: UDP-N-acetylglucosamine4,6-dehydratase/5-epimerase

Chain E:



• Molecule 1: UDP-N-acetylglucosamine4,6-dehydratase/5-epimerase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.93Å 114.54Å 215.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 2.65 24.86 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.86-2.65) 96.8 (24.86-2.65)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.160 , 0.202 0.161 , 0.202	Depositor DCC
$R_{free}$ test set	2320 reflections (3.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 75313 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.52	0/2507	0.65	0/3356
1	B	0.54	0/2495	0.67	0/3342
1	C	0.48	0/2518	0.64	0/3370
1	D	0.47	0/2481	0.62	0/3317
1	E	0.45	0/2415	0.58	0/3233
1	F	0.44	0/2388	0.59	0/3195
All	All	0.48	0/14804	0.63	0/19813

There are no bond length outliers.

There are no bond angle outliers.

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	A	2480	0	0	11	0
1	B	2468	0	0	9	0
1	C	2491	0	0	7	0
1	D	2457	0	0	11	0
1	E	2389	0	0	6	0
1	F	2364	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
2	E	48	0	25	1	0
2	F	48	0	25	5	0
3	A	38	0	0	2	0
3	B	38	0	0	4	0
3	C	25	0	0	0	0
3	D	22	0	0	1	0
3	E	22	0	0	0	0
3	F	15	0	0	1	0
All	All	15097	0	150	57	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (57) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:27:THR:O	1:C:53:LYS:NZ	2.18	0.77
1:B:27:THR:O	1:B:53:LYS:NZ	2.18	0.77
1:B:1:MSE:N	3:B:518:HOH:O	2.23	0.70
1:E:23:ARG:NH2	1:E:207:ASP:OD1	2.25	0.69
1:C:23:ARG:NH1	1:C:207:ASP:OD1	2.25	0.69
1:B:281:ARG:NH1	3:B:536:HOH:O	2.27	0.68
1:A:150:ARG:NH2	1:A:285:ASP:O	2.27	0.67
1:C:236:GLU:OE2	1:C:240:GLN:NE2	2.29	0.66
1:F:164:TYR:O	2:F:400:NAP:H5N	1.96	0.65
1:C:90:GLU:OE2	1:C:133:ALA:N	2.35	0.60
1:B:225:LYS:NZ	1:B:275:ASP:OD2	2.36	0.59
1:F:27:THR:O	1:F:53:LYS:NZ	2.36	0.58
1:D:105:GLU:OE2	1:D:148:LYS:NZ	2.38	0.57
1:A:329:ASP:OD1	1:A:332:ARG:NH1	2.38	0.56
1:A:72:ARG:NH1	3:A:511:HOH:O	2.40	0.55
1:F:23:ARG:NH2	1:F:207:ASP:OD1	2.40	0.55
1:F:62:ARG:NH2	1:F:95:GLU:OE1	2.41	0.54
1:D:307:ASP:OD1	1:D:309:ASN:ND2	2.41	0.54
1:A:105:GLU:OE2	1:A:148:LYS:NZ	2.41	0.53
1:D:164:TYR:O	2:D:400:NAP:H5N	2.08	0.53
1:C:105:GLU:OE2	1:C:148:LYS:NZ	2.41	0.53
1:E:90:GLU:OE2	1:E:133:ALA:N	2.42	0.53
1:D:90:GLU:OE2	1:D:133:ALA:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:ASP:N	1:A:28:ASP:OD1	2.44	0.51
1:B:105:GLU:OE1	1:B:148:LYS:NZ	2.44	0.50
1:F:28:ASP:N	1:F:28:ASP:OD1	2.46	0.49
1:F:151:ASN:ND2	3:F:511:HOH:O	2.44	0.49
1:F:16:PHE:N	2:F:400:NAP:O2N	2.45	0.49
1:F:220:ASP:OD2	1:F:281:ARG:NE	2.46	0.49
2:F:400:NAP:H2N	2:F:400:NAP:H52N	1.96	0.47
1:D:75:ASP:OD1	1:D:117:LYS:NZ	2.47	0.47
1:C:150:ARG:NH2	1:C:285:ASP:O	2.48	0.47
1:A:18:ASN:OD1	1:A:49:TYR:OH	2.33	0.46
1:A:90:GLU:OE2	1:A:133:ALA:N	2.49	0.46
1:A:154:GLY:N	3:A:501:HOH:O	2.48	0.46
1:F:198:PHE:N	1:F:262:GLU:OE2	2.49	0.46
1:D:41:LYS:NZ	3:D:522:HOH:O	2.49	0.46
1:A:41:LYS:NZ	2:A:400:NAP:O3X	2.50	0.45
1:D:27:THR:O	1:D:53:LYS:NZ	2.49	0.45
1:B:28:ASP:N	1:B:28:ASP:OD2	2.50	0.45
1:F:326:LEU:O	1:F:332:ARG:NE	2.50	0.44
1:B:224:GLN:N	3:B:528:HOH:O	2.51	0.44
1:B:40:LYS:NZ	2:F:400:NAP:O2A	2.51	0.44
1:F:90:GLU:OE2	1:F:133:ALA:N	2.51	0.43
1:B:276:GLN:NE2	3:B:535:HOH:O	2.51	0.43
1:D:163:ARG:NH1	1:D:264:LEU:O	2.52	0.43
1:E:124:THR:CB	2:E:400:NAP:H6N	2.48	0.43
1:D:203:GLU:N	1:D:203:GLU:OE1	2.52	0.42
1:E:329:ASP:OD1	1:E:332:ARG:NH1	2.52	0.42
1:A:29:ILE:O	1:A:53:LYS:NZ	2.52	0.42
1:C:29:ILE:O	1:C:53:LYS:NZ	2.52	0.42
1:F:274:PHE:CD2	1:F:281:ARG:NH1	2.88	0.42
1:D:252:MSE:N	1:D:252:MSE:SE	3.03	0.42
1:E:236:GLU:OE2	1:E:240:GLN:NE2	2.52	0.41
1:E:129:TYR:O	1:E:259:LYS:NZ	2.54	0.41
2:F:400:NAP:H2N	2:F:400:NAP:H2D	1.87	0.40
1:A:98:LYS:NZ	1:D:63:ASP:OD2	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/363 (86%)	303 (97%)	8 (3%)	0	100	100
1	B	307/363 (85%)	300 (98%)	6 (2%)	1 (0%)	50	80
1	C	312/363 (86%)	304 (97%)	7 (2%)	1 (0%)	50	80
1	D	306/363 (84%)	299 (98%)	7 (2%)	0	100	100
1	E	297/363 (82%)	289 (97%)	6 (2%)	2 (1%)	30	59
1	F	294/363 (81%)	288 (98%)	5 (2%)	1 (0%)	50	80
All	All	1827/2178 (84%)	1783 (98%)	39 (2%)	5 (0%)	50	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	GLY
1	E	151	ASN
1	E	172	GLY
1	F	151	ASN
1	B	246	ASP

### 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	A	269/296 (91%)	267 (99%)	2 (1%)	91	98
1	B	268/296 (90%)	266 (99%)	2 (1%)	91	98
1	C	270/296 (91%)	265 (98%)	5 (2%)	69	91
1	D	266/296 (90%)	263 (99%)	3 (1%)	84	96
1	E	259/296 (88%)	255 (98%)	4 (2%)	76	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	256/296 (86%)	253 (99%)	3 (1%)	82	95
All	All	1588/1776 (89%)	1569 (99%)	19 (1%)	82	95

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	244	VAL
1	B	124	THR
1	B	156	ASP
1	C	23	ARG
1	C	124	THR
1	C	140	MSE
1	C	153	GLU
1	C	244	VAL
1	D	51	SER
1	D	124	THR
1	D	140	MSE
1	E	23	ARG
1	E	124	THR
1	E	140	MSE
1	E	141	MSE
1	F	23	ARG
1	F	51	SER
1	F	124	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

6 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	A	400	-	52,52,52	2.43	17 (32%)	80,80,80	2.11	18 (22%)
2	NAP	B	400	-	52,52,52	2.42	18 (34%)	80,80,80	2.25	19 (23%)
2	NAP	C	400	-	52,52,52	2.45	17 (32%)	80,80,80	2.29	18 (22%)
2	NAP	D	400	-	52,52,52	2.37	16 (30%)	80,80,80	2.24	15 (18%)
2	NAP	E	400	-	52,52,52	2.39	17 (32%)	80,80,80	2.17	17 (21%)
2	NAP	F	400	-	52,52,52	2.39	18 (34%)	80,80,80	2.27	14 (17%)

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	A	400	-	-	0/35/67/67	0/3/5/5
2	NAP	B	400	-	-	0/35/67/67	0/3/5/5
2	NAP	C	400	-	-	0/35/67/67	0/3/5/5
2	NAP	D	400	-	-	0/35/67/67	0/3/5/5
2	NAP	E	400	-	-	0/35/67/67	0/3/5/5
2	NAP	F	400	-	-	0/35/67/67	0/3/5/5

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	NAP	C2D-C1D	-6.71	1.43	1.53
2	D	400	NAP	C2D-C1D	-6.59	1.44	1.53
2	E	400	NAP	C2N-N1N	6.41	1.43	1.35
2	B	400	NAP	C2N-N1N	6.16	1.43	1.35
2	D	400	NAP	C2N-N1N	6.13	1.43	1.35
2	B	400	NAP	C2D-C1D	-6.10	1.44	1.53
2	C	400	NAP	C2D-C1D	-6.09	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NAP	C2D-C1D	-6.06	1.44	1.53
2	F	400	NAP	C2N-N1N	5.99	1.43	1.35
2	C	400	NAP	C2N-N1N	5.91	1.42	1.35
2	E	400	NAP	C2D-C1D	-5.77	1.45	1.53
2	A	400	NAP	C2N-N1N	5.69	1.42	1.35
2	C	400	NAP	O4D-C1D	5.19	1.49	1.41
2	A	400	NAP	C4A-N9A	5.17	1.45	1.37
2	F	400	NAP	O4D-C1D	5.16	1.49	1.41
2	C	400	NAP	C4A-N9A	4.99	1.45	1.37
2	E	400	NAP	O4D-C1D	4.98	1.49	1.41
2	B	400	NAP	O4D-C1D	4.95	1.49	1.41
2	E	400	NAP	C4A-N9A	4.84	1.44	1.37
2	A	400	NAP	O4D-C1D	4.78	1.48	1.41
2	A	400	NAP	C7N-N7N	4.54	1.43	1.33
2	D	400	NAP	C3B-C2B	-4.52	1.42	1.53
2	B	400	NAP	C7N-N7N	4.48	1.43	1.33
2	B	400	NAP	C4A-N9A	4.44	1.44	1.37
2	C	400	NAP	C7N-N7N	4.42	1.42	1.33
2	B	400	NAP	C2B-C1B	-4.41	1.45	1.52
2	D	400	NAP	C4A-N9A	4.37	1.44	1.37
2	F	400	NAP	C7N-N7N	4.36	1.42	1.33
2	D	400	NAP	C7N-N7N	4.35	1.42	1.33
2	E	400	NAP	C3B-C2B	-4.29	1.43	1.53
2	F	400	NAP	C3B-C2B	-4.28	1.43	1.53
2	E	400	NAP	C7N-N7N	4.26	1.42	1.33
2	C	400	NAP	C2B-C1B	-4.17	1.45	1.52
2	D	400	NAP	O4D-C1D	4.15	1.47	1.41
2	D	400	NAP	C2B-C1B	-4.12	1.45	1.52
2	B	400	NAP	C3B-C2B	-4.08	1.43	1.53
2	C	400	NAP	C3B-C2B	-4.02	1.43	1.53
2	A	400	NAP	C2A-N3A	4.00	1.40	1.32
2	B	400	NAP	C2A-N3A	3.98	1.40	1.32
2	A	400	NAP	C3B-C2B	-3.97	1.43	1.53
2	E	400	NAP	C2A-N3A	3.95	1.40	1.32
2	F	400	NAP	C2B-C1B	-3.89	1.45	1.52
2	C	400	NAP	C2A-N3A	3.83	1.39	1.32
2	E	400	NAP	C2B-C1B	-3.81	1.46	1.52
2	A	400	NAP	C2B-C1B	-3.76	1.46	1.52
2	C	400	NAP	C6A-N6A	3.72	1.47	1.35
2	D	400	NAP	C6A-N6A	3.71	1.47	1.35
2	E	400	NAP	C6A-N6A	3.68	1.46	1.35
2	A	400	NAP	C6A-N6A	3.67	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	NAP	C3D-C4D	-3.66	1.42	1.53
2	F	400	NAP	C4A-N9A	3.63	1.43	1.37
2	F	400	NAP	C2A-N3A	3.60	1.39	1.32
2	A	400	NAP	C3D-C4D	-3.58	1.43	1.53
2	A	400	NAP	C2D-C3D	-3.58	1.43	1.53
2	A	400	NAP	C1B-N9A	-3.54	1.37	1.48
2	C	400	NAP	C2D-C3D	-3.45	1.43	1.53
2	D	400	NAP	C2A-N3A	3.43	1.38	1.32
2	E	400	NAP	O4B-C1B	3.41	1.46	1.41
2	C	400	NAP	C3N-C7N	3.40	1.56	1.50
2	F	400	NAP	C6A-N6A	3.35	1.45	1.35
2	D	400	NAP	C1B-N9A	-3.33	1.38	1.48
2	E	400	NAP	C3D-C4D	-3.32	1.43	1.53
2	D	400	NAP	C2D-C3D	-3.30	1.44	1.53
2	B	400	NAP	C3N-C7N	3.27	1.56	1.50
2	F	400	NAP	C1B-N9A	-3.27	1.38	1.48
2	E	400	NAP	C2D-C3D	-3.26	1.44	1.53
2	B	400	NAP	C2D-C3D	-3.25	1.44	1.53
2	B	400	NAP	C6A-N6A	3.24	1.45	1.35
2	B	400	NAP	C1B-N9A	-3.24	1.38	1.48
2	F	400	NAP	O4B-C1B	3.23	1.46	1.41
2	B	400	NAP	C3D-C4D	-3.23	1.44	1.53
2	C	400	NAP	C3D-C4D	-3.20	1.44	1.53
2	F	400	NAP	C2D-C3D	-3.20	1.44	1.53
2	D	400	NAP	O4B-C1B	3.18	1.46	1.41
2	D	400	NAP	C3D-C4D	-3.12	1.44	1.53
2	C	400	NAP	C1B-N9A	-3.05	1.39	1.48
2	A	400	NAP	O4B-C1B	3.04	1.46	1.41
2	C	400	NAP	O4B-C1B	3.01	1.46	1.41
2	C	400	NAP	C4A-N3A	3.01	1.40	1.35
2	A	400	NAP	C3N-C7N	2.95	1.55	1.50
2	D	400	NAP	C1D-N1N	-2.85	1.39	1.48
2	A	400	NAP	C3B-C4B	-2.84	1.45	1.53
2	C	400	NAP	C3B-C4B	-2.83	1.45	1.53
2	F	400	NAP	C1D-N1N	-2.82	1.39	1.48
2	E	400	NAP	C3N-C7N	2.82	1.55	1.50
2	E	400	NAP	C1B-N9A	-2.78	1.40	1.48
2	E	400	NAP	C3B-C4B	-2.73	1.45	1.53
2	B	400	NAP	C3B-C4B	-2.70	1.45	1.53
2	D	400	NAP	C3B-C4B	-2.64	1.45	1.53
2	B	400	NAP	O4B-C1B	2.57	1.45	1.41
2	F	400	NAP	C3N-C7N	2.56	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	NAP	C4A-N3A	2.50	1.39	1.35
2	E	400	NAP	C4A-N3A	2.44	1.39	1.35
2	A	400	NAP	C1D-N1N	-2.44	1.41	1.48
2	F	400	NAP	C3B-C4B	-2.42	1.46	1.53
2	B	400	NAP	C1D-N1N	-2.41	1.41	1.48
2	D	400	NAP	C3N-C7N	2.35	1.54	1.50
2	C	400	NAP	C1D-N1N	-2.30	1.41	1.48
2	F	400	NAP	PA-O3	-2.11	1.56	1.59
2	F	400	NAP	C4A-N3A	2.05	1.38	1.35
2	B	400	NAP	C2A-N1A	2.04	1.37	1.33
2	E	400	NAP	C1D-N1N	-2.02	1.42	1.48
2	A	400	NAP	C8A-N9A	2.01	1.39	1.36

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	NAP	N3A-C2A-N1A	-11.07	119.45	128.71
2	C	400	NAP	N3A-C2A-N1A	-10.97	119.54	128.71
2	D	400	NAP	N3A-C2A-N1A	-10.91	119.59	128.71
2	B	400	NAP	N3A-C2A-N1A	-10.67	119.79	128.71
2	E	400	NAP	N3A-C2A-N1A	-8.98	121.20	128.71
2	F	400	NAP	C4B-O4B-C1B	-8.78	100.21	109.75
2	A	400	NAP	N3A-C2A-N1A	-8.54	121.57	128.71
2	D	400	NAP	C4B-O4B-C1B	-7.63	101.46	109.75
2	C	400	NAP	C4B-O4B-C1B	-7.12	102.02	109.75
2	D	400	NAP	C4D-O4D-C1D	-6.56	102.63	109.75
2	E	400	NAP	O2N-PN-O1N	-6.51	99.09	118.72
2	B	400	NAP	C4B-O4B-C1B	-6.48	102.70	109.75
2	A	400	NAP	O2N-PN-O1N	-6.45	99.27	118.72
2	F	400	NAP	C4D-O4D-C1D	-6.34	102.86	109.75
2	A	400	NAP	C4B-O4B-C1B	-6.08	103.15	109.75
2	E	400	NAP	C4B-O4B-C1B	-5.84	103.40	109.75
2	B	400	NAP	O2N-PN-O1N	-5.77	101.31	118.72
2	C	400	NAP	N3A-C4A-N9A	5.72	135.76	125.43
2	E	400	NAP	N3A-C4A-N9A	5.45	135.27	125.43
2	C	400	NAP	O2N-PN-O1N	-5.44	102.31	118.72
2	B	400	NAP	N3A-C4A-N9A	5.32	135.04	125.43
2	F	400	NAP	N3A-C4A-N9A	5.15	134.74	125.43
2	A	400	NAP	N3A-C4A-N9A	5.15	134.74	125.43
2	D	400	NAP	N3A-C4A-N9A	5.11	134.65	125.43
2	C	400	NAP	C3D-C2D-C1D	4.96	108.68	100.91
2	D	400	NAP	O2N-PN-O1N	-4.83	104.14	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	NAP	O4D-C1D-N1N	4.80	112.86	107.95
2	B	400	NAP	C3D-C2D-C1D	4.79	108.41	100.91
2	E	400	NAP	C3D-C2D-C1D	4.74	108.33	100.91
2	F	400	NAP	O2N-PN-O1N	-4.71	104.50	118.72
2	A	400	NAP	C4D-O4D-C1D	-4.67	104.68	109.75
2	A	400	NAP	O4B-C1B-N9A	-4.57	104.19	108.44
2	A	400	NAP	C3D-C2D-C1D	4.54	108.01	100.91
2	B	400	NAP	O4D-C1D-N1N	4.49	112.54	107.95
2	E	400	NAP	C4D-O4D-C1D	-4.35	105.02	109.75
2	B	400	NAP	C4D-O4D-C1D	-4.08	105.31	109.75
2	F	400	NAP	O4D-C1D-N1N	3.93	111.97	107.95
2	D	400	NAP	O4D-C1D-N1N	3.92	111.96	107.95
2	C	400	NAP	C4D-O4D-C1D	-3.68	105.75	109.75
2	D	400	NAP	C3D-C2D-C1D	3.46	106.32	100.91
2	B	400	NAP	C3N-C7N-N7N	3.44	121.68	117.77
2	F	400	NAP	PN-O3-PA	-3.41	118.32	132.95
2	C	400	NAP	C3N-C7N-N7N	3.35	121.58	117.77
2	E	400	NAP	C6N-N1N-C2N	-3.34	118.27	122.04
2	B	400	NAP	O2N-PN-O3	3.33	117.77	108.79
2	B	400	NAP	C2D-C1D-N1N	-3.28	108.31	113.86
2	E	400	NAP	C3N-C7N-N7N	3.15	121.36	117.77
2	C	400	NAP	C2D-C3D-C4D	3.14	108.92	102.65
2	C	400	NAP	O4D-C1D-N1N	2.99	111.00	107.95
2	E	400	NAP	C2D-C3D-C4D	2.93	108.48	102.65
2	E	400	NAP	O7N-C7N-N7N	-2.92	118.38	122.59
2	C	400	NAP	O7N-C7N-N7N	-2.85	118.48	122.59
2	A	400	NAP	C6N-N1N-C2N	-2.82	118.85	122.04
2	A	400	NAP	C5A-C4A-N3A	-2.81	119.58	125.70
2	A	400	NAP	C3N-C7N-N7N	2.78	120.94	117.77
2	B	400	NAP	O7N-C7N-N7N	-2.77	118.59	122.59
2	F	400	NAP	C3N-C7N-N7N	2.76	120.91	117.77
2	B	400	NAP	C2D-C3D-C4D	2.76	108.16	102.65
2	C	400	NAP	O2N-PN-O3	2.73	116.15	108.79
2	B	400	NAP	C8A-N9A-C4A	2.70	108.96	106.90
2	E	400	NAP	C5A-C4A-N3A	-2.67	119.88	125.70
2	C	400	NAP	O4B-C1B-N9A	-2.64	105.99	108.44
2	A	400	NAP	PN-O3-PA	-2.59	121.84	132.95
2	F	400	NAP	C8A-N9A-C4A	2.59	108.87	106.90
2	E	400	NAP	O2N-PN-O3	2.54	115.63	108.79
2	C	400	NAP	C5A-C4A-N3A	-2.50	120.26	125.70
2	D	400	NAP	C2D-C1D-N1N	-2.50	109.63	113.86
2	C	400	NAP	C6N-N1N-C2N	-2.49	119.23	122.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	NAP	C5A-C4A-N3A	-2.47	120.33	125.70
2	D	400	NAP	O2N-PN-O3	2.44	115.37	108.79
2	C	400	NAP	C2D-C1D-N1N	-2.44	109.73	113.86
2	B	400	NAP	C5A-C4A-N3A	-2.40	120.47	125.70
2	A	400	NAP	C3B-C2B-C1B	2.34	107.27	102.73
2	B	400	NAP	C6N-N1N-C2N	-2.34	119.40	122.04
2	A	400	NAP	O2N-PN-O3	2.32	115.04	108.79
2	E	400	NAP	C2B-C3B-C4B	2.31	107.43	101.94
2	B	400	NAP	PN-O3-PA	-2.25	123.27	132.95
2	F	400	NAP	O3-PN-O5D	2.24	110.35	101.36
2	E	400	NAP	C3B-C2B-C1B	2.24	107.08	102.73
2	A	400	NAP	O4D-C1D-N1N	2.23	110.23	107.95
2	D	400	NAP	O4D-C4D-C3D	2.21	109.65	105.17
2	C	400	NAP	C5A-C4A-N9A	-2.21	103.98	107.16
2	D	400	NAP	C2B-C3B-C4B	2.20	107.17	101.94
2	A	400	NAP	C2D-C1D-N1N	-2.19	110.15	113.86
2	F	400	NAP	C5A-C4A-N3A	-2.19	120.94	125.70
2	A	400	NAP	O3-PN-O5D	2.17	110.06	101.36
2	D	400	NAP	C2A-N3A-C4A	2.17	120.18	114.01
2	B	400	NAP	C2A-N3A-C4A	2.14	120.10	114.01
2	E	400	NAP	PN-O3-PA	-2.13	123.81	132.95
2	C	400	NAP	C8A-N9A-C4A	2.11	108.51	106.90
2	E	400	NAP	O4D-C4D-C3D	2.10	109.42	105.17
2	D	400	NAP	O2A-PA-O3	2.09	115.08	105.14
2	A	400	NAP	C2D-C3D-C4D	2.05	106.74	102.65
2	F	400	NAP	O7N-C7N-N7N	-2.04	119.64	122.59
2	F	400	NAP	C2A-N3A-C4A	2.04	119.81	114.01
2	F	400	NAP	C5D-C4D-C3D	-2.03	107.09	115.21
2	C	400	NAP	C2A-N3A-C4A	2.02	119.77	114.01
2	A	400	NAP	C2B-C3B-C4B	2.02	106.74	101.94
2	B	400	NAP	C3B-C2B-C1B	2.02	106.66	102.73
2	B	400	NAP	C2B-C3B-C4B	2.02	106.73	101.94
2	D	400	NAP	PN-O3-PA	-2.01	124.31	132.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	315/363 (86%)	-0.23	9 (2%)	49	53	35, 58, 100, 139	0
1	B	313/363 (86%)	-0.30	3 (0%)	79	83	32, 57, 92, 138	0
1	C	316/363 (87%)	-0.17	9 (2%)	50	54	39, 68, 108, 147	0
1	D	312/363 (85%)	-0.08	15 (4%)	29	31	34, 68, 122, 149	0
1	E	303/363 (83%)	0.04	20 (6%)	18	19	40, 71, 152, 189	0
1	F	300/363 (82%)	0.25	31 (10%)	7	6	41, 74, 162, 183	0
All	All	1859/2178 (85%)	-0.08	87 (4%)	30	32	32, 65, 131, 189	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	256	HIS	4.6
1	F	154	GLY	4.6
1	A	256	HIS	4.5
1	E	180	ASP	4.5
1	F	185	GLY	4.3
1	F	333	ALA	4.3
1	F	153	GLU	4.3
1	D	336	ARG	4.0
1	D	1	MSE	4.0
1	E	26	GLU	3.9
1	E	319	GLU	3.7
1	B	246	ASP	3.7
1	D	252	MSE	3.6
1	F	194	ASN	3.6
1	E	246	ASP	3.6
1	F	186	LYS	3.5
1	B	26	GLU	3.5
1	B	260	ALA	3.4
1	F	156	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	259	LYS	3.4
1	A	255	ARG	3.3
1	F	191	THR	3.3
1	C	306	GLU	3.3
1	F	236	GLU	3.3
1	F	171	ARG	3.2
1	F	183	ARG	3.1
1	D	256	HIS	3.1
1	F	187	PRO	3.1
1	C	171	ARG	3.0
1	F	244	VAL	3.0
1	F	180	ASP	3.0
1	A	257	GLY	2.9
1	F	152	LEU	2.9
1	D	285	ASP	2.9
1	F	184	GLN	2.8
1	F	329	ASP	2.8
1	E	171	ARG	2.8
1	A	153	GLU	2.7
1	E	329	ASP	2.7
1	F	327	LYS	2.7
1	F	179	VAL	2.7
1	A	171	ARG	2.7
1	E	243	ASN	2.7
1	E	153	GLU	2.6
1	F	181	GLN	2.6
1	D	254	THR	2.6
1	C	255	ARG	2.6
1	F	260	ALA	2.6
1	C	253	GLY	2.6
1	E	184	GLN	2.6
1	F	155	LEU	2.6
1	A	154	GLY	2.6
1	E	194	ASN	2.6
1	E	183	ARG	2.5
1	C	154	GLY	2.5
1	A	183	ARG	2.5
1	D	243	ASN	2.5
1	A	286	GLN	2.5
1	C	1	MSE	2.5
1	F	172	GLY	2.5
1	F	307	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	336	ARG	2.4
1	E	249	ILE	2.4
1	F	245	GLU	2.4
1	F	261	PHE	2.4
1	C	153	GLU	2.3
1	D	156	ASP	2.3
1	D	171	ARG	2.3
1	E	248	PRO	2.3
1	E	259	LYS	2.3
1	F	182	ILE	2.3
1	F	334	LEU	2.3
1	E	245	GLU	2.3
1	E	191	THR	2.2
1	F	26	GLU	2.2
1	D	184	GLN	2.2
1	D	245	GLU	2.2
1	D	253	GLY	2.2
1	E	187	PRO	2.2
1	D	327	LYS	2.1
1	A	155	LEU	2.1
1	E	8	LEU	2.1
1	F	177	LEU	2.1
1	D	251	ILE	2.1
1	E	326	LEU	2.0
1	D	236	GLU	2.0
1	E	185	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	A	400	48/48	0.12	-0.44	33,57,104,123	0
2	NAP	E	400	48/48	0.14	-0.46	44,71,146,156	0
2	NAP	C	400	48/48	0.13	-0.49	43,79,123,125	0
2	NAP	F	400	48/48	0.12	-0.77	43,70,118,177	0
2	NAP	D	400	48/48	0.11	-0.91	37,58,88,108	0
2	NAP	B	400	48/48	0.11	-0.97	38,68,107,140	0

## 6.5 Other polymers

There are no such residues in this entry.