



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 01:09 AM EDT

PDB ID : 3MAP  
Title : Crystal structure of homodimeric R132H mutant of human cytosolic NADP(+)-dependent isocitrate dehydrogenase in complex with NADP and isocitrate  
Authors : Yang, B.; Peng, Y.; Ding, J.  
Deposited on : 2010-03-24  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

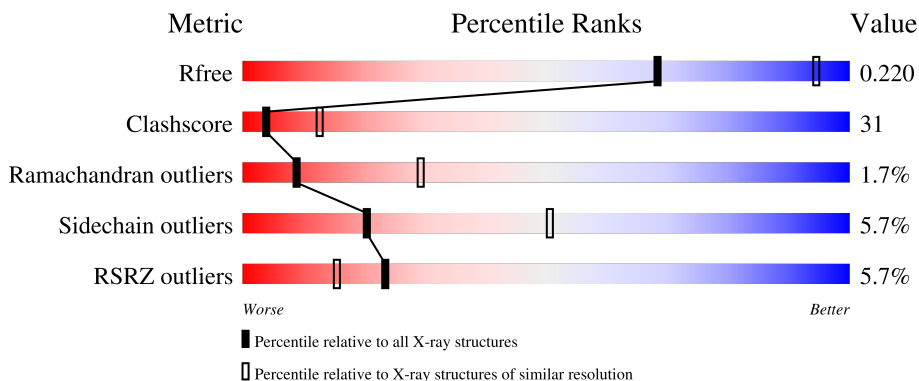
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>5%</div> <div> <div></div> <div>47%</div> <div>43%</div> <div>• 6%</div> </div> </div>
1	B	422	<div> <div>5%</div> <div> <div></div> <div>44%</div> <div>47%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6377 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3125	1990	532	585	18			
1	B	398	Total	C	N	O	S	0	0	0
			3130	1993	533	586	18			

There are 18 discrepancies between the modelled and reference sequences:

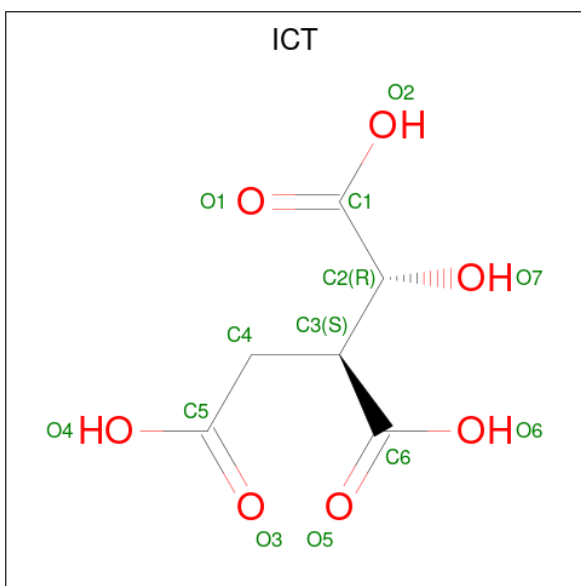
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	HIS	ARG	engineered mutation	UNP O75874
A	415	LEU	-	expression tag	UNP O75874
A	416	GLU	-	expression tag	UNP O75874
A	417	HIS	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
B	132	HIS	ARG	engineered mutation	UNP O75874
B	415	LEU	-	expression tag	UNP O75874
B	416	GLU	-	expression tag	UNP O75874
B	417	HIS	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (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>).



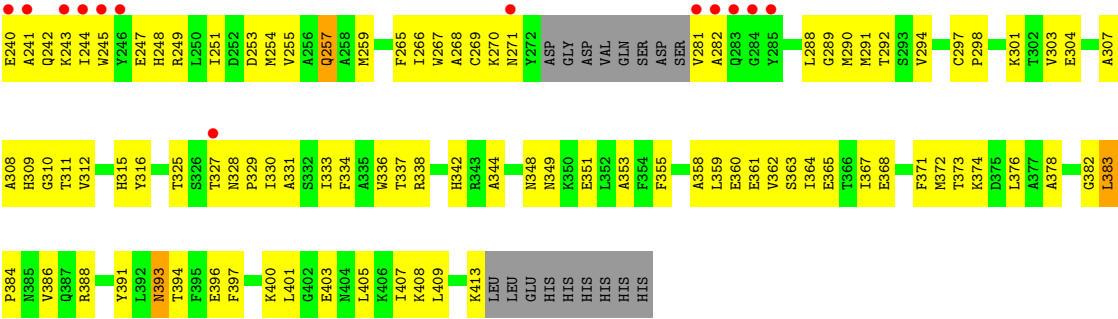
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is ISOCITRIC ACID (three-letter code: ICT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.84Å 79.84Å 295.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.92 – 2.80 47.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (39.92-2.80) 100.0 (47.55-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, $R_{free}$	0.224 , 0.269 0.225 , 0.220	Depositor DCC
$R_{free}$ test set	1258 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.27	0/3188	0.44	0/4295
1	B	0.27	0/3193	0.45	0/4302
All	All	0.27	0/6381	0.44	0/8597

There are no bond length outliers.

There are no bond angle outliers.

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	A	3125	0	3105	193	0
1	B	3130	0	3107	206	0
2	A	48	0	25	10	0
2	B	48	0	25	6	0
3	A	13	0	7	0	0
3	B	13	0	7	0	0
All	All	6377	0	6276	387	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TYR:HA	1:B:178:VAL:HG21	1.39	1.04
1:A:178:VAL:HG21	1:B:219:TYR:HA	1.38	1.03
1:B:117:ILE:HD13	1:B:376:LEU:HD22	1.45	0.97
1:B:9:SER:HB2	1:B:40:HIS:HE1	1.26	0.97
1:A:393:ASN:ND2	1:A:396:GLU:H	1.64	0.94
1:B:315:HIS:HE1	2:B:423:NAP:O2X	1.50	0.93
1:A:155:THR:HG21	1:A:164:LYS:HE2	1.54	0.89
1:B:244:ILE:HG12	1:B:245:TRP:H	1.39	0.88
2:A:423:NAP:H8A	2:A:423:NAP:H51A	1.56	0.87
1:B:9:SER:HB2	1:B:40:HIS:CE1	2.08	0.87
1:A:9:SER:HB2	1:A:40:HIS:HE1	1.42	0.85
1:B:338:ARG:HG3	1:B:338:ARG:HH11	1.43	0.82
1:A:393:ASN:HD21	1:A:396:GLU:H	1.27	0.81
1:A:218:LYS:HE3	1:B:145:VAL:HG23	1.62	0.80
1:B:116:ASN:H	1:B:116:ASN:HD22	1.27	0.80
1:A:314:ARG:NE	2:A:423:NAP:O3X	2.14	0.80
1:B:393:ASN:ND2	1:B:396:GLU:H	1.79	0.79
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.64	0.79
1:B:211:THR:HB	1:B:220:ASP:HB3	1.67	0.77
1:A:219:TYR:HA	1:B:178:VAL:CG2	2.16	0.75
1:A:393:ASN:C	1:A:393:ASN:HD22	1.90	0.75
1:A:219:TYR:HB2	1:B:143:ASP:HB2	1.67	0.75
1:B:212:LYS:HE3	1:B:251:ILE:HG13	1.69	0.74
1:A:116:ASN:ND2	1:A:368:GLU:HA	2.02	0.74
1:A:9:SER:HB2	1:A:40:HIS:CE1	2.22	0.74
1:A:207:LEU:HD22	1:A:208:TYR:H	1.54	0.72
1:B:291:MET:HB3	1:B:308:ALA:HB3	1.71	0.72
1:B:315:HIS:CE1	2:B:423:NAP:O2X	2.39	0.71
1:A:145:VAL:HG23	1:A:146:VAL:H	1.55	0.71
1:B:393:ASN:HD22	1:B:393:ASN:C	1.93	0.71
1:B:196:SER:HB3	1:B:207:LEU:HD11	1.73	0.70
1:B:109:ARG:HD2	1:B:282:ALA:CB	2.22	0.70
1:B:117:ILE:HD11	1:B:367:ILE:HG21	1.72	0.70
1:A:16:ASP:HB2	1:A:311:THR:HG21	1.72	0.69
1:B:397:PHE:CE2	1:B:401:LEU:HD11	2.28	0.69
1:A:309:HIS:HD2	1:A:310:GLY:O	1.76	0.69
1:B:244:ILE:HG12	1:B:245:TRP:N	2.06	0.69
1:B:64:ILE:HD13	1:B:304:GLU:HG3	1.74	0.69
1:B:248:HIS:CG	1:B:249:ARG:H	2.11	0.69
1:B:255:VAL:O	1:B:259:MET:HG2	1.93	0.69
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:HIS:HB2	1:B:183:TYR:CD2	2.28	0.68
1:A:210:SER:HA	1:A:249:ARG:O	1.94	0.68
1:B:205:TRP:HB3	1:B:265:PHE:HA	1.75	0.68
1:B:383:LEU:HB3	1:B:384:PRO:HD3	1.76	0.68
1:B:249:ARG:HB3	1:B:254:MET:HG2	1.76	0.67
1:A:9:SER:HA	1:A:38:ASP:HB2	1.77	0.67
1:A:198:GLN:HG2	1:A:300:GLY:HA2	1.77	0.67
1:B:358:ALA:O	1:B:362:VAL:HG23	1.95	0.67
1:A:116:ASN:HD22	1:A:116:ASN:H	1.43	0.66
1:A:200:ALA:HB1	1:A:244:ILE:HD11	1.76	0.66
1:B:200:ALA:HA	1:B:266:ILE:HG13	1.78	0.66
1:A:200:ALA:HA	1:A:266:ILE:HG13	1.76	0.65
1:B:309:HIS:CE1	1:B:331:ALA:HB3	2.30	0.65
1:A:210:SER:HB3	1:A:254:MET:HG2	1.78	0.65
1:A:330:ILE:HG13	1:A:367:ILE:HD11	1.79	0.65
1:B:93:LYS:H	1:B:93:LYS:HD2	1.60	0.64
1:B:14:GLN:HE22	1:B:41:SER:HB3	1.62	0.64
1:B:129:ILE:CD1	1:B:203:LYS:HD3	2.28	0.64
1:B:309:HIS:HE1	1:B:331:ALA:HB3	1.61	0.64
1:B:393:ASN:HD21	1:B:396:GLU:H	1.44	0.64
1:A:127:PRO:HG2	1:A:205:TRP:CH2	2.33	0.64
1:B:242:GLN:HB3	1:B:244:ILE:HG22	1.79	0.64
1:B:403:GLU:O	1:B:407:ILE:HD13	1.96	0.64
1:A:315:HIS:HE1	2:A:423:NAP:O2X	1.81	0.63
1:A:301:LYS:O	1:A:342:HIS:NE2	2.30	0.63
1:A:155:THR:CG2	1:A:164:LYS:HE2	2.29	0.63
1:B:7:GLY:HA3	1:B:37:LEU:HD23	1.80	0.62
1:B:338:ARG:HG3	1:B:338:ARG:NH1	2.08	0.62
1:A:17:GLU:HB2	1:A:311:THR:HB	1.80	0.62
1:A:207:LEU:HD22	1:A:208:TYR:N	2.15	0.62
1:B:95:PRO:O	1:B:99:ILE:HG12	1.99	0.62
1:B:23:TRP:CD2	1:B:73:CYS:HB2	2.35	0.61
1:B:152:VAL:O	1:B:169:VAL:HG13	2.00	0.61
1:B:93:LYS:HD2	1:B:93:LYS:N	2.16	0.61
1:B:158:PRO:HG2	1:B:163:GLN:HG2	1.80	0.61
1:A:127:PRO:HG2	1:A:205:TRP:HH2	1.66	0.61
1:B:128:ILE:HD12	1:B:128:ILE:N	2.15	0.61
1:A:113:ILE:HG23	1:A:119:ARG:HD2	1.82	0.61
1:A:192:PHE:CZ	1:A:268:ALA:HB1	2.36	0.61
1:B:116:ASN:ND2	1:B:368:GLU:HA	2.16	0.61
1:A:60:ALA:O	1:A:64:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HB3	1:A:215:ILE:HG22	1.83	0.60
1:A:251:ILE:O	1:A:255:VAL:HG13	2.01	0.60
1:B:75:THR:O	2:B:423:NAP:H2N	2.01	0.60
1:B:334:PHE:O	1:B:338:ARG:HG2	2.00	0.60
1:A:270:LYS:O	1:A:270:LYS:HD3	2.01	0.60
1:B:15:GLY:O	1:B:20:ARG:HD2	2.02	0.60
1:A:242:GLN:HB3	1:A:244:ILE:HG22	1.84	0.59
1:B:362:VAL:HG21	1:B:405:LEU:HA	1.84	0.59
1:B:71:VAL:O	1:B:71:VAL:HG23	2.01	0.59
1:A:381:LYS:HD2	1:A:390:ASP:OD1	2.02	0.59
1:A:116:ASN:HD21	1:A:368:GLU:HA	1.67	0.59
1:B:75:THR:OG1	1:B:95:PRO:HG2	2.02	0.59
1:A:359:LEU:HD13	1:A:405:LEU:HD22	1.84	0.59
1:B:382:GLY:O	1:B:386:VAL:HG23	2.03	0.59
1:A:207:LEU:HD23	1:A:266:ILE:HB	1.84	0.58
1:B:289:GLY:HA3	1:B:328:ASN:HB3	1.83	0.58
1:B:120:LEU:HB3	1:B:124:TRP:CZ3	2.38	0.58
1:B:212:LYS:HB2	1:B:220:ASP:OD1	2.02	0.58
1:A:121:VAL:HG12	1:A:123:GLY:H	1.68	0.58
1:B:13:MET:SD	1:B:64:ILE:HD11	2.43	0.58
1:B:309:HIS:HD2	1:B:310:GLY:O	1.87	0.58
1:A:15:GLY:HA3	1:A:74:ALA:O	2.03	0.58
1:A:29:LYS:HE3	1:A:399:ASP:OD1	2.03	0.58
1:A:112:ILE:HD11	1:A:330:ILE:HG21	1.85	0.58
1:A:344:ALA:HA	1:A:349:ASN:HB3	1.86	0.58
1:A:357:ASN:O	1:A:361:GLU:HG2	2.03	0.58
1:A:167:TYR:HB3	1:B:142:THR:HG21	1.86	0.57
1:A:309:HIS:CE1	1:A:331:ALA:HB3	2.39	0.57
1:A:46:ILE:HD11	1:A:78:PRO:HG3	1.86	0.56
1:A:291:MET:HB3	1:A:308:ALA:HB3	1.87	0.56
1:A:403:GLU:O	1:A:407:ILE:HG12	2.06	0.56
1:B:105:GLY:HA2	1:B:298:PRO:HD3	1.87	0.56
1:B:26:ILE:HG22	1:B:31:ILE:HD13	1.88	0.56
1:B:197:PHE:HA	1:B:207:LEU:HD12	1.88	0.56
1:A:72:LYS:HE2	1:A:96:ASN:OD1	2.06	0.56
1:A:209:LEU:HD22	1:A:227:PHE:CG	2.41	0.56
1:A:334:PHE:HA	1:A:337:THR:OG1	2.06	0.56
1:A:15:GLY:HA2	1:A:75:THR:HG22	1.86	0.55
1:A:57:THR:HG21	1:A:95:PRO:HA	1.87	0.55
1:A:194:HIS:O	1:A:198:GLN:HB2	2.07	0.55
1:B:117:ILE:HD11	1:B:367:ILE:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:CD1	1:A:401:LEU:HD13	2.36	0.55
1:B:4:LYS:HD2	1:B:36:GLU:OE1	2.07	0.55
1:A:382:GLY:O	1:A:386:VAL:HG23	2.06	0.55
1:A:397:PHE:CE2	1:A:401:LEU:HD11	2.42	0.55
1:B:330:ILE:HG13	1:B:367:ILE:HD11	1.89	0.55
1:B:248:HIS:CG	1:B:249:ARG:N	2.70	0.54
1:B:210:SER:HB3	1:B:254:MET:HG3	1.90	0.54
1:B:98:THR:O	1:B:102:ILE:HG12	2.08	0.54
1:B:109:ARG:HD2	1:B:282:ALA:HB1	1.90	0.54
1:A:271:ASN:N	1:A:271:ASN:HD22	2.06	0.54
1:A:413:LYS:HB2	1:A:413:LYS:NZ	2.21	0.54
1:A:249:ARG:HB3	1:A:254:MET:HB2	1.89	0.54
1:A:270:LYS:HD3	1:A:270:LYS:C	2.27	0.54
1:A:362:VAL:HG21	1:A:405:LEU:HA	1.90	0.54
1:A:208:TYR:OH	1:A:245:TRP:HH2	1.91	0.53
1:B:288:LEU:HB3	1:B:309:HIS:HB3	1.90	0.53
1:A:23:TRP:CD2	1:A:73:CYS:HB2	2.43	0.53
1:A:207:LEU:CD2	1:A:208:TYR:H	2.21	0.53
1:B:205:TRP:O	1:B:244:ILE:HD11	2.08	0.53
1:A:117:ILE:O	1:A:119:ARG:HD3	2.08	0.53
1:B:334:PHE:HA	1:B:337:THR:OG1	2.09	0.53
1:B:215:ILE:HG23	1:B:216:LEU:N	2.23	0.53
1:A:128:ILE:N	1:A:128:ILE:HD12	2.24	0.52
1:A:75:THR:OG1	1:A:95:PRO:HG2	2.09	0.52
1:A:208:TYR:OH	1:A:245:TRP:CH2	2.61	0.52
1:A:363:SER:HA	1:A:401:LEU:HD21	1.91	0.52
1:B:359:LEU:HD13	1:B:405:LEU:HD22	1.90	0.52
1:B:378:ALA:HA	1:B:386:VAL:HG21	1.90	0.52
1:A:367:ILE:HA	1:A:371:PHE:O	2.10	0.52
1:A:66:LYS:HE3	1:A:67:HIS:CE1	2.44	0.52
1:A:211:THR:OG1	1:A:248:HIS:HE1	1.93	0.52
1:B:312:VAL:HG12	1:B:315:HIS:HB2	1.90	0.52
1:A:15:GLY:N	1:A:73:CYS:HB3	2.24	0.52
1:A:79:ASP:H	1:A:82:ARG:HB2	1.74	0.52
1:A:330:ILE:CD1	1:A:363:SER:HB3	2.39	0.52
1:B:69:VAL:HG22	1:B:342:HIS:HD2	1.75	0.52
1:B:165:VAL:HG11	1:B:167:TYR:CZ	2.45	0.51
1:A:207:LEU:HD13	1:A:246:TYR:CD2	2.45	0.51
1:B:248:HIS:CD2	1:B:249:ARG:H	2.28	0.51
1:A:212:LYS:HB3	1:A:215:ILE:CG2	2.41	0.51
1:A:226:ILE:O	1:A:230:ILE:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:HD2	1:B:245:TRP:CA	2.24	0.51
1:B:231:TYR:CE1	1:B:236:LYS:HA	2.45	0.50
1:B:19:THR:O	1:B:23:TRP:HB2	2.11	0.50
1:B:145:VAL:O	1:B:146:VAL:HB	2.11	0.50
1:B:270:LYS:HD3	1:B:270:LYS:O	2.11	0.50
1:A:144:PHE:HE1	1:B:154:ILE:HD13	1.76	0.50
1:A:246:TYR:CG	1:A:247:GLU:N	2.79	0.50
1:B:327:THR:O	1:B:329:PRO:HD3	2.12	0.50
1:B:117:ILE:HD11	1:B:376:LEU:HD13	1.94	0.50
1:B:129:ILE:HD12	1:B:266:ILE:CD1	2.42	0.50
1:B:46:ILE:HG21	1:B:86:PHE:CZ	2.47	0.49
1:B:270:LYS:HD3	1:B:270:LYS:C	2.33	0.49
1:A:70:GLY:O	1:A:304:GLU:HA	2.13	0.49
1:A:30:LEU:O	1:A:355:PHE:HZ	1.95	0.49
1:A:75:THR:H	2:A:423:NAP:H71N	1.58	0.49
1:A:197:PHE:CZ	1:A:231:TYR:HB2	2.46	0.49
1:A:310:GLY:HA3	2:A:423:NAP:C6N	2.42	0.49
1:A:393:ASN:ND2	1:A:393:ASN:C	2.61	0.49
1:B:393:ASN:ND2	1:B:393:ASN:C	2.65	0.49
1:B:11:VAL:HG21	1:B:63:ALA:C	2.33	0.49
1:B:337:THR:CB	1:B:360:GLU:HG3	2.42	0.49
1:B:344:ALA:HB1	1:B:353:ALA:HB2	1.94	0.49
1:A:311:THR:OG1	2:A:423:NAP:H4D	2.13	0.49
1:B:112:ILE:HG12	1:B:330:ILE:HG21	1.95	0.49
1:B:333:ILE:O	1:B:337:THR:HG23	2.13	0.49
1:A:239:PHE:O	1:A:244:ILE:HG22	2.12	0.49
1:A:334:PHE:CE2	1:A:360:GLU:HG2	2.47	0.49
1:B:15:GLY:HA2	1:B:75:THR:HG22	1.94	0.49
1:B:15:GLY:N	1:B:73:CYS:HB3	2.27	0.49
1:B:328:ASN:OD1	1:B:330:ILE:HG12	2.13	0.49
1:B:145:VAL:O	1:B:177:GLY:O	2.30	0.49
1:A:371:PHE:CD1	1:A:400:LYS:HE2	2.48	0.48
1:B:133:HIS:O	1:B:134:ALA:HB3	2.12	0.48
1:A:219:TYR:HE2	1:A:270:LYS:HE3	1.77	0.48
1:B:240:GLU:C	1:B:242:GLN:H	2.15	0.48
1:A:183:TYR:CD2	1:B:170:HIS:HB2	2.49	0.48
1:A:327:THR:O	1:A:373:THR:HG21	2.13	0.48
1:B:19:THR:OG1	1:B:74:ALA:HB3	2.13	0.48
1:B:374:LYS:HD2	1:B:391:TYR:CZ	2.49	0.48
2:B:423:NAP:O1A	2:B:423:NAP:O1N	2.30	0.48
1:B:212:LYS:HE2	1:B:212:LYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ALA:HB1	1:B:309:HIS:CE1	2.48	0.48
1:B:112:ILE:O	1:B:112:ILE:HG13	2.14	0.48
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.49	0.48
1:A:183:TYR:HA	1:B:179:ALA:HA	1.94	0.47
1:B:207:LEU:HD23	1:B:208:TYR:N	2.29	0.47
1:A:309:HIS:HE1	1:A:331:ALA:HB3	1.79	0.47
1:B:325:THR:O	1:B:393:ASN:HB2	2.14	0.47
1:B:9:SER:HA	1:B:38:ASP:HB2	1.95	0.47
1:A:5:ILE:HG12	1:A:34:TYR:O	2.15	0.47
1:B:208:TYR:HH	1:B:245:TRP:HH2	1.63	0.47
1:A:20:ARG:HH22	1:A:43:ASP:CG	2.16	0.47
1:A:46:ILE:CD1	1:A:78:PRO:HG3	2.44	0.47
1:B:197:PHE:HB3	1:B:235:TYR:CD2	2.50	0.47
1:B:239:PHE:HD2	1:B:245:TRP:C	2.17	0.47
1:B:249:ARG:HH21	1:B:257:GLN:HB2	1.79	0.47
1:B:12:GLU:HG3	1:B:336:TRP:CZ2	2.50	0.47
1:B:364:ILE:O	1:B:368:GLU:HG3	2.15	0.47
1:A:5:ILE:HG21	1:A:351:GLU:HB3	1.97	0.47
1:B:193:ALA:HB3	1:B:230:ILE:HD12	1.97	0.47
1:B:337:THR:HB	1:B:360:GLU:HG3	1.97	0.47
1:A:378:ALA:HB1	1:A:383:LEU:HD22	1.97	0.47
1:A:86:PHE:HB2	1:A:88:LEU:HG	1.97	0.46
1:A:219:TYR:CD2	1:B:180:MET:HE2	2.51	0.46
1:B:281:VAL:O	1:B:282:ALA:HB3	2.15	0.46
1:B:367:ILE:HA	1:B:371:PHE:O	2.16	0.46
1:B:294:VAL:HG13	1:B:303:VAL:HG13	1.98	0.46
1:B:71:VAL:O	1:B:71:VAL:CG2	2.63	0.46
1:B:112:ILE:HG12	1:B:330:ILE:CG2	2.46	0.46
1:B:400:LYS:HD2	1:B:400:LYS:HA	1.68	0.46
1:B:310:GLY:HA3	2:B:423:NAP:C6N	2.46	0.46
1:A:115:LYS:HA	1:A:119:ARG:HH12	1.80	0.46
1:A:255:VAL:O	1:A:259:MET:HG2	2.16	0.46
1:B:208:TYR:OH	1:B:245:TRP:HH2	1.98	0.46
1:B:291:MET:CB	1:B:308:ALA:HB3	2.43	0.46
1:B:361:GLU:HB3	1:B:408:LYS:NZ	2.31	0.46
1:B:147:PRO:O	1:B:176:GLY:HA3	2.16	0.45
1:A:307:ALA:HB1	1:A:309:HIS:CE1	2.50	0.45
1:A:46:ILE:HG13	1:A:88:LEU:HD21	1.98	0.45
1:B:117:ILE:CD1	1:B:367:ILE:HG21	2.45	0.45
1:B:383:LEU:CB	1:B:384:PRO:HD3	2.45	0.45
1:A:160:ASP:OD1	1:A:162:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:HG3	1:A:338:ARG:HH11	1.81	0.45
1:B:17:GLU:CG	1:B:76:ILE:HD11	2.47	0.45
1:B:114:CYS:HB2	1:B:117:ILE:HD12	1.99	0.45
1:A:146:VAL:N	1:A:147:PRO:HD3	2.31	0.45
1:B:16:ASP:HB2	1:B:311:THR:HG21	1.97	0.45
1:B:361:GLU:O	1:B:365:GLU:HG3	2.16	0.45
1:A:242:GLN:C	1:A:244:ILE:H	2.20	0.45
1:B:152:VAL:HG11	1:B:179:ALA:CB	2.46	0.45
1:A:19:THR:OG1	1:A:311:THR:HA	2.17	0.45
1:B:239:PHE:HA	1:B:244:ILE:HG23	1.99	0.45
1:B:367:ILE:HD13	1:B:376:LEU:CD1	2.47	0.45
1:A:69:VAL:HG22	1:A:342:HIS:HD2	1.82	0.45
1:A:381:LYS:O	1:A:385:ASN:HB2	2.15	0.45
1:B:9:SER:HA	1:B:38:ASP:O	2.17	0.45
1:A:271:ASN:N	1:A:271:ASN:ND2	2.65	0.45
1:B:226:ILE:O	1:B:230:ILE:HG13	2.17	0.45
1:A:13:MET:SD	1:A:64:ILE:HD11	2.58	0.44
1:A:209:LEU:HD22	1:A:227:PHE:CD1	2.53	0.44
1:A:244:ILE:HG12	1:A:245:TRP:N	2.33	0.44
1:B:351:GLU:H	1:B:351:GLU:CD	2.21	0.44
1:A:197:PHE:CD2	1:A:207:LEU:HD12	2.51	0.44
1:A:407:ILE:O	1:A:411:GLN:HG3	2.17	0.44
1:B:127:PRO:HG2	1:B:205:TRP:CH2	2.52	0.44
1:B:248:HIS:O	1:B:249:ARG:HB2	2.17	0.44
1:B:124:TRP:CG	1:B:128:ILE:HD11	2.53	0.44
1:B:212:LYS:O	1:B:214:THR:N	2.50	0.44
1:B:242:GLN:O	1:B:242:GLN:HG2	2.17	0.44
1:A:171:ASN:C	1:A:171:ASN:HD22	2.19	0.44
1:A:205:TRP:O	1:A:244:ILE:HD11	2.17	0.44
1:A:230:ILE:O	1:A:234:GLN:HB3	2.18	0.44
1:B:200:ALA:CA	1:B:266:ILE:HG13	2.47	0.44
1:B:60:ALA:O	1:B:64:ILE:HG13	2.18	0.44
1:B:315:HIS:O	1:B:325:THR:HG21	2.17	0.44
1:B:327:THR:O	1:B:373:THR:HG21	2.18	0.44
1:A:112:ILE:CD1	1:A:330:ILE:HG21	2.47	0.44
1:A:159:SER:OG	1:B:149:PRO:HB2	2.17	0.44
1:B:265:PHE:HE1	1:B:267:TRP:HB2	1.83	0.44
1:A:312:VAL:HA	2:A:423:NAP:O2A	2.18	0.44
1:A:324:GLU:OE2	1:A:388:ARG:NH1	2.50	0.44
1:A:12:GLU:HG3	1:A:336:TRP:CZ2	2.53	0.43
1:A:48:ASN:O	1:A:52:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:VAL:O	1:B:70:GLY:HA2	2.18	0.43
1:B:156:TYR:CE1	1:B:158:PRO:HG3	2.53	0.43
1:A:4:LYS:HD3	1:A:32:PHE:O	2.17	0.43
1:A:231:TYR:CE1	1:A:246:TYR:HB3	2.53	0.43
1:B:27:LYS:HD2	1:B:336:TRP:HZ2	1.83	0.43
1:B:116:ASN:HD22	1:B:116:ASN:N	2.00	0.43
1:B:393:ASN:O	1:B:394:THR:C	2.55	0.43
1:A:208:TYR:CE2	1:A:245:TRP:HZ3	2.36	0.43
1:A:329:PRO:O	1:A:333:ILE:HG13	2.19	0.43
1:A:363:SER:HA	1:A:401:LEU:CD2	2.48	0.43
1:A:75:THR:O	2:A:423:NAP:H2N	2.19	0.43
1:A:210:SER:HB2	1:A:251:ILE:HA	2.01	0.43
1:A:388:ARG:O	1:A:388:ARG:NE	2.49	0.43
1:A:105:GLY:HA2	1:A:298:PRO:HD3	2.01	0.43
1:B:265:PHE:CE1	1:B:267:TRP:HB2	2.54	0.43
1:A:26:ILE:HD11	1:A:332:SER:HB2	2.00	0.43
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.76	0.43
1:B:26:ILE:CG2	1:B:31:ILE:HD13	2.48	0.43
1:B:206:PRO:HB3	1:B:245:TRP:CE2	2.54	0.43
1:A:114:CYS:O	1:A:117:ILE:HB	2.19	0.43
1:A:205:TRP:HB3	1:A:265:PHE:HA	2.00	0.43
1:B:113:ILE:HG21	1:B:125:VAL:O	2.17	0.43
1:A:13:MET:HA	1:A:42:TYR:O	2.19	0.42
1:A:15:GLY:O	1:A:20:ARG:NH1	2.45	0.42
1:A:53:ASN:HA	1:A:92:TRP:CH2	2.53	0.42
1:A:170:HIS:HB2	1:B:183:TYR:CE2	2.54	0.42
1:A:413:LYS:HB2	1:A:413:LYS:HZ2	1.84	0.42
1:B:43:ASP:HB3	1:B:48:ASN:ND2	2.33	0.42
1:B:211:THR:OG1	1:B:213:ASN:HB2	2.19	0.42
1:A:19:THR:OG1	1:A:74:ALA:HB3	2.19	0.42
1:A:23:TRP:HZ2	1:A:71:VAL:HG23	1.83	0.42
1:B:6:SER:O	1:B:349:ASN:ND2	2.49	0.42
1:A:16:ASP:OD1	1:A:45:GLY:HA2	2.20	0.42
1:B:109:ARG:CD	1:B:282:ALA:CB	2.97	0.42
1:B:253:ASP:O	1:B:257:GLN:HB3	2.19	0.42
1:B:378:ALA:HA	1:B:386:VAL:CG2	2.48	0.42
1:A:124:TRP:CG	1:A:128:ILE:HD11	2.55	0.42
1:A:205:TRP:C	1:A:244:ILE:HG13	2.40	0.42
1:B:20:ARG:O	1:B:24:GLU:HG2	2.18	0.42
1:B:123:GLY:O	1:B:125:VAL:HG23	2.20	0.42
1:B:251:ILE:O	1:B:255:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HD3	1:A:119:ARG:N	2.35	0.42
1:B:309:HIS:CD2	1:B:310:GLY:O	2.71	0.42
1:A:23:TRP:CZ2	1:A:71:VAL:HG23	2.55	0.42
1:A:108:PHE:CD1	1:A:131:GLY:HA3	2.55	0.42
1:A:289:GLY:HA3	1:A:328:ASN:HB3	2.01	0.42
1:A:13:MET:CE	1:A:64:ILE:HD11	2.50	0.41
1:A:295:LEU:HB3	1:A:304:GLU:HB3	2.01	0.41
1:A:378:ALA:HA	1:A:386:VAL:CG2	2.50	0.41
1:B:209:LEU:HD12	1:B:268:ALA:O	2.20	0.41
1:A:64:ILE:HD13	1:A:304:GLU:HG3	2.02	0.41
1:A:305:ALA:HB1	1:A:335:ALA:HA	2.02	0.41
1:B:112:ILE:CD1	1:B:364:ILE:HG12	2.50	0.41
1:B:239:PHE:HB3	1:B:245:TRP:HA	2.02	0.41
1:A:85:GLU:OE2	1:A:317:ARG:NH2	2.52	0.41
1:B:215:ILE:HG23	1:B:216:LEU:H	1.83	0.41
1:B:372:MET:HB2	1:B:376:LEU:HD12	2.02	0.41
1:A:12:GLU:OE2	1:A:23:TRP:NE1	2.52	0.41
1:A:201:LEU:HD21	1:A:239:PHE:CD1	2.55	0.41
1:A:365:GLU:O	1:A:369:ALA:N	2.54	0.41
1:B:330:ILE:CD1	1:B:363:SER:HB3	2.49	0.41
1:A:32:PHE:HB2	1:A:33:PRO:HD3	2.02	0.41
1:A:108:PHE:CE1	1:A:131:GLY:HA3	2.55	0.41
1:B:190:GLU:HA	1:B:230:ILE:CD1	2.51	0.41
1:B:355:PHE:CD1	1:B:409:LEU:HD11	2.56	0.41
1:A:312:VAL:N	2:A:423:NAP:O2A	2.51	0.41
2:B:423:NAP:H6N	2:B:423:NAP:H2D	1.86	0.41
1:B:190:GLU:HG2	1:B:230:ILE:HD11	2.03	0.41
1:A:240:GLU:C	1:A:242:GLN:H	2.24	0.41
1:A:265:PHE:HE1	1:A:267:TRP:HB2	1.86	0.41
1:A:120:LEU:HD22	1:A:121:VAL:HG23	2.03	0.41
1:A:169:VAL:O	1:A:170:HIS:HB2	2.21	0.41
1:A:179:ALA:HA	1:B:183:TYR:HA	2.02	0.41
1:A:200:ALA:CA	1:A:266:ILE:HG13	2.47	0.41
1:B:57:THR:HG21	1:B:95:PRO:HA	2.03	0.41
1:B:112:ILE:HD11	1:B:290:MET:HE1	2.01	0.41
1:A:14:GLN:HB2	1:A:43:ASP:HA	2.02	0.41
1:A:129:ILE:HG13	1:A:266:ILE:CD1	2.51	0.41
1:B:116:ASN:H	1:B:116:ASN:ND2	2.07	0.41
1:B:217:LYS:HB3	1:B:218:LYS:H	1.66	0.41
1:A:40:HIS:NE2	1:A:67:HIS:NE2	2.69	0.40
1:A:116:ASN:HD22	1:A:116:ASN:N	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LYS:HD2	1:B:336:TRP:CZ2	2.56	0.40
1:B:153:GLU:HB3	1:B:168:LEU:HA	2.03	0.40
1:A:156:TYR:CE1	1:B:147:PRO:HD2	2.56	0.40
1:B:17:GLU:HB3	1:B:316:TYR:CG	2.56	0.40
1:B:39:LEU:HD23	1:B:39:LEU:HA	1.93	0.40
1:B:78:PRO:HA	1:B:82:ARG:HG3	2.03	0.40
1:B:247:GLU:HG2	1:B:248:HIS:O	2.21	0.40
1:B:383:LEU:HB3	1:B:384:PRO:CD	2.48	0.40
1:A:393:ASN:HD21	1:A:396:GLU:N	2.05	0.40
1:B:27:LYS:HG2	1:B:32:PHE:CZ	2.57	0.40
1:A:123:GLY:O	1:A:262:GLU:HA	2.21	0.40
1:A:210:SER:HB2	1:A:251:ILE:HD13	2.04	0.40
2:A:423:NAP:H8A	2:A:423:NAP:C5B	2.39	0.40
1:A:79:ASP:O	1:A:83:VAL:HG23	2.22	0.40
1:A:154:ILE:CG2	1:B:144:PHE:HE2	2.35	0.40
1:A:207:LEU:HB3	1:A:246:TYR:HD2	1.86	0.40
1:B:105:GLY:HA3	1:B:297:CYS:HA	2.04	0.40
1:B:239:PHE:O	1:B:244:ILE:HG22	2.21	0.40

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	A	391/422 (93%)	351 (90%)	33 (8%)	7 (2%)	8	28
1	B	392/422 (93%)	349 (89%)	37 (9%)	6 (2%)	10	33
All	All	783/844 (93%)	700 (89%)	70 (9%)	13 (2%)	9	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	VAL
1	A	242	GLN
1	B	213	ASN
1	B	217	LYS
1	A	282	ALA
1	B	124	TRP
1	A	234	GLN
1	B	147	PRO
1	B	218	LYS
1	A	241	ALA
1	B	241	ALA
1	A	175	GLY
1	A	382	GLY

### 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	331/358 (92%)	314 (95%)	17 (5%)	24	55
1	B	331/358 (92%)	310 (94%)	21 (6%)	18	46
All	All	662/716 (92%)	624 (94%)	38 (6%)	20	50

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	39	LEU
1	A	71	VAL
1	A	80	GLU
1	A	116	ASN
1	A	119	ARG
1	A	171	ASN
1	A	184	ASN
1	A	207	LEU
1	A	217	LYS
1	A	234	GLN

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Mol	Chain	Res	Type
1	A	249	ARG
1	A	348	ASN
1	A	383	LEU
1	A	388	ARG
1	A	393	ASN
1	A	413	LYS
1	B	62	GLU
1	B	112	ILE
1	B	113	ILE
1	B	116	ASN
1	B	119	ARG
1	B	157	THR
1	B	166	THR
1	B	168	LEU
1	B	169	VAL
1	B	212	LYS
1	B	243	LYS
1	B	257	GLN
1	B	269	CYS
1	B	271	ASN
1	B	292	THR
1	B	301	LYS
1	B	348	ASN
1	B	383	LEU
1	B	388	ARG
1	B	393	ASN
1	B	413	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	116	ASN
1	A	163	GLN
1	A	171	ASN
1	A	228	GLN
1	A	234	GLN
1	A	238	GLN
1	A	248	HIS
1	A	257	GLN
1	A	271	ASN
1	A	309	HIS

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Mol	Chain	Res	Type
1	A	315	HIS
1	A	393	ASN
1	A	404	ASN
1	B	14	GLN
1	B	90	GLN
1	B	96	ASN
1	B	101	ASN
1	B	116	ASN
1	B	228	GLN
1	B	248	HIS
1	B	257	GLN
1	B	271	ASN
1	B	309	HIS
1	B	315	HIS
1	B	348	ASN
1	B	393	ASN
1	B	404	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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
3	ICT	A	424	-	2,12,12	1.49	0	5,16,16	1.55	0
2	NAP	A	423	-	45,52,52	1.93	13 (28%)	56,80,80	1.55	9 (16%)
2	NAP	B	423	-	45,52,52	2.30	19 (42%)	56,80,80	1.76	13 (23%)
3	ICT	B	424	-	2,12,12	1.57	1 (50%)	5,16,16	1.54	1 (20%)

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
3	ICT	A	424	-	-	2/6/16/16	-
2	NAP	A	423	-	-	14/31/67/67	0/5/5/5
2	NAP	B	423	-	-	11/31/67/67	0/5/5/5
3	ICT	B	424	-	-	4/6/16/16	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	423	NAP	P2B-O2B	-4.68	1.50	1.59
2	B	423	NAP	O4D-C1D	-4.41	1.34	1.41
2	B	423	NAP	C2D-C1D	-4.34	1.47	1.53
2	A	423	NAP	O4D-C4D	-4.21	1.35	1.45
2	B	423	NAP	O4D-C4D	-4.08	1.35	1.45
2	B	423	NAP	PA-O5B	-3.97	1.43	1.59
2	A	423	NAP	C2D-C1D	-3.97	1.47	1.53
2	B	423	NAP	O4B-C4B	-3.82	1.36	1.45
2	A	423	NAP	P2B-O2B	-3.74	1.52	1.59
2	B	423	NAP	PN-O5D	-3.54	1.45	1.59
2	B	423	NAP	P2B-O2X	-3.35	1.41	1.54
2	A	423	NAP	PA-O5B	-3.27	1.46	1.59
2	B	423	NAP	C4A-N3A	-3.09	1.31	1.35
2	A	423	NAP	P2B-O2X	-3.08	1.43	1.54
2	B	423	NAP	PA-O1A	-3.01	1.40	1.50
2	B	423	NAP	PN-O2N	-2.95	1.41	1.55
2	A	423	NAP	PN-O5D	-2.84	1.47	1.59
2	A	423	NAP	PN-O2N	-2.68	1.42	1.55
2	B	423	NAP	PN-O1N	-2.66	1.41	1.50
2	A	423	NAP	PA-O2A	-2.62	1.43	1.55
2	A	423	NAP	PA-O1A	-2.53	1.41	1.50
2	A	423	NAP	C5A-N7A	-2.50	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	423	NAP	PA-O2A	-2.48	1.43	1.55
2	B	423	NAP	C5A-N7A	-2.47	1.30	1.39
2	A	423	NAP	O4B-C4B	-2.44	1.39	1.45
2	A	423	NAP	C4A-N3A	-2.29	1.32	1.35
2	B	423	NAP	C8A-N7A	-2.28	1.30	1.34
2	A	423	NAP	PN-O1N	-2.21	1.43	1.50
2	B	423	NAP	C2D-C3D	-2.07	1.47	1.53
2	B	423	NAP	C3B-C4B	-2.05	1.47	1.53
3	B	424	ICT	O7-C2	-2.03	1.38	1.42
2	B	423	NAP	O5D-C5D	-2.03	1.37	1.44
2	B	423	NAP	C5A-C4A	-2.02	1.35	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	423	NAP	O4D-C1D-C2D	-5.56	98.80	106.93
2	A	423	NAP	O4D-C1D-C2D	-4.58	100.23	106.93
2	A	423	NAP	N3A-C2A-N1A	-4.44	121.73	128.68
2	B	423	NAP	N3A-C2A-N1A	-4.00	122.43	128.68
2	A	423	NAP	O4D-C4D-C5D	-3.74	97.06	109.37
2	B	423	NAP	PN-O3-PA	-3.57	120.58	132.83
2	B	423	NAP	C3D-C2D-C1D	-3.49	95.72	100.98
2	B	423	NAP	C4A-C5A-N7A	-3.25	106.01	109.40
2	B	423	NAP	O2X-P2B-O2B	2.93	119.14	105.99
2	B	423	NAP	C5A-C6A-N6A	2.78	124.58	120.35
2	A	423	NAP	C3B-C2B-C1B	-2.50	98.19	102.89
2	A	423	NAP	C4A-C5A-N7A	-2.50	106.79	109.40
2	B	423	NAP	C5B-C4B-C3B	-2.47	105.94	115.18
2	B	423	NAP	O3D-C3D-C2D	-2.37	104.15	111.82
2	A	423	NAP	O4B-C4B-C5B	-2.36	101.62	109.37
2	A	423	NAP	O3X-P2B-O1X	-2.30	101.68	110.68
2	B	423	NAP	C2N-C3N-C4N	2.23	120.79	118.26
2	A	423	NAP	PN-O3-PA	-2.20	125.28	132.83
2	B	423	NAP	O3X-P2B-O2B	-2.11	96.55	105.99
3	B	424	ICT	C1-C2-C3	2.10	114.62	112.25
2	B	423	NAP	O3X-P2B-O2X	2.09	115.61	107.64
2	A	423	NAP	O3D-C3D-C2D	-2.04	105.21	111.82
2	B	423	NAP	C5D-C4D-C3D	-2.02	107.60	115.18

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	423	NAP	C5B-O5B-PA-O1A
2	A	423	NAP	C2B-O2B-P2B-O1X
2	A	423	NAP	C5D-O5D-PN-O1N
2	A	423	NAP	C5D-O5D-PN-O2N
2	A	423	NAP	O4D-C1D-N1N-C6N
2	B	423	NAP	C5B-O5B-PA-O1A
2	B	423	NAP	C5B-O5B-PA-O3
2	B	423	NAP	C2B-O2B-P2B-O1X
2	B	423	NAP	O4D-C1D-N1N-C6N
2	B	423	NAP	C2D-C1D-N1N-C2N
2	B	423	NAP	C2D-C1D-N1N-C6N
3	A	424	ICT	C2-C3-C4-C5
3	B	424	ICT	C1-C2-C3-C4
3	B	424	ICT	C2-C3-C4-C5
2	A	423	NAP	O4B-C4B-C5B-O5B
2	B	423	NAP	O4D-C4D-C5D-O5D
2	B	423	NAP	O4B-C4B-C5B-O5B
2	A	423	NAP	C5B-O5B-PA-O3
2	A	423	NAP	C3B-C4B-C5B-O5B
2	A	423	NAP	C5B-O5B-PA-O2A
2	B	423	NAP	C5B-O5B-PA-O2A
3	A	424	ICT	C6-C3-C4-C5
3	B	424	ICT	C6-C3-C4-C5
2	A	423	NAP	PA-O3-PN-O1N
3	B	424	ICT	O7-C2-C3-C4
2	A	423	NAP	C5D-O5D-PN-O3
2	A	423	NAP	C2D-C1D-N1N-C2N
2	B	423	NAP	C3D-C4D-C5D-O5D
2	A	423	NAP	PA-O3-PN-O2N
2	B	423	NAP	C5D-O5D-PN-O1N
2	A	423	NAP	O4D-C4D-C5D-O5D

There are no ring outliers.

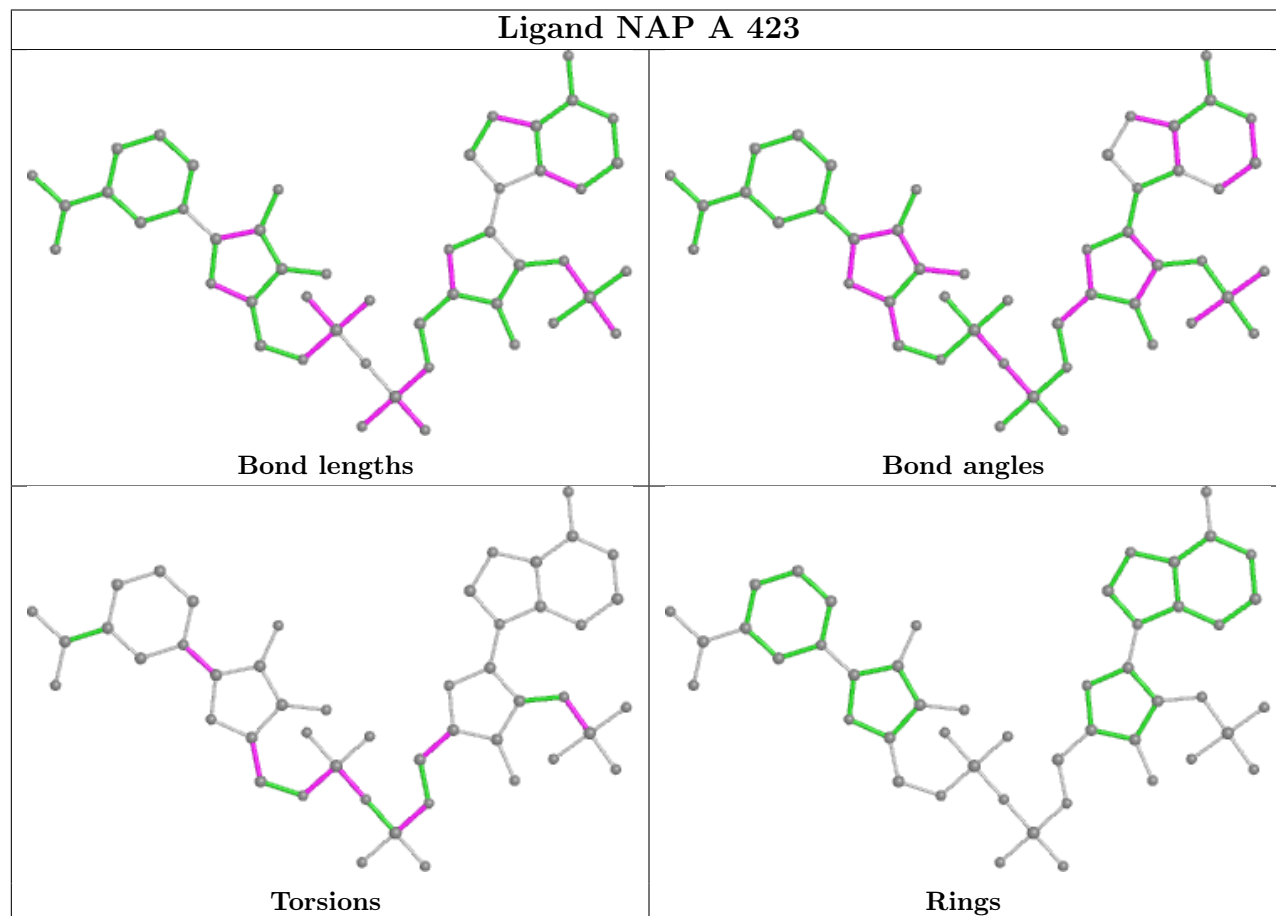
2 monomers are involved in 16 short contacts:

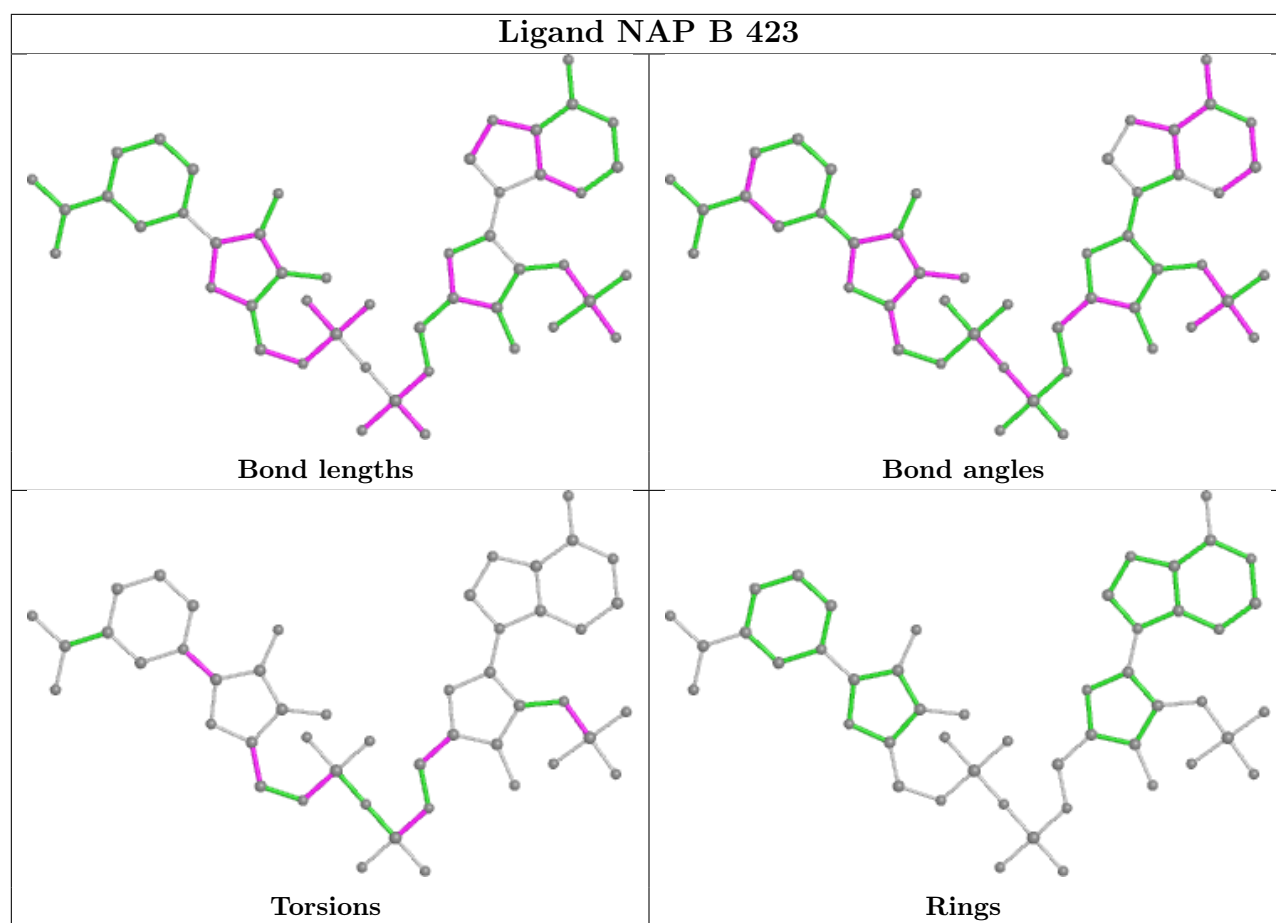
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	423	NAP	10	0
2	B	423	NAP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is



within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	397/422 (94%)	0.50	22 (5%) 25 16	39, 63, 110, 149	0
1	B	398/422 (94%)	0.50	23 (5%) 23 15	37, 63, 116, 154	0
All	All	795/844 (94%)	0.50	45 (5%) 23 15	37, 63, 114, 154	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	VAL	8.8
1	A	281	VAL	7.3
1	A	284	GLY	7.2
1	A	282	ALA	6.2
1	A	285	TYR	5.4
1	B	284	GLY	5.1
1	B	282	ALA	4.7
1	A	283	GLN	4.4
1	B	285	TYR	4.3
1	B	283	GLN	3.8
1	B	236	LYS	3.8
1	B	235	TYR	3.7
1	A	134	ALA	3.4
1	B	244	ILE	3.2
1	B	239	PHE	3.2
1	A	237	SER	3.1
1	A	244	ILE	3.1
1	A	245	TRP	3.1
1	B	202	SER	3.0
1	B	231	TYR	3.0
1	B	241	ALA	3.0
1	B	245	TRP	3.0
1	A	236	LYS	2.8
1	A	240	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	133	HIS	2.7
1	A	174	GLU	2.6
1	A	286	GLY	2.6
1	A	271	ASN	2.6
1	B	246	TYR	2.5
1	B	207	LEU	2.4
1	A	235	TYR	2.3
1	A	246	TYR	2.3
1	B	237	SER	2.3
1	B	213	ASN	2.3
1	A	241	ALA	2.3
1	B	240	GLU	2.3
1	B	327	THR	2.3
1	A	238	GLN	2.2
1	A	201	LEU	2.2
1	A	145	VAL	2.1
1	B	271	ASN	2.1
1	B	243	LYS	2.1
1	B	154	ILE	2.1
1	A	322	GLY	2.0
1	B	189	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

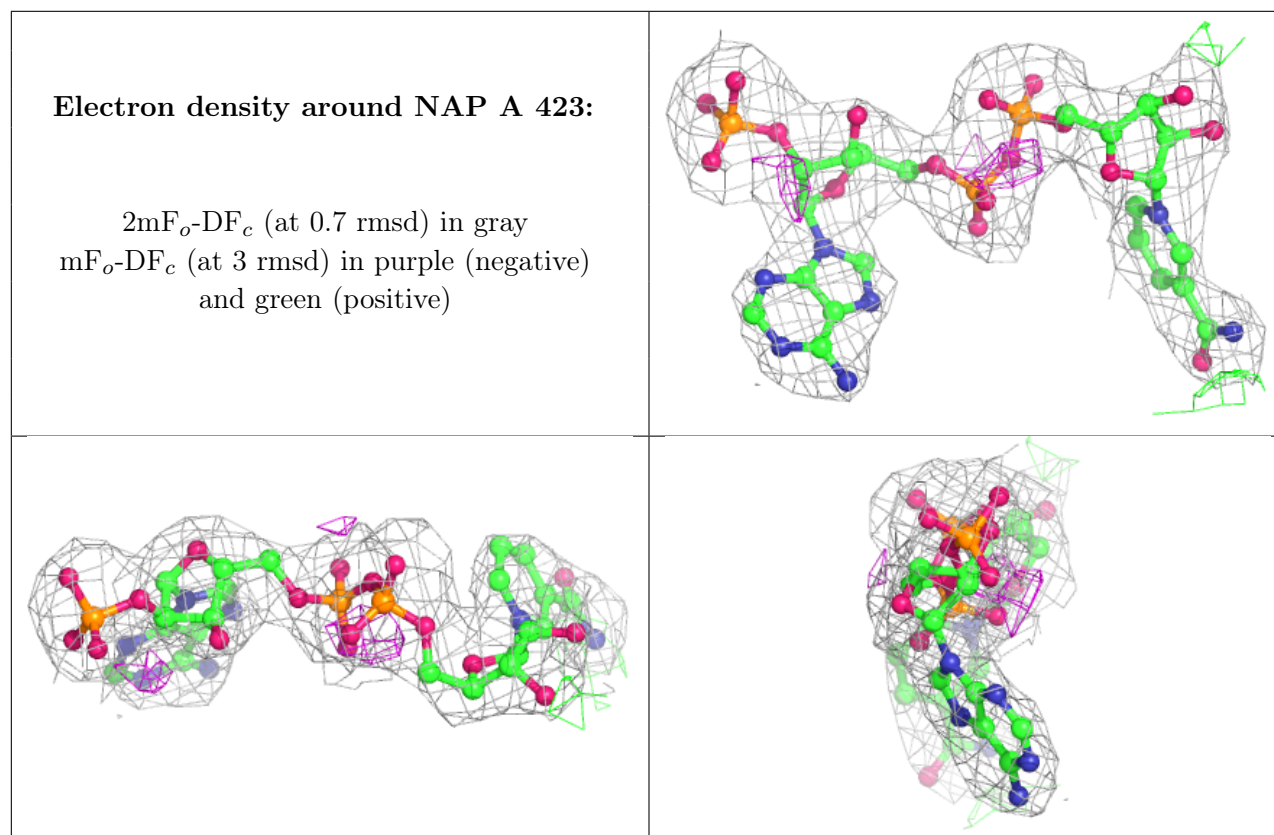
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ICT	B	424	13/13	0.66	0.39	106,111,111,112	0
3	ICT	A	424	13/13	0.81	0.37	118,120,121,122	0

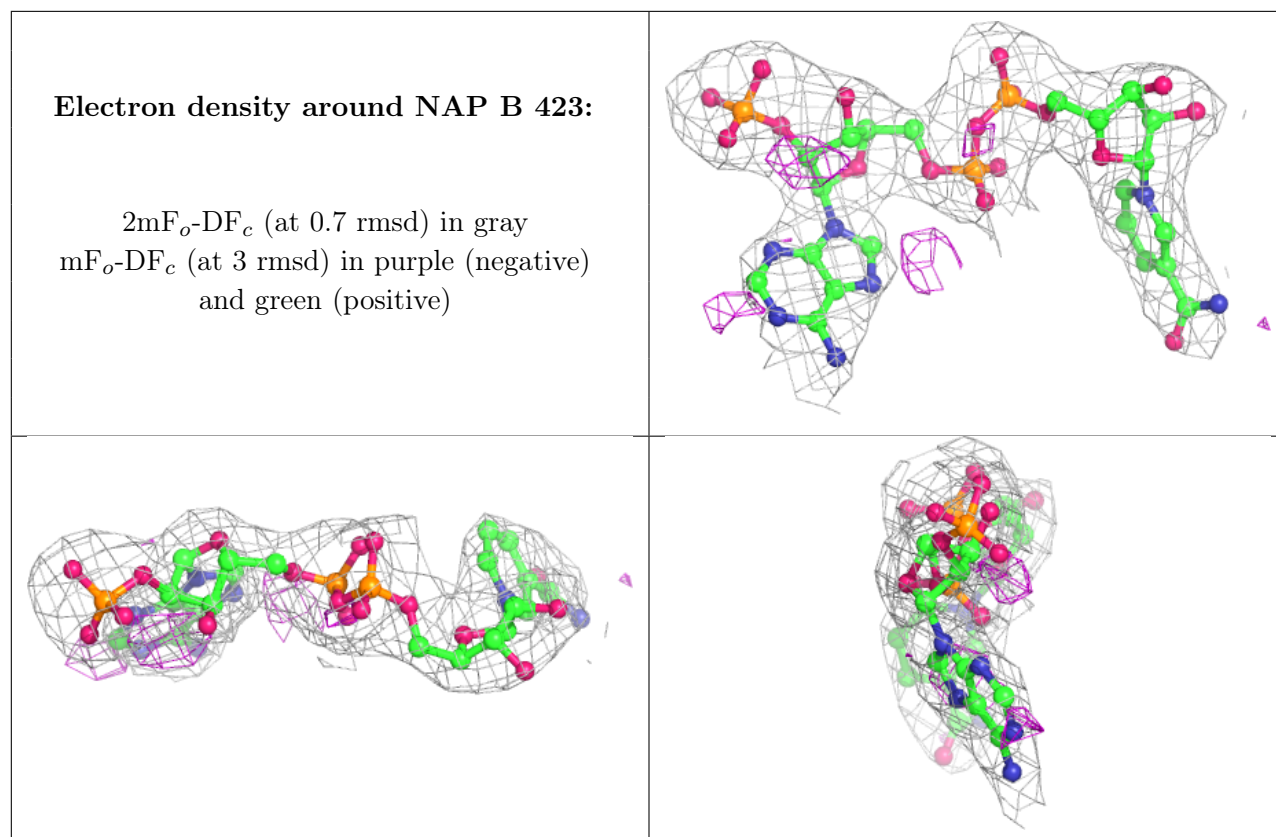
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	A	423	48/48	0.94	0.18	61,67,78,82	0
2	NAP	B	423	48/48	0.96	0.17	46,58,68,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.