Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2023 – 03:22 AM EDT

PDB ID	:	3WBB
Title	:	Crystal Structures of meso-diaminopimelate dehydrogenase from Symbiobacterium thermophilum
Authors	:	Liu, W.D.; Li, Z.; Huang, C.H.; Guo, R.T.; Wu, Q.Q.; Zhu, D.M.
Deposited on	:	2013-05-14
Resolution	:	1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

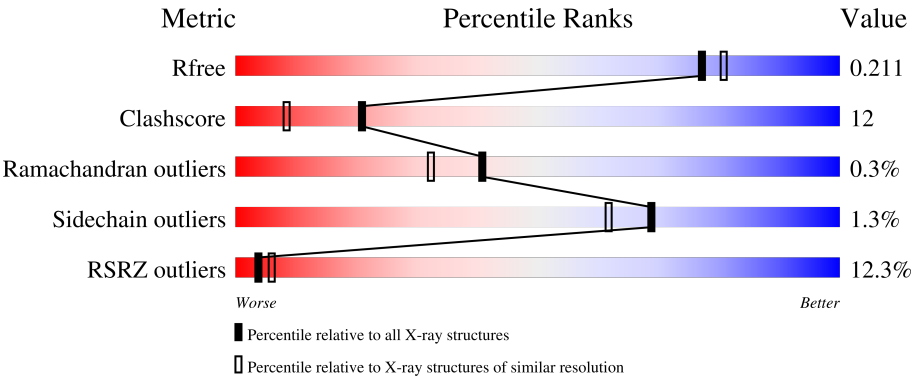
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	305	13% 77% 20%
1	B	305	12% 76% 20%
1	C	305	11% 73% 23%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	301	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8354 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.

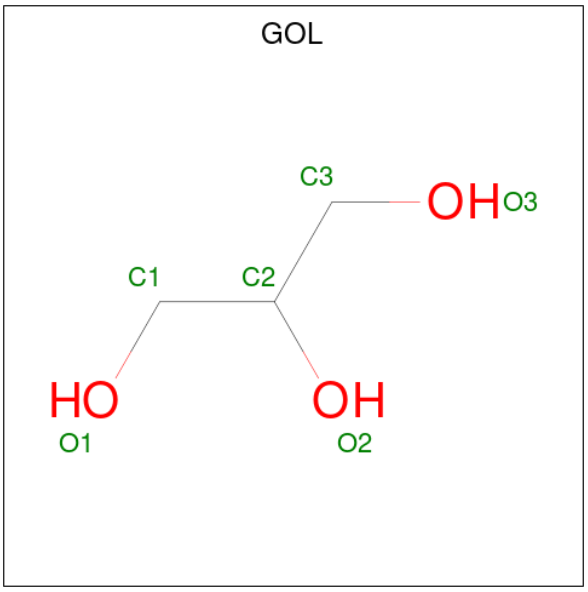
- Molecule 1 is a protein called Diaminopimelate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2259	1423	409	413	14			
1	B	297	Total	C	N	O	S	0	0	0
			2259	1423	409	413	14			
1	C	297	Total	C	N	O	S	0	0	0
			2259	1423	409	413	14			

There are 18 discrepancies between the modelled and reference sequences:

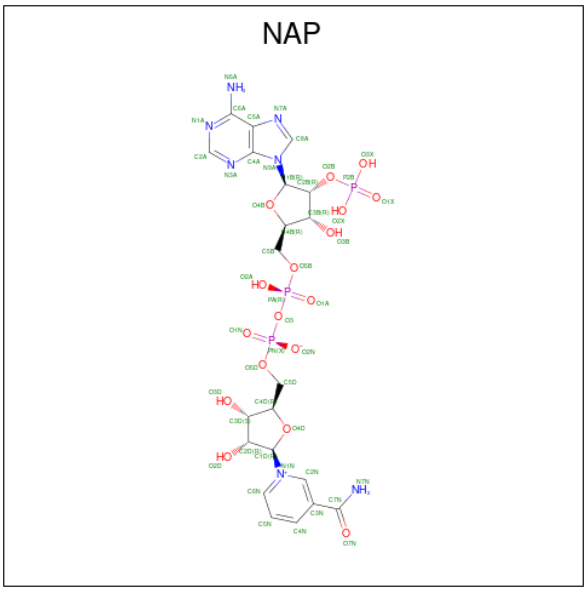
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q67PI3
A	-4	HIS	-	expression tag	UNP Q67PI3
A	-3	HIS	-	expression tag	UNP Q67PI3
A	-2	HIS	-	expression tag	UNP Q67PI3
A	-1	HIS	-	expression tag	UNP Q67PI3
A	0	HIS	-	expression tag	UNP Q67PI3
B	-5	HIS	-	expression tag	UNP Q67PI3
B	-4	HIS	-	expression tag	UNP Q67PI3
B	-3	HIS	-	expression tag	UNP Q67PI3
B	-2	HIS	-	expression tag	UNP Q67PI3
B	-1	HIS	-	expression tag	UNP Q67PI3
B	0	HIS	-	expression tag	UNP Q67PI3
C	-5	HIS	-	expression tag	UNP Q67PI3
C	-4	HIS	-	expression tag	UNP Q67PI3
C	-3	HIS	-	expression tag	UNP Q67PI3
C	-2	HIS	-	expression tag	UNP Q67PI3
C	-1	HIS	-	expression tag	UNP Q67PI3
C	0	HIS	-	expression tag	UNP Q67PI3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is water.

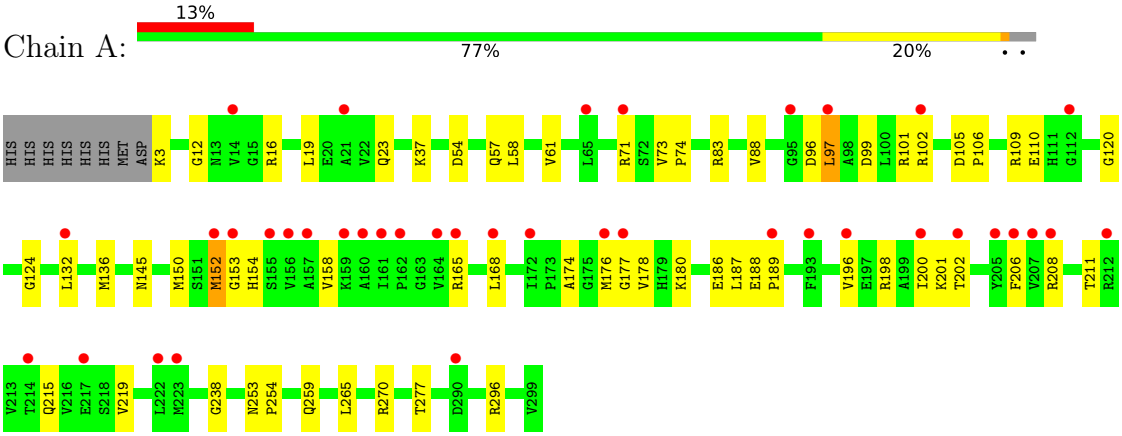
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	451	Total	O	0	0
			451	451		
4	B	444	Total	O	0	0
			444	444		
4	C	472	Total	O	0	0
			472	472		

3 Residue-property plots (i)

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

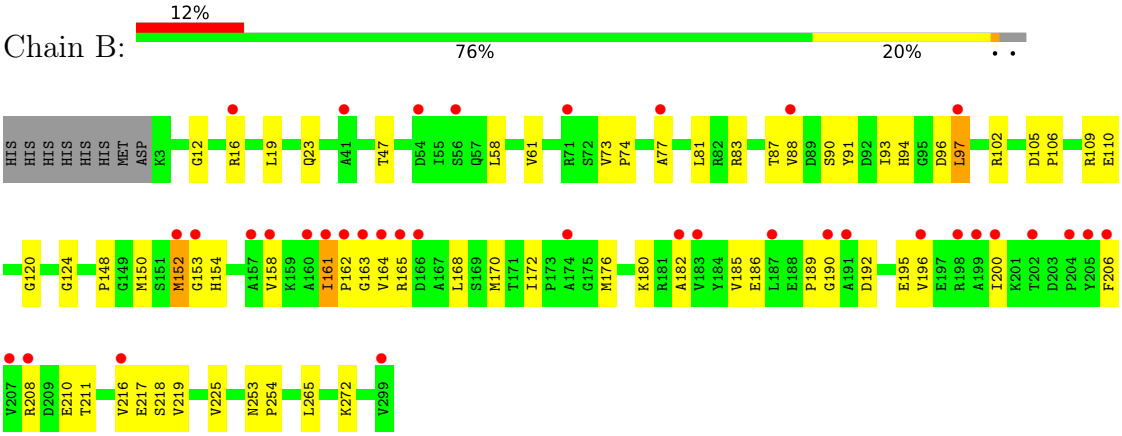
• Molecule 1: Diaminopimelate dehydrogenase

Chain A:



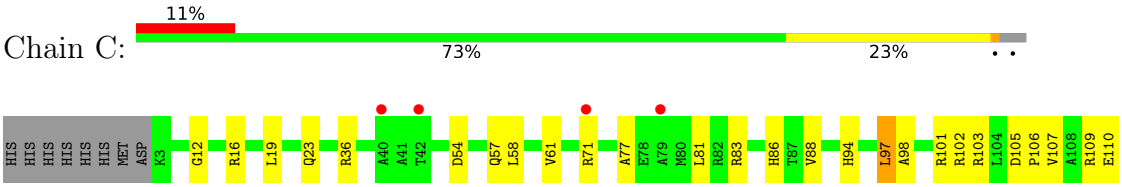
• Molecule 1: Diaminopimelate dehydrogenase

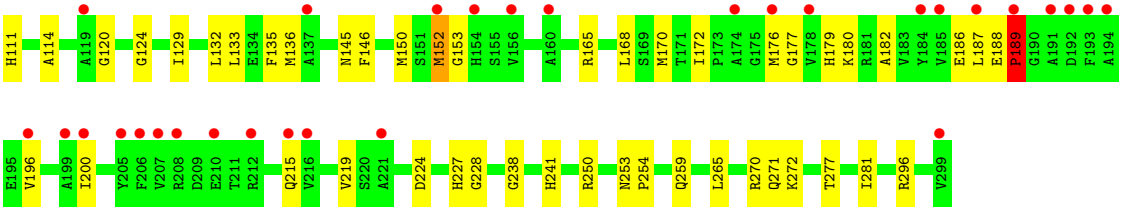
Chain B:



• Molecule 1: Diaminopimelate dehydrogenase

Chain C:




H111
A114
A119
G120
G124
I129
L132
L133
E134
F135
M136
A137
N145
F146
M150
S151
M152
G153
H154
S155
V156
A160
R165
L168
S169
M170
T171
I172
P173
A174
G175
M176
G177
V178
H179
K180
R181
A182
V183
Y184
V185
E186
L187
E188
P189
G190
A191
D192
F193
A194
E196
V196
A199
I200
Y205
F206
V207
R208
D209
E210
T211
R212
Q215
V216
V219
S220
A221
D224
H227
G228
G238
H241
R250
N253
P254
Q259
L265
R270
Q271
K272
T277
I281
R296
V299

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.82Å 99.95Å 84.83Å 90.00° 112.25° 90.00°	Depositor
Resolution (Å)	50.00 – 1.93 41.04 – 1.93	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-1.93) 93.4 (41.04-1.93)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	16.90 (at 1.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.216 0.173 , 0.211	Depositor DCC
R_{free} test set	3984 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.457 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.460 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8354	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.29	0/2301	0.62	0/3123
1	B	0.29	0/2301	0.62	0/3123
1	C	0.29	0/2301	0.63	0/3123
All	All	0.29	0/6903	0.62	0/9369

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

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	2259	0	2298	51	0
1	B	2259	0	2298	58	0
1	C	2259	0	2298	72	0
2	A	24	0	32	0	0
2	B	18	0	24	0	0
2	C	24	0	32	1	0
3	A	48	0	25	1	0
3	B	48	0	25	2	0
3	C	48	0	25	5	0
4	A	451	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	444	0	0	6	0
4	C	472	0	0	7	0
All	All	8354	0	7057	171	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 12.

All (171) 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:C:146:PHE:H	1:C:179:HIS:HE1	0.98	0.96
1:B:225:VAL:H	1:C:241:HIS:HD2	1.16	0.93
1:C:146:PHE:H	1:C:179:HIS:CE1	1.88	0.90
1:B:165:ARG:HH21	1:B:189:PRO:HD3	1.36	0.88
1:C:188:GLU:HB3	1:C:189:PRO:HD2	1.56	0.87
1:B:93:ILE:O	1:B:97:LEU:HD13	1.79	0.83
1:A:238:GLY:H	1:C:259:GLN:HE21	1.27	0.79
1:C:86:HIS:HD2	1:C:114:ALA:H	1.31	0.79
1:A:102:ARG:HH22	1:C:296:ARG:NH2	1.81	0.78
1:B:152:MET:HG3	1:B:153:GLY:H	1.48	0.78
1:B:225:VAL:H	1:C:241:HIS:CD2	2.02	0.77
1:A:259:GLN:HE21	1:C:238:GLY:H	1.33	0.76
1:A:97:LEU:HD11	4:C:461:HOH:O	1.86	0.75
3:C:305:NAP:H3B	3:C:305:NAP:H8A	1.69	0.75
1:C:188:GLU:HB3	1:C:189:PRO:CD	2.16	0.74
1:B:91:TYR:HD2	1:B:97:LEU:HD12	1.54	0.70
1:A:187:LEU:HD22	1:A:215:GLN:NE2	2.05	0.70
1:C:146:PHE:N	1:C:179:HIS:HE1	1.82	0.69
1:C:145:ASN:ND2	1:C:177:GLY:H	1.91	0.67
1:C:227:HIS:HD2	1:C:228:GLY:H	1.39	0.67
1:C:152:MET:CE	1:C:153:GLY:H	2.08	0.66
1:C:227:HIS:CD2	1:C:228:GLY:H	2.14	0.66
1:A:238:GLY:H	1:C:259:GLN:NE2	1.94	0.66
1:C:172:ILE:HB	1:C:180:LYS:HG3	1.78	0.65
1:B:158:VAL:O	1:B:161:ILE:HG23	1.98	0.63
1:A:259:GLN:NE2	1:C:238:GLY:H	1.96	0.63
1:C:54:ASP:HB3	1:C:57:GLN:NE2	2.14	0.62
1:A:102:ARG:NH2	1:C:296:ARG:NH2	2.46	0.62
1:B:192:ASP:OD2	1:B:195:GLU:HG3	1.99	0.62
1:B:12:GLY:O	1:B:16:ARG:HG3	1.99	0.61
1:B:91:TYR:CD2	1:B:97:LEU:HD12	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASN:HD21	1:C:177:GLY:H	1.47	0.61
1:C:187:LEU:HD13	1:C:215:GLN:HG3	1.82	0.61
1:A:152:MET:HG3	1:A:153:GLY:H	1.67	0.60
4:A:457:HOH:O	1:C:97:LEU:HD11	2.00	0.60
1:C:150:MET:HE3	1:C:224:ASP:H	1.65	0.60
1:B:164:VAL:HG13	1:B:185:VAL:HG13	1.84	0.58
3:B:404:NAP:H3B	3:B:404:NAP:N3A	2.18	0.58
1:C:270:ARG:HD3	4:C:835:HOH:O	2.03	0.57
1:B:272:LYS:HE2	4:B:833:HOH:O	2.04	0.57
1:B:206:PHE:HB3	1:B:211:THR:OG1	2.05	0.57
1:C:129:ILE:O	1:C:133:LEU:HD13	2.05	0.57
1:B:87:THR:HG23	4:B:503:HOH:O	2.03	0.57
1:B:83:ARG:HH11	1:B:83:ARG:HG3	1.69	0.57
1:C:152:MET:HE2	1:C:153:GLY:H	1.69	0.57
1:C:152:MET:HG2	1:C:153:GLY:N	2.20	0.56
1:B:208:ARG:HG2	4:B:850:HOH:O	2.07	0.55
1:C:94:HIS:HA	1:C:97:LEU:HD12	1.87	0.55
1:B:148:PRO:HB3	1:C:176:MET:HE2	1.89	0.54
1:A:188:GLU:HG3	1:A:189:PRO:HD2	1.89	0.54
1:A:196:VAL:O	1:A:200:ILE:HG13	2.07	0.54
1:B:172:ILE:HD12	1:C:176:MET:HE2	1.90	0.54
3:A:305:NAP:H3B	3:A:305:NAP:N3A	2.22	0.53
1:A:105:ASP:OD2	1:A:109:ARG:NH2	2.40	0.53
1:B:225:VAL:N	1:C:241:HIS:HD2	1.97	0.53
1:C:150:MET:HG2	4:C:473:HOH:O	2.10	0.52
1:B:161:ILE:HD12	1:B:163:GLY:H	1.74	0.52
1:A:54:ASP:HB3	1:A:57:GLN:NE2	2.25	0.52
1:B:81:LEU:HD21	1:B:87:THR:HG22	1.90	0.52
1:B:172:ILE:HD12	1:C:176:MET:CE	2.40	0.52
1:C:186:GLU:HB2	1:C:219:VAL:HG23	1.92	0.51
1:C:272:LYS:HE2	4:C:790:HOH:O	2.09	0.51
1:B:164:VAL:HG22	1:B:185:VAL:HG11	1.92	0.51
1:C:19:LEU:O	1:C:23:GLN:HG3	2.10	0.51
1:A:83:ARG:HD3	4:A:638:HOH:O	2.11	0.51
1:C:83:ARG:HH11	1:C:83:ARG:HG3	1.75	0.51
1:B:88:VAL:HG21	1:B:265:LEU:CA	2.40	0.51
1:C:120:GLY:O	1:C:124:GLY:HA3	2.11	0.51
1:B:154:HIS:O	1:B:158:VAL:HG23	2.12	0.50
1:C:88:VAL:HG21	1:C:265:LEU:CA	2.42	0.50
1:C:189:PRO:HA	4:C:787:HOH:O	2.12	0.50
1:C:86:HIS:CD2	1:C:114:ALA:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:NH2	1:A:189:PRO:HD3	2.27	0.50
1:A:37:LYS:HE3	4:A:630:HOH:O	2.12	0.49
1:A:176:MET:HG3	1:A:178:VAL:HG23	1.94	0.49
1:B:90:SER:O	3:B:404:NAP:H2N	2.13	0.49
1:B:94:HIS:HA	1:B:97:LEU:HD22	1.94	0.49
3:C:305:NAP:H8A	3:C:305:NAP:C3B	2.41	0.49
1:A:88:VAL:HG21	1:A:265:LEU:CA	2.43	0.49
1:C:196:VAL:O	1:C:200:ILE:HG13	2.13	0.49
1:C:132:LEU:C	1:C:136:MET:HE2	2.33	0.48
1:C:106:PRO:O	1:C:110:GLU:HG3	2.14	0.48
1:B:105:ASP:OD2	1:B:109:ARG:NH2	2.45	0.48
1:A:106:PRO:O	1:A:110:GLU:HG3	2.13	0.48
1:A:198:ARG:O	1:A:202:THR:HG22	2.13	0.48
1:B:192:ASP:HB3	1:B:195:GLU:OE1	2.14	0.48
1:A:174:ALA:HB2	1:A:180:LYS:HG3	1.96	0.48
1:C:152:MET:HG2	1:C:153:GLY:H	1.79	0.48
1:C:101:ARG:HD2	1:C:277:THR:HG23	1.96	0.48
1:A:58:LEU:O	1:A:61:VAL:HG23	2.14	0.47
1:B:180:LYS:HE3	1:B:210:GLU:OE2	2.14	0.47
1:B:216:VAL:HG12	1:B:218:SER:H	1.79	0.47
3:C:305:NAP:H3B	3:C:305:NAP:C8A	2.42	0.47
1:A:145:ASN:HD21	1:A:177:GLY:H	1.60	0.47
1:A:186:GLU:HB2	1:A:219:VAL:HG23	1.95	0.47
1:A:145:ASN:ND2	1:A:177:GLY:H	2.12	0.47
1:B:19:LEU:O	1:B:23:GLN:HG3	2.15	0.47
1:A:150:MET:HG2	1:A:168:LEU:HD11	1.95	0.47
1:A:270:ARG:HD3	4:A:411:HOH:O	2.14	0.47
1:A:102:ARG:NH2	1:C:296:ARG:HH21	2.12	0.47
1:C:36:ARG:NH2	3:C:305:NAP:H2B	2.30	0.47
1:B:176:MET:HE2	4:B:719:HOH:O	2.13	0.46
1:C:105:ASP:OD2	1:C:109:ARG:NH2	2.47	0.46
1:C:152:MET:SD	1:C:152:MET:N	2.86	0.46
1:C:12:GLY:O	1:C:16:ARG:HG3	2.14	0.46
1:A:132:LEU:C	1:A:136:MET:HE2	2.36	0.46
1:B:186:GLU:HB2	1:B:219:VAL:HG23	1.97	0.46
1:B:253:ASN:HB3	1:B:254:PRO:CD	2.45	0.46
3:C:305:NAP:C3B	3:C:305:NAP:C8A	2.94	0.46
1:A:296:ARG:NH2	1:C:102:ARG:HH12	2.13	0.46
1:A:19:LEU:O	1:A:23:GLN:HG3	2.15	0.46
1:A:12:GLY:O	1:A:16:ARG:HG3	2.15	0.46
1:B:161:ILE:CD1	1:B:163:GLY:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:MET:HE3	1:C:224:ASP:N	2.32	0.45
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.81	0.45
1:B:106:PRO:O	1:B:110:GLU:HG3	2.15	0.45
1:A:120:GLY:O	1:A:124:GLY:HA3	2.15	0.45
1:B:120:GLY:O	1:B:124:GLY:HA3	2.16	0.45
1:A:201:LYS:HE3	1:A:211:THR:O	2.17	0.45
1:B:225:VAL:CG2	1:B:254:PRO:CD	2.94	0.45
1:A:187:LEU:HB2	1:A:215:GLN:HE21	1.82	0.45
1:B:216:VAL:HG12	1:B:217:GLU:N	2.30	0.45
1:B:225:VAL:HG22	1:B:254:PRO:HD3	1.99	0.45
1:C:97:LEU:HD22	1:C:98:ALA:N	2.31	0.45
1:B:225:VAL:CG2	1:B:254:PRO:HD3	2.47	0.45
1:A:165:ARG:HH22	1:A:189:PRO:HD3	1.81	0.45
1:A:253:ASN:HB3	1:A:254:PRO:CD	2.47	0.45
1:C:103:ARG:HH11	2:C:302:GOL:H12	1.82	0.44
1:A:165:ARG:HD2	1:A:186:GLU:OE2	2.17	0.44
1:B:152:MET:HB3	4:B:555:HOH:O	2.18	0.44
1:C:77:ALA:O	1:C:81:LEU:HG	2.17	0.44
1:A:154:HIS:O	1:A:158:VAL:HG23	2.18	0.44
1:B:225:VAL:HG22	1:B:254:PRO:CD	2.48	0.43
1:C:253:ASN:HB3	1:C:254:PRO:CD	2.48	0.43
1:C:107:VAL:O	1:C:111:HIS:HD2	2.01	0.43
1:B:161:ILE:HD12	1:B:162:PRO:N	2.34	0.43
1:C:152:MET:HG3	4:C:871:HOH:O	2.17	0.43
1:C:97:LEU:HD13	1:C:97:LEU:H	1.82	0.43
1:C:165:ARG:HD2	1:C:186:GLU:OE2	2.18	0.43
1:A:206:PHE:HB3	1:A:211:THR:OG1	2.19	0.43
1:B:58:LEU:O	1:B:61:VAL:HG23	2.19	0.43
1:C:250:ARG:HA	1:C:250:ARG:HD3	1.87	0.42
1:A:102:ARG:HD2	4:A:754:HOH:O	2.20	0.42
1:B:196:VAL:O	1:B:200:ILE:HG13	2.19	0.42
1:A:208:ARG:HH11	1:A:208:ARG:HG2	1.84	0.42
4:A:802:HOH:O	1:B:47:THR:HG21	2.19	0.42
1:C:58:LEU:O	1:C:61:VAL:HG23	2.20	0.42
1:B:192:ASP:O	1:B:196:VAL:HG23	2.20	0.42
1:A:102:ARG:HH22	1:C:296:ARG:HH21	1.60	0.42
1:C:271:GLN:CD	1:C:281:ILE:HD12	2.39	0.42
1:B:172:ILE:CG2	1:C:176:MET:HG3	2.50	0.42
1:B:190:GLY:HA3	4:B:869:HOH:O	2.20	0.42
1:B:73:VAL:HB	1:B:74:PRO:HD3	2.02	0.41
1:A:101:ARG:HD2	1:A:277:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MET:HB3	4:A:739:HOH:O	2.20	0.41
1:A:73:VAL:HB	1:A:74:PRO:HD3	2.02	0.41
1:B:91:TYR:HD2	1:B:97:LEU:CD1	2.28	0.41
1:A:71:ARG:NH1	1:A:71:ARG:HG3	2.35	0.41
1:C:152:MET:CG	1:C:153:GLY:N	2.84	0.41
1:A:3:LYS:HE3	1:A:3:LYS:HB2	1.95	0.41
1:C:150:MET:HE1	1:C:168:LEU:CD1	2.50	0.41
1:C:102:ARG:NH2	4:C:712:HOH:O	2.53	0.41
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.86	0.41
1:B:170:MET:HB2	1:B:182:ALA:HB3	2.03	0.41
1:C:170:MET:HB2	1:C:182:ALA:HB3	2.03	0.41
1:B:77:ALA:O	1:B:81:LEU:HG	2.21	0.40
1:B:150:MET:HG2	1:B:168:LEU:HD11	2.04	0.40
1:C:132:LEU:HD23	1:C:135:PHE:CE2	2.56	0.40
1:B:83:ARG:HG3	1:B:83:ARG:NH1	2.34	0.40
1:A:99:ASP:OD1	1:A:102:ARG:NH2	2.54	0.40
1:A:152:MET:CG	1:A:153:GLY:H	2.33	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	295/305 (97%)	285 (97%)	9 (3%)	1 (0%)	41	32
1	B	295/305 (97%)	285 (97%)	9 (3%)	1 (0%)	41	32
1	C	295/305 (97%)	285 (97%)	9 (3%)	1 (0%)	41	32
All	All	885/915 (97%)	855 (97%)	27 (3%)	3 (0%)	41	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	MET
1	B	152	MET
1	C	189	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/243 (97%)	233 (99%)	2 (1%)	78	75
1	B	235/243 (97%)	232 (99%)	3 (1%)	69	62
1	C	235/243 (97%)	231 (98%)	4 (2%)	60	49
All	All	705/729 (97%)	696 (99%)	9 (1%)	69	62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASP
1	A	97	LEU
1	B	96	ASP
1	B	97	LEU
1	B	161	ILE
1	C	71	ARG
1	C	97	LEU
1	C	152	MET
1	C	189	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	57	GLN
1	A	145	ASN
1	A	215	GLN
1	A	242	ASN
1	A	259	GLN

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Mol	Chain	Res	Type
1	C	57	GLN
1	C	86	HIS
1	C	111	HIS
1	C	145	ASN
1	C	179	HIS
1	C	227	HIS
1	C	241	HIS
1	C	242	ASN
1	C	259	GLN

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)

14 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	GOL	A	302	-	5,5,5	0.30	0	5,5,5	0.28	0
2	GOL	B	402	-	5,5,5	0.30	0	5,5,5	0.24	0
2	GOL	A	304	-	5,5,5	0.30	0	5,5,5	0.27	0
2	GOL	B	401	-	5,5,5	0.30	0	5,5,5	0.27	0
2	GOL	C	302	-	5,5,5	0.31	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	A	301	-	5,5,5	0.30	0	5,5,5	0.28	0
2	GOL	C	303	-	5,5,5	0.30	0	5,5,5	0.29	0
2	GOL	B	403	-	5,5,5	0.31	0	5,5,5	0.31	0
2	GOL	C	301	-	5,5,5	0.31	0	5,5,5	0.27	0
3	NAP	A	305	-	45,52,52	1.90	9 (20%)	56,80,80	1.42	6 (10%)
2	GOL	A	303	-	5,5,5	0.31	0	5,5,5	0.27	0
3	NAP	B	404	-	45,52,52	1.91	9 (20%)	56,80,80	1.39	5 (8%)
3	NAP	C	305	-	45,52,52	1.90	9 (20%)	56,80,80	1.45	6 (10%)
2	GOL	C	304	-	5,5,5	0.30	0	5,5,5	0.27	0

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	GOL	A	302	-	-	0/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	A	304	-	-	0/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	C	302	-	-	0/4/4/4	-
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	C	303	-	-	0/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
3	NAP	A	305	-	-	1/31/67/67	0/5/5/5
2	GOL	A	303	-	-	0/4/4/4	-
3	NAP	B	404	-	-	7/31/67/67	0/5/5/5
3	NAP	C	305	-	-	1/31/67/67	0/5/5/5
2	GOL	C	304	-	-	0/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	NAP	C3N-C7N	-7.40	1.39	1.50
3	C	305	NAP	C3N-C7N	-7.35	1.39	1.50
3	A	305	NAP	C3N-C7N	-7.32	1.39	1.50
3	B	404	NAP	C2A-N3A	5.19	1.40	1.32
3	A	305	NAP	C2A-N3A	5.17	1.40	1.32
3	C	305	NAP	C2A-N3A	5.12	1.40	1.32
3	A	305	NAP	C2N-N1N	4.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	305	NAP	C2N-N1N	4.47	1.40	1.35
3	B	404	NAP	C2N-N1N	4.44	1.40	1.35
3	A	305	NAP	C2A-N1A	3.46	1.40	1.33
3	C	305	NAP	C2A-N1A	3.46	1.40	1.33
3	B	404	NAP	C2A-N1A	3.44	1.40	1.33
3	B	404	NAP	C5A-C4A	-2.78	1.33	1.40
3	A	305	NAP	C5A-C4A	-2.77	1.33	1.40
3	C	305	NAP	C5A-C4A	-2.76	1.33	1.40
3	C	305	NAP	C6A-C5A	-2.63	1.33	1.43
3	B	404	NAP	C6A-C5A	-2.63	1.33	1.43
3	A	305	NAP	C6A-C5A	-2.62	1.33	1.43
3	B	404	NAP	O4D-C1D	2.38	1.44	1.41
3	C	305	NAP	O4B-C1B	2.35	1.44	1.41
3	A	305	NAP	O4B-C1B	2.32	1.44	1.41
3	B	404	NAP	O4B-C1B	2.28	1.44	1.41
3	A	305	NAP	O4D-C1D	2.25	1.44	1.41
3	C	305	NAP	O4D-C1D	2.18	1.44	1.41
3	B	404	NAP	C6N-N1N	2.12	1.40	1.35
3	A	305	NAP	C6N-N1N	2.07	1.40	1.35
3	C	305	NAP	C6N-N1N	2.07	1.40	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	305	NAP	N3A-C2A-N1A	-7.01	117.72	128.68
3	B	404	NAP	N3A-C2A-N1A	-6.95	117.82	128.68
3	C	305	NAP	N3A-C2A-N1A	-6.87	117.94	128.68
3	C	305	NAP	PN-O3-PA	-3.50	120.80	132.83
3	A	305	NAP	PN-O3-PA	-3.34	121.37	132.83
3	C	305	NAP	C5A-C6A-N6A	-2.69	116.26	120.35
3	B	404	NAP	C5A-C6A-N6A	-2.67	116.30	120.35
3	A	305	NAP	C5A-C6A-N6A	-2.62	116.37	120.35
3	B	404	NAP	C6N-N1N-C2N	-2.44	119.75	121.97
3	B	404	NAP	C3N-C7N-N7N	-2.40	114.87	117.75
3	B	404	NAP	PN-O3-PA	-2.39	124.64	132.83
3	C	305	NAP	C3N-C7N-N7N	-2.30	114.99	117.75
3	A	305	NAP	O4D-C4D-C3D	-2.26	100.65	105.11
3	C	305	NAP	O4D-C4D-C3D	-2.23	100.71	105.11
3	A	305	NAP	C3N-C7N-N7N	-2.19	115.12	117.75
3	C	305	NAP	C6N-N1N-C2N	-2.19	119.98	121.97
3	A	305	NAP	C6N-N1N-C2N	-2.18	119.99	121.97

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	NAP	C5B-O5B-PA-O1A
3	B	404	NAP	C5B-O5B-PA-O2A
3	B	404	NAP	PA-O3-PN-O5D
3	B	404	NAP	C2B-O2B-P2B-O2X
3	B	404	NAP	O4B-C4B-C5B-O5B
3	B	404	NAP	C5B-O5B-PA-O3
3	A	305	NAP	O4B-C4B-C5B-O5B
3	C	305	NAP	O4B-C4B-C5B-O5B
3	B	404	NAP	O4D-C4D-C5D-O5D

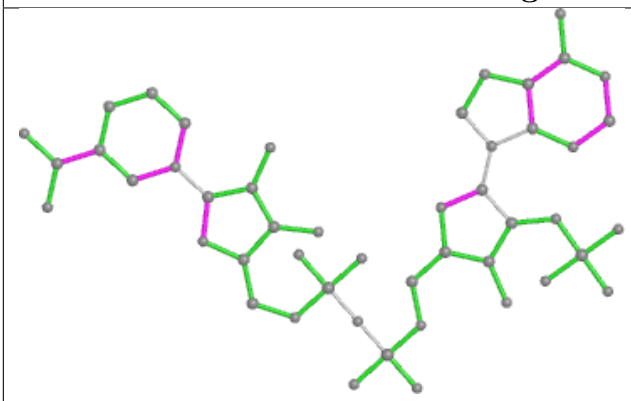
There are no ring outliers.

4 monomers are involved in 9 short contacts:

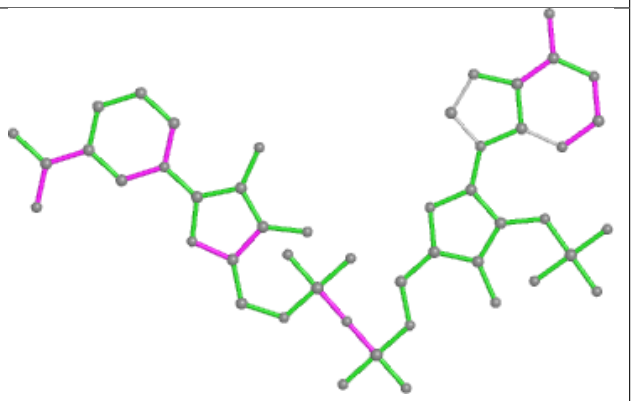
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	GOL	1	0
3	A	305	NAP	1	0
3	B	404	NAP	2	0
3	C	305	NAP	5	0

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 then 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.

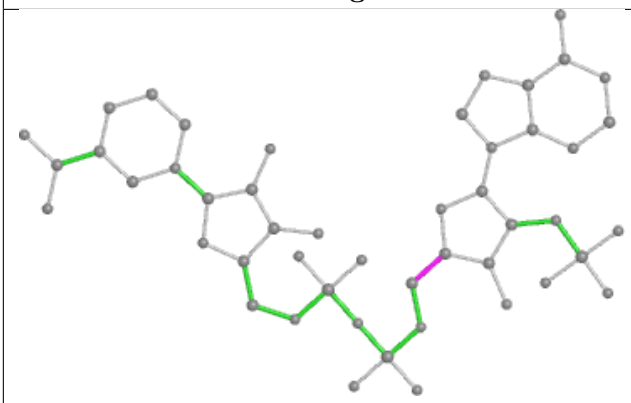
Ligand NAP A 305



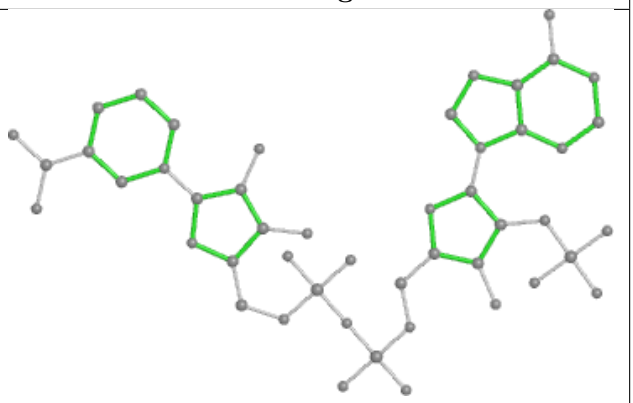
Bond lengths



Bond angles

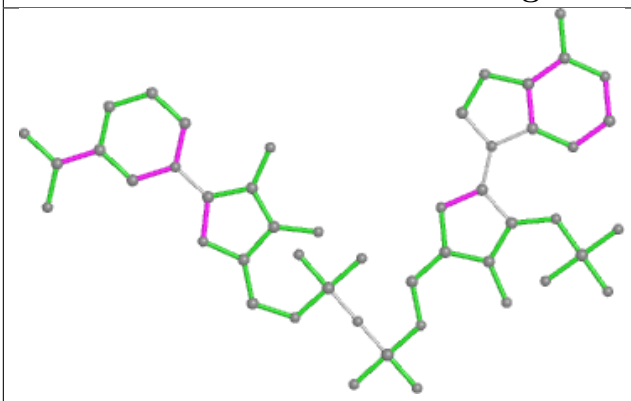


Torsions

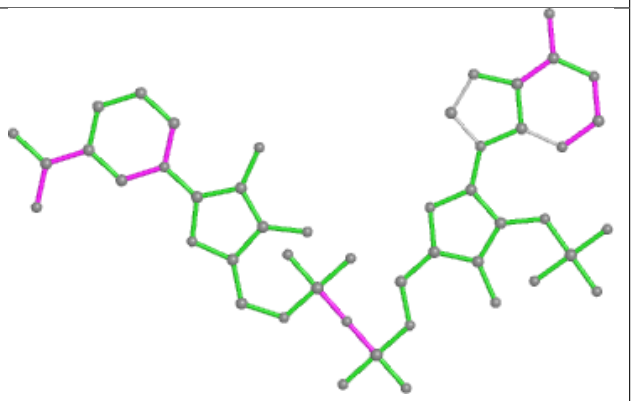


Rings

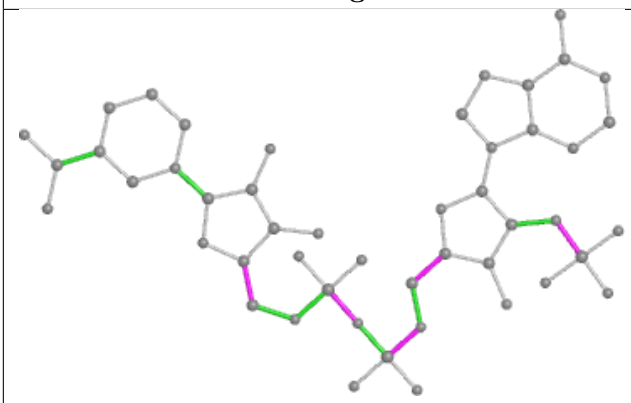
Ligand NAP B 404



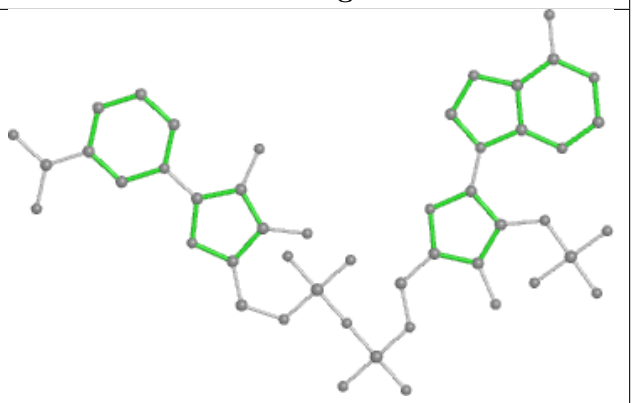
Bond lengths



Bond angles

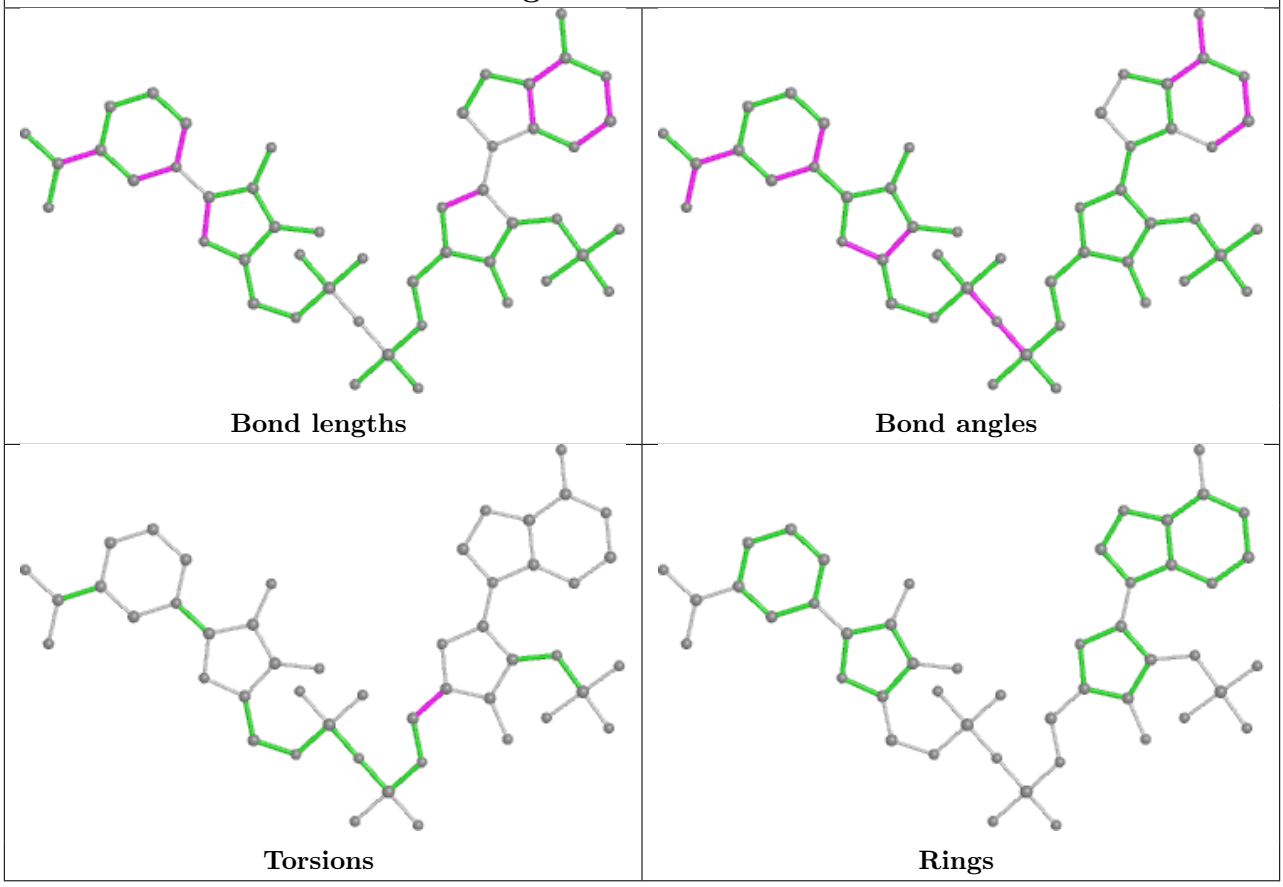


Torsions



Rings

Ligand NAP C 305



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	297/305 (97%)	0.98	39 (13%)	3 5	19, 26, 59, 67	0
1	B	297/305 (97%)	1.04	37 (12%)	3 5	18, 26, 58, 68	0
1	C	297/305 (97%)	1.00	34 (11%)	5 7	19, 26, 59, 68	0
All	All	891/915 (97%)	1.01	110 (12%)	4 6	18, 26, 59, 68	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ALA	7.9
1	A	205	TYR	7.7
1	C	205	TYR	7.3
1	C	189	PRO	6.7
1	C	206	PHE	6.3
1	B	152	MET	6.2
1	B	163	GLY	5.9
1	B	205	TYR	5.2
1	B	191	ALA	5.0
1	C	174	ALA	4.6
1	B	202	THR	4.5
1	A	164	VAL	4.4
1	B	206	PHE	4.2
1	A	189	PRO	4.2
1	C	196	VAL	4.2
1	B	208	ARG	4.1
1	B	153	GLY	4.0
1	A	152	MET	4.0
1	B	190	GLY	3.9
1	C	208	ARG	3.8
1	B	161	ILE	3.8
1	A	200	ILE	3.8
1	C	207	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	162	PRO	3.7
1	B	97	LEU	3.7
1	B	187	LEU	3.6
1	C	156	VAL	3.6
1	C	154	HIS	3.6
1	B	77	ALA	3.6
1	C	187	LEU	3.5
1	B	198	ARG	3.4
1	A	21	ALA	3.3
1	B	158	VAL	3.3
1	A	177	GLY	3.1
1	B	166	ASP	3.1
1	A	112	GLY	3.1
1	C	221	ALA	3.1
1	A	208	ARG	3.1
1	C	176	MET	3.0
1	C	193	PHE	3.0
1	A	97	LEU	2.9
1	A	217	GLU	2.9
1	A	132	LEU	2.9
1	B	183	VAL	2.9
1	C	216	VAL	2.9
1	A	196	VAL	2.8
1	A	159	LYS	2.8
1	A	14	VAL	2.8
1	B	196	VAL	2.8
1	A	214	THR	2.8
1	C	160	ALA	2.7
1	C	194	ALA	2.7
1	A	168	LEU	2.7
1	A	165	ARG	2.7
1	B	299	VAL	2.7
1	C	212	ARG	2.7
1	B	204	PRO	2.7
1	B	164	VAL	2.7
1	C	178	VAL	2.7
1	A	160	ALA	2.7
1	C	79	ALA	2.6
1	C	191	ALA	2.6
1	C	210	GLU	2.6
1	A	71	ARG	2.6
1	A	65	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	2.5
1	C	137	ALA	2.5
1	A	172	ILE	2.5
1	A	222	LEU	2.5
1	B	200	ILE	2.4
1	A	290	ASP	2.4
1	C	192	ASP	2.4
1	A	155	SER	2.4
1	B	165	ARG	2.4
1	A	156	VAL	2.3
1	A	161	ILE	2.3
1	A	212	ARG	2.3
1	C	71	ARG	2.3
1	A	176	MET	2.3
1	A	206	PHE	2.3
1	A	95	GLY	2.3
1	A	102	ARG	2.3
1	C	152	MET	2.3
1	A	202	THR	2.3
1	C	200	ILE	2.2
1	C	184	TYR	2.2
1	A	223	MET	2.2
1	C	119	ALA	2.2
1	C	199	ALA	2.2
1	B	174	ALA	2.2
1	B	16	ARG	2.1
1	B	216	VAL	2.1
1	A	157	ALA	2.1
1	B	54	ASP	2.1
1	C	299	VAL	2.1
1	A	162	PRO	2.1
1	A	153	GLY	2.1
1	C	42	THR	2.1
1	A	193	PHE	2.1
1	B	41	ALA	2.1
1	C	215	GLN	2.1
1	B	157	ALA	2.0
1	B	88	VAL	2.0
1	B	207	VAL	2.0
1	C	185	VAL	2.0
1	B	182	ALA	2.0
1	B	199	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	40	ALA	2.0
1	B	56	SER	2.0
1	B	71	ARG	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)

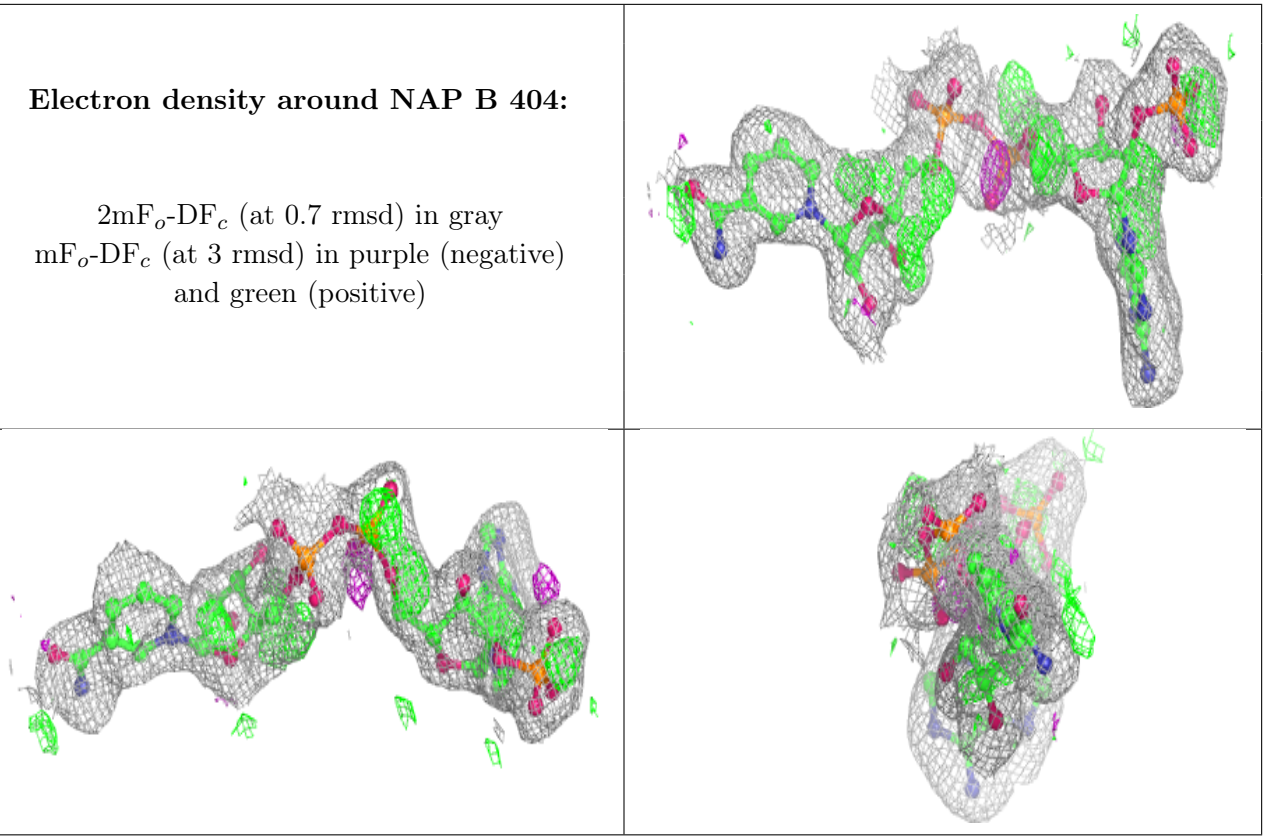
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	304	6/6	0.58	0.23	63,63,64,64	0
2	GOL	C	301	6/6	0.62	0.41	71,72,72,73	0
2	GOL	A	304	6/6	0.65	0.25	70,71,71,71	0
2	GOL	A	301	6/6	0.66	0.26	70,71,71,72	0
2	GOL	A	303	6/6	0.69	0.32	70,70,71,71	0
2	GOL	A	302	6/6	0.72	0.18	47,50,53,54	0
2	GOL	B	402	6/6	0.76	0.22	72,72,73,74	0
2	GOL	B	401	6/6	0.77	0.22	60,61,61,62	0
2	GOL	C	303	6/6	0.78	0.19	43,46,48,51	0
2	GOL	C	302	6/6	0.79	0.23	69,70,70,70	0
3	NAP	B	404	48/48	0.83	0.16	22,29,41,45	0
3	NAP	A	305	48/48	0.84	0.16	23,28,30,31	0
3	NAP	C	305	48/48	0.85	0.15	22,27,40,43	0
2	GOL	B	403	6/6	0.88	0.20	41,45,48,49	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.

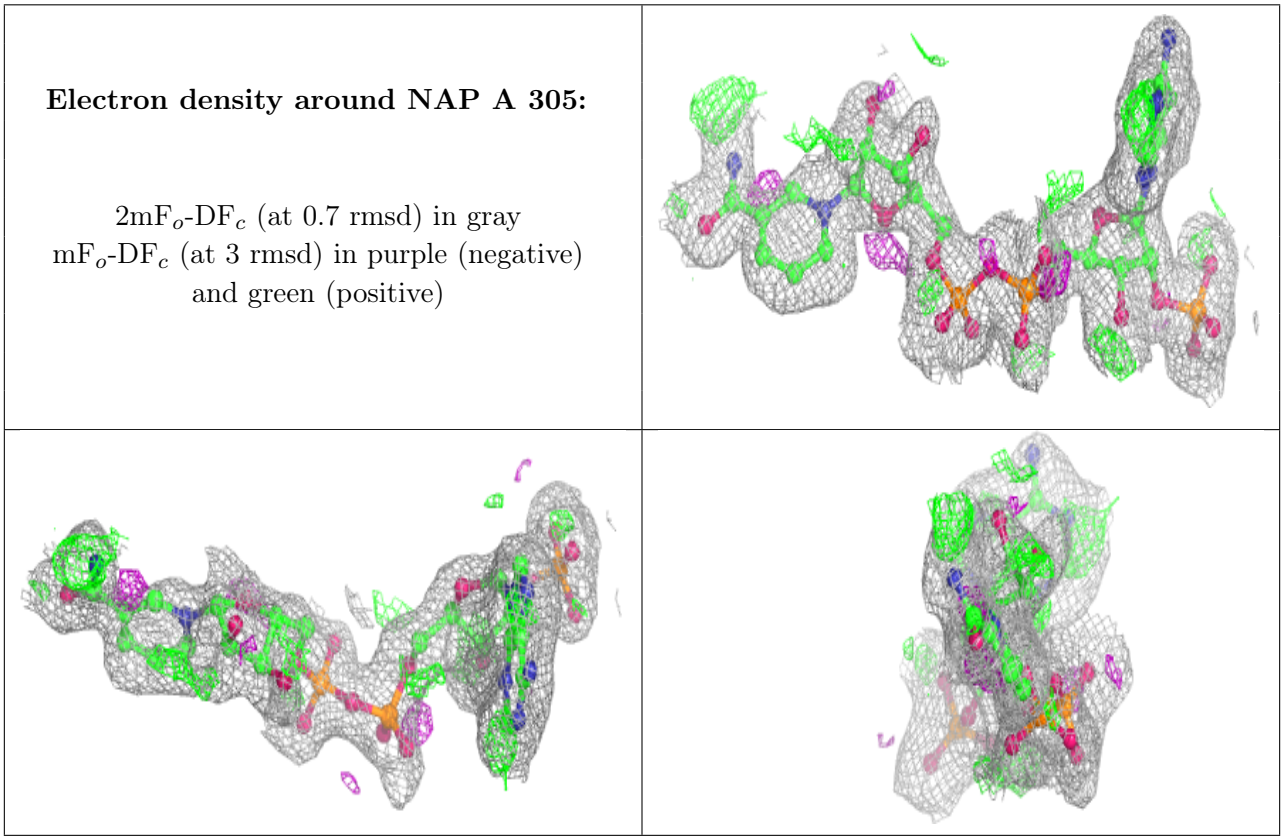
Electron density around NAP B 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



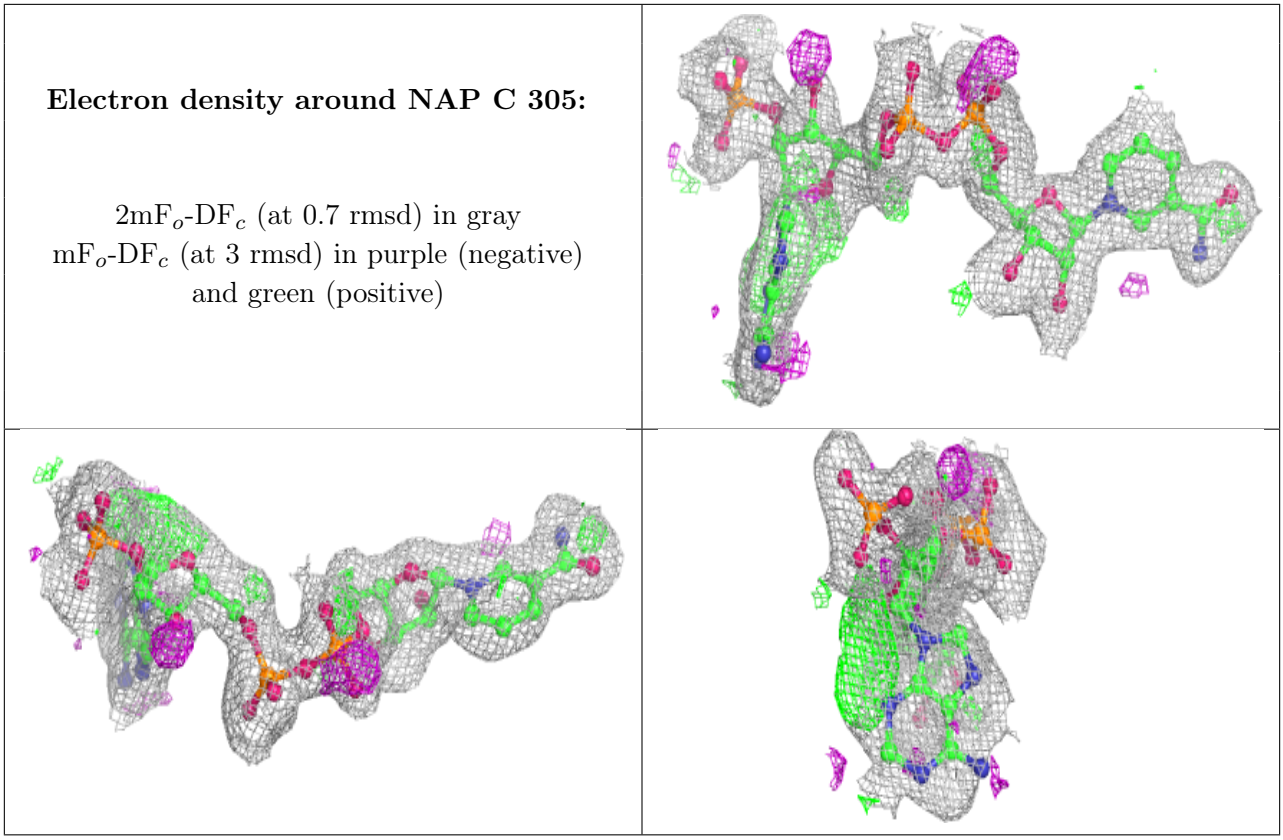
Electron density around NAP A 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAP C 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.