



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 05:05 PM EDT

PDB ID : 2HK9  
Title : Crystal structure of shikimate dehydrogenase from aquifex aeolicus in complex with shikimate and NADP+ at 2.2 angstrom resolution  
Authors : Gan, J.H.; Prabakaran, P.; Gu, Y.J.; Andrykovitch, M.; Li, Y.; Liu, H.H.; Yan, H.; Ji, X.  
Deposited on : 2006-07-03  
Resolution : 2.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

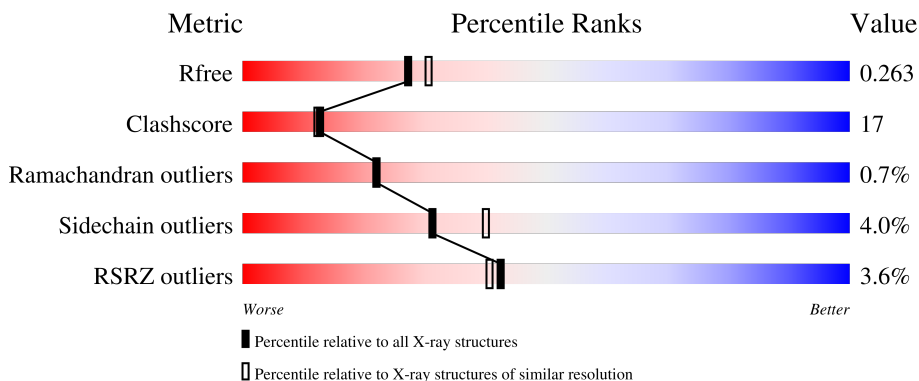
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	275	
1	B	275	
1	C	275	
1	D	275	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8871 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 Shikimate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	Total 2127	C 1392	N 346	O 386	S 3	0	0	0
1	B	267	Total 2111	C 1384	N 341	O 383	S 3	0	0	0
1	C	266	Total 2103	C 1378	N 340	O 382	S 3	0	0	0
1	D	266	Total 2103	C 1378	N 340	O 382	S 3	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

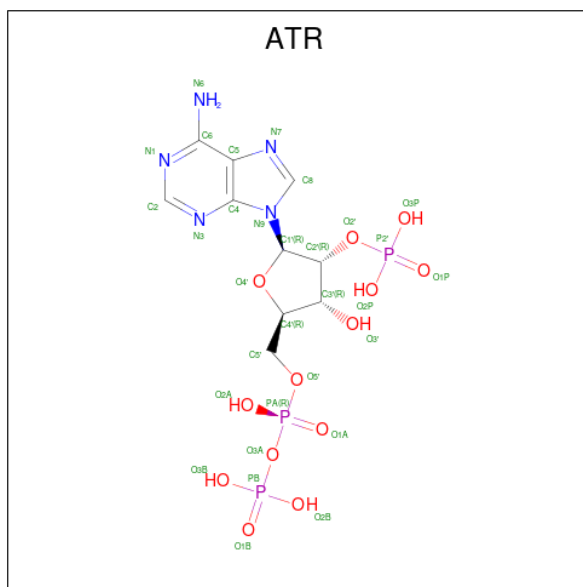
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP O67049
A	-4	HIS	-	expression tag	UNP O67049
A	-3	HIS	-	expression tag	UNP O67049
A	-2	HIS	-	expression tag	UNP O67049
A	-1	HIS	-	expression tag	UNP O67049
A	0	HIS	-	expression tag	UNP O67049
A	195	GLU	LYS	SEE REMARK 999	UNP O67049
A	233	LEU	PHE	SEE REMARK 999	UNP O67049
B	-5	HIS	-	expression tag	UNP O67049
B	-4	HIS	-	expression tag	UNP O67049
B	-3	HIS	-	expression tag	UNP O67049
B	-2	HIS	-	expression tag	UNP O67049
B	-1	HIS	-	expression tag	UNP O67049
B	0	HIS	-	expression tag	UNP O67049
B	195	GLU	LYS	SEE REMARK 999	UNP O67049
B	233	LEU	PHE	SEE REMARK 999	UNP O67049
C	-5	HIS	-	expression tag	UNP O67049
C	-4	HIS	-	expression tag	UNP O67049
C	-3	HIS	-	expression tag	UNP O67049
C	-2	HIS	-	expression tag	UNP O67049
C	-1	HIS	-	expression tag	UNP O67049

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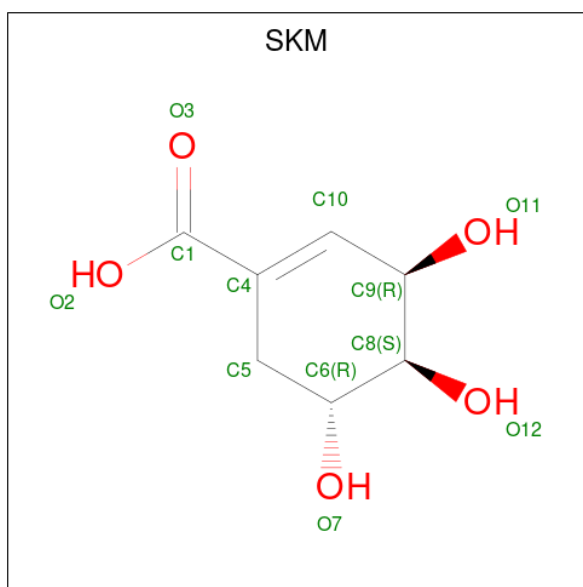
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP O67049
C	195	GLU	LYS	SEE REMARK 999	UNP O67049
C	233	LEU	PHE	SEE REMARK 999	UNP O67049
D	-5	HIS	-	expression tag	UNP O67049
D	-4	HIS	-	expression tag	UNP O67049
D	-3	HIS	-	expression tag	UNP O67049
D	-2	HIS	-	expression tag	UNP O67049
D	-1	HIS	-	expression tag	UNP O67049
D	0	HIS	-	expression tag	UNP O67049
D	195	GLU	LYS	SEE REMARK 999	UNP O67049
D	233	LEU	PHE	SEE REMARK 999	UNP O67049

- Molecule 2 is 2'-MONOPHOSPHOADENOSINE-5'-DIPHOSPHATE (three-letter code: ATR) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



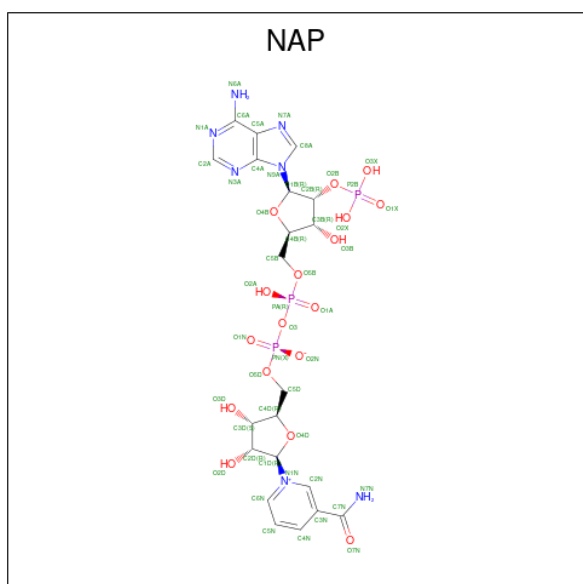
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0

- Molecule 3 is (3R,4S,5R)-3,4,5-TRIHIDROXYCYCLOHEX-1-ENE-1-CARBOXYLIC ACID (three-letter code: SKM) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 7 5	0	0
3	B	1	Total C O 12 7 5	0	0
3	C	1	Total C O 12 7 5	0	0
3	D	1	Total C O 12 7 5	0	0

- Molecule 4 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
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

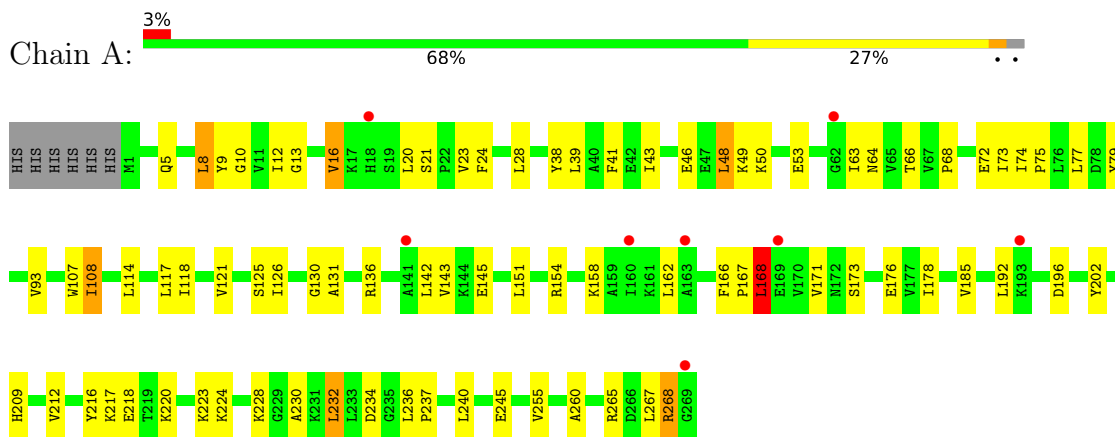
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	46	Total	O	0	0
			46	46		
5	C	56	Total	O	0	0
			56	56		
5	D	46	Total	O	0	0
			46	46		

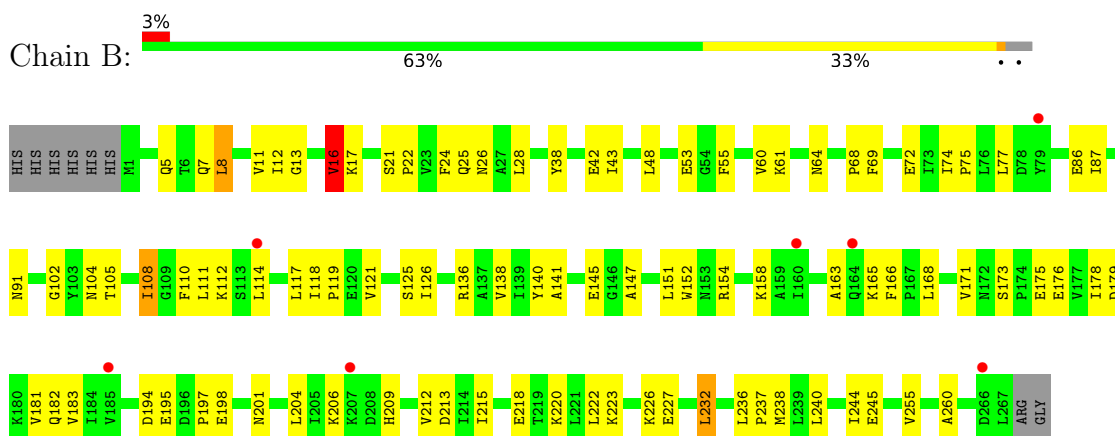
### 3 Residue-property plots [i](#)

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.

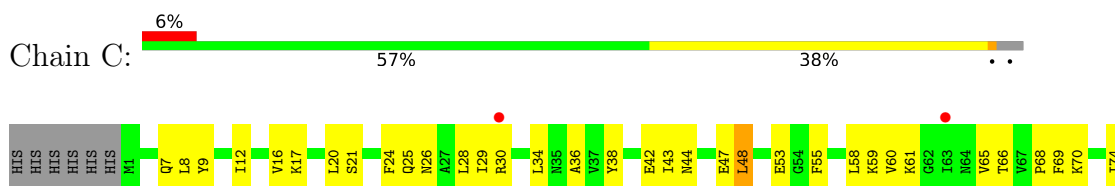
- Molecule 1: Shikimate dehydrogenase

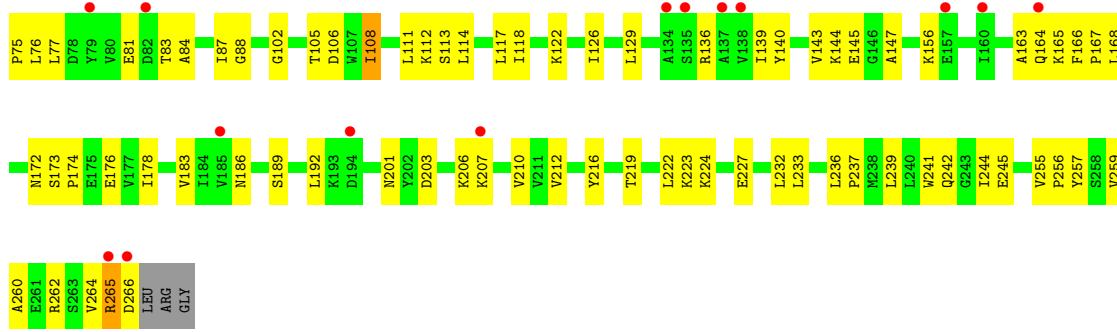


- Molecule 1: Shikimate dehydrogenase

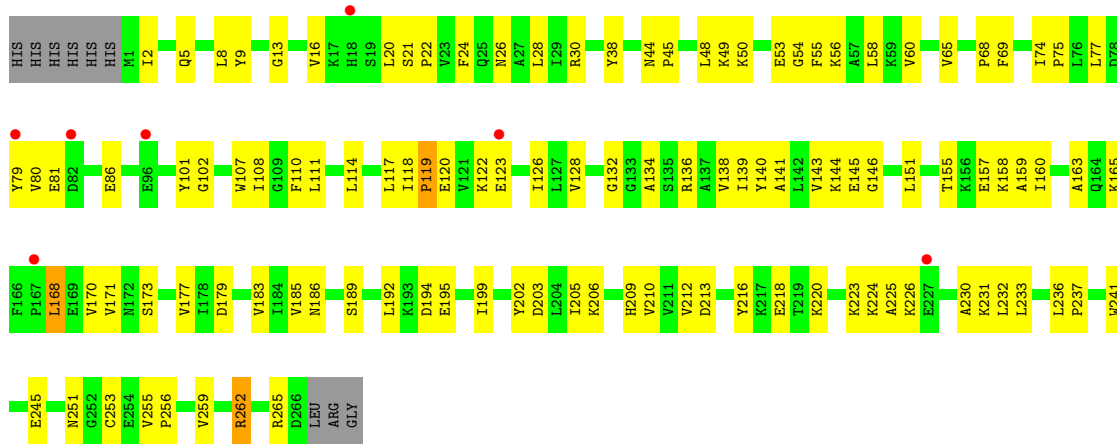


- Molecule 1: Shikimate dehydrogenase





● Molecule 1: Shikimate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.00Å 119.80Å 128.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 2.20 30.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	82.3 (29.41-2.20) 82.5 (30.01-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.271 0.198 , 0.263	Depositor DCC
$R_{free}$ test set	2407 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: ATR, SKM, 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	0.38	0/2169	0.63	1/2930 (0.0%)
1	B	0.38	0/2153	0.61	0/2911
1	C	0.38	0/2145	0.63	0/2900
1	D	0.37	0/2145	0.61	0/2900
All	All	0.38	0/8612	0.62	1/11641 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LEU	CA-CB-CG	5.04	126.89	115.30

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	2127	0	2222	67	0
1	B	2111	0	2206	80	0
1	C	2103	0	2195	79	0
1	D	2103	0	2195	81	0
2	A	31	0	11	1	0
3	A	12	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	9	0	0
3	C	12	0	9	0	0
3	D	12	0	9	0	0
4	B	48	0	25	2	0
4	C	48	0	25	0	0
4	D	48	0	25	2	0
5	A	56	0	0	0	0
5	B	46	0	0	2	0
5	C	56	0	0	3	0
5	D	46	0	0	2	0
All	All	8871	0	8940	293	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 17.

All (293) 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:D:118:ILE:HD11	1:D:210:VAL:HG11	1.34	1.04
1:C:28:LEU:HD22	1:C:255:VAL:HG11	1.40	1.03
1:D:111:LEU:HD13	1:D:141:ALA:HB1	1.41	1.00
1:C:206:LYS:HG2	1:C:207:LYS:N	1.91	0.86
1:C:206:LYS:HG2	1:C:207:LYS:H	1.41	0.84
1:A:13:GLY:HA3	1:A:66:THR:HG22	1.62	0.81
1:C:108:ILE:HD11	1:C:112:LYS:HE2	1.62	0.81
1:C:118:ILE:HD11	1:C:210:VAL:HG11	1.67	0.76
1:C:105:THR:HG23	5:C:1355:HOH:O	1.86	0.75
1:A:108:ILE:HG13	1:D:195:GLU:HG2	1.69	0.74
1:A:178:ILE:HG23	1:A:209:HIS:CE1	2.23	0.73
1:A:268:ARG:HH11	1:A:268:ARG:HB2	1.54	0.73
1:B:121:VAL:HG22	1:B:147:ALA:HB2	1.70	0.73
1:B:226:LYS:HB2	1:B:232:LEU:HD13	1.70	0.73
1:D:55:PHE:HD1	1:D:60:VAL:HG21	1.54	0.72
1:D:185:VAL:HG13	1:D:212:VAL:HG23	1.70	0.72
1:B:195:GLU:HG3	1:C:108:ILE:HG12	1.71	0.72
1:B:28:LEU:HD22	1:B:255:VAL:HG11	1.72	0.71
1:D:185:VAL:HG13	1:D:212:VAL:CG2	2.20	0.71
1:A:5:GLN:NE2	1:B:17:LYS:HD2	2.06	0.71
1:C:28:LEU:HD22	1:C:255:VAL:CG1	2.18	0.70
1:B:121:VAL:HG11	1:B:145:GLU:HB3	1.71	0.70
1:C:108:ILE:HD12	1:C:245:GLU:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:SER:O	1:B:181:VAL:HG13	1.90	0.69
1:A:232:LEU:HD13	1:A:232:LEU:H	1.57	0.69
1:A:50:LYS:HE2	1:B:53:GLU:O	1.94	0.68
1:A:13:GLY:HA3	1:A:66:THR:CG2	2.22	0.68
1:D:256:PRO:HG2	1:D:259:VAL:HG23	1.76	0.67
1:B:86:GLU:HG2	1:B:140:TYR:CE2	2.30	0.67
1:D:107:TRP:CE2	1:D:108:ILE:HG13	2.28	0.67
1:C:256:PRO:HB2	1:C:259:VAL:HG23	1.75	0.67
1:D:236:LEU:HD23	1:D:265:ARG:NH2	2.10	0.67
1:A:178:ILE:HG23	1:A:209:HIS:HE1	1.58	0.66
1:D:256:PRO:HG2	1:D:259:VAL:CG2	2.26	0.66
1:B:236:LEU:HB3	1:B:237:PRO:HD3	1.78	0.66
1:B:125:SER:HB2	1:B:182:GLN:OE1	1.96	0.66
1:B:163:ALA:HB2	1:B:168:LEU:HD11	1.79	0.65
1:B:121:VAL:CG1	1:B:145:GLU:HB3	2.25	0.65
1:B:218:GLU:HG2	1:B:223:LYS:NZ	2.12	0.64
1:C:28:LEU:CD2	1:C:255:VAL:HG11	2.22	0.64
1:C:55:PHE:HD1	1:C:60:VAL:HG21	1.63	0.64
1:D:136:ARG:NH2	1:D:165:LYS:NZ	2.45	0.64
1:B:171:VAL:HG12	1:B:173:SER:H	1.62	0.64
1:A:166:PHE:O	1:A:168:LEU:HD13	1.98	0.64
1:C:173:SER:OG	1:C:176:GLU:HG3	1.98	0.64
1:C:108:ILE:HD13	1:C:108:ILE:C	2.19	0.64
1:C:88:GLY:HA3	1:C:136:ARG:HH21	1.64	0.63
1:D:183:VAL:HG22	1:D:210:VAL:HB	1.81	0.63
1:B:197:PRO:HG3	1:C:144:LYS:HB3	1.80	0.63
1:B:48:LEU:HD22	1:B:69:PHE:CD1	2.34	0.62
1:A:118:ILE:O	1:A:121:VAL:HG13	2.00	0.62
1:C:244:ILE:HD11	1:C:257:TYR:HA	1.81	0.62
1:D:195:GLU:HB2	5:D:1434:HOH:O	1.98	0.62
1:A:236:LEU:HB3	1:A:237:PRO:HD3	1.82	0.62
1:C:12:ILE:HB	1:C:43:ILE:HD12	1.81	0.62
1:B:213:ASP:OD1	1:B:215:ILE:HB	2.00	0.61
1:B:108:ILE:HD13	1:B:108:ILE:O	2.00	0.61
1:D:136:ARG:HH22	1:D:165:LYS:HZ1	1.49	0.61
1:D:49:LYS:O	1:D:53:GLU:HG2	2.02	0.60
1:C:122:LYS:HG2	1:C:145:GLU:OE1	2.02	0.60
1:B:201:ASN:HD22	1:B:204:LEU:HG	1.67	0.59
1:A:240:LEU:HD22	1:A:260:ALA:HB1	1.83	0.59
1:C:236:LEU:HB3	1:C:237:PRO:HD3	1.84	0.59
1:B:168:LEU:HD12	1:B:168:LEU:C	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PHE:CD1	1:C:60:VAL:HG21	2.38	0.59
1:C:143:VAL:HG11	1:C:167:PRO:HD2	1.84	0.59
1:B:179:ASP:OD1	1:B:206:LYS:HE3	2.03	0.59
1:B:171:VAL:HG11	1:B:176:GLU:HB3	1.85	0.59
1:B:121:VAL:HG11	1:B:145:GLU:CB	2.34	0.58
1:D:185:VAL:HG22	1:D:212:VAL:HG22	1.85	0.58
1:C:24:PHE:O	1:C:28:LEU:HG	2.04	0.58
1:C:219:THR:O	1:C:223:LYS:HG3	2.04	0.58
1:D:155:THR:HG23	4:D:1401:NAP:O2X	2.05	0.57
1:A:108:ILE:CG2	1:A:245:GLU:HG3	2.34	0.57
1:D:55:PHE:CD1	1:D:60:VAL:HG21	2.38	0.57
1:C:224:LYS:O	1:C:227:GLU:HB3	2.04	0.57
1:A:108:ILE:HG21	1:A:245:GLU:HG3	1.87	0.57
1:C:126:ILE:HD12	1:C:147:ALA:HB1	1.85	0.56
1:D:54:GLY:O	1:D:58:LEU:HD13	2.04	0.56
1:A:20:LEU:HD12	1:A:216:TYR:CE1	2.39	0.56
1:D:171:VAL:HG12	1:D:173:SER:H	1.70	0.56
1:B:110:PHE:HB2	1:B:238:MET:CE	2.35	0.56
1:C:239:LEU:HD12	1:C:242:GLN:HE21	1.70	0.56
1:C:140:TYR:CE2	1:C:144:LYS:HE3	2.41	0.56
1:C:28:LEU:HD21	1:C:260:ALA:HB2	1.86	0.56
1:A:21:SER:HA	1:A:24:PHE:CE2	2.41	0.55
1:D:236:LEU:HB3	1:D:237:PRO:HD3	1.88	0.55
1:D:189:SER:O	1:D:192:LEU:HG	2.07	0.55
1:B:163:ALA:CB	1:B:168:LEU:HD11	2.36	0.55
1:D:136:ARG:HH22	1:D:165:LYS:NZ	2.03	0.55
1:A:185:VAL:HG22	1:A:212:VAL:CG1	2.37	0.55
1:D:163:ALA:HA	1:D:168:LEU:HD21	1.89	0.55
1:D:218:GLU:HG2	1:D:223:LYS:HG3	1.88	0.55
1:B:213:ASP:HB3	1:B:222:LEU:HD11	1.89	0.55
1:A:46:GLU:O	1:A:46:GLU:HG2	2.07	0.55
1:A:48:LEU:HD12	1:A:72:GLU:CD	2.28	0.54
1:B:12:ILE:HB	1:B:43:ILE:HD12	1.90	0.54
1:A:209:HIS:O	1:A:230:ALA:HB1	2.07	0.54
1:D:122:LYS:O	1:D:123:GLU:HB2	2.07	0.54
1:D:179:ASP:OD1	1:D:206:LYS:HE3	2.08	0.54
1:C:48:LEU:HD13	1:C:76:LEU:HD11	1.90	0.54
1:B:110:PHE:HB2	1:B:238:MET:HE1	1.89	0.54
1:B:28:LEU:HD21	1:B:260:ALA:HB2	1.89	0.54
1:B:126:ILE:HG13	1:B:183:VAL:HB	1.89	0.54
1:D:136:ARG:NH2	1:D:165:LYS:HZ1	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ILE:CD1	1:D:183:VAL:HB	2.39	0.53
1:A:202:TYR:CB	1:A:224:LYS:HG2	2.39	0.53
1:D:220:LYS:O	1:D:224:LYS:HD3	2.09	0.53
1:A:171:VAL:HG12	1:A:173:SER:H	1.73	0.53
1:A:218:GLU:OE1	1:A:223:LYS:HG2	2.09	0.53
1:B:86:GLU:HG2	1:B:140:TYR:HE2	1.71	0.53
1:B:218:GLU:HG2	1:B:223:LYS:HZ1	1.73	0.53
1:B:13:GLY:HA3	1:B:16:VAL:HG13	1.90	0.53
1:B:108:ILE:HG21	1:B:245:GLU:HG2	1.91	0.53
1:B:201:ASN:ND2	1:B:204:LEU:HG	2.24	0.52
1:B:126:ILE:HD12	1:B:126:ILE:N	2.24	0.52
1:C:114:LEU:HD11	1:C:118:ILE:HD12	1.91	0.52
1:D:53:GLU:OE1	1:D:56:LYS:HD2	2.10	0.52
1:C:201:ASN:ND2	1:C:203:ASP:HB2	2.24	0.52
1:D:199:ILE:HG13	1:D:202:TYR:OH	2.10	0.52
1:D:158:LYS:HD2	4:D:1401:NAP:O1X	2.10	0.52
1:D:186:ASN:HD22	1:D:213:ASP:CG	2.12	0.52
1:A:49:LYS:O	1:A:53:GLU:HG2	2.10	0.52
1:B:108:ILE:CD1	1:B:112:LYS:HE2	2.41	0.51
1:B:178:ILE:HG23	1:B:179:ASP:N	2.26	0.51
1:C:9:TYR:CZ	1:C:61:LYS:HB2	2.45	0.51
1:D:226:LYS:HB2	1:D:232:LEU:HD23	1.92	0.51
1:A:79:TYR:CZ	1:D:45:PRO:HD2	2.46	0.51
1:D:139:ILE:O	1:D:143:VAL:HG23	2.09	0.51
1:B:74:ILE:HB	1:B:75:PRO:HD3	1.92	0.51
1:D:79:TYR:HB2	1:D:101:TYR:CD2	2.44	0.51
1:A:173:SER:OG	1:A:176:GLU:HG3	2.11	0.50
1:C:21:SER:HA	1:C:24:PHE:CE2	2.46	0.50
1:C:232:LEU:N	1:C:232:LEU:HD23	2.25	0.50
1:D:165:LYS:HD3	5:D:1417:HOH:O	2.10	0.50
1:C:9:TYR:CE2	1:C:61:LYS:HB2	2.46	0.50
1:D:117:LEU:HD23	1:D:117:LEU:O	2.11	0.50
1:D:117:LEU:HD21	1:D:231:LYS:HE2	1.93	0.50
1:D:126:ILE:HD13	1:D:183:VAL:HB	1.94	0.50
1:D:134:ALA:O	1:D:138:VAL:HG23	2.11	0.50
1:A:20:LEU:HD12	1:A:216:TYR:CD1	2.47	0.50
1:A:126:ILE:HD12	1:A:142:LEU:HD22	1.94	0.49
1:B:165:LYS:HD3	1:B:166:PHE:CZ	2.47	0.49
1:C:219:THR:HG23	1:C:222:LEU:H	1.76	0.49
1:D:132:GLY:O	1:D:136:ARG:HG3	2.12	0.49
1:D:28:LEU:HD22	1:D:255:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LYS:HG2	1:B:42:GLU:OE2	2.13	0.49
1:B:117:LEU:O	1:B:119:PRO:HD3	2.11	0.49
1:B:77:LEU:HD13	1:B:102:GLY:HA3	1.95	0.49
1:B:110:PHE:CE2	1:B:138:VAL:HG13	2.48	0.49
1:B:64:ASN:HA	1:B:91:ASN:O	2.12	0.48
1:B:72:GLU:O	1:B:75:PRO:HD2	2.13	0.48
1:A:50:LYS:HE3	1:B:53:GLU:HB3	1.95	0.48
1:A:202:TYR:HB2	1:A:224:LYS:HG2	1.94	0.48
1:D:77:LEU:HD13	1:D:102:GLY:HA3	1.95	0.48
1:D:117:LEU:HD12	1:D:233:LEU:HB2	1.94	0.48
1:C:126:ILE:HG12	1:C:183:VAL:HB	1.94	0.48
1:A:41:PHE:HE1	1:B:8:LEU:HD12	1.78	0.48
1:C:20:LEU:HD12	1:C:216:TYR:CD2	2.49	0.48
1:A:28:LEU:HD22	1:A:255:VAL:HG11	1.95	0.48
1:A:131:ALA:O	1:A:158:LYS:HE2	2.13	0.47
1:A:108:ILE:CG1	1:D:195:GLU:HG2	2.40	0.47
1:C:74:ILE:HB	1:C:75:PRO:HD3	1.95	0.47
1:C:77:LEU:HD13	1:C:102:GLY:HA3	1.97	0.47
1:D:20:LEU:HD12	1:D:216:TYR:CD2	2.49	0.47
1:D:157:GLU:HA	1:D:160:ILE:HD12	1.95	0.47
1:D:205:ILE:HD13	1:D:225:ALA:HB2	1.97	0.47
1:C:117:LEU:HD11	1:C:233:LEU:HB2	1.96	0.47
1:C:189:SER:O	1:C:192:LEU:HG	2.14	0.47
1:A:107:TRP:CH2	1:A:108:ILE:HG12	2.50	0.47
1:B:154:ARG:HB3	4:B:1201:NAP:O2X	2.14	0.47
1:C:25:GLN:HG3	1:C:38:TYR:CZ	2.50	0.47
1:D:21:SER:N	1:D:22:PRO:HD2	2.30	0.47
1:B:232:LEU:HG	5:B:1237:HOH:O	2.14	0.47
1:B:105:THR:O	1:B:108:ILE:HG22	2.15	0.47
1:D:74:ILE:HB	1:D:75:PRO:HD3	1.96	0.47
1:D:209:HIS:O	1:D:230:ALA:HB1	2.14	0.47
1:A:8:LEU:HD22	1:A:9:TYR:N	2.30	0.46
1:A:39:LEU:CD1	1:B:8:LEU:HG	2.46	0.46
1:A:234:ASP:OD2	1:A:268:ARG:NH2	2.47	0.46
1:C:241:TRP:O	1:C:245:GLU:HG2	2.14	0.46
1:A:178:ILE:CG2	1:A:209:HIS:HE1	2.26	0.46
1:C:26:ASN:OD1	5:C:1314:HOH:O	2.21	0.46
1:D:185:VAL:HG22	1:D:212:VAL:CG2	2.44	0.46
1:A:154:ARG:HB3	2:A:1101:ATR:O1P	2.15	0.46
1:A:232:LEU:C	1:A:232:LEU:HD22	2.36	0.46
1:B:7:GLN:NE2	1:B:61:LYS:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ILE:HD13	1:C:108:ILE:O	2.15	0.46
1:A:5:GLN:HE22	1:B:17:LYS:HD2	1.77	0.46
1:D:122:LYS:HG2	1:D:123:GLU:HG2	1.98	0.46
1:D:163:ALA:HA	1:D:168:LEU:CD2	2.45	0.46
1:C:156:LYS:NZ	1:C:172:ASN:HD21	2.15	0.45
1:D:5:GLN:O	1:D:5:GLN:HG2	2.16	0.45
1:D:21:SER:HA	1:D:24:PHE:CE2	2.51	0.45
1:C:139:ILE:O	1:C:143:VAL:HG23	2.16	0.45
1:B:87:ILE:O	1:B:136:ARG:HD3	2.15	0.45
1:C:83:THR:O	1:C:87:ILE:HG13	2.16	0.45
1:C:262:ARG:HG2	1:C:262:ARG:HH11	1.81	0.45
1:D:117:LEU:CD2	1:D:231:LYS:HE2	2.46	0.45
1:B:218:GLU:HG3	1:B:223:LYS:HG3	1.99	0.45
1:C:70:LYS:HE3	1:C:106:ASP:OD2	2.16	0.45
1:D:262:ARG:HH11	1:D:262:ARG:HG2	1.82	0.45
1:C:17:LYS:HD3	1:C:42:GLU:OE2	2.17	0.45
1:A:79:TYR:CE2	1:D:44:ASN:HB3	2.52	0.45
1:A:232:LEU:CD1	1:A:232:LEU:N	2.80	0.45
1:B:158:LYS:HD3	4:B:1201:NAP:O1X	2.17	0.45
1:C:48:LEU:HD13	1:C:76:LEU:CD1	2.47	0.44
1:C:7:GLN:HB2	1:C:36:ALA:HB2	1.97	0.44
1:C:201:ASN:HD21	1:C:203:ASP:HB2	1.79	0.44
1:C:264:VAL:HG23	1:C:265:ARG:N	2.31	0.44
1:A:64:ASN:HD22	1:A:64:ASN:HA	1.61	0.44
1:B:111:LEU:HD13	1:B:141:ALA:HB1	2.00	0.44
1:C:29:ILE:HG23	1:C:34:LEU:HB2	1.99	0.44
1:C:232:LEU:HD23	5:C:1335:HOH:O	2.16	0.44
1:C:129:LEU:HB2	1:C:186:ASN:HA	1.98	0.44
1:A:23:VAL:HG11	1:A:267:LEU:HD12	1.99	0.44
1:C:53:GLU:HB3	1:D:50:LYS:HD3	1.99	0.44
1:C:164:GLN:O	1:C:165:LYS:HD3	2.18	0.44
1:A:143:VAL:HG11	1:A:167:PRO:HD2	1.99	0.44
1:B:194:ASP:O	1:B:220:LYS:HE3	2.17	0.44
1:A:202:TYR:HB3	1:A:224:LYS:HG2	2.00	0.44
1:C:168:LEU:C	1:C:168:LEU:HD12	2.38	0.44
1:D:110:PHE:CZ	1:D:114:LEU:HD11	2.53	0.44
1:C:126:ILE:HD12	1:C:147:ALA:CB	2.47	0.43
1:B:25:GLN:HG3	1:B:38:TYR:CE2	2.53	0.43
1:D:65:VAL:CG1	1:D:69:PHE:HB2	2.47	0.43
1:A:72:GLU:O	1:A:75:PRO:HD2	2.18	0.43
1:D:111:LEU:HD12	1:D:111:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:TRP:O	1:D:245:GLU:HG2	2.17	0.43
1:C:174:PRO:O	1:C:178:ILE:HB	2.18	0.43
1:A:73:ILE:O	1:A:77:LEU:HG	2.19	0.43
1:A:118:ILE:HB	1:A:121:VAL:HG12	2.01	0.43
1:A:196:ASP:O	1:A:220:LYS:NZ	2.51	0.43
1:C:113:SER:OG	1:C:233:LEU:HD21	2.19	0.43
1:B:227:GLU:O	1:B:227:GLU:HG2	2.19	0.43
1:C:111:LEU:HD11	1:C:145:GLU:HG3	2.01	0.42
1:C:65:VAL:CG1	1:C:69:PHE:HB2	2.49	0.42
1:C:264:VAL:C	1:C:266:ASP:H	2.22	0.42
1:D:9:TYR:O	1:D:38:TYR:HA	2.18	0.42
1:A:108:ILE:CD1	1:D:195:GLU:HG2	2.49	0.42
1:D:80:VAL:O	1:D:81:GLU:C	2.57	0.42
1:B:21:SER:HA	1:B:24:PHE:CE2	2.54	0.42
1:B:175:GLU:HG2	1:B:204:LEU:HD12	2.02	0.42
1:C:166:PHE:HA	1:C:167:PRO:HD3	1.84	0.42
1:C:239:LEU:HD12	1:C:242:GLN:NE2	2.33	0.42
1:A:108:ILE:HA	1:A:108:ILE:HD13	1.82	0.42
1:A:192:LEU:O	1:A:217:LYS:NZ	2.48	0.42
1:B:22:PRO:O	1:B:26:ASN:ND2	2.52	0.42
1:D:171:VAL:HG21	1:D:177:VAL:HG11	2.02	0.42
1:A:43:ILE:O	1:A:43:ILE:HG13	2.19	0.42
1:A:74:ILE:HB	1:A:75:PRO:HD3	2.01	0.42
1:C:108:ILE:HD11	1:C:112:LYS:CE	2.39	0.42
1:A:136:ARG:HG2	1:A:162:LEU:HD21	2.01	0.42
1:B:175:GLU:O	1:B:178:ILE:HG22	2.20	0.42
1:C:29:ILE:HG21	1:C:36:ALA:O	2.19	0.42
1:D:13:GLY:C	1:D:16:VAL:HG13	2.40	0.42
1:B:24:PHE:O	1:B:28:LEU:HG	2.20	0.42
1:C:58:LEU:O	1:C:59:LYS:HB2	2.19	0.42
1:D:26:ASN:HB3	1:D:30:ARG:HH22	1.85	0.42
1:B:110:PHE:CE2	1:B:114:LEU:HD11	2.55	0.41
1:D:126:ILE:HG23	1:D:183:VAL:HG12	2.01	0.41
1:A:63:ILE:HG12	1:A:93:VAL:HB	2.02	0.41
1:D:13:GLY:CA	1:D:16:VAL:CG1	2.98	0.41
1:A:12:ILE:O	1:A:66:THR:HG22	2.19	0.41
1:B:151:LEU:HD12	1:B:152:TRP:N	2.35	0.41
1:A:10:GLY:O	1:A:63:ILE:HA	2.20	0.41
1:B:55:PHE:HD1	1:B:60:VAL:HG21	1.86	0.41
1:B:91:ASN:OD1	1:B:104:ASN:HA	2.19	0.41
1:D:86:GLU:OE2	1:D:140:TYR:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ASN:ND2	1:C:47:GLU:OE2	2.47	0.41
1:D:122:LYS:HA	1:D:146:GLY:O	2.21	0.41
1:A:121:VAL:CG2	1:A:145:GLU:HG2	2.51	0.41
1:A:130:GLY:O	1:A:151:LEU:HD11	2.21	0.41
1:B:12:ILE:HG21	1:B:55:PHE:HE2	1.85	0.41
1:B:110:PHE:HB2	1:B:238:MET:HE3	2.03	0.41
1:C:163:ALA:HB2	1:C:168:LEU:HD11	2.01	0.41
1:C:264:VAL:O	1:C:266:ASP:N	2.54	0.41
1:D:159:ALA:HB1	1:D:170:VAL:HG13	2.03	0.41
1:B:11:VAL:HB	1:B:38:TYR:OH	2.20	0.41
1:D:128:VAL:O	1:D:151:LEU:HD12	2.21	0.41
1:A:9:TYR:O	1:A:38:TYR:HA	2.21	0.40
1:B:126:ILE:HD13	1:B:147:ALA:HB1	2.03	0.40
1:B:198:GLU:HG3	5:B:1231:HOH:O	2.22	0.40
1:C:66:THR:HA	1:C:70:LYS:NZ	2.36	0.40
1:D:120:GLU:O	1:D:120:GLU:HG3	2.21	0.40
1:A:171:VAL:HG12	1:A:173:SER:N	2.36	0.40
1:B:28:LEU:HD22	1:B:255:VAL:CG1	2.48	0.40
1:B:181:VAL:HG12	1:B:183:VAL:H	1.86	0.40
1:B:240:LEU:O	1:B:244:ILE:HG13	2.20	0.40
1:C:81:GLU:O	1:C:84:ALA:HB3	2.20	0.40
1:D:251:ASN:C	1:D:253:CYS:H	2.24	0.40
1:A:185:VAL:HG22	1:A:212:VAL:HG13	2.03	0.40
1:B:114:LEU:HD22	1:B:118:ILE:HD12	2.04	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	267/275 (97%)	257 (96%)	9 (3%)	1 (0%)	34 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	265/275 (96%)	248 (94%)	15 (6%)	2 (1%)	19	19
1	C	264/275 (96%)	251 (95%)	11 (4%)	2 (1%)	19	19
1	D	264/275 (96%)	241 (91%)	21 (8%)	2 (1%)	19	19
All	All	1060/1100 (96%)	997 (94%)	56 (5%)	7 (1%)	22	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	HIS
1	C	265	ARG
1	D	119	PRO
1	A	16	VAL
1	B	16	VAL
1	C	16	VAL
1	D	2	ILE

### 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	229/235 (97%)	216 (94%)	13 (6%)	20	24
1	B	228/235 (97%)	221 (97%)	7 (3%)	40	51
1	C	227/235 (97%)	221 (97%)	6 (3%)	46	58
1	D	227/235 (97%)	217 (96%)	10 (4%)	28	35
All	All	911/940 (97%)	875 (96%)	36 (4%)	31	40

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	16	VAL
1	A	48	LEU
1	A	68	PRO

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Mol	Chain	Res	Type
1	A	108	ILE
1	A	114	LEU
1	A	117	LEU
1	A	125	SER
1	A	168	LEU
1	A	228	LYS
1	A	232	LEU
1	A	265	ARG
1	A	268	ARG
1	B	5	GLN
1	B	8	LEU
1	B	16	VAL
1	B	68	PRO
1	B	108	ILE
1	B	212	VAL
1	B	232	LEU
1	C	8	LEU
1	C	30	ARG
1	C	48	LEU
1	C	68	PRO
1	C	108	ILE
1	C	212	VAL
1	D	8	LEU
1	D	48	LEU
1	D	68	PRO
1	D	119	PRO
1	D	144	LYS
1	D	145	GLU
1	D	168	LEU
1	D	194	ASP
1	D	203	ASP
1	D	262	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	64	ASN
1	A	97	ASN
1	A	251	ASN
1	B	5	GLN
1	B	201	ASN

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Mol	Chain	Res	Type
1	C	172	ASN
1	C	201	ASN
1	C	242	GLN
1	D	5	GLN
1	D	186	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](#)

8 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	SKM	D	1402	-	12,12,12	2.08	5 (41%)	16,17,17	1.90	4 (25%)
3	SKM	B	1202	-	12,12,12	2.29	5 (41%)	16,17,17	2.00	5 (31%)
2	ATR	A	1101	-	27,33,33	1.99	9 (33%)	35,52,52	2.00	9 (25%)
3	SKM	A	1102	-	12,12,12	2.29	5 (41%)	16,17,17	2.01	5 (31%)
3	SKM	C	1302	-	12,12,12	2.18	5 (41%)	16,17,17	2.04	7 (43%)
4	NAP	B	1201	-	45,52,52	1.44	7 (15%)	56,80,80	1.11	3 (5%)
4	NAP	C	1301	-	45,52,52	1.39	7 (15%)	56,80,80	1.10	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	D	1401	-	45,52,52	1.43	6 (13%)	56,80,80	1.09	4 (7%)

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	SKM	D	1402	-	-	0/4/20/20	0/1/1/1
3	SKM	B	1202	-	-	0/4/20/20	0/1/1/1
2	ATR	A	1101	-	-	5/17/37/37	0/3/3/3
3	SKM	A	1102	-	-	0/4/20/20	0/1/1/1
3	SKM	C	1302	-	-	0/4/20/20	0/1/1/1
4	NAP	B	1201	-	-	10/31/67/67	0/5/5/5
4	NAP	C	1301	-	-	12/31/67/67	0/5/5/5
4	NAP	D	1401	-	-	9/31/67/67	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ATR	PB-O1B	5.96	1.69	1.50
3	B	1202	SKM	C9-C10	4.28	1.55	1.50
3	A	1102	SKM	C9-C10	4.27	1.55	1.50
3	C	1302	SKM	C9-C10	4.13	1.55	1.50
2	A	1101	ATR	P2'-O3P	3.78	1.69	1.54
4	B	1201	NAP	O4B-C1B	3.68	1.46	1.41
4	D	1401	NAP	O4B-C1B	3.61	1.46	1.41
3	D	1402	SKM	C9-C10	3.60	1.55	1.50
4	C	1301	NAP	C2A-N3A	3.50	1.37	1.32
4	C	1301	NAP	C4N-C3N	3.50	1.45	1.39
4	B	1201	NAP	C4N-C3N	3.48	1.45	1.39
4	D	1401	NAP	C4N-C3N	3.47	1.45	1.39
4	B	1201	NAP	C6N-N1N	3.46	1.43	1.35
4	C	1301	NAP	C6N-N1N	3.42	1.43	1.35
4	D	1401	NAP	C6N-N1N	3.34	1.43	1.35
3	A	1102	SKM	C10-C4	3.33	1.41	1.33
4	C	1301	NAP	O4B-C1B	3.31	1.45	1.41
4	D	1401	NAP	C2A-N3A	3.31	1.37	1.32
3	B	1202	SKM	C10-C4	3.31	1.41	1.33
2	A	1101	ATR	PA-O2A	3.30	1.70	1.55
3	B	1202	SKM	O7-C6	3.29	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1401	NAP	C4A-N3A	3.21	1.40	1.35
4	B	1201	NAP	C4A-N3A	3.20	1.40	1.35
4	B	1201	NAP	C2A-N3A	3.13	1.37	1.32
3	D	1402	SKM	C10-C4	3.12	1.41	1.33
4	B	1201	NAP	P2B-O2B	3.03	1.65	1.59
3	A	1102	SKM	O7-C6	3.03	1.49	1.43
3	D	1402	SKM	O3-C1	2.94	1.30	1.22
3	C	1302	SKM	C5-C4	-2.92	1.46	1.51
4	C	1301	NAP	C4A-N3A	2.88	1.39	1.35
3	C	1302	SKM	O7-C6	2.86	1.49	1.43
4	D	1401	NAP	C2N-N1N	2.78	1.38	1.35
3	A	1102	SKM	O3-C1	2.75	1.29	1.22
3	B	1202	SKM	O3-C1	2.72	1.29	1.22
3	C	1302	SKM	O3-C1	2.70	1.29	1.22
3	A	1102	SKM	C5-C4	-2.69	1.46	1.51
3	C	1302	SKM	C10-C4	2.68	1.40	1.33
3	D	1402	SKM	O7-C6	2.59	1.48	1.43
4	C	1301	NAP	C2N-N1N	2.58	1.38	1.35
2	A	1101	ATR	C3'-C2'	-2.57	1.47	1.52
3	D	1402	SKM	C5-C4	-2.56	1.47	1.51
2	A	1101	ATR	O4'-C1'	2.56	1.44	1.41
3	B	1202	SKM	C5-C4	-2.51	1.47	1.51
4	B	1201	NAP	C2N-N1N	2.47	1.38	1.35
2	A	1101	ATR	P2'-O2P	2.43	1.64	1.54
2	A	1101	ATR	C2-N3	2.23	1.35	1.32
2	A	1101	ATR	C6-C5	2.22	1.51	1.43
4	C	1301	NAP	P2B-O2B	2.15	1.63	1.59
2	A	1101	ATR	C5-C4	2.07	1.46	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ATR	C1'-N9-C4	-6.16	115.82	126.64
3	A	1102	SKM	O3-C1-C4	-4.99	112.98	121.59
3	C	1302	SKM	O3-C1-C4	-4.80	113.31	121.59
3	B	1202	SKM	O3-C1-C4	-4.62	113.62	121.59
2	A	1101	ATR	O2'-C2'-C3'	4.46	127.85	111.68
3	D	1402	SKM	O3-C1-C4	-4.46	113.91	121.59
2	A	1101	ATR	N3-C2-N1	-3.93	122.53	128.68
2	A	1101	ATR	O3'-C3'-C2'	-3.44	101.40	111.17
3	B	1202	SKM	C5-C6-C8	-2.98	106.72	110.30
2	A	1101	ATR	C2'-C3'-C4'	2.82	108.12	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1301	NAP	C6N-N1N-C2N	-2.75	119.47	121.97
3	C	1302	SKM	C5-C6-C8	-2.72	107.03	110.30
4	B	1201	NAP	C6N-N1N-C2N	-2.67	119.54	121.97
3	D	1402	SKM	C5-C6-C8	-2.53	107.26	110.30
3	C	1302	SKM	C8-C9-C10	2.46	116.18	111.84
3	D	1402	SKM	C8-C9-C10	2.44	116.13	111.84
2	A	1101	ATR	PA-O3A-PB	-2.42	124.53	132.83
3	A	1102	SKM	O11-C9-C8	-2.38	105.82	110.29
3	B	1202	SKM	C8-C9-C10	2.28	115.85	111.84
3	A	1102	SKM	C8-C9-C10	2.27	115.84	111.84
3	A	1102	SKM	C5-C6-C8	-2.26	107.58	110.30
3	D	1402	SKM	O11-C9-C8	-2.25	106.05	110.29
2	A	1101	ATR	C2-N1-C6	2.25	122.60	118.75
4	D	1401	NAP	C6N-N1N-C2N	-2.24	119.94	121.97
4	B	1201	NAP	C2A-N1A-C6A	2.19	122.50	118.75
3	B	1202	SKM	O11-C9-C8	-2.19	106.18	110.29
3	C	1302	SKM	O11-C9-C8	-2.18	106.18	110.29
2	A	1101	ATR	O3'-C3'-C4'	2.17	117.32	111.05
3	C	1302	SKM	C6-C5-C4	2.15	115.97	111.78
4	C	1301	NAP	C2A-N1A-C6A	2.14	122.42	118.75
4	D	1401	NAP	C2A-N1A-C6A	2.14	122.42	118.75
4	B	1201	NAP	PN-O3-PA	2.11	140.07	132.83
3	A	1102	SKM	O2-C1-C4	2.11	119.96	115.49
3	C	1302	SKM	O2-C1-C4	2.10	119.95	115.49
2	A	1101	ATR	O4'-C4'-C5'	-2.09	102.48	109.37
4	D	1401	NAP	O2A-PA-O1A	2.07	122.49	112.24
3	B	1202	SKM	O2-C1-C4	2.06	119.85	115.49
3	C	1302	SKM	C5-C4-C10	-2.06	119.48	122.23
4	D	1401	NAP	C3N-C2N-N1N	2.01	122.39	120.43

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1201	NAP	C5B-O5B-PA-O1A
4	B	1201	NAP	O4D-C1D-N1N-C6N
4	C	1301	NAP	C5B-O5B-PA-O1A
4	C	1301	NAP	C5D-O5D-PN-O2N
4	C	1301	NAP	O4D-C1D-N1N-C6N
4	D	1401	NAP	C5B-O5B-PA-O1A
4	D	1401	NAP	O4D-C1D-N1N-C6N
4	B	1201	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	C	1301	NAP	O4B-C4B-C5B-O5B
4	C	1301	NAP	C3B-C4B-C5B-O5B
4	D	1401	NAP	O4B-C4B-C5B-O5B
4	D	1401	NAP	C3B-C4B-C5B-O5B
4	B	1201	NAP	C3B-C4B-C5B-O5B
4	C	1301	NAP	O4D-C4D-C5D-O5D
4	C	1301	NAP	C3D-C4D-C5D-O5D
2	A	1101	ATR	C3'-C2'-O2'-P2'
4	D	1401	NAP	O4D-C4D-C5D-O5D
4	D	1401	NAP	C3D-C4D-C5D-O5D
4	B	1201	NAP	O4D-C4D-C5D-O5D
4	B	1201	NAP	C5B-O5B-PA-O3
4	C	1301	NAP	C5B-O5B-PA-O3
4	D	1401	NAP	C5B-O5B-PA-O3
4	B	1201	NAP	C5B-O5B-PA-O2A
4	C	1301	NAP	C5B-O5B-PA-O2A
4	C	1301	NAP	C5D-O5D-PN-O1N
4	D	1401	NAP	C5B-O5B-PA-O2A
2	A	1101	ATR	PB-O3A-PA-O1A
2	A	1101	ATR	PB-O3A-PA-O2A
4	B	1201	NAP	C3B-C2B-O2B-P2B
4	B	1201	NAP	C2B-O2B-P2B-O1X
4	B	1201	NAP	C2B-O2B-P2B-O2X
4	C	1301	NAP	C2B-O2B-P2B-O2X
4	C	1301	NAP	C5D-O5D-PN-O3
4	D	1401	NAP	C2B-O2B-P2B-O2X
2	A	1101	ATR	C5'-O5'-PA-O1A
2	A	1101	ATR	O4'-C4'-C5'-O5'

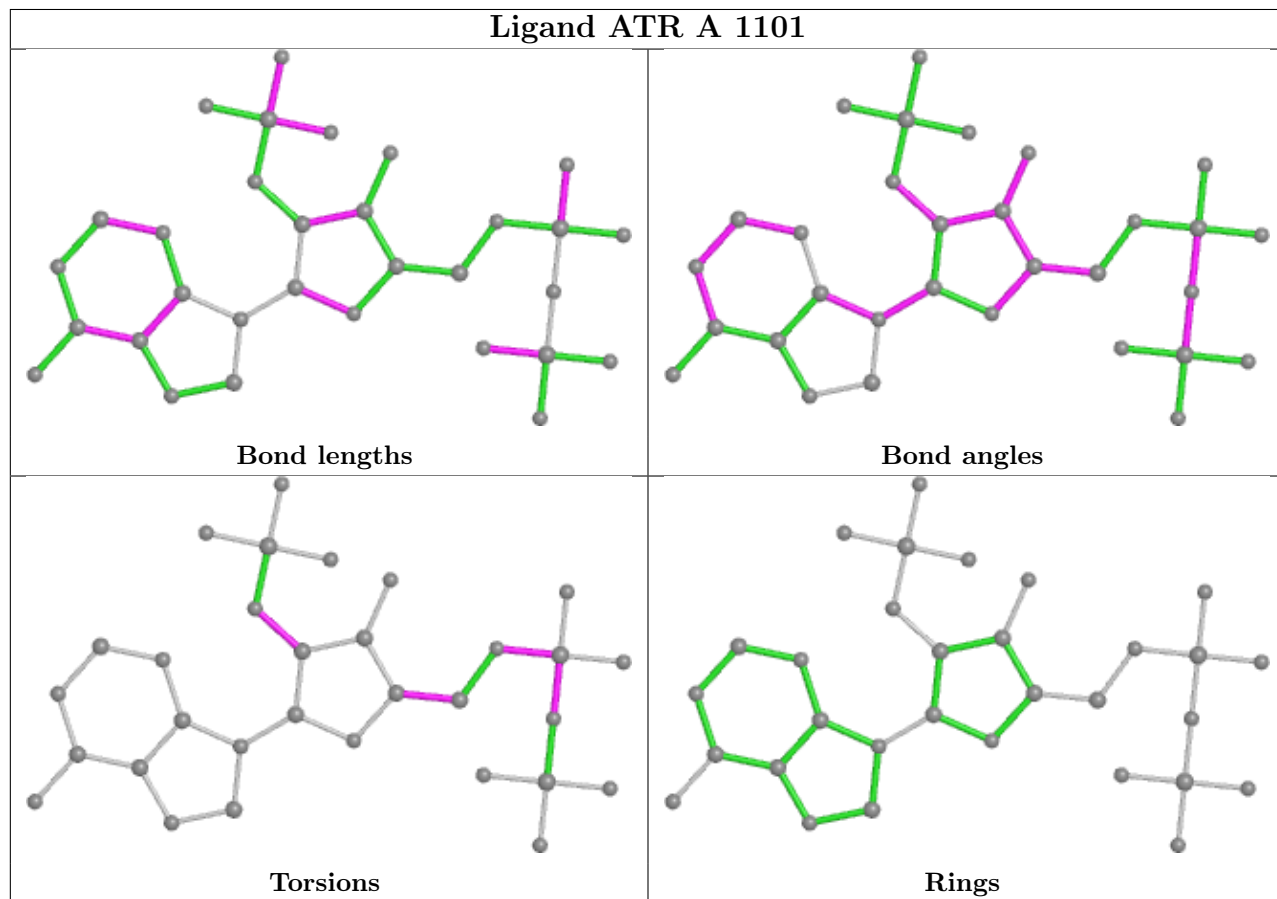
There are no ring outliers.

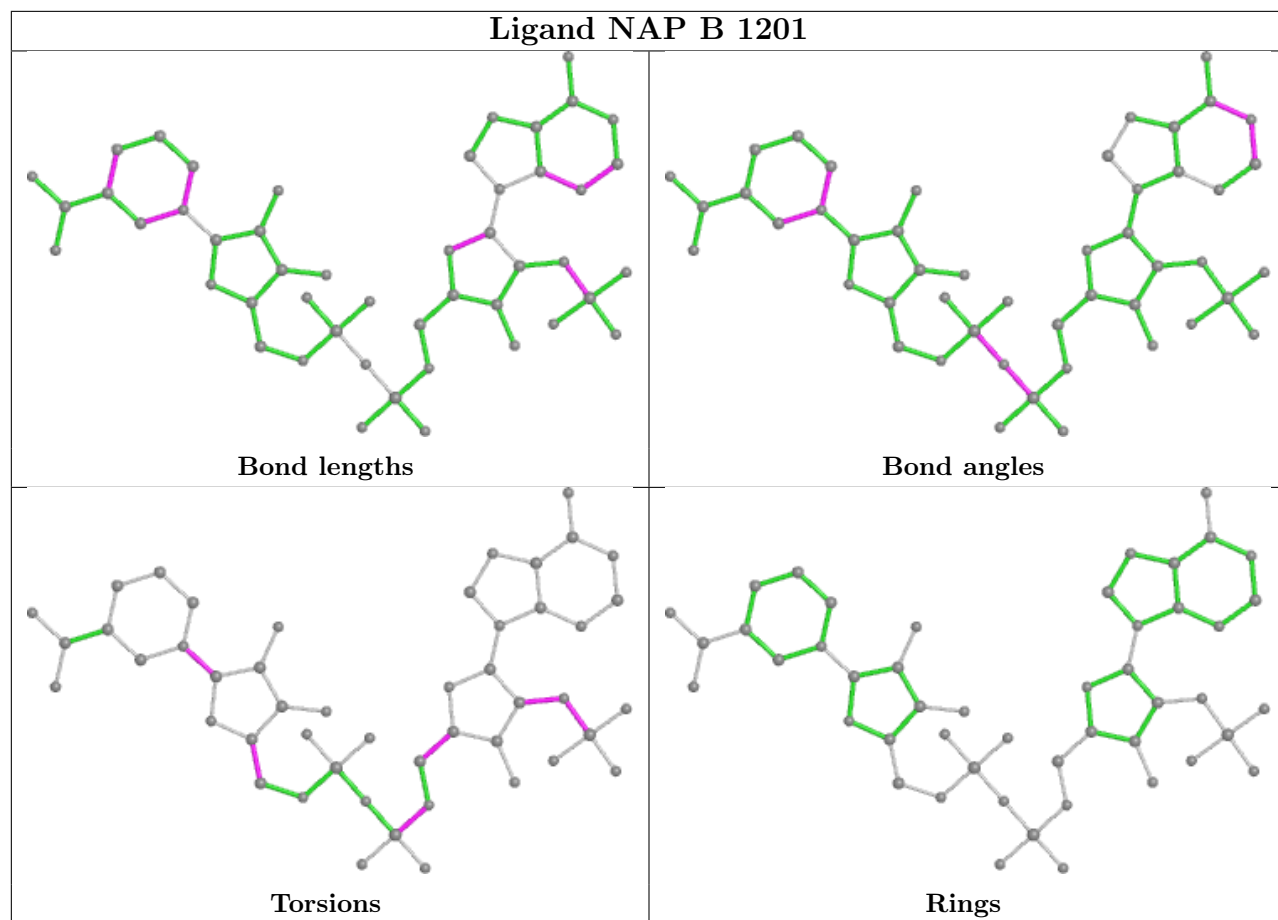
3 monomers are involved in 5 short contacts:

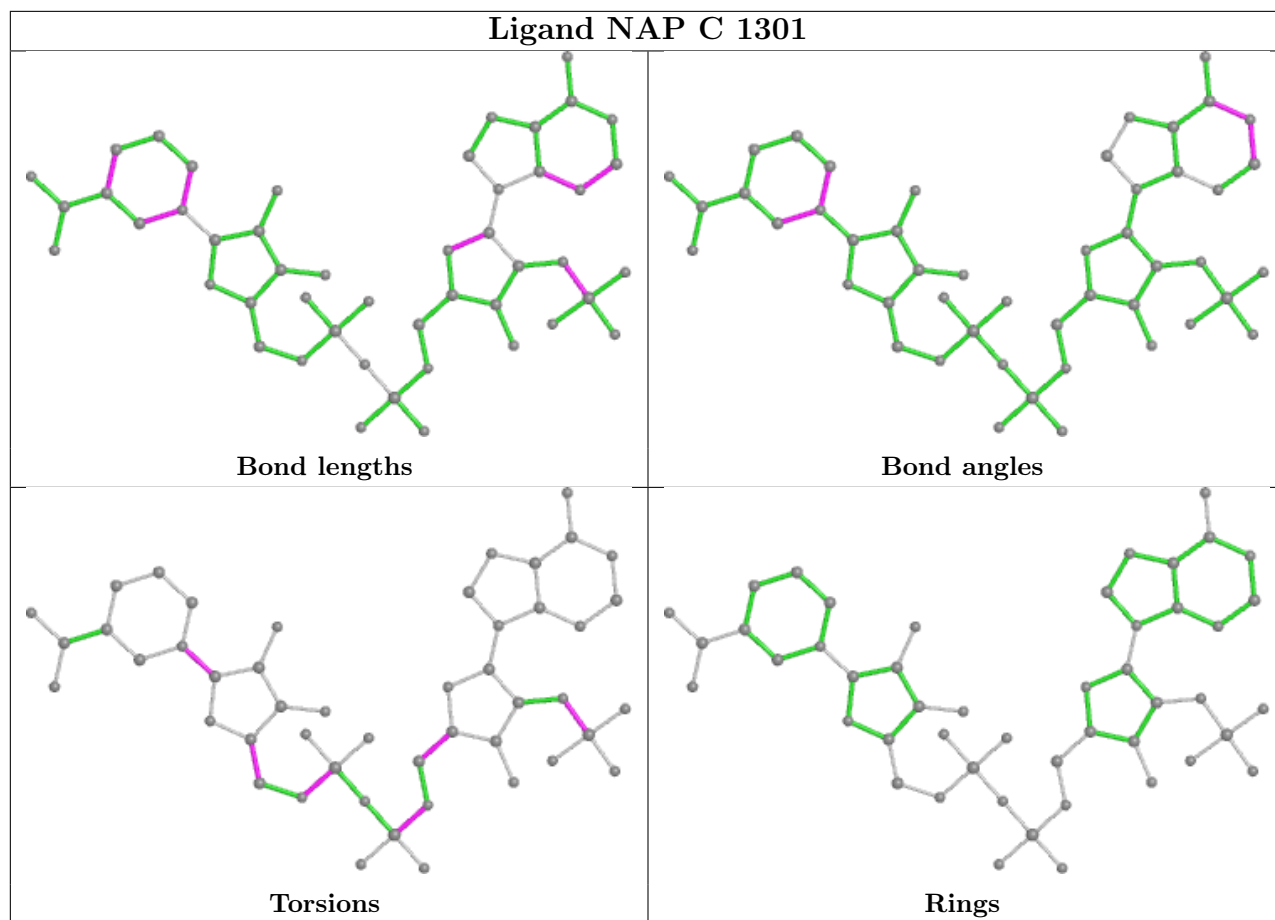
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ATR	1	0
4	B	1201	NAP	2	0
4	D	1401	NAP	2	0

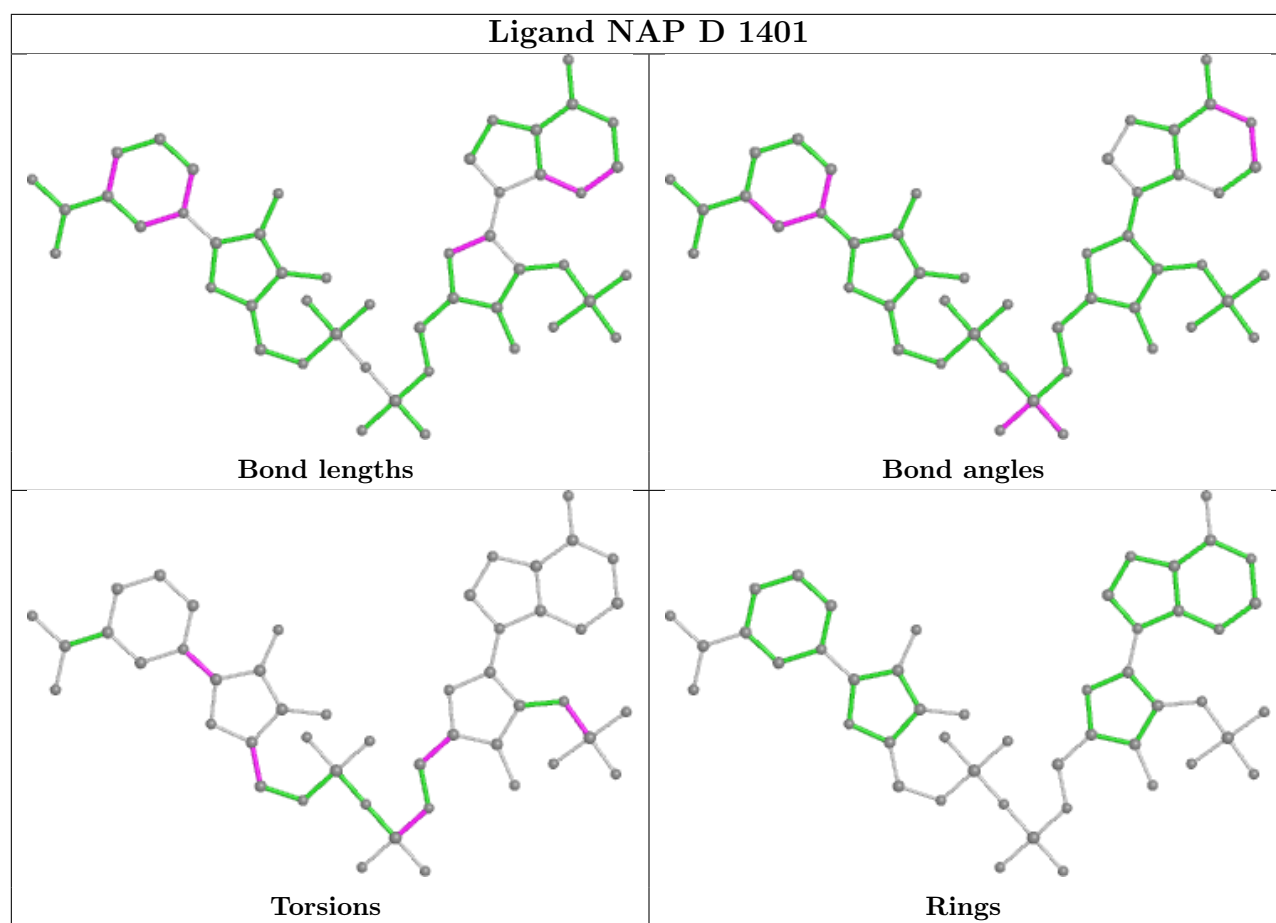
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	269/275 (97%)	-0.03	8 (2%) 50 48	26, 43, 71, 89	0
1	B	267/275 (97%)	0.17	7 (2%) 56 53	26, 47, 77, 95	0
1	C	266/275 (96%)	0.21	16 (6%) 21 20	31, 46, 71, 99	0
1	D	266/275 (96%)	0.12	7 (2%) 56 53	29, 48, 76, 98	0
All	All	1068/1100 (97%)	0.12	38 (3%) 42 41	26, 46, 75, 99	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	GLY	4.3
1	B	160	ILE	4.2
1	D	79	TYR	4.1
1	C	265	ARG	3.8
1	C	82	ASP	3.6
1	B	164	GLN	3.6
1	C	135	SER	3.3
1	B	185	VAL	3.1
1	D	167	PRO	3.1
1	C	266	ASP	3.1
1	A	193	LYS	3.0
1	B	79	TYR	2.8
1	C	157	GLU	2.7
1	C	164	GLN	2.6
1	C	207	LYS	2.6
1	A	141	ALA	2.5
1	B	266	ASP	2.5
1	C	194	ASP	2.5
1	B	114	LEU	2.5
1	C	30	ARG	2.4
1	C	79	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	82	ASP	2.4
1	D	227	GLU	2.4
1	C	138	VAL	2.3
1	C	134	ALA	2.3
1	C	185	VAL	2.3
1	C	137	ALA	2.3
1	A	18	HIS	2.3
1	A	160	ILE	2.3
1	D	96	GLU	2.2
1	A	163	ALA	2.2
1	C	63	ILE	2.2
1	A	169	GLU	2.1
1	C	160	ILE	2.1
1	D	123	GLU	2.1
1	D	18	HIS	2.0
1	A	62	GLY	2.0
1	B	207	LYS	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.

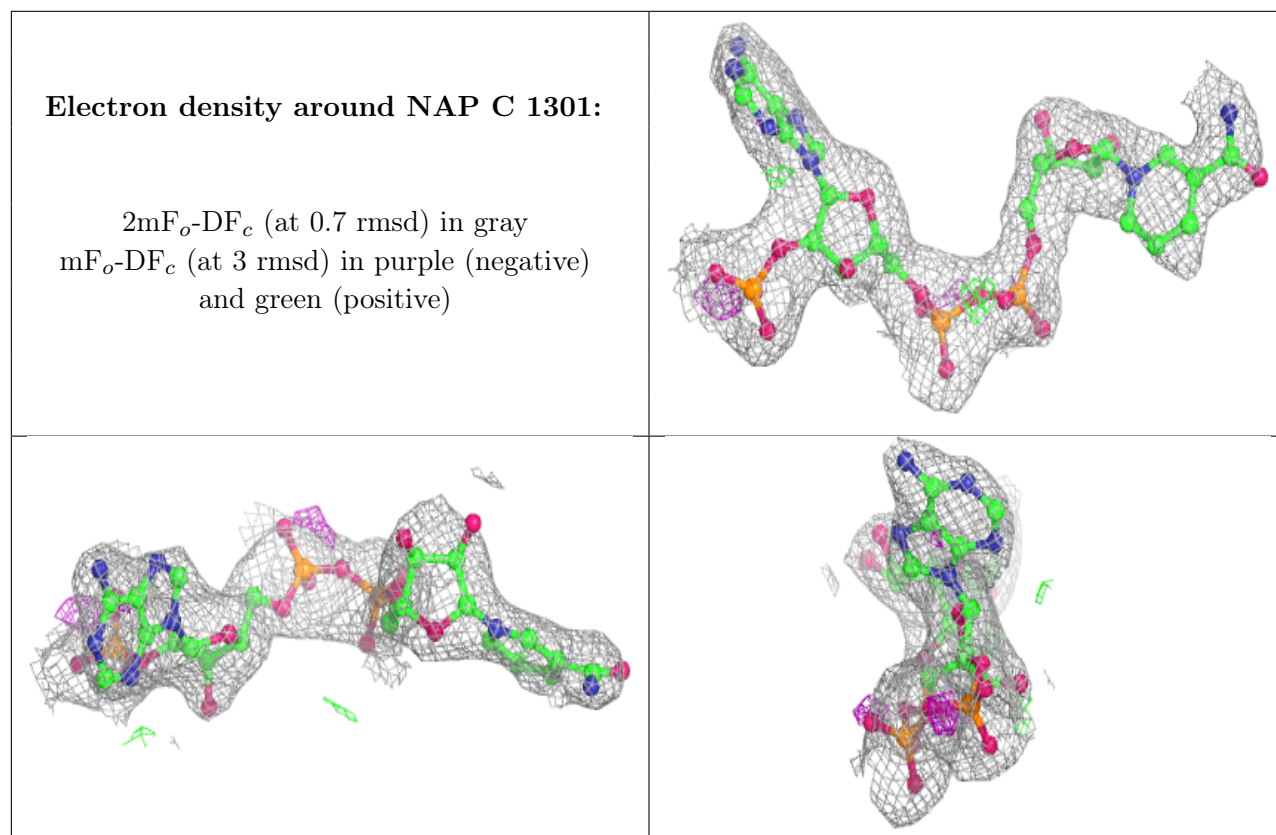
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAP	C	1301	48/48	0.87	0.17	58,71,89,89	0
4	NAP	B	1201	48/48	0.89	0.14	48,58,72,77	0
3	SKM	C	1302	12/12	0.91	0.16	32,41,52,53	0
3	SKM	B	1202	12/12	0.92	0.17	32,49,55,58	0
2	ATR	A	1101	31/31	0.93	0.12	34,54,89,93	0
3	SKM	A	1102	12/12	0.94	0.13	47,53,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SKM	D	1402	12/12	0.95	0.14	33,39,45,50	0
4	NAP	D	1401	48/48	0.96	0.11	37,46,57,59	0

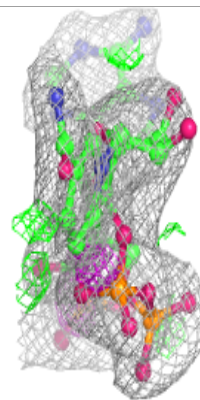
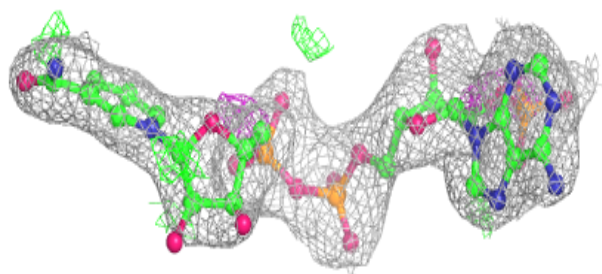
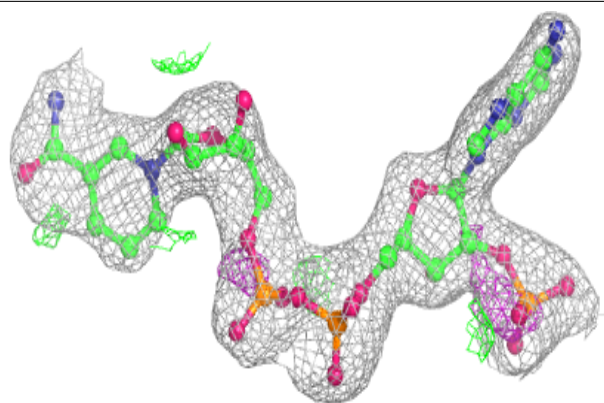
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



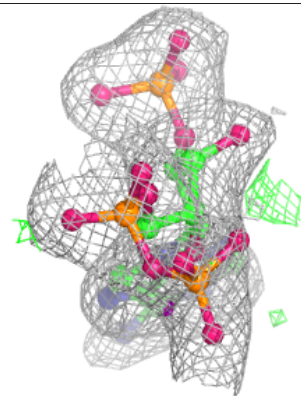
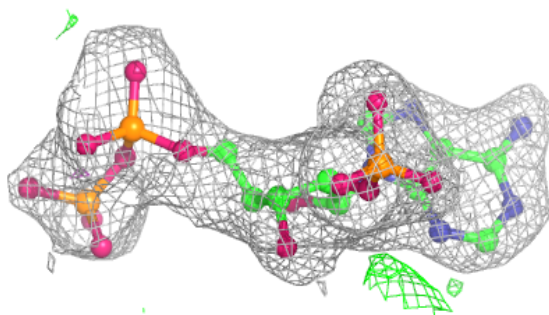
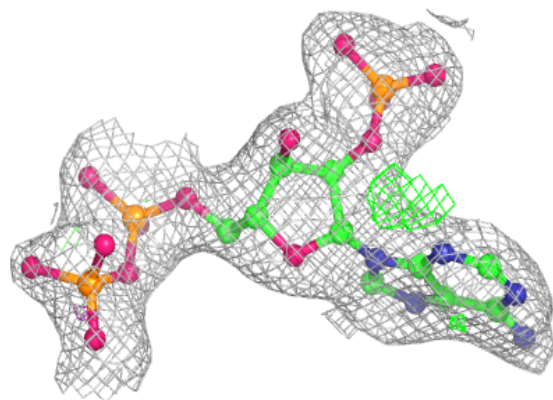


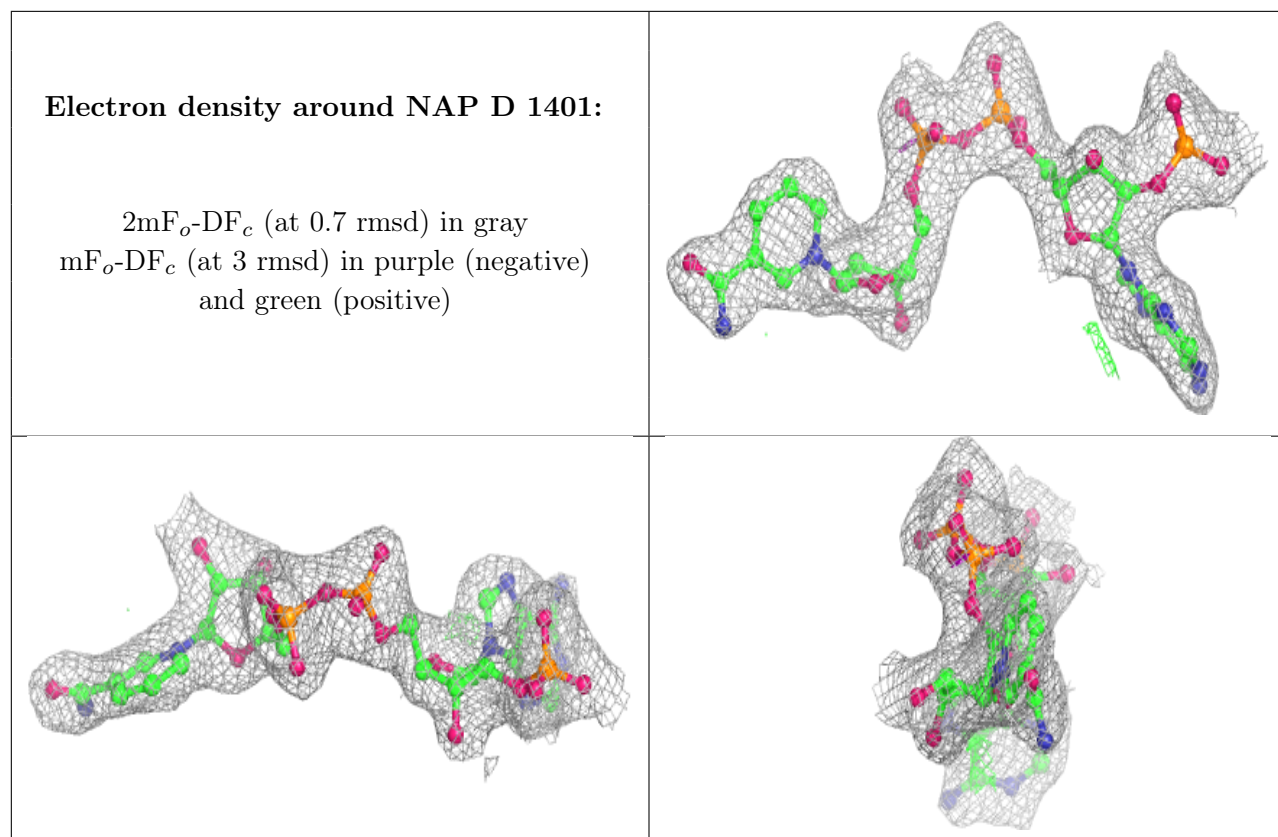
**Electron density around NAP B 1201:**

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

**Electron density around ATR A 1101:**

$2mF_o-DF_c$  (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.