



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:25 am BST

PDB ID : 2B7Q
Title : Crystal structure of quinolinic acid phosphoribosyltransferase from *Helicobacter pylori* with nicotinate mononucleotide
Authors : Kim, M.K.; Im, Y.J.; Lee, J.H.; Eom, S.H.
Deposited on : 2005-10-05
Resolution : 3.31 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 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 : 2.11
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) : 2.11

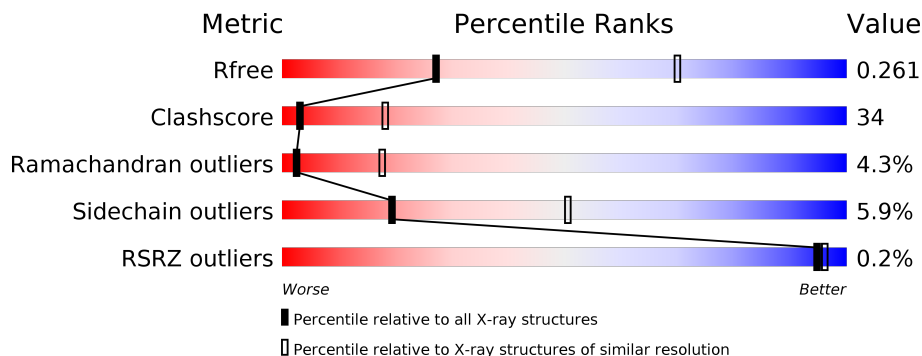
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	273	
1	B	273	
1	C	273	

2 Entry composition i

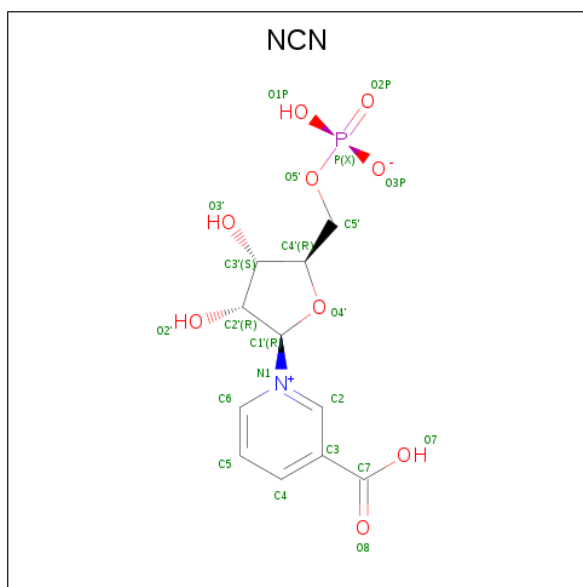
There are 3 unique types of molecules in this entry. The entry contains 6564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable nicotinate-nucleotide pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	Total 2160	C 1367	N 377	O 403	S 13	0	0	0
1	B	273	Total 2160	C 1367	N 377	O 403	S 13	0	0	0
1	C	273	Total 2160	C 1367	N 377	O 403	S 13	0	0	0

- Molecule 2 is NICOTINATE MONONUCLEOTIDE (three-letter code: NCN) (formula: C₁₁H₁₄NO₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 22	C 11	N 1	O 9	P 1	0	0
2	B	1	Total 22	C 11	N 1	O 9	P 1	0	0
2	C	1	Total 22	C 11	N 1	O 9	P 1	0	0

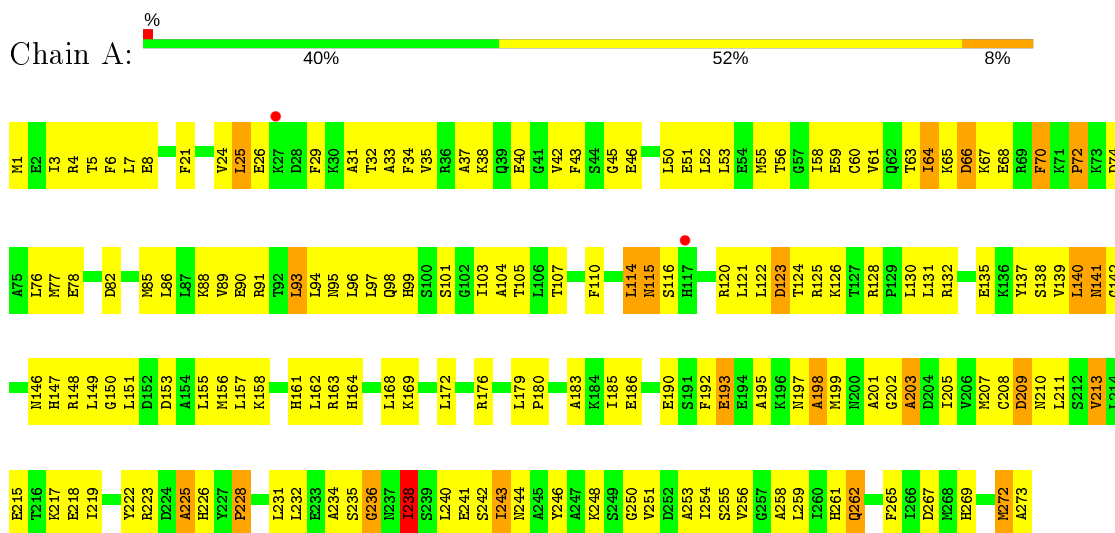
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	5	Total O 5 5	0	0
3	C	10	Total O 10 10	0	0

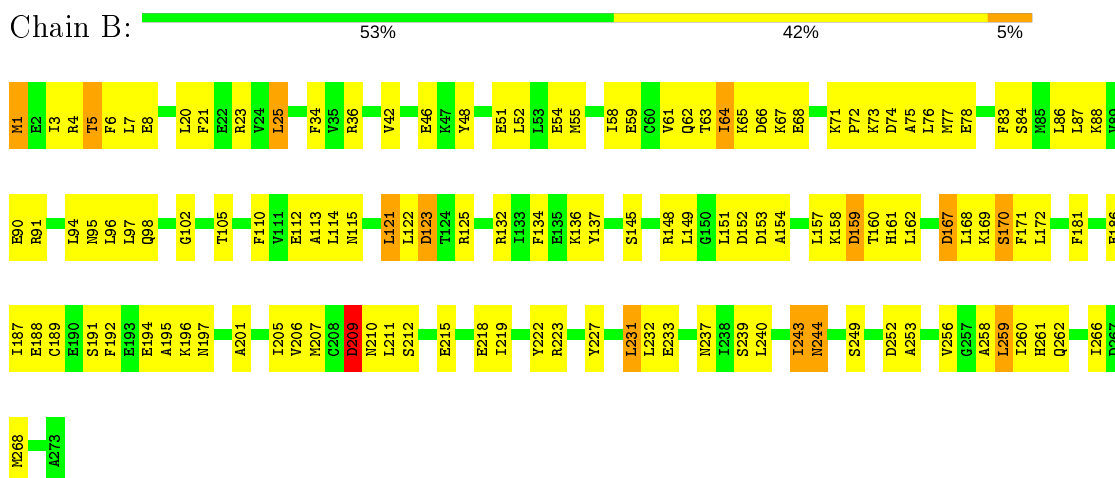
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Probable nicotinate-nucleotide pyrophosphorylase



- Molecule 1: Probable nicotinate-nucleotide pyrophosphorylase



- Molecule 1: Probable nicotinate-nucleotide pyrophosphorylase



M1	M85	H164	H261
E2	L86	D167	Q262
I3	L87	L168	A263
R4	K88	K169	T264
F21	V89	S170	F265
E22	E90	F171	I266
R23	R91	L172	D267
V24	T92	R176	M268
L25	L93	L179	H269
E26	L94	L186	M270
K27	N95	I187	A273
D28	L96	E188	
F29	L97	E197	
K30	Q98	E198	
A31	H99	N197	
T32	G102	A201	
A33	I103	D204	
F34	A104	I205	
V35	T105	V206	
R36	L106	M207	
A37	T107	S212	
K38	F110	V213	
Q39	F114	L214	
V42	L114	E215	
F43	M115	T216	
S44	S116	K217	
G45	L121	R223	
E46	R125	Y227	
K47	R132	V230	
Y48	I133	L231	
A49	F134	L232	
L50	E135	I238	
E51	K136	E241	
M55	Y137	S242	
I58	L140	I243	
T63	M141	A247	
I64	M146	K248	
K65	H147	S249	
D66	R148	G250	
K67	L149	V251	
F70	L150	I254	
K71	L151	S255	
D74	D152	V256	
A75	A153	G257	
L76	A154	A258	
M77	L155	L259	
E78	M156	I260	
I79	L157		
R80	K158		
G81	H161		
D82	L162		
F83	R163		
S84			

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	148.85Å 148.85Å 145.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.31 29.95 – 3.32	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.95-3.31) 91.0 (29.95-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.13 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.286 0.196 , 0.261	Depositor DCC
R_{free} test set	2249 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for -h,-l,-k 0.037 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6564	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: NCN

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	0.39	0/2192	0.60	0/2940
1	B	0.43	0/2192	0.66	0/2940
1	C	0.44	0/2192	0.68	0/2940
All	All	0.42	0/6576	0.65	0/8820

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	2160	0	2203	174	0
1	B	2160	0	2203	129	0
1	C	2160	0	2203	146	0
2	A	22	0	12	2	0
2	B	22	0	12	0	0
2	C	22	0	12	0	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
All	All	6564	0	6645	442	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 34.

All (442) 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:1:MET:HG3	1:C:2:GLU:H	0.99	1.14
1:C:1:MET:HG2	1:C:4:ARG:HG3	1.30	1.14
1:A:7:LEU:HD12	1:A:52:LEU:HB2	1.42	1.01
1:A:146:ASN:HD22	1:C:23:ARG:NH2	1.60	0.98
1:C:1:MET:HG3	1:C:2:GLU:N	1.75	0.96
1:C:158:LYS:H	1:C:161:HIS:HD2	1.08	0.95
1:B:23:ARG:HH22	1:C:146:ASN:HD22	1.12	0.94
1:B:64:ILE:HD11	1:B:76:LEU:HA	1.47	0.94
1:A:155:LEU:HD12	1:A:179:LEU:HD21	1.54	0.90
1:C:1:MET:CG	1:C:2:GLU:H	1.79	0.90
1:A:42:VAL:HG22	1:A:43:PHE:H	1.36	0.89
1:C:85:MET:CE	1:C:88:LYS:HD2	2.03	0.89
1:A:234:ALA:HB3	1:A:254:ILE:HG23	1.59	0.85
1:C:51:GLU:O	1:C:55:MET:HB2	1.78	0.84
1:B:3:ILE:O	1:B:7:LEU:HD23	1.77	0.83
1:C:213:VAL:O	1:C:217:LYS:HG3	1.78	0.82
1:A:256:VAL:HG13	1:A:259:LEU:HG	1.59	0.81
1:C:39:GLN:NE2	1:C:267:ASP:H	1.79	0.81
1:A:1:MET:HB2	1:A:4:ARG:HE	1.47	0.80
1:B:91:ARG:HH22	1:B:98:GLN:NE2	1.79	0.79
1:C:91:ARG:HA	1:C:91:ARG:HE	1.48	0.78
1:A:146:ASN:HD22	1:C:23:ARG:HH22	1.30	0.78
1:A:21:PHE:O	1:A:24:VAL:HG22	1.83	0.78
1:B:42:VAL:HG12	1:B:105:THR:HA	1.63	0.78
1:B:46:GLU:OE1	1:B:65:LYS:HA	1.84	0.77
1:C:76:LEU:HD22	1:C:268:MET:CE	2.15	0.76
1:A:146:ASN:ND2	1:C:23:ARG:HH22	1.84	0.76
1:A:146:ASN:ND2	1:C:23:ARG:NH2	2.33	0.76
1:A:157:LEU:HD13	1:A:162:LEU:HD21	1.67	0.75
1:B:42:VAL:CG1	1:B:105:THR:HA	2.17	0.75
1:B:91:ARG:NH2	1:B:98:GLN:NE2	2.35	0.74
1:A:96:LEU:HD12	1:A:97:LEU:N	2.02	0.74
1:C:158:LYS:H	1:C:161:HIS:CD2	2.00	0.73
1:B:51:GLU:O	1:B:55:MET:HB2	1.88	0.73
1:A:91:ARG:HG3	1:A:95:ASN:HD21	1.53	0.72
1:B:91:ARG:NH2	1:B:98:GLN:HE21	1.88	0.72
1:C:158:LYS:N	1:C:161:HIS:HD2	1.87	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.55	0.71
1:C:227:TYR:HB3	1:C:230:VAL:CG2	2.20	0.71
1:B:158:LYS:H	1:B:161:HIS:HD2	1.37	0.71
1:A:1:MET:HE3	1:A:51:GLU:HB2	1.72	0.70
1:C:58:ILE:HD13	1:C:86:LEU:HD23	1.71	0.70
1:C:132:ARG:HG3	1:C:133:ILE:HD12	1.73	0.70
1:B:34:PHE:CE2	1:B:78:GLU:HG3	2.27	0.70
1:C:258:ALA:HA	1:C:261:HIS:CE1	2.26	0.70
1:B:121:LEU:HD21	1:B:256:VAL:HG12	1.73	0.69
1:B:61:VAL:HG12	1:B:62:GLN:HG3	1.72	0.69
1:B:261:HIS:HD2	1:B:262:GLN:HE21	1.40	0.69
1:A:120:ARG:HB2	1:A:253:ALA:HB2	1.72	0.69
1:C:1:MET:N	1:C:4:ARG:HD2	2.07	0.69
1:A:258:ALA:HA	1:A:261:HIS:CE1	2.28	0.69
1:A:91:ARG:HG3	1:A:95:ASN:ND2	2.08	0.68
1:B:1:MET:HB3	1:B:4:ARG:HG3	1.73	0.68
1:A:3:ILE:O	1:A:7:LEU:HD23	1.92	0.68
1:A:125:ARG:NH1	1:A:151:LEU:HD21	2.09	0.68
1:C:4:ARG:HG2	1:C:51:GLU:OE2	1.92	0.68
1:B:158:LYS:HG3	1:B:160:THR:HG22	1.76	0.68
1:A:140:LEU:HD12	1:A:146:ASN:HD21	1.59	0.67
1:C:1:MET:H1	1:C:4:ARG:HD2	1.58	0.67
1:A:226:HIS:O	1:A:228:PRO:HD3	1.94	0.67
1:B:232:LEU:O	1:B:252:ASP:HB2	1.95	0.67
1:C:121:LEU:CD2	1:C:259:LEU:HD11	2.25	0.67
1:C:66:ASP:O	1:C:67:LYS:HB2	1.94	0.67
1:A:190:GLU:O	1:A:211:LEU:HD21	1.95	0.67
1:C:223:ARG:HD2	1:C:227:TYR:O	1.95	0.66
1:A:232:LEU:HB3	1:A:251:VAL:HG23	1.77	0.66
1:A:99:HIS:O	1:A:103:ILE:HG13	1.95	0.66
1:B:64:ILE:HD11	1:B:76:LEU:CA	2.25	0.66
1:A:38:LYS:HD2	1:A:269:HIS:ND1	2.11	0.66
1:C:227:TYR:HB3	1:C:230:VAL:HG21	1.77	0.66
1:A:124:THR:HG22	1:A:126:LYS:H	1.61	0.66
1:C:155:LEU:HD12	1:C:156:MET:N	2.11	0.66
1:B:132:ARG:NH1	1:B:149:LEU:O	2.30	0.65
1:A:42:VAL:HG22	1:A:43:PHE:N	2.11	0.64
1:C:30:LYS:HE2	1:C:80:ARG:NH2	2.13	0.64
1:A:256:VAL:O	1:A:256:VAL:HG13	1.98	0.64
1:C:168:LEU:HD23	1:C:172:LEU:HG	1.78	0.64
1:C:34:PHE:CZ	1:C:78:GLU:HG3	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CE1	1:A:218:GLU:HB3	2.32	0.64
1:B:6:PHE:HD2	1:B:7:LEU:HD22	1.62	0.64
1:A:124:THR:CG2	1:A:126:LYS:HG3	2.28	0.64
1:A:66:ASP:O	1:A:68:GLU:N	2.31	0.63
1:C:162:LEU:O	1:C:164:HIS:N	2.32	0.63
1:A:158:LYS:H	1:A:161:HIS:CD2	2.15	0.63
1:A:29:PHE:HE1	1:A:31:ALA:HB2	1.62	0.63
1:B:102:GLY:HA2	1:B:266:ILE:HG13	1.80	0.63
1:A:85:MET:HA	1:A:88:LYS:HE3	1.81	0.62
1:C:32:THR:HG22	1:C:33:ALA:N	2.15	0.62
1:C:1:MET:HG2	1:C:4:ARG:CG	2.17	0.62
1:A:146:ASN:HD22	1:C:23:ARG:HH21	1.47	0.62
1:A:56:THR:HG21	1:A:89:VAL:CG2	2.29	0.62
1:C:114:LEU:HD23	1:C:243:ILE:HG22	1.80	0.62
1:C:30:LYS:HE2	1:C:80:ARG:HH21	1.64	0.62
1:B:232:LEU:N	1:B:252:ASP:OD1	2.33	0.62
1:C:94:LEU:HB3	1:C:98:GLN:HE21	1.65	0.61
1:A:124:THR:HG21	1:A:126:LYS:HG3	1.82	0.61
1:A:140:LEU:CD1	1:A:146:ASN:HD21	2.13	0.61
1:C:39:GLN:HE21	1:C:267:ASP:H	1.48	0.61
1:A:156:MET:HG3	1:A:186:GLU:OE1	2.01	0.61
1:A:56:THR:HG21	1:A:89:VAL:HG21	1.83	0.61
1:B:64:ILE:CD1	1:B:76:LEU:HD23	2.30	0.61
1:B:58:ILE:HD13	1:B:86:LEU:HD23	1.82	0.61
1:B:239:SER:O	1:B:243:ILE:HB	2.00	0.60
1:C:168:LEU:CD2	1:C:172:LEU:HG	2.31	0.60
1:A:46:GLU:HB3	1:A:66:ASP:OD2	2.00	0.60
1:B:256:VAL:O	1:B:259:LEU:HG	2.02	0.60
1:B:77:MET:HE1	1:B:97:LEU:HD11	1.84	0.60
1:A:261:HIS:O	1:A:262:GLN:HG2	2.00	0.60
1:A:94:LEU:HB3	1:A:98:GLN:HE21	1.67	0.60
1:B:110:PHE:HE2	1:B:256:VAL:HG21	1.66	0.60
1:C:37:ALA:HB2	1:C:76:LEU:HD11	1.82	0.60
1:C:34:PHE:HA	1:C:77:MET:O	2.02	0.60
1:A:59:GLU:OE2	1:A:61:VAL:HG22	2.01	0.59
1:A:124:THR:CG2	1:A:125:ARG:N	2.65	0.59
1:A:66:ASP:HB3	1:A:141:ASN:ND2	2.18	0.59
1:A:140:LEU:C	1:A:142:GLY:H	2.06	0.59
1:A:172:LEU:O	1:A:176:ARG:HG2	2.02	0.59
1:A:107:THR:HG23	1:A:259:LEU:HD22	1.84	0.59
1:B:206:VAL:HB	1:B:232:LEU:HD23	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD22	1:A:185:ILE:HG21	1.84	0.59
1:C:110:PHE:HB3	1:C:121:LEU:HD11	1.85	0.59
1:B:192:PHE:CE1	1:B:218:GLU:HG2	2.38	0.59
1:B:258:ALA:HA	1:B:261:HIS:CE1	2.38	0.59
1:A:53:LEU:HD22	1:A:58:ILE:HG21	1.84	0.58
1:A:130:LEU:O	1:A:131:LEU:HD23	2.03	0.58
1:B:102:GLY:HA2	1:B:266:ILE:CG1	2.33	0.58
1:A:243:ILE:O	1:A:243:ILE:HD13	2.03	0.58
1:C:188:GLU:HA	1:C:207:MET:HB2	1.86	0.58
1:A:195:ALA:HB2	1:A:219:ILE:HD13	1.85	0.58
1:C:85:MET:HE3	1:C:88:LYS:HD2	1.84	0.58
1:C:115:ASN:O	1:C:116:SER:HB2	2.03	0.58
1:B:162:LEU:HD22	1:B:162:LEU:H	1.69	0.57
1:A:124:THR:HG22	1:A:125:ARG:N	2.18	0.57
1:A:40:GLU:N	1:A:72:PRO:HD3	2.19	0.57
1:A:124:THR:HG22	1:A:126:LYS:N	2.20	0.57
1:B:215:GLU:O	1:B:219:ILE:HG13	2.04	0.57
1:B:132:ARG:NH1	1:B:132:ARG:HG2	2.19	0.57
1:C:230:VAL:O	1:C:231:LEU:HB2	2.04	0.57
1:C:94:LEU:O	1:C:98:GLN:HG3	2.04	0.57
1:A:122:LEU:HB2	1:A:255:SER:HB3	1.85	0.57
1:B:77:MET:CE	1:B:97:LEU:HD11	2.34	0.57
1:A:240:LEU:O	1:A:240:LEU:HD23	2.05	0.57
1:A:93:LEU:HD22	1:A:97:LEU:HD12	1.86	0.57
1:C:76:LEU:HD22	1:C:268:MET:HE3	1.87	0.57
1:A:234:ALA:CB	1:A:254:ILE:HG23	2.33	0.57
1:C:1:MET:CE	1:C:3:ILE:HG12	2.35	0.56
1:C:63:THR:HG22	1:C:64:ILE:O	2.05	0.56
1:B:36:ARG:HG2	1:B:75:ALA:HA	1.88	0.56
1:C:136:LYS:HG3	1:C:149:LEU:HD23	1.87	0.56
1:A:186:GLU:HG3	1:A:205:ILE:HG22	1.86	0.56
1:C:121:LEU:HD22	1:C:259:LEU:HD11	1.88	0.56
1:A:180:PRO:HG2	1:A:183:ALA:HB2	1.88	0.56
1:C:204:ASP:C	1:C:205:ILE:HG13	2.24	0.56
1:C:152:ASP:N	1:C:152:ASP:OD2	2.36	0.56
1:C:42:VAL:HG12	1:C:105:THR:HA	1.88	0.56
1:B:231:LEU:HA	1:B:252:ASP:OD1	2.06	0.56
1:C:96:LEU:C	1:C:96:LEU:HD12	2.26	0.56
1:C:67:LYS:HG2	1:C:141:ASN:O	2.06	0.55
1:B:102:GLY:HA2	1:B:266:ILE:HD11	1.88	0.55
1:A:24:VAL:HG23	1:A:25:LEU:N	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:NE	1:B:95:ASN:OD1	2.36	0.55
1:A:272:MET:O	1:A:273:ALA:HB3	2.06	0.55
1:C:125:ARG:CZ	1:C:151:LEU:HD21	2.37	0.55
1:B:102:GLY:HA2	1:B:266:ILE:CD1	2.37	0.55
1:C:155:LEU:HD11	1:C:157:LEU:CD2	2.37	0.55
1:B:122:LEU:HA	1:B:145:SER:O	2.06	0.55
1:A:53:LEU:HD22	1:A:58:ILE:CG2	2.37	0.55
1:B:266:ILE:O	1:B:268:MET:HG3	2.07	0.55
1:A:210:ASN:O	1:A:211:LEU:HD23	2.07	0.54
1:B:167:ASP:OD2	1:B:170:SER:HB3	2.07	0.54
1:B:21:PHE:CE2	1:B:25:LEU:HD23	2.42	0.54
1:A:91:ARG:HE	1:A:95:ASN:HD21	1.53	0.54
1:B:123:ASP:OD1	1:B:136:LYS:NZ	2.41	0.54
1:B:209:ASP:O	1:B:211:LEU:N	2.40	0.54
1:B:23:ARG:HH22	1:C:146:ASN:ND2	1.93	0.54
1:C:157:LEU:HA	1:C:161:HIS:CD2	2.42	0.54
1:A:60:CYS:SG	1:A:63:THR:OG1	2.65	0.54
1:B:158:LYS:H	1:B:161:HIS:CD2	2.22	0.54
1:B:233:GLU:HA	1:B:253:ALA:O	2.08	0.54
1:C:85:MET:O	1:C:87:LEU:N	2.41	0.54
1:A:135:GLU:O	1:A:138:SER:N	2.40	0.54
1:C:204:ASP:O	1:C:230:VAL:O	2.25	0.54
1:A:132:ARG:HD3	1:A:132:ARG:O	2.07	0.54
1:C:230:VAL:O	1:C:231:LEU:CB	2.56	0.54
1:B:206:VAL:HB	1:B:232:LEU:CD2	2.38	0.53
1:A:94:LEU:O	1:A:98:GLN:HG3	2.08	0.53
1:B:125:ARG:CZ	1:B:151:LEU:HD21	2.38	0.53
1:C:162:LEU:C	1:C:164:HIS:H	2.11	0.53
1:C:249:SER:OG	1:C:251:VAL:HG13	2.08	0.53
1:A:168:LEU:HD22	1:A:201:ALA:CB	2.39	0.53
1:A:56:THR:HG22	1:A:85:MET:SD	2.49	0.53
1:C:21:PHE:CE2	1:C:25:LEU:HD23	2.44	0.53
1:B:168:LEU:O	1:B:171:PHE:N	2.41	0.53
1:B:94:LEU:O	1:B:98:GLN:HG3	2.09	0.53
1:C:155:LEU:HD11	1:C:157:LEU:HD23	1.91	0.53
1:C:238:ILE:HG22	1:C:243:ILE:HD13	1.91	0.53
1:A:32:THR:HG22	1:A:33:ALA:N	2.24	0.52
1:C:46:GLU:HB3	1:C:66:ASP:OD2	2.10	0.52
1:A:42:VAL:HG12	1:A:105:THR:OG1	2.09	0.52
1:A:5:THR:HA	1:A:8:GLU:HB2	1.90	0.52
1:B:256:VAL:O	1:B:256:VAL:HG13	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ARG:HB2	1:C:153:ASP:HB3	1.92	0.52
1:C:76:LEU:N	1:C:76:LEU:HD12	2.25	0.52
1:B:110:PHE:CE1	1:B:240:LEU:HG	2.45	0.51
1:B:34:PHE:HA	1:B:77:MET:O	2.09	0.51
1:C:227:TYR:CB	1:C:230:VAL:HG21	2.40	0.51
1:A:38:LYS:HB2	1:A:267:ASP:HB3	1.93	0.51
1:B:244:ASN:C	1:B:244:ASN:HD22	2.13	0.51
1:A:125:ARG:CZ	1:A:151:LEU:HD21	2.41	0.51
1:A:202:GLY:O	1:A:203:ALA:C	2.49	0.51
1:C:172:LEU:O	1:C:176:ARG:HG2	2.10	0.51
1:C:1:MET:CG	1:C:2:GLU:N	2.51	0.51
1:A:7:LEU:CD1	1:A:52:LEU:HB2	2.26	0.51
1:C:121:LEU:HD21	1:C:259:LEU:HD11	1.92	0.51
1:A:162:LEU:C	1:A:164:HIS:H	2.14	0.51
1:B:192:PHE:CE2	1:B:196:LYS:HD2	2.46	0.51
1:A:186:GLU:HG3	1:A:205:ILE:CG2	2.41	0.51
1:A:91:ARG:HE	1:A:95:ASN:ND2	2.08	0.51
1:B:121:LEU:HD22	1:B:259:LEU:HD11	1.93	0.51
1:B:157:LEU:HA	1:B:161:HIS:CD2	2.46	0.51
1:B:6:PHE:CD2	1:B:7:LEU:HD22	2.42	0.51
1:C:21:PHE:CZ	1:C:25:LEU:HD23	2.47	0.50
1:A:207:MET:HG2	1:A:208:CYS:H	1.75	0.50
1:A:242:SER:O	1:A:246:TYR:HD1	1.94	0.50
1:C:134:PHE:O	1:C:137:TYR:HB3	2.11	0.50
1:B:169:LYS:HA	1:B:201:ALA:HB1	1.94	0.50
1:B:186:GLU:HA	1:B:205:ILE:O	2.10	0.50
1:B:121:LEU:HD21	1:B:256:VAL:CG1	2.38	0.50
1:C:91:ARG:HH21	1:C:94:LEU:CB	2.24	0.50
1:A:110:PHE:HE2	1:A:256:VAL:HG21	1.76	0.50
1:A:258:ALA:O	1:A:262:GLN:HB2	2.11	0.50
1:C:147:HIS:ND1	1:C:148:ARG:N	2.56	0.50
1:B:21:PHE:CZ	1:B:25:LEU:HD23	2.46	0.50
1:C:212:SER:OG	1:C:215:GLU:HG3	2.12	0.50
1:C:1:MET:HE2	1:C:3:ILE:HG12	1.93	0.50
1:C:25:LEU:HD13	1:C:26:GLU:N	2.27	0.50
1:A:209:ASP:HA	1:A:235:SER:O	2.12	0.50
1:C:85:MET:O	1:C:88:LYS:N	2.44	0.50
1:C:238:ILE:HG22	1:C:243:ILE:CD1	2.42	0.49
1:C:1:MET:H1	1:C:4:ARG:CD	2.24	0.49
1:A:34:PHE:CE2	1:A:78:GLU:HG3	2.46	0.49
1:B:21:PHE:CE2	1:B:87:LEU:HD12	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ALA:O	1:A:198:ALA:HB3	2.13	0.49
1:A:110:PHE:CE2	1:A:256:VAL:HG21	2.47	0.49
1:B:212:SER:OG	1:B:215:GLU:HG3	2.11	0.49
1:B:110:PHE:CE2	1:B:256:VAL:HG21	2.46	0.49
1:B:72:PRO:O	1:B:73:LYS:HB2	2.12	0.49
1:A:231:LEU:H	1:A:231:LEU:HD22	1.77	0.49
1:B:71:LYS:O	1:B:74:ASP:HB2	2.13	0.49
1:A:198:ALA:O	1:A:199:MET:C	2.51	0.49
1:C:186:GLU:HG3	1:C:205:ILE:HB	1.95	0.49
1:A:248:LYS:C	1:A:250:GLY:H	2.17	0.49
1:A:235:SER:HB2	1:A:255:SER:OG	2.13	0.49
1:B:91:ARG:HH22	1:B:98:GLN:HE22	1.57	0.49
1:A:34:PHE:HA	1:A:77:MET:O	2.13	0.49
1:A:128:ARG:HG3	1:A:128:ARG:HH11	1.77	0.48
1:A:66:ASP:C	1:A:68:GLU:H	2.17	0.48
1:B:63:THR:HG23	1:B:77:MET:HG2	1.95	0.48
1:C:71:LYS:O	1:C:74:ASP:HB2	2.13	0.48
1:A:236:GLY:H	1:A:238:ILE:HD11	1.78	0.48
1:B:20:LEU:O	1:B:23:ARG:HB2	2.12	0.48
1:C:91:ARG:HH22	1:C:98:GLN:HE22	1.60	0.48
1:A:238:ILE:HD13	1:A:238:ILE:H	1.77	0.48
1:B:66:ASP:O	1:B:67:LYS:HB2	2.14	0.48
1:C:44:SER:HA	1:C:66:ASP:OD1	2.14	0.48
1:A:243:ILE:C	1:A:243:ILE:HD13	2.34	0.48
1:A:25:LEU:HD13	1:A:26:GLU:N	2.28	0.48
1:A:243:ILE:HG23	1:A:244:ASN:N	2.27	0.48
1:B:64:ILE:HD11	1:B:76:LEU:HD23	1.95	0.48
1:C:91:ARG:HH21	1:C:94:LEU:HB2	1.79	0.48
1:B:244:ASN:ND2	1:B:244:ASN:C	2.67	0.48
1:B:258:ALA:C	1:B:260:ILE:H	2.17	0.48
1:B:188:GLU:HA	1:B:207:MET:HB3	1.94	0.48
1:C:85:MET:O	1:C:86:LEU:C	2.51	0.48
1:A:179:LEU:HB3	1:A:180:PRO:HD2	1.97	0.47
1:A:140:LEU:O	1:A:142:GLY:N	2.46	0.47
1:A:241:GLU:C	1:A:243:ILE:H	2.18	0.47
1:A:238:ILE:HD13	1:A:238:ILE:N	2.29	0.47
1:A:6:PHE:HD2	1:A:7:LEU:HD22	1.80	0.47
1:A:261:HIS:O	1:A:262:GLN:CG	2.63	0.47
1:B:96:LEU:C	1:B:96:LEU:HD12	2.35	0.47
1:C:223:ARG:HG3	1:C:232:LEU:HD11	1.96	0.47
1:A:162:LEU:HD22	1:A:162:LEU:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:PHE:HE2	1:B:196:LYS:HD2	1.80	0.47
1:A:29:PHE:CE1	1:A:31:ALA:HB2	2.47	0.47
1:A:42:VAL:CG2	1:A:43:PHE:H	2.19	0.47
1:C:168:LEU:HD23	1:C:168:LEU:O	2.15	0.47
1:C:223:ARG:HG3	1:C:232:LEU:CD1	2.45	0.47
1:A:158:LYS:H	1:A:161:HIS:HD2	1.61	0.47
1:C:79:ILE:HD11	1:C:270:MET:CE	2.45	0.47
1:A:124:THR:C	1:A:126:LYS:H	2.16	0.46
1:A:256:VAL:HG13	1:A:259:LEU:CG	2.39	0.46
1:A:43:PHE:HE2	1:A:46:GLU:HB2	1.79	0.46
1:B:162:LEU:N	1:B:162:LEU:HD22	2.30	0.46
1:A:45:GLY:HA2	1:A:137:TYR:HE2	1.80	0.46
1:A:114:LEU:HD22	1:A:116:SER:HB3	1.97	0.46
1:A:5:THR:O	1:A:6:PHE:C	2.51	0.46
1:A:63:THR:HG22	1:A:64:ILE:N	2.30	0.46
1:B:54:GLU:HG2	1:B:54:GLU:O	2.16	0.46
1:C:32:THR:HG22	1:C:33:ALA:H	1.78	0.46
1:C:64:ILE:HD11	1:C:76:LEU:HB3	1.96	0.46
1:A:40:GLU:H	1:A:72:PRO:HD3	1.79	0.46
1:C:99:HIS:O	1:C:103:ILE:HG13	2.16	0.46
1:A:169:LYS:HA	1:A:201:ALA:HB1	1.98	0.46
1:B:102:GLY:CA	1:B:266:ILE:HG13	2.45	0.46
1:C:256:VAL:O	1:C:259:LEU:HG	2.15	0.46
1:A:261:HIS:HE1	2:A:1002:NCN:O1P	1.99	0.46
1:A:63:THR:CG2	1:A:64:ILE:N	2.79	0.46
1:B:48:TYR:CZ	1:B:134:PHE:HD1	2.34	0.46
1:B:205:ILE:HG12	1:B:231:LEU:CB	2.45	0.46
1:C:223:ARG:C	1:C:223:ARG:HD2	2.36	0.46
1:C:97:LEU:HA	1:C:97:LEU:HD23	1.80	0.46
1:C:107:THR:HG23	1:C:259:LEU:HD13	1.97	0.45
1:B:168:LEU:HD22	1:B:201:ALA:CB	2.46	0.45
1:C:85:MET:C	1:C:87:LEU:N	2.68	0.45
1:C:155:LEU:HD23	1:C:179:LEU:HD11	1.97	0.45
1:C:45:GLY:O	1:C:46:GLU:C	2.53	0.45
1:B:187:ILE:HG22	1:B:189:CYS:SG	2.57	0.45
1:C:91:ARG:HE	1:C:91:ARG:CA	2.26	0.45
1:A:124:THR:HG22	1:A:126:LYS:HG3	1.99	0.45
1:A:223:ARG:C	1:A:225:ALA:N	2.67	0.45
1:A:43:PHE:C	1:A:43:PHE:CD2	2.89	0.45
1:B:195:ALA:HB2	1:B:219:ILE:HD13	1.99	0.45
1:C:32:THR:CG2	1:C:33:ALA:N	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TYR:O	1:A:225:ALA:HB3	2.16	0.45
1:C:102:GLY:HA2	1:C:266:ILE:HG12	1.98	0.45
1:C:223:ARG:CD	1:C:227:TYR:O	2.63	0.45
1:C:36:ARG:HB2	1:C:269:HIS:CE1	2.51	0.45
1:A:124:THR:HG23	2:A:1002:NCN:C2	2.47	0.45
1:A:222:TYR:HE1	1:A:226:HIS:HD2	1.64	0.45
1:A:52:LEU:O	1:A:55:MET:HB3	2.17	0.45
1:B:192:PHE:O	1:B:195:ALA:HB3	2.17	0.45
1:A:24:VAL:CG2	1:A:25:LEU:N	2.80	0.44
1:B:243:ILE:HD13	1:B:243:ILE:O	2.18	0.44
1:A:213:VAL:CG1	1:A:217:LYS:HE3	2.47	0.44
1:B:148:ARG:NH1	1:B:154:ALA:O	2.49	0.44
1:A:149:LEU:HB2	1:A:153:ASP:OD2	2.18	0.44
1:C:102:GLY:HA3	1:C:264:THR:O	2.18	0.44
1:C:63:THR:HG23	1:C:77:MET:HG2	2.00	0.44
1:B:169:LYS:HG3	1:B:201:ALA:HA	2.00	0.44
1:A:33:ALA:HB2	1:A:272:MET:HE1	2.00	0.44
1:B:134:PHE:O	1:B:137:TYR:HB3	2.17	0.44
1:C:3:ILE:HD12	1:C:48:TYR:CD2	2.52	0.43
1:A:261:HIS:CG	1:A:261:HIS:O	2.71	0.43
1:A:96:LEU:HD12	1:A:96:LEU:C	2.38	0.43
1:B:261:HIS:CD2	1:B:262:GLN:HG2	2.53	0.43
1:C:223:ARG:O	1:C:227:TYR:O	2.36	0.43
1:C:85:MET:HE1	1:C:88:LYS:HD2	1.97	0.43
1:B:258:ALA:C	1:B:260:ILE:N	2.71	0.43
1:C:91:ARG:HH21	1:C:94:LEU:CD1	2.31	0.43
1:A:70:PHE:C	1:A:70:PHE:CD1	2.92	0.43
1:B:191:SER:OG	1:B:194:GLU:HG3	2.19	0.43
1:B:61:VAL:HB	1:B:78:GLU:HB3	2.00	0.43
1:A:198:ALA:O	1:A:201:ALA:N	2.51	0.43
1:B:114:LEU:HD13	1:B:115:ASN:N	2.34	0.43
1:C:256:VAL:HG13	1:C:256:VAL:O	2.18	0.43
1:A:101:SER:O	1:A:104:ALA:HB3	2.19	0.43
1:A:64:ILE:HG22	1:A:76:LEU:O	2.18	0.43
1:B:110:PHE:C	1:B:112:GLU:N	2.72	0.43
1:C:76:LEU:HD12	1:C:76:LEU:H	1.84	0.43
1:C:76:LEU:HD22	1:C:268:MET:HE1	1.96	0.43
1:B:256:VAL:O	1:B:256:VAL:HG22	2.19	0.42
1:A:140:LEU:C	1:A:142:GLY:N	2.72	0.42
1:A:243:ILE:CG2	1:A:244:ASN:N	2.83	0.42
1:B:207:MET:HG3	1:B:233:GLU:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:CB	1:A:251:VAL:HG23	2.46	0.42
1:C:39:GLN:O	1:C:70:PHE:HE1	2.02	0.42
1:A:120:ARG:HB2	1:A:253:ALA:CB	2.45	0.42
1:A:207:MET:HG2	1:A:208:CYS:N	2.34	0.42
1:B:91:ARG:O	1:B:95:ASN:HB2	2.20	0.42
1:C:169:LYS:HA	1:C:201:ALA:HA	2.02	0.42
1:C:258:ALA:O	1:C:262:GLN:HB2	2.19	0.42
1:C:28:ASP:OD1	1:C:84:SER:HB3	2.18	0.42
1:A:193:GLU:HA	1:A:193:GLU:OE1	2.20	0.42
1:A:70:PHE:HD1	1:A:70:PHE:C	2.23	0.42
1:C:42:VAL:CG1	1:C:105:THR:HA	2.50	0.42
1:A:46:GLU:HG2	1:A:50:LEU:HD23	2.01	0.42
1:C:70:PHE:C	1:C:70:PHE:CD1	2.93	0.42
1:C:85:MET:HE2	1:C:88:LYS:HB2	2.02	0.42
1:C:84:SER:OG	1:C:85:MET:N	2.52	0.42
1:A:123:ASP:OD2	1:A:139:VAL:HG11	2.20	0.42
1:A:85:MET:O	1:A:85:MET:HE3	2.20	0.42
1:C:204:ASP:O	1:C:205:ILE:HG13	2.19	0.41
1:A:236:GLY:N	1:A:238:ILE:HD11	2.34	0.41
1:A:91:ARG:O	1:A:95:ASN:ND2	2.51	0.41
1:B:158:LYS:O	1:B:162:LEU:HD22	2.20	0.41
1:B:205:ILE:HG23	1:B:231:LEU:HB3	2.02	0.41
1:B:34:PHE:CD2	1:B:78:GLU:HG3	2.54	0.41
1:C:247:ALA:HA	1:C:254:ILE:HD11	2.02	0.41
1:C:39:GLN:HB3	1:C:266:ILE:HG23	2.02	0.41
1:B:157:LEU:HD22	1:B:161:HIS:HB3	2.02	0.41
1:B:196:LYS:HG2	1:B:222:TYR:CZ	2.55	0.41
1:C:110:PHE:O	1:C:114:LEU:HB2	2.20	0.41
1:C:162:LEU:C	1:C:164:HIS:N	2.73	0.41
1:A:35:VAL:O	1:A:35:VAL:HG12	2.21	0.41
1:A:7:LEU:HD22	1:A:7:LEU:N	2.36	0.41
1:A:89:VAL:O	1:A:90:GLU:C	2.58	0.41
1:B:152:ASP:OD1	1:B:153:ASP:N	2.53	0.41
1:B:42:VAL:CG1	1:B:105:THR:CA	2.94	0.41
1:B:64:ILE:HG13	1:B:76:LEU:O	2.19	0.41
1:B:7:LEU:HD12	1:B:52:LEU:HB2	2.01	0.41
1:B:84:SER:O	1:B:88:LYS:HG3	2.19	0.41
1:B:5:THR:HA	1:B:8:GLU:HB2	2.02	0.41
1:A:231:LEU:N	1:A:231:LEU:HD22	2.35	0.41
1:A:1:MET:HB2	1:A:4:ARG:NE	2.26	0.41
1:A:244:ASN:OD1	1:A:248:LYS:HE2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:HG22	1:B:68:GLU:CD	2.40	0.41
1:A:37:ALA:HB2	1:A:76:LEU:HD11	2.03	0.41
1:B:261:HIS:CD2	1:B:262:GLN:HE21	2.29	0.41
1:C:105:THR:O	1:C:106:LEU:C	2.58	0.41
1:C:28:ASP:OD2	1:C:82:ASP:HB3	2.21	0.41
1:A:148:ARG:HD2	1:A:150:GLY:O	2.21	0.41
1:B:192:PHE:CE2	1:B:196:LYS:CD	3.04	0.41
1:A:157:LEU:HD12	1:A:157:LEU:C	2.41	0.41
1:B:192:PHE:CD1	1:B:218:GLU:HG2	2.56	0.41
1:B:36:ARG:CG	1:B:75:ALA:HA	2.51	0.41
1:C:106:LEU:O	1:C:106:LEU:HD23	2.21	0.41
1:C:48:TYR:CZ	1:C:134:PHE:HD1	2.38	0.41
1:C:79:ILE:HD11	1:C:270:MET:HE2	2.02	0.41
1:C:46:GLU:HG2	1:C:50:LEU:HD12	2.03	0.41
1:A:82:ASP:O	1:A:86:LEU:HG	2.21	0.41
1:B:168:LEU:CD2	1:B:172:LEU:HG	2.51	0.41
1:B:223:ARG:HG2	1:B:227:TYR:O	2.21	0.41
1:B:1:MET:HB2	1:B:4:ARG:NE	2.36	0.41
1:B:205:ILE:HG12	1:B:231:LEU:HB2	2.02	0.40
1:A:128:ARG:HG3	1:A:128:ARG:NH1	2.35	0.40
1:A:66:ASP:CB	1:A:141:ASN:ND2	2.85	0.40
1:A:147:HIS:ND1	1:A:148:ARG:N	2.61	0.40
1:A:29:PHE:C	1:A:29:PHE:CD1	2.94	0.40
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.88	0.40
1:A:186:GLU:OE2	1:A:205:ILE:HG21	2.21	0.40
1:A:231:LEU:H	1:A:231:LEU:CD2	2.33	0.40
1:A:33:ALA:HB2	1:A:272:MET:CE	2.52	0.40
1:B:83:PHE:CZ	1:B:87:LEU:HD11	2.56	0.40
1:C:155:LEU:HD12	1:C:156:MET:H	1.83	0.40
1:C:170:SER:OG	1:C:171:PHE:N	2.55	0.40
1:C:256:VAL:HG13	1:C:259:LEU:HG	2.04	0.40
1:C:66:ASP:O	1:C:67:LYS:CB	2.65	0.40
1:A:56:THR:CG2	1:A:85:MET:SD	3.09	0.40
1:B:113:ALA:O	1:B:114:LEU:C	2.59	0.40
1:B:121:LEU:CD2	1:B:259:LEU:HD11	2.51	0.40
1:B:91:ARG:NH2	1:B:94:LEU:HB3	2.36	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	271/273 (99%)	207 (76%)	47 (17%)	17 (6%)	1	10
1	B	271/273 (99%)	216 (80%)	46 (17%)	9 (3%)	4	23
1	C	271/273 (99%)	234 (86%)	28 (10%)	9 (3%)	4	23
All	All	813/819 (99%)	657 (81%)	121 (15%)	35 (4%)	2	18

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	198	ALA
1	A	272	MET
1	B	181	PHE
1	C	163	ARG
1	A	66	ASP
1	A	141	ASN
1	A	203	ALA
1	A	225	ALA
1	A	262	GLN
1	A	265	PHE
1	B	209	ASP
1	B	210	ASN
1	C	116	SER
1	A	115	ASN
1	A	236	GLY
1	B	167	ASP
1	C	86	LEU
1	C	115	ASN
1	C	242	SER
1	A	163	ARG
1	B	237	ASN
1	B	249	SER
1	C	231	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	90	GLU
1	B	159	ASP
1	C	90	GLU
1	C	167	ASP
1	A	65	LYS
1	B	259	LEU
1	C	241	GLU
1	A	228	PRO
1	A	238	ILE
1	A	213	VAL
1	A	72	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	233/233 (100%)	217 (93%)	16 (7%)	15	45
1	B	233/233 (100%)	219 (94%)	14 (6%)	19	50
1	C	233/233 (100%)	222 (95%)	11 (5%)	26	59
All	All	699/699 (100%)	658 (94%)	41 (6%)	19	50

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	64	ILE
1	A	70	PHE
1	A	74	ASP
1	A	93	LEU
1	A	114	LEU
1	A	115	ASN
1	A	121	LEU
1	A	123	ASP
1	A	140	LEU
1	A	193	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	ASN
1	A	209	ASP
1	A	215	GLU
1	A	238	ILE
1	A	243	ILE
1	B	1	MET
1	B	5	THR
1	B	25	LEU
1	B	59	GLU
1	B	64	ILE
1	B	121	LEU
1	B	123	ASP
1	B	159	ASP
1	B	170	SER
1	B	197	ASN
1	B	209	ASP
1	B	231	LEU
1	B	243	ILE
1	B	244	ASN
1	C	2	GLU
1	C	36	ARG
1	C	85	MET
1	C	91	ARG
1	C	93	LEU
1	C	106	LEU
1	C	140	LEU
1	C	153	ASP
1	C	158	LYS
1	C	197	ASN
1	C	231	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	95	ASN
1	A	98	GLN
1	A	115	ASN
1	A	141	ASN
1	A	146	ASN
1	A	161	HIS
1	A	197	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	HIS
1	B	39	GLN
1	B	98	GLN
1	B	161	HIS
1	B	197	ASN
1	B	244	ASN
1	B	261	HIS
1	C	39	GLN
1	C	62	GLN
1	C	98	GLN
1	C	146	ASN
1	C	161	HIS
1	C	197	ASN
1	C	210	ASN
1	C	226	HIS
1	C	262	GLN
1	C	269	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	NCN	C	1001	-	20,23,23	4.83	13 (65%)	27,34,34	1.92	9 (33%)
2	NCN	B	1003	-	20,23,23	4.80	11 (55%)	27,34,34	1.95	8 (29%)
2	NCN	A	1002	-	20,23,23	4.32	12 (60%)	27,34,34	1.94	9 (33%)

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	NCN	C	1001	-	-	6/10/30/30	0/2/2/2
2	NCN	B	1003	-	-	4/10/30/30	0/2/2/2
2	NCN	A	1002	-	-	4/10/30/30	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	NCN	C2-N1	10.88	1.48	1.35
2	C	1001	NCN	C2-N1	10.74	1.48	1.35
2	B	1003	NCN	O4'-C1'	10.28	1.55	1.41
2	C	1001	NCN	O4'-C1'	10.04	1.55	1.41
2	C	1001	NCN	C3-C7	9.77	1.56	1.47
2	A	1002	NCN	O4'-C1'	9.43	1.54	1.41
2	A	1002	NCN	C2-N1	9.13	1.46	1.35
2	B	1003	NCN	C3-C7	8.34	1.55	1.47
2	A	1002	NCN	C3-C7	7.02	1.54	1.47
2	B	1003	NCN	C2'-C1'	6.75	1.64	1.53
2	A	1002	NCN	C2'-C1'	6.00	1.62	1.53
2	B	1003	NCN	C6-N1	5.52	1.48	1.35
2	A	1002	NCN	C6-N1	5.32	1.48	1.35
2	C	1001	NCN	C2'-C1'	5.05	1.61	1.53
2	C	1001	NCN	C6-N1	4.99	1.47	1.35
2	C	1001	NCN	O3'-C3'	4.31	1.53	1.43
2	B	1003	NCN	O2'-C2'	4.27	1.53	1.43
2	A	1002	NCN	O3'-C3'	4.00	1.52	1.43
2	B	1003	NCN	O3'-C3'	3.98	1.52	1.43
2	C	1001	NCN	C3'-C4'	3.93	1.63	1.53
2	B	1003	NCN	C6-C5	3.91	1.47	1.38
2	A	1002	NCN	O2'-C2'	3.86	1.52	1.43
2	C	1001	NCN	O2'-C2'	3.77	1.51	1.43
2	C	1001	NCN	C6-C5	3.73	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	NCN	C6-C5	3.61	1.46	1.38
2	B	1003	NCN	C3'-C4'	3.49	1.61	1.53
2	C	1001	NCN	C4-C3	3.46	1.46	1.39
2	C	1001	NCN	P-O5'	3.39	1.71	1.60
2	A	1002	NCN	C3'-C4'	3.39	1.61	1.53
2	B	1003	NCN	C4-C3	3.22	1.46	1.39
2	A	1002	NCN	P-O5'	3.12	1.70	1.60
2	A	1002	NCN	C4-C3	3.06	1.45	1.39
2	C	1001	NCN	C5'-C4'	2.82	1.60	1.51
2	B	1003	NCN	P-O5'	2.58	1.68	1.60
2	A	1002	NCN	C5'-C4'	2.06	1.58	1.51
2	C	1001	NCN	C5-C4	2.04	1.43	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	NCN	C6-N1-C2	-4.31	118.05	121.97
2	A	1002	NCN	O3'-C3'-C4'	4.11	122.93	111.05
2	A	1002	NCN	C6-N1-C2	-4.09	118.24	121.97
2	C	1001	NCN	O3'-C3'-C4'	3.96	122.49	111.05
2	B	1003	NCN	O3'-C3'-C4'	3.80	122.05	111.05
2	C	1001	NCN	C6-N1-C2	-3.54	118.74	121.97
2	B	1003	NCN	O2'-C2'-C1'	3.28	122.98	110.85
2	A	1002	NCN	O2'-C2'-C1'	3.25	122.86	110.85
2	A	1002	NCN	C3'-C2'-C1'	-3.23	96.12	100.98
2	B	1003	NCN	C3'-C2'-C1'	-3.19	96.17	100.98
2	C	1001	NCN	C3'-C2'-C1'	-3.14	96.25	100.98
2	B	1003	NCN	C2-C3-C7	3.09	125.80	119.84
2	C	1001	NCN	C2-C3-C7	3.05	125.72	119.84
2	C	1001	NCN	O2'-C2'-C1'	3.04	122.08	110.85
2	B	1003	NCN	O5'-C5'-C4'	2.90	118.99	108.99
2	B	1003	NCN	C4-C3-C7	-2.83	116.57	120.37
2	A	1002	NCN	C4-C3-C7	-2.79	116.62	120.37
2	A	1002	NCN	C2-C3-C7	2.79	125.22	119.84
2	C	1001	NCN	O5'-C5'-C4'	2.76	118.48	108.99
2	C	1001	NCN	P-O5'-C5'	2.71	125.76	118.30
2	A	1002	NCN	O5'-C5'-C4'	2.58	117.86	108.99
2	B	1003	NCN	C5-C4-C3	2.56	123.77	120.56
2	C	1001	NCN	C4-C3-C7	-2.40	117.15	120.37
2	A	1002	NCN	C5-C4-C3	2.37	123.54	120.56
2	C	1001	NCN	C5-C4-C3	2.33	123.49	120.56
2	A	1002	NCN	P-O5'-C5'	2.32	124.68	118.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

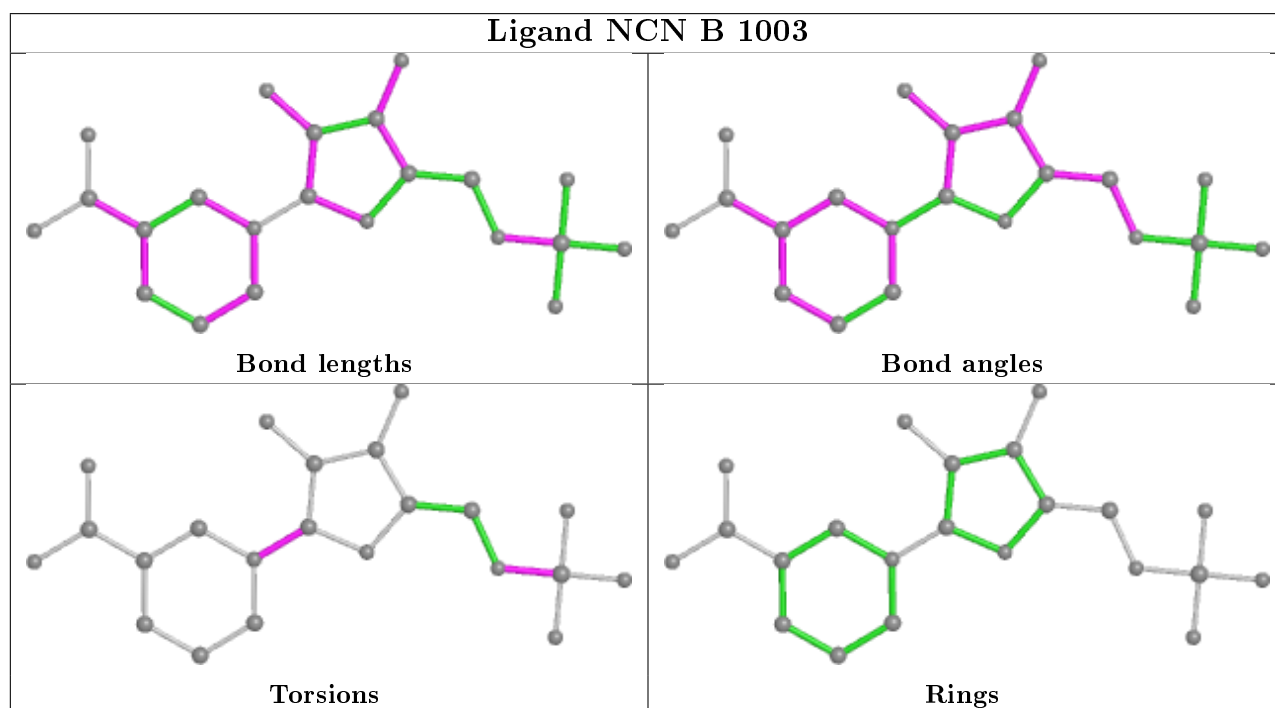
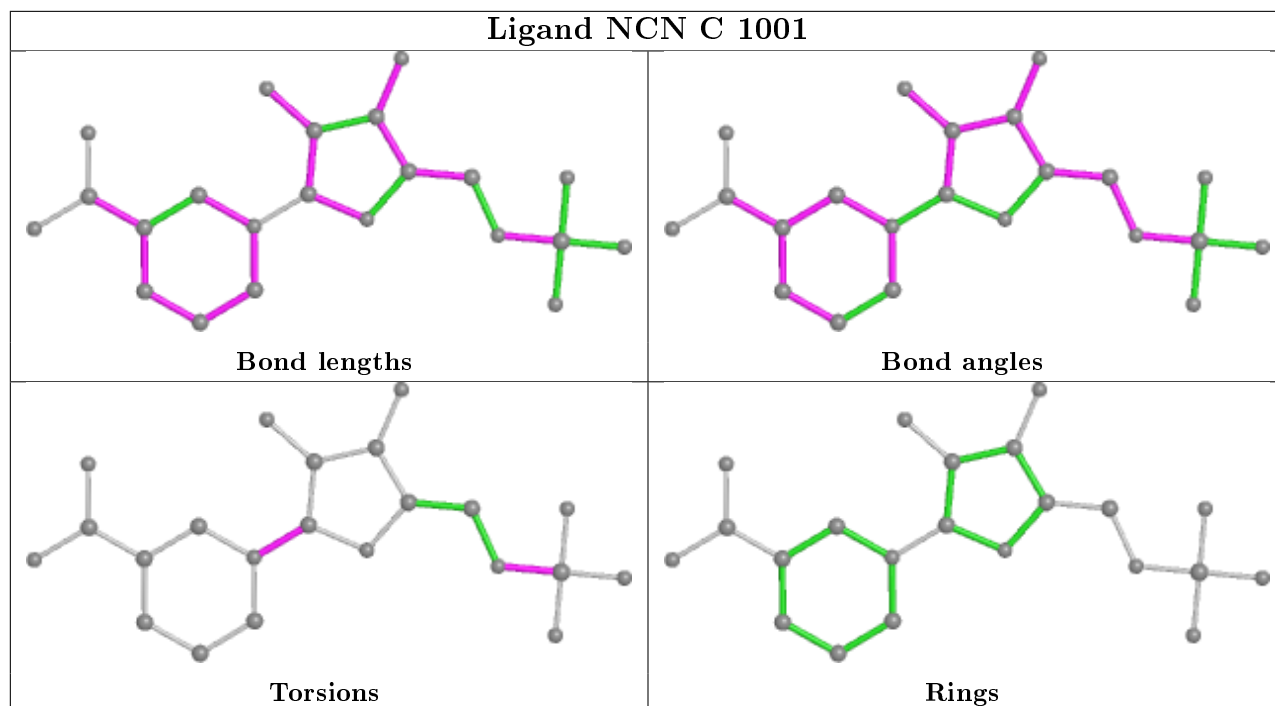
Mol	Chain	Res	Type	Atoms
2	C	1001	NCN	C5'-O5'-P-O1P
2	C	1001	NCN	C5'-O5'-P-O2P
2	C	1001	NCN	C5'-O5'-P-O3P
2	C	1001	NCN	O4'-C1'-N1-C6
2	C	1001	NCN	O4'-C1'-N1-C2
2	B	1003	NCN	C5'-O5'-P-O1P
2	B	1003	NCN	C5'-O5'-P-O2P
2	B	1003	NCN	C5'-O5'-P-O3P
2	B	1003	NCN	O4'-C1'-N1-C6
2	A	1002	NCN	C5'-O5'-P-O1P
2	A	1002	NCN	C5'-O5'-P-O3P
2	A	1002	NCN	O4'-C1'-N1-C6
2	A	1002	NCN	C5'-O5'-P-O2P
2	C	1001	NCN	C2'-C1'-N1-C2

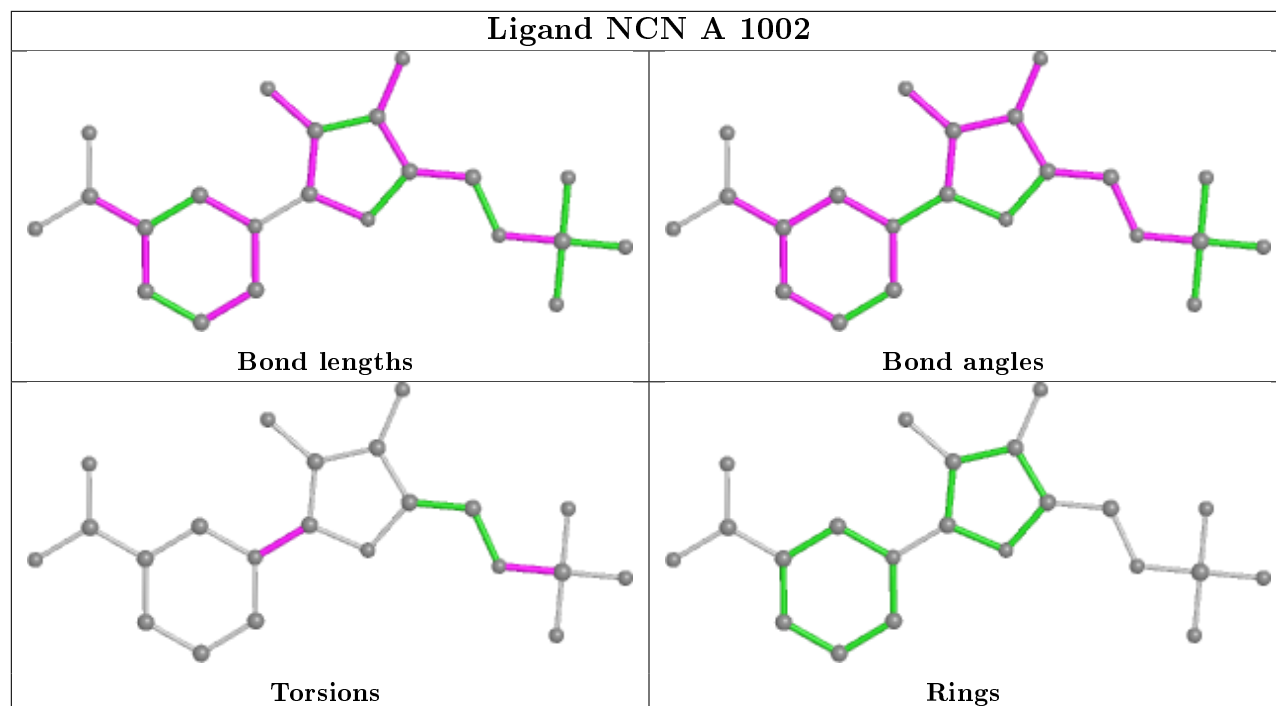
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	NCN	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	273/273 (100%)	-0.37	2 (0%) 87 89	17, 64, 134, 168	0
1	B	273/273 (100%)	-0.52	0 100 100	4, 47, 87, 122	0
1	C	273/273 (100%)	-0.60	0 100 100	12, 40, 97, 122	0
All	All	819/819 (100%)	-0.50	2 (0%) 95 96	4, 50, 112, 168	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	LYS	2.8
1	A	117	HIS	2.2

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 carbohydrates 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, 95th 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.

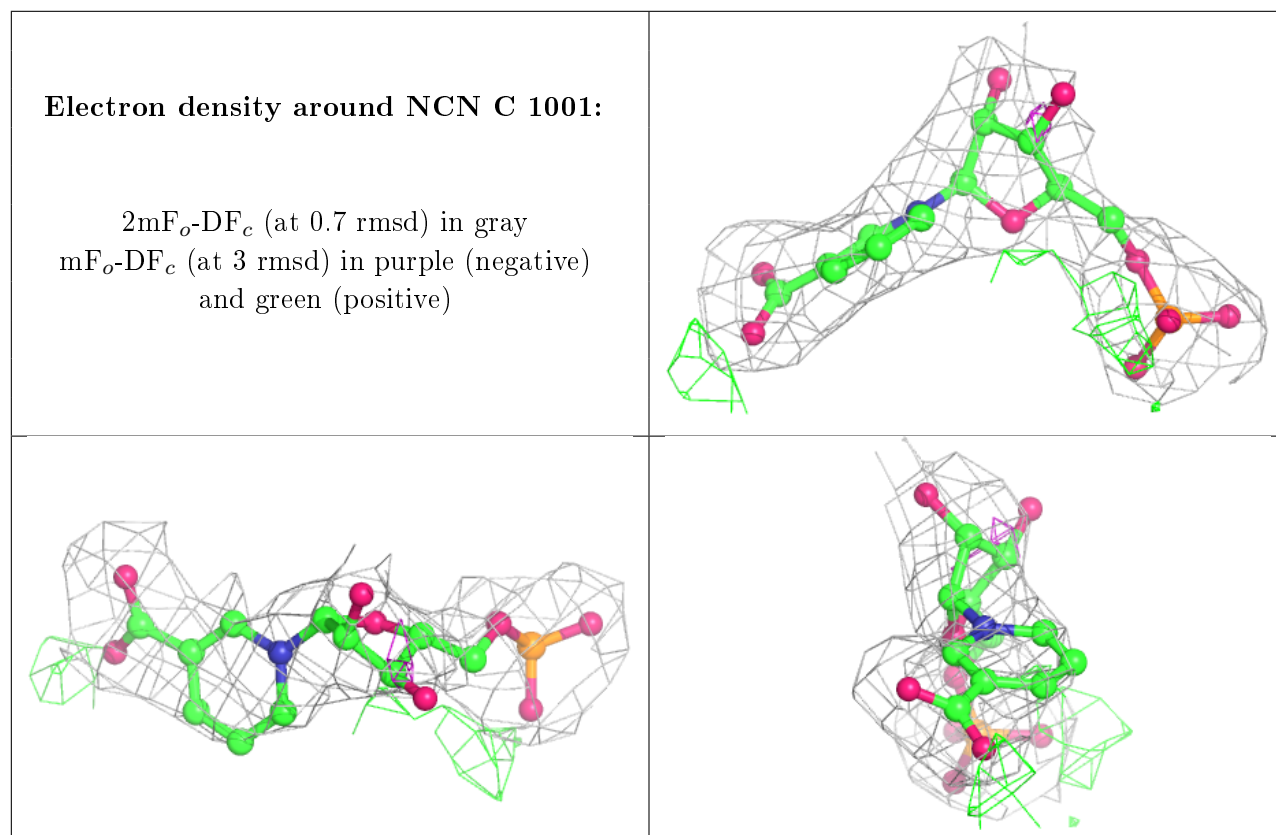
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NCN	C	1001	22/22	0.88	0.24	35,56,61,62	0

Continued on next page...

Continued from previous page...

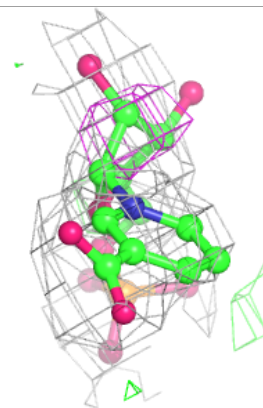
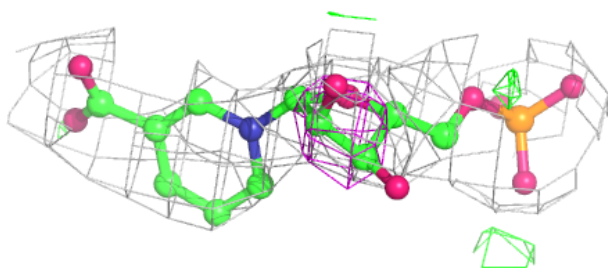
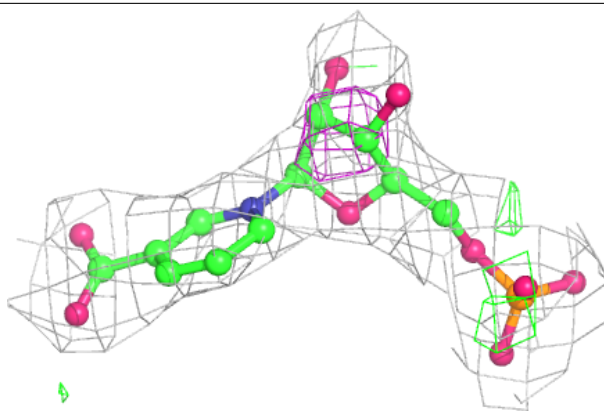
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NCN	B	1003	22/22	0.91	0.24	36,44,52,55	0
2	NCN	A	1002	22/22	0.93	0.18	46,53,54,54	0

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.

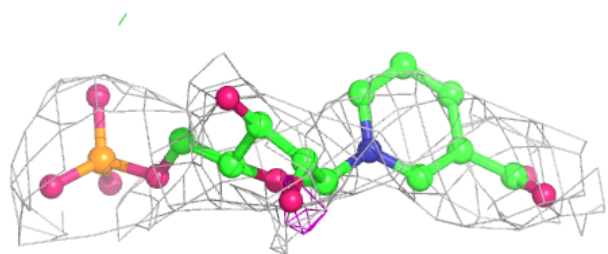
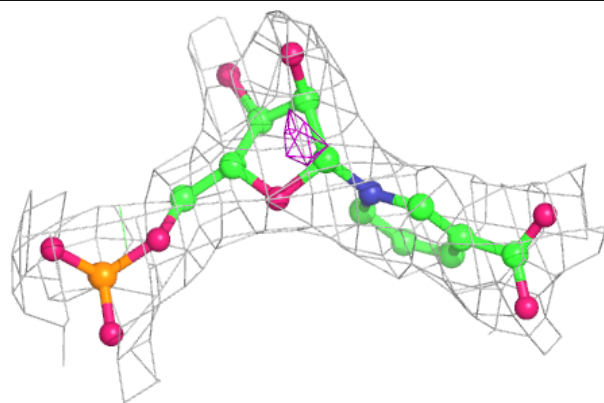


Electron density around NCN B 1003:

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

**Electron density around NCN A 1002:**

$2mF_o-DF_c$ (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.