



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:43 AM UTC

PDB ID : 2B7Q / pdb_00002b7q
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

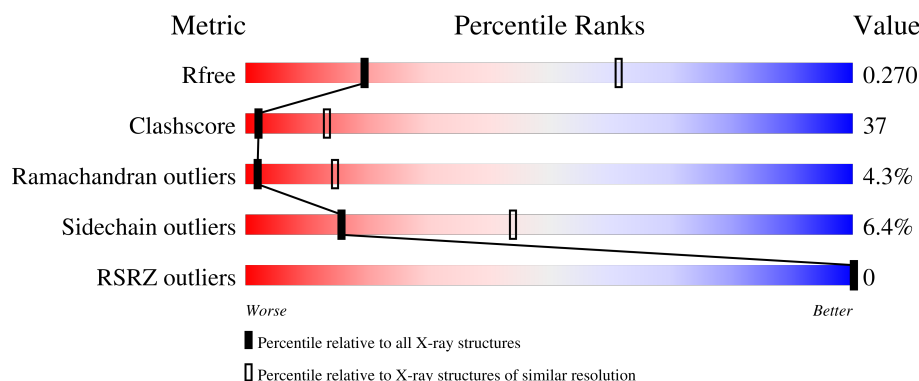
1 Overall quality at a glance

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}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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 $\leq 5\%$. 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	36% 53% 10%
1	B	273	46% 47% 6% .
1	C	273	49% 45% 5% .

2 Entry composition [i](#)

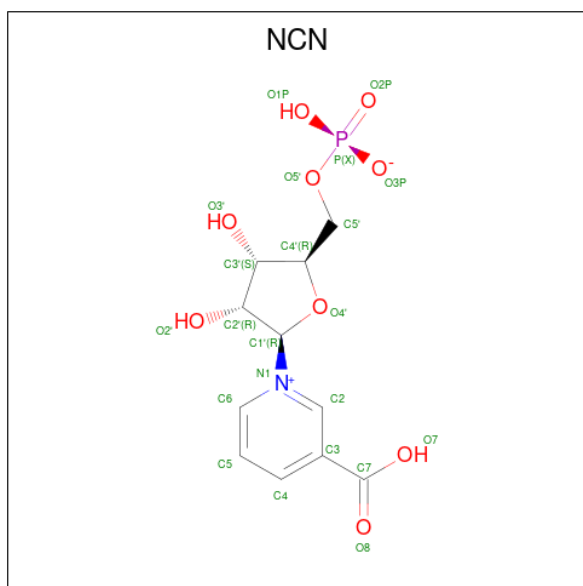
There are 3 unique types of molecules in this entry. The entry contains 6564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	273	Total	C	N	O	S	0	0	0
			2160	1367	377	403	13			
1	B	273	Total	C	N	O	S	0	0	0
			2160	1367	377	403	13			
1	C	273	Total	C	N	O	S	0	0	0
			2160	1367	377	403	13			

- Molecule 2 is NICOTINATE MONONUCLEOTIDE (CCD ID: NCN) (formula: $C_{11}H_{14}NO_9P$).



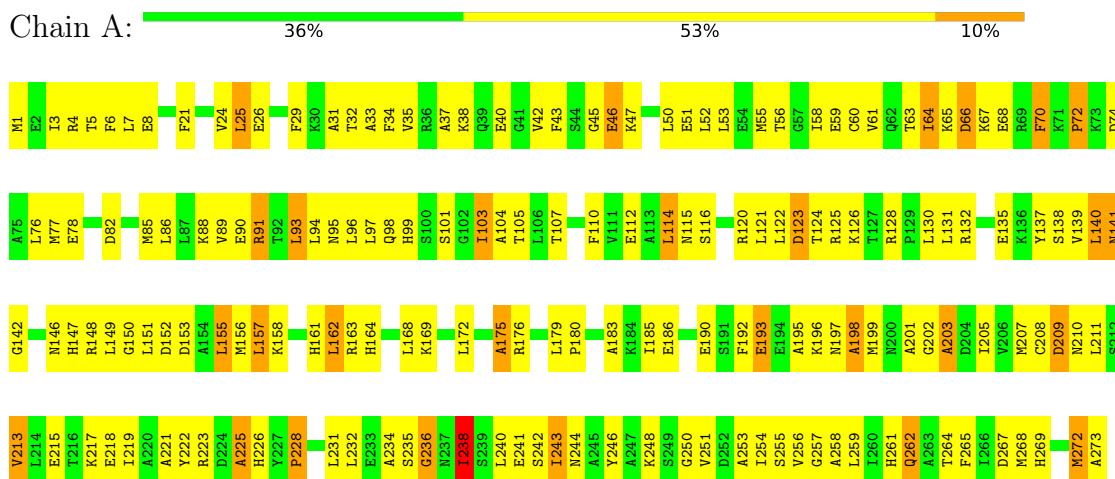
- Molecule 3 is water.

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

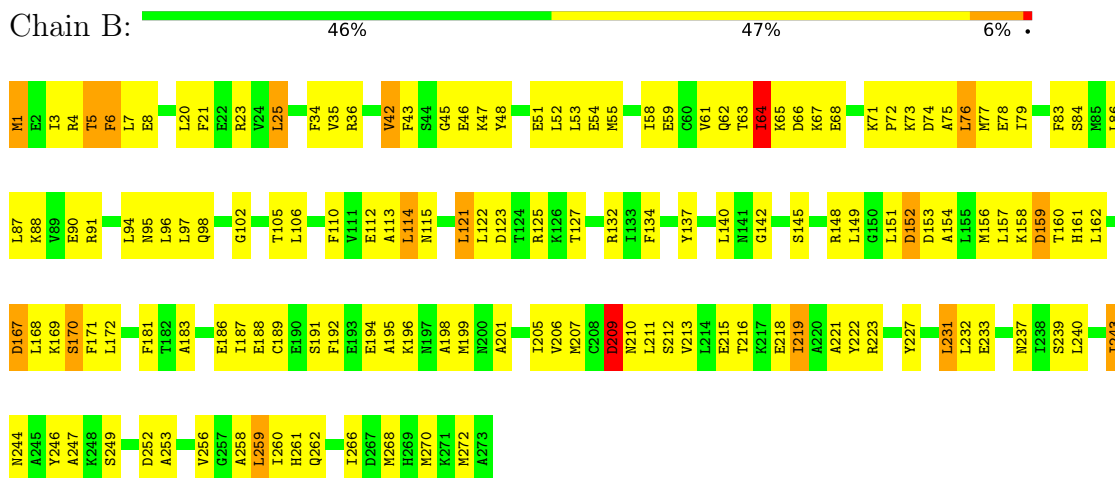
3 Residue-property plots

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: Probable nicotinate-nucleotide pyrophosphorylase



- Molecule 1: Probable nicotinate-nucleotide pyrophosphorylase



- Molecule 1: Probable nicotinate-nucleotide pyrophosphorylase



K248	S249	G250	V251	I254	S255	V256	G257	A258	L259	I260	H261	Q262	A263	T264	F265	I266	D267	M268	H269	M270	A273	S84	M85	L86	L87	K88	V89	E90	R91	T92	L93	L94	N95	L96	L97	Q98	H99	G102	I103	A104	T105	L106	T107	F110	L114	N115	S116	L121	R125	R132	I133	F134	E135	K136	Y137	L140	N141	G142	G143	N146	H147	R148	L149	G150	L151	D152	D153	A154	L155	M156	L157	K158	D159	T160	H161	L162	R163	H164	V165	K166	D167	L168	K169	S170	F171	L172	A175	R176	L179	E186	T187	E188	N197	A198	K199	M200	A201	G202	A203	D204	I205	V206	M207	S212	V213	L214	E215	T216	K217	A221	Y222	R223	Y227	V230	L231	L232	I238	E241	S242	I243	M244	A247	F21	E22	R23	V24	L25	E26	K27	D28	F29	K30	A31	T32	A33	F34	V35	R36	A37	K38	Q39	V42	F43	S44	G45	E46	K47	Y48	A49	L50	E51	M55	I58	T63	I64	K65	D66	K67	F70	K71	P72	K73	D74	A75	L76	M77	E78	I79	R80	G81	D82	F83
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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 – 3.31	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.95-3.31) 90.8 (29.95-3.31)	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 0.209 , 0.270	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)	0.32 , 78.4	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	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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	0.45	0/2192	0.90	5/2940 (0.2%)
1	B	0.51	0/2192	0.93	7/2940 (0.2%)
1	C	0.54	0/2192	1.02	11/2940 (0.4%)
All	All	0.50	0/6576	0.95	23/8820 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	ALA	N-CA-C	-8.22	105.25	114.62
1	B	183	ALA	N-CA-C	6.19	119.59	110.30
1	A	91	ARG	N-CA-C	6.18	117.69	111.07
1	C	147	HIS	N-CA-C	-6.08	100.68	109.31
1	C	43	PHE	N-CA-C	6.06	118.53	109.25
1	C	230	VAL	N-CA-C	5.86	117.24	111.67
1	C	162	LEU	N-CA-C	5.84	117.72	111.36
1	A	152	ASP	N-CA-C	-5.74	106.26	113.72
1	B	6	PHE	N-CA-C	-5.73	104.72	110.97
1	C	165	VAL	N-CA-C	5.65	115.46	106.88
1	B	35	VAL	N-CA-C	-5.64	100.30	108.36
1	B	43	PHE	N-CA-C	5.62	118.70	109.76
1	B	152	ASP	N-CA-C	-5.57	107.12	114.31
1	C	136	LYS	N-CA-C	-5.49	105.19	111.07
1	B	64	ILE	CB-CA-C	-5.43	104.73	111.08
1	B	219	ILE	N-CA-C	-5.37	104.53	112.04
1	C	25	LEU	N-CA-C	-5.32	103.12	110.35
1	C	227	TYR	CA-C-N	5.20	126.34	119.84
1	C	227	TYR	C-N-CA	5.20	126.34	119.84
1	C	166	LYS	N-CA-C	-5.16	102.22	109.96
1	A	157	LEU	N-CA-C	5.10	116.43	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	N-CA-C	-5.09	105.90	112.68
1	A	46	GLU	N-CA-C	-5.06	105.45	110.97

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	2160	0	2203	195	0
1	B	2160	0	2203	149	0
1	C	2160	0	2203	156	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	493	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 37.

All (493) 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:1:MET:H3	1:C:4:ARG:HD2	1.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE	1:C:91:ARG:HA	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:33:ALA:HB2	1:A:272:MET:HE2	1.68	0.76
1:A:146:ASN:ND2	1:C:23:ARG:NH2	2.33	0.76
1:A:146:ASN:ND2	1:C:23:ARG:HH22	1.84	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:79:ILE:HD11	1:C:270:MET:HE2	1.70	0.71
1:C:158:LYS:N	1:C:161:HIS:HD2	1.87	0.71
1:C:1:MET:HE2	1:C:3:ILE:HG12	1.71	0.71
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:C:58:ILE:HD13	1:C:86:LEU:HD23	1.71	0.70
1:B:156:MET:HE2	1:B:186:GLU:OE1	1.92	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:61:VAL:HG12	1:B:62:GLN:HG3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD21	1:B:256:VAL:HG12	1.73	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: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:B:77:MET:HE2	1:B:97:LEU:HD11	1.74	0.67
1:C:76:LEU:HD22	1:C:268:MET:HE3	1.75	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:66:ASP:O	1:C:67:LYS:HB2	1.94	0.67
1:C:121:LEU:CD2	1:C:259:LEU:HD11	2.25	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:99:HIS:O	1:A:103:ILE:HG13	1.95	0.66
1:A:232:LEU:HB3	1:A:251:VAL:HG23	1.77	0.66
1:B:64:ILE:HD11	1:B:76:LEU:CA	2.25	0.66
1:C:1:MET:N	1:C:4:ARG:HD2	2.07	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:C:1:MET:H3	1:C:4:ARG:CD	2.05	0.65
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:A:140:LEU:C	1:A:142:GLY:H	2.06	0.64
1:C:30:LYS:HE2	1:C:80:ARG:NH2	2.13	0.64
1:A:1:MET:HE3	1:A:51:GLU:OE1	1.97	0.64
1:C:34:PHE:CZ	1:C:78:GLU:HG3	2.33	0.64
1:C:168:LEU:HD23	1:C:172:LEU:HG	1.78	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD13	1:B:268:MET:HE2	1.80	0.63
1:A:29:PHE:HE1	1:A:31:ALA:HB2	1.62	0.63
1:B:83:PHE:HE1	1:B:272:MET:HE2	1.64	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:A:256:VAL:HG13	1:A:256:VAL:O	1.98	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:56:THR:HG21	1:A:89:VAL:CG2	2.29	0.62
1:A:146:ASN:HD22	1:C:23:ARG:HH21	1.47	0.62
1:C:30:LYS:HE2	1:C:80:ARG:HH21	1.64	0.62
1:C:114:LEU:HD23	1:C:243:ILE:HG22	1.80	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:B:83:PHE:CE1	1:B:272:MET:HE2	2.34	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:56:THR:HG21	1:A:89:VAL:HG21	1.83	0.61
1:A:156:MET:HG3	1:A:186:GLU:OE1	2.01	0.61
1:B:64:ILE:CD1	1:B:76:LEU:HD23	2.30	0.61
1:C:204:ASP:C	1:C:205:ILE:HG13	2.24	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:C:96:LEU:C	1:C:96:LEU:HD12	2.26	0.60
1:A:94:LEU:HB3	1:A:98:GLN:HE21	1.67	0.60
1:A:261:HIS:O	1:A:262:GLN:HG2	2.00	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:A:243:ILE:O	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:115:ASN:O	1:C:116:SER:HB2	2.03	0.58
1:B:162:LEU:H	1:B:162:LEU:HD22	1.69	0.57
1:C:162:LEU:C	1:C:164:HIS:H	2.11	0.57
1:A:40:GLU:N	1:A:72:PRO:HD3	2.19	0.57
1:A:124:THR:HG22	1:A:125:ARG:N	2.18	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:HG2	1:B:132:ARG:NH1	2.19	0.57
1:C:94:LEU:O	1:C:98:GLN:HG3	2.04	0.57
1:C:230:VAL:O	1:C:231:LEU:HB2	2.04	0.57
1:A:122:LEU:HB2	1:A:255:SER:HB3	1.85	0.57
1:A:93:LEU:HD22	1:A:97:LEU:HD12	1.86	0.57
1:A:240:LEU:HD23	1:A:240:LEU:O	2.05	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:77:MET:HE1	1:A:97:LEU:HD11	1.88	0.56
1:A:186:GLU:HG3	1:A:205:ILE:HG22	1.86	0.56
1:A:195:ALA:O	1:A:199:MET:HE3	2.06	0.56
1:C:121:LEU:HD22	1:C:259:LEU:HD11	1.88	0.56
1:B:77:MET:CE	1:B:97:LEU:HD11	2.34	0.56
1:A:180:PRO:HG2	1:A:183:ALA:HB2	1.88	0.56
1:B:244:ASN:C	1:B:244:ASN:HD22	2.13	0.56
1:A:202:GLY:O	1:A:203:ALA:C	2.49	0.56
1:C:42:VAL:HG12	1:C:105:THR:HA	1.88	0.56
1:C:152:ASP:OD2	1:C:152:ASP:N	2.36	0.56
1:B:231:LEU:HA	1:B:252:ASP:OD1	2.06	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
1:B:91:ARG:NE	1:B:95:ASN:OD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:MET:HE2	1:A:89:VAL:HG23	1.89	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:A:162:LEU:C	1:A:164:HIS:H	2.14	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:O	1:A:132:ARG:HD3	2.07	0.54
1:A:198:ALA:O	1:A:199:MET:C	2.51	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:A:66:ASP:C	1:A:68:GLU:H	2.17	0.53
1:C:85:MET:HE3	1:C:88:LYS:HD2	1.86	0.53
1:C:249:SER:OG	1:C:251:VAL:HG13	2.08	0.53
1:A:56:THR:HG22	1:A:85:MET:SD	2.49	0.53
1:A:168:LEU:HD22	1:A:201:ALA:CB	2.39	0.53
1:B:79:ILE:HD11	1:B:270:MET:HE2	1.90	0.53
1:A:243:ILE:HD13	1:A:243:ILE:C	2.34	0.53
1:C:21:PHE:CE2	1:C:25:LEU:HD23	2.44	0.53
1:B:94:LEU:O	1:B:98:GLN:HG3	2.09	0.53
1:B:168:LEU:O	1:B:171:PHE:N	2.41	0.53
1:B:244:ASN:C	1:B:244:ASN:ND2	2.67	0.53
1:B:258:ALA:C	1:B:260:ILE:H	2.17	0.53
1:C:155:LEU:HD11	1:C:157:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:248:LYS:C	1:A:250:GLY:H	2.17	0.52
1:C:85:MET:O	1:C:86:LEU:C	2.51	0.52
1:C:79:ILE:CD1	1:C:270:MET:HE2	2.38	0.52
1:A:124:THR:C	1:A:126:LYS:H	2.16	0.52
1:C:46:GLU:HB3	1:C:66:ASP:OD2	2.10	0.52
1:A:5:THR:HA	1:A:8:GLU:HB2	1.90	0.52
1:A:42:VAL:HG12	1:A:105:THR:OG1	2.09	0.52
1:B:256:VAL:O	1:B:256:VAL:HG13	2.10	0.52
1:B:96:LEU:C	1:B:96:LEU:HD12	2.35	0.52
1:C:76:LEU:N	1:C:76:LEU:HD12	2.25	0.52
1:C:148:ARG:HB2	1:C:153:ASP:HB3	1.92	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:207:MET:HE2	1:B:233:GLU:OE2	2.10	0.51
1:A:125:ARG:CZ	1:A:151:LEU:HD21	2.41	0.51
1:C:1:MET:CG	1:C:2:GLU:N	2.51	0.51
1:C:172:LEU:O	1:C:176:ARG:HG2	2.10	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:5:THR:O	1:A:6:PHE:C	2.51	0.51
1:B:192:PHE:CE2	1:B:196:LYS:HD2	2.46	0.51
1:C:223:ARG:HD2	1:C:223:ARG:C	2.36	0.51
1:A:91:ARG:HE	1:A:95:ASN:ND2	2.08	0.51
1:A:186:GLU:HG3	1:A:205:ILE:CG2	2.41	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:A:241:GLU:C	1:A:243:ILE:H	2.18	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:121:LEU:HD21	1:B:256:VAL:CG1	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:156:MET:HE2	1:C:186:GLU:CD	2.35	0.50
1:B:21:PHE:CZ	1:B:25:LEU:HD23	2.46	0.50
1:C:45:GLY:O	1:C:46:GLU:C	2.53	0.50
1:C:212:SER:OG	1:C:215:GLU:HG3	2.12	0.50
1:C:25:LEU:HD13	1:C:26:GLU:N	2.27	0.50
1:A:43:PHE:C	1:A:43:PHE:CD2	2.89	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: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
1:A:195:ALA:O	1:A:198:ALA:HB3	2.13	0.49
1:A:223:ARG:C	1:A:225:ALA:N	2.67	0.49
1:A:110:PHE:CE2	1:A:256:VAL:HG21	2.47	0.49
1:B:72:PRO:O	1:B:73:LYS:HB2	2.12	0.49
1:B:110:PHE:CE2	1:B:256:VAL:HG21	2.46	0.49
1:B:212:SER:OG	1:B:215:GLU:HG3	2.11	0.49
1:A:231:LEU:HD22	1:A:231:LEU:H	1.77	0.49
1:B:71:LYS:O	1:B:74:ASP:HB2	2.13	0.49
1:C:186:GLU:HG3	1:C:205:ILE:HB	1.95	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:HH11	1:A:128:ARG:HG3	1.77	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: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:85:MET:HE3	1:C:85:MET:HA	1.95	0.48
1:C:91:ARG:HH21	1:C:94:LEU:HB2	1.79	0.48
1:A:96:LEU:HD12	1:A:96:LEU:C	2.38	0.48
1:B:77:MET:HE2	1:B:97:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CD1	1:A:70:PHE:C	2.92	0.48
1:C:76:LEU:CD2	1:C:268:MET:HE3	2.42	0.48
1:B:188:GLU:HA	1:B:207:MET:HB3	1.94	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:85:MET:HE3	1:A:88:LYS:HE3	1.96	0.47
1:C:85:MET:C	1:C:87:LEU:N	2.68	0.47
1:A:6:PHE:HD2	1:A:7:LEU:HD22	1.80	0.47
1:A:140:LEU:C	1:A:142:GLY:N	2.72	0.47
1:A:238:ILE:HD13	1:A:238:ILE:N	2.29	0.47
1:A:85:MET:HE3	1:A:88:LYS:HB2	1.95	0.47
1:A:162:LEU:N	1:A:162:LEU:HD22	2.29	0.47
1:A:261:HIS:O	1:A:262:GLN:CG	2.63	0.47
1:B:192:PHE:HE2	1:B:196:LYS:HD2	1.80	0.47
1:C:223:ARG:HG3	1:C:232:LEU:HD11	1.96	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:70:PHE:C	1:A:70:PHE:HD1	2.23	0.47
1:A:158:LYS:H	1:A:161:HIS:HD2	1.61	0.47
1:C:70:PHE:CD1	1:C:70:PHE:C	2.93	0.47
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:HD22	1:B:162:LEU:N	2.30	0.46
1:A:45:GLY:HA2	1:A:137:TYR:HE2	1.80	0.46
1:A:63:THR:HG22	1:A:64:ILE:N	2.30	0.46
1:A:114:LEU:HD22	1:A:116:SER:HB3	1.97	0.46
1:B:54:GLU:O	1:B:54:GLU:HG2	2.16	0.46
1:B:258:ALA:C	1:B:260:ILE:N	2.71	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:89:VAL:O	1:A:90:GLU:C	2.58	0.46
1:A:40:GLU:H	1:A:72:PRO:HD3	1.79	0.46
1:B:64:ILE:HG22	1:B:68:GLU:CD	2.40	0.46
1:C:99:HIS:O	1:C:103:ILE:HG13	2.16	0.46
1:A:157:LEU:HD12	1:A:157:LEU:C	2.41	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:63:THR:CG2	1:A:64:ILE:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:HIS:HE1	2:A:1002:NCN:O1P	1.99	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:97:LEU:HD23	1:C:97:LEU:HA	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:155:LEU:HD23	1:C:179:LEU:HD11	1.97	0.45
1:A:29:PHE:CD1	1:A:29:PHE:C	2.94	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: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
1:C:105:THR:O	1:C:106:LEU:C	2.58	0.45
1:A:222:TYR:O	1:A:225:ALA:HB3	2.16	0.45
1:B:113:ALA:O	1:B:114:LEU:C	2.59	0.45
1:C:36:ARG:HB2	1:C:269:HIS:CE1	2.51	0.45
1:C:85:MET:HE1	1:C:88:LYS:HD2	1.93	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:A:52:LEU:O	1:A:55:MET:HB3	2.17	0.45
1:A:124:THR:HG23	2:A:1002:NCN:C2	2.47	0.45
1:A:155:LEU:C	1:A:155:LEU:CD2	2.90	0.45
1:A:222:TYR:HE1	1:A:226:HIS:HD2	1.64	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:A:155:LEU:C	1:A:155:LEU:HD23	2.42	0.44
1:B:243:ILE:HD13	1:B:243:ILE:O	2.18	0.44
1:C:141:ASN:C	1:C:143:GLY:N	2.75	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:B:158:LYS:O	1:B:159:ASP:C	2.59	0.44
1:A:98:GLN:HA	1:A:268:MET:HE3	1.99	0.44
1:A:149:LEU:HB2	1:A:153:ASP:OD2	2.18	0.44
1:A:175:ALA:C	1:A:179:LEU:HD12	2.43	0.44
1:B:221:ALA:O	1:B:222:TYR:C	2.59	0.44
1:C:102:GLY:HA3	1:C:264:THR:O	2.18	0.44
1:C:197:ASN:O	1:C:198:ALA:C	2.59	0.44
1:C:63:THR:HG23	1:C:77:MET:HG2	2.00	0.44
1:C:72:PRO:C	1:C:74:ASP:H	2.24	0.44
1:B:169:LYS:HG3	1:B:201:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TYR:O	1:B:247:ALA:C	2.59	0.44
1:B:45:GLY:O	1:B:46:GLU:C	2.60	0.44
1:B:134:PHE:O	1:B:137:TYR:HB3	2.17	0.44
1:B:53:LEU:C	1:B:55:MET:N	2.76	0.43
1:C:3:ILE:HD12	1:C:48:TYR:CD2	2.52	0.43
1:C:79:ILE:HD11	1:C:270:MET:CE	2.45	0.43
1:A:248:LYS:C	1:A:250:GLY:N	2.74	0.43
1:B:212:SER:O	1:B:213:VAL:C	2.59	0.43
1:A:261:HIS:O	1:A:261:HIS:CG	2.71	0.43
1:B:243:ILE:HD13	1:B:243:ILE:C	2.43	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:91:ARG:HH21	1:C:94:LEU:CD1	2.31	0.43
1:B:61:VAL:HB	1:B:78:GLU:HB3	2.00	0.43
1:B:191:SER:OG	1:B:194:GLU:HG3	2.19	0.43
1:A:198:ALA:O	1:A:201:ALA:N	2.51	0.43
1:B:114:LEU:C	1:B:114:LEU:HD13	2.44	0.43
1:B:114:LEU:HD13	1:B:115:ASN:N	2.34	0.43
1:C:256:VAL:O	1:C:256:VAL:HG13	2.18	0.43
1:A:64:ILE:HG22	1:A:76:LEU:O	2.18	0.43
1:A:101:SER:O	1:A:104:ALA:HB3	2.19	0.43
1:A:196:LYS:O	1:A:197:ASN:C	2.60	0.43
1:B:140:LEU:C	1:B:142:GLY:H	2.26	0.43
1:C:76:LEU:HD12	1:C:76:LEU:H	1.84	0.43
1:A:66:ASP:C	1:A:68:GLU:N	2.77	0.42
1:B:256:VAL:O	1:B:256:VAL:HG22	2.19	0.42
1:A:162:LEU:C	1:A:164:HIS:N	2.78	0.42
1:A:223:ARG:C	1:A:225:ALA:H	2.26	0.42
1:A:243:ILE:CG2	1:A:244:ASN:N	2.83	0.42
1:A:46:GLU:O	1:A:47:LYS:C	2.62	0.42
1:A:112:GLU:C	1:A:114:LEU:H	2.26	0.42
1:B:110:PHE:C	1:B:112:GLU:N	2.72	0.42
1:B:207:MET:HG3	1:B:233:GLU:HG3	2.00	0.42
1:A:42:VAL:HG11	1:A:104:ALA:C	2.44	0.42
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:C:141:ASN:C	1:C:143:GLY:H	2.26	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:28:ASP:OD1	1:C:84:SER:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:193:GLU:HA	1:A:193:GLU:OE1	2.20	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:A:86:LEU:HD13	1:A:272:MET:HE1	2.02	0.42
1:A:124:THR:C	1:A:126:LYS:N	2.76	0.42
1:A:241:GLU:C	1:A:243:ILE:N	2.78	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:C:204:ASP:O	1:C:205:ILE:HG13	2.19	0.41
1:C:243:ILE:O	1:C:244:ASN:C	2.62	0.41
1:A:91:ARG:O	1:A:95:ASN:ND2	2.51	0.41
1:A:236:GLY:N	1:A:238:ILE:HD11	2.34	0.41
1:B:34:PHE:CD2	1:B:78:GLU:HG3	2.54	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:216:THR:C	1:B:218:GLU:N	2.75	0.41
1:C:39:GLN:HB3	1:C:266:ILE:HG23	2.02	0.41
1:C:247:ALA:HA	1:C:254:ILE:HD11	2.02	0.41
1:B:46:GLU:O	1:B:47:LYS:C	2.62	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:A:7:LEU:HD22	1:A:7:LEU:N	2.36	0.41
1:B:5:THR:HA	1:B:8:GLU:HB2	2.02	0.41
1:B:7:LEU:HD12	1:B:52:LEU:HB2	2.01	0.41
1:B:42:VAL:CG1	1:B:105:THR:CA	2.94	0.41
1:B:53:LEU:C	1:B:55:MET:H	2.28	0.41
1:B:64:ILE:HG13	1:B:76:LEU:O	2.19	0.41
1:B:84:SER:O	1:B:88:LYS:HG3	2.19	0.41
1:B:152:ASP:OD1	1:B:153:ASP:N	2.53	0.41
1:C:85:MET:HE2	1:C:88:LYS:HB2	2.01	0.41
1:A:85:MET:HA	1:A:85:MET:HE3	2.03	0.41
1:A:231:LEU:HD22	1:A:231:LEU:N	2.35	0.41
1:A:257:GLY:C	1:A:259:LEU:N	2.78	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
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:28:ASP:OD2	1:C:82:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:200:ASN:C	1:C:202:GLY:N	2.76	0.41
1:B:36:ARG:CG	1:B:75:ALA:HA	2.51	0.41
1:B:192:PHE:CD1	1:B:218:GLU:HG2	2.56	0.41
1:C:46:GLU:HG2	1:C:50:LEU:HD12	2.03	0.41
1:C:48:TYR:CZ	1:C:134:PHE:HD1	2.38	0.41
1:C:106:LEU:HD23	1:C:106:LEU:O	2.21	0.41
1:C:159:ASP:O	1:C:160:THR:C	2.64	0.41
1:A:82:ASP:O	1:A:86:LEU:HG	2.21	0.41
1:B:1:MET:HB2	1:B:4:ARG:NE	2.36	0.41
1:B:168:LEU:CD2	1:B:172:LEU:HG	2.51	0.41
1:B:198:ALA:O	1:B:199:MET:C	2.64	0.41
1:B:223:ARG:HG2	1:B:227:TYR:O	2.21	0.41
1:A:221:ALA:C	1:A:223:ARG:N	2.77	0.40
1:B:205:ILE:HG12	1:B:231:LEU:HB2	2.02	0.40
1:C:221:ALA:C	1:C:223:ARG:N	2.76	0.40
1:A:66:ASP:CB	1:A:141:ASN:ND2	2.85	0.40
1:A:128:ARG:HG3	1:A:128:ARG:NH1	2.35	0.40
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.88	0.40
1:A:147:HIS:ND1	1:A:148:ARG:N	2.61	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:B:83:PHE:CZ	1:B:87:LEU:HD11	2.56	0.40
1:C:66:ASP:O	1:C:67:LYS:CB	2.65	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:A:35:VAL:O	1:A:35:VAL:HG12	2.21	0.40
1:A:56:THR:CG2	1:A:85:MET:SD	3.09	0.40
1:B:91:ARG:NH2	1:B:94:LEU:HB3	2.36	0.40
1:B:112:GLU:O	1:B:113:ALA:C	2.64	0.40
1:B:121:LEU:CD2	1:B:259:LEU:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/273 (99%)	207 (76%)	47 (17%)	17 (6%)	1	8
1	B	271/273 (99%)	216 (80%)	46 (17%)	9 (3%)	3	19
1	C	271/273 (99%)	234 (86%)	28 (10%)	9 (3%)	3	19
All	All	813/819 (99%)	657 (81%)	121 (15%)	35 (4%)	2	15

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

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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 ⓘ

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%)	215 (92%)	18 (8%)	12	38
1	B	233/233 (100%)	217 (93%)	16 (7%)	14	42
1	C	233/233 (100%)	222 (95%)	11 (5%)	23	52
All	All	699/699 (100%)	654 (94%)	45 (6%)	16	44

All (45) 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	103	ILE
1	A	114	LEU
1	A	121	LEU
1	A	123	ASP
1	A	140	LEU
1	A	155	LEU

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Mol	Chain	Res	Type
1	A	162	LEU
1	A	193	GLU
1	A	209	ASP
1	A	215	GLU
1	A	238	ILE
1	A	243	ILE
1	A	264	THR
1	B	1	MET
1	B	5	THR
1	B	25	LEU
1	B	42	VAL
1	B	59	GLU
1	B	64	ILE
1	B	76	LEU
1	B	106	LEU
1	B	114	LEU
1	B	121	LEU
1	B	123	ASP
1	B	127	THR
1	B	170	SER
1	B	209	ASP
1	B	231	LEU
1	B	243	ILE
1	C	2	GLU
1	C	25	LEU
1	C	64	ILE
1	C	85	MET
1	C	93	LEU
1	C	96	LEU
1	C	106	LEU
1	C	140	LEU
1	C	153	ASP
1	C	158	LYS
1	C	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	39	GLN
1	A	95	ASN
1	A	98	GLN

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Mol	Chain	Res	Type
1	A	115	ASN
1	A	146	ASN
1	A	161	HIS
1	A	197	ASN
1	A	226	HIS
1	A	237	ASN
1	A	262	GLN
1	B	39	GLN
1	B	98	GLN
1	B	161	HIS
1	B	197	ASN
1	B	200	ASN
1	B	244	ASN
1	B	261	HIS
1	B	262	GLN
1	B	269	HIS
1	C	39	GLN
1	C	98	GLN
1	C	146	ASN
1	C	161	HIS
1	C	164	HIS
1	C	178	ASN
1	C	197	ASN
1	C	210	ASN
1	C	226	HIS
1	C	262	GLN
1	C	269	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A	1002	-	21,23,23	4.11	14 (66%)	27,34,34	1.99	7 (25%)
2	NCN	C	1001	-	21,23,23	4.57	14 (66%)	27,34,34	1.98	7 (25%)
2	NCN	B	1003	-	21,23,23	4.51	13 (61%)	27,34,34	2.09	7 (25%)

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	A	1002	-	-	9/14/30/30	0/2/2/2
2	NCN	C	1001	-	-	6/14/30/30	0/2/2/2
2	NCN	B	1003	-	-	9/14/30/30	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	NCN	C2-N1	12.04	1.48	1.35
2	C	1001	NCN	C2-N1	11.89	1.48	1.35
2	B	1003	NCN	O4'-C1'	11.07	1.55	1.40
2	C	1001	NCN	O4'-C1'	10.82	1.55	1.40
2	A	1002	NCN	O4'-C1'	10.17	1.54	1.40
2	A	1002	NCN	C2-N1	10.10	1.46	1.35
2	B	1003	NCN	C6-N1	5.94	1.48	1.35
2	A	1002	NCN	C6-N1	5.73	1.48	1.35
2	C	1001	NCN	C6-N1	5.38	1.47	1.35
2	C	1001	NCN	C4-C3	4.81	1.46	1.39
2	B	1003	NCN	C4-C3	4.47	1.46	1.39
2	A	1002	NCN	C4-C3	4.24	1.45	1.39
2	B	1003	NCN	C6-C5	4.17	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	NCN	O3'-C3'	4.11	1.53	1.43
2	B	1003	NCN	O2'-C2'	4.07	1.53	1.43
2	C	1001	NCN	C6-C5	3.98	1.46	1.38
2	C	1001	NCN	C3'-C4'	3.96	1.63	1.53
2	A	1002	NCN	C6-C5	3.85	1.46	1.38
2	A	1002	NCN	O3'-C3'	3.81	1.52	1.43
2	B	1003	NCN	O3'-C3'	3.80	1.52	1.43
2	C	1001	NCN	O8-C7	3.75	1.33	1.22
2	A	1002	NCN	O2'-C2'	3.68	1.52	1.43
2	C	1001	NCN	O2'-C2'	3.60	1.51	1.43
2	B	1003	NCN	C3'-C4'	3.51	1.61	1.53
2	C	1001	NCN	C3-C7	3.49	1.56	1.49
2	C	1001	NCN	P-O5'	3.43	1.71	1.60
2	A	1002	NCN	C3'-C4'	3.42	1.61	1.53
2	A	1002	NCN	O8-C7	3.23	1.32	1.22
2	A	1002	NCN	P-O5'	3.15	1.70	1.60
2	C	1001	NCN	C2-C3	2.94	1.43	1.39
2	C	1001	NCN	C5'-C4'	2.94	1.60	1.51
2	B	1003	NCN	O8-C7	2.85	1.31	1.22
2	B	1003	NCN	C3-C7	2.84	1.55	1.49
2	B	1003	NCN	C2-C3	2.81	1.43	1.39
2	B	1003	NCN	P-O5'	2.60	1.68	1.60
2	C	1001	NCN	C5-C4	2.52	1.43	1.38
2	A	1002	NCN	C3-C7	2.24	1.54	1.49
2	B	1003	NCN	C5-C4	2.17	1.42	1.38
2	A	1002	NCN	C5'-C4'	2.15	1.58	1.51
2	A	1002	NCN	P-O2P	2.09	1.57	1.50
2	A	1002	NCN	C2-C3	2.07	1.42	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	NCN	C4'-O4'-C1'	-5.22	105.14	109.92
2	A	1002	NCN	C4'-O4'-C1'	-4.69	105.63	109.92
2	C	1001	NCN	C4'-O4'-C1'	-4.63	105.68	109.92
2	B	1003	NCN	C6-N1-C2	-4.50	118.05	121.88
2	A	1002	NCN	C6-N1-C2	-4.27	118.24	121.88
2	A	1002	NCN	O3'-C3'-C4'	4.13	122.93	111.08
2	C	1001	NCN	O3'-C3'-C4'	3.97	122.49	111.08
2	B	1003	NCN	O3'-C3'-C4'	3.82	122.05	111.08
2	C	1001	NCN	C6-N1-C2	-3.68	118.74	121.88
2	B	1003	NCN	C2-C3-C7	3.51	125.80	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	NCN	C5-C4-C3	3.47	123.77	120.36
2	C	1001	NCN	C2-C3-C7	3.46	125.72	119.78
2	A	1002	NCN	C5-C4-C3	3.23	123.54	120.36
2	C	1001	NCN	C5-C4-C3	3.18	123.49	120.36
2	A	1002	NCN	C2-C3-C7	3.17	125.22	119.78
2	B	1003	NCN	O5'-C5'-C4'	2.93	118.99	108.99
2	C	1001	NCN	O5'-C5'-C4'	2.79	118.48	108.99
2	A	1002	NCN	O5'-C5'-C4'	2.60	117.86	108.99
2	B	1003	NCN	O8-C7-C3	-2.09	115.97	121.46
2	C	1001	NCN	O8-C7-C3	-2.05	116.10	121.46
2	A	1002	NCN	O8-C7-C3	-2.01	116.17	121.46

There are no chirality outliers.

All (24) torsion outliers are listed below:

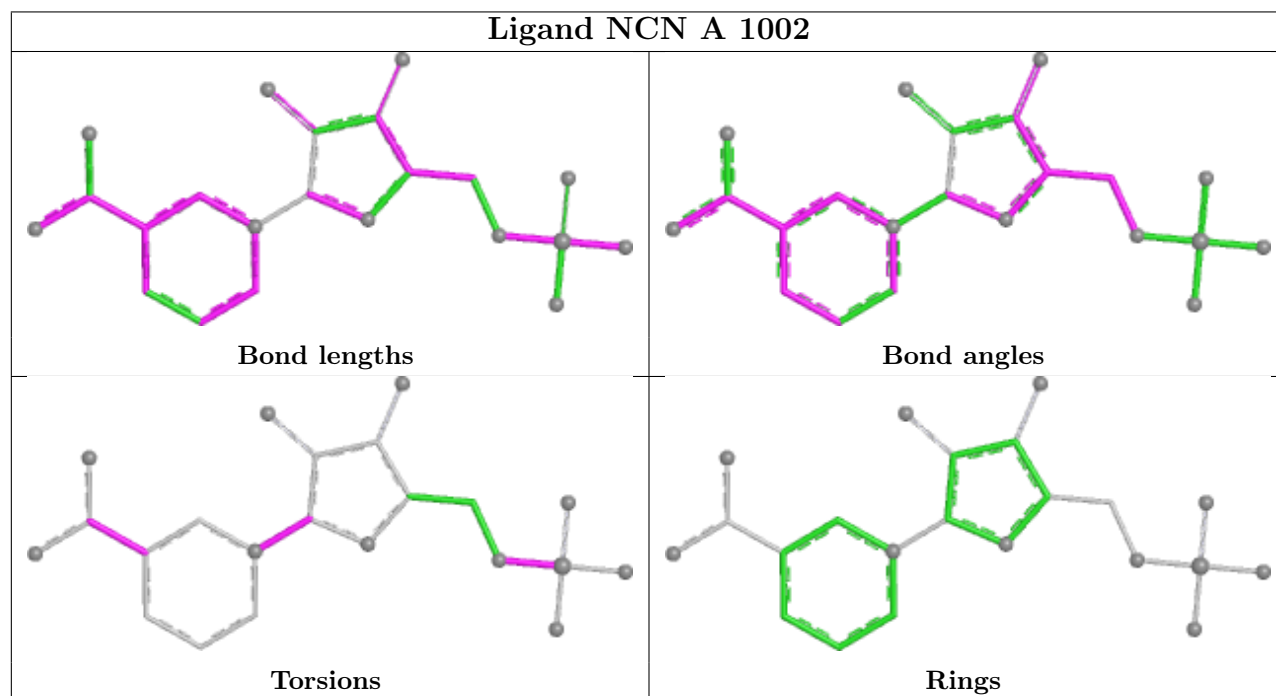
Mol	Chain	Res	Type	Atoms
2	A	1002	NCN	C5'-O5'-P-O1P
2	A	1002	NCN	C5'-O5'-P-O3P
2	A	1002	NCN	O4'-C1'-N1-C6
2	A	1002	NCN	C2-C3-C7-O7
2	A	1002	NCN	C2-C3-C7-O8
2	B	1003	NCN	C5'-O5'-P-O1P
2	B	1003	NCN	C5'-O5'-P-O2P
2	B	1003	NCN	C5'-O5'-P-O3P
2	B	1003	NCN	O4'-C1'-N1-C6
2	C	1001	NCN	C5'-O5'-P-O1P
2	C	1001	NCN	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	A	1002	NCN	C4-C3-C7-O8
2	A	1002	NCN	C4-C3-C7-O7
2	A	1002	NCN	C5'-O5'-P-O2P
2	B	1003	NCN	C4-C3-C7-O7
2	B	1003	NCN	C4-C3-C7-O8
2	C	1001	NCN	C2'-C1'-N1-C2
2	B	1003	NCN	C2-C3-C7-O8
2	A	1002	NCN	O4'-C1'-N1-C2
2	B	1003	NCN	O4'-C1'-N1-C2
2	B	1003	NCN	C2-C3-C7-O7

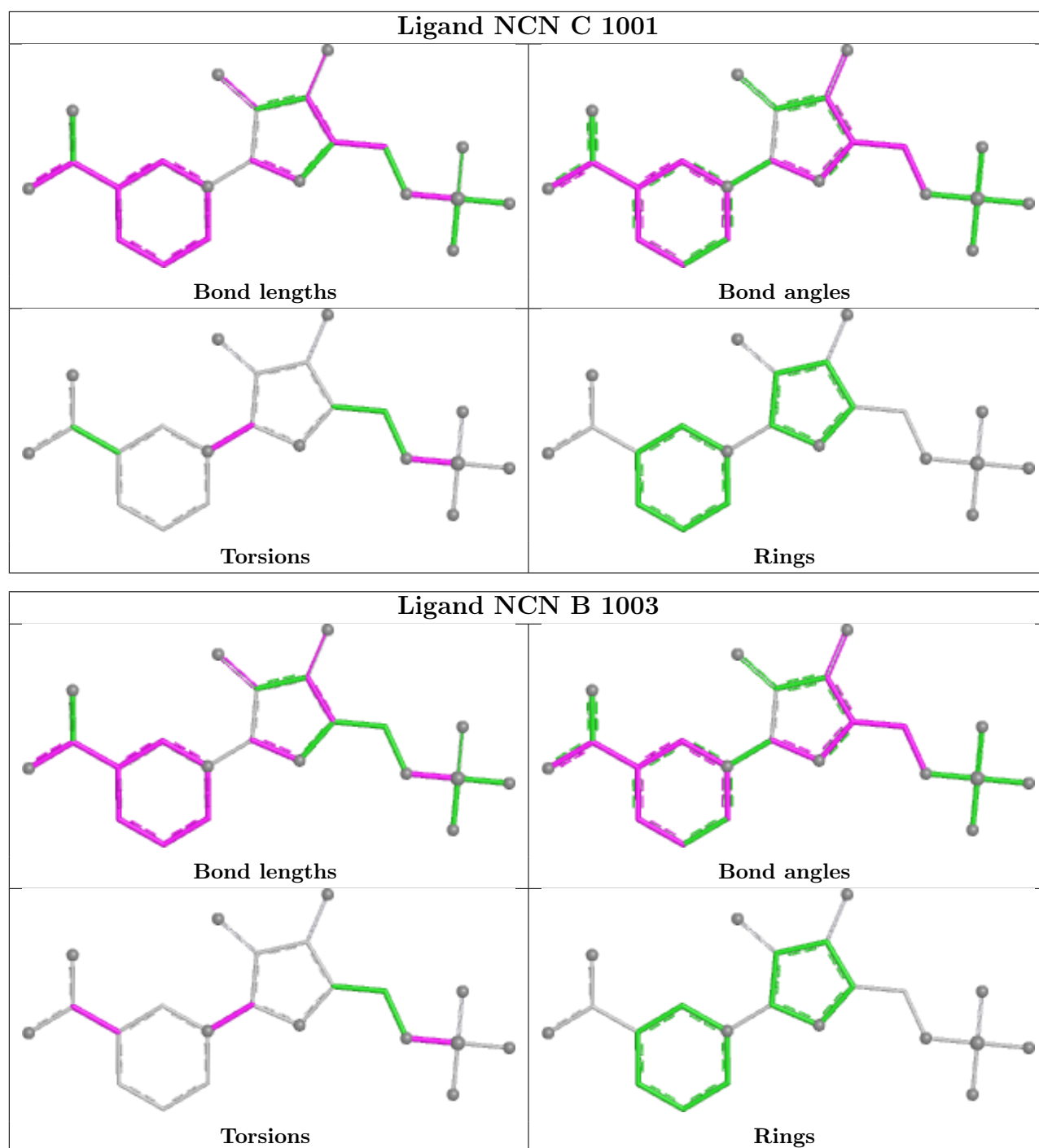
There are no ring outliers.

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%)	-0.11	0 100 100	17, 64, 134, 168	0
1	B	273/273 (100%)	-0.46	0 100 100	4, 47, 87, 122	0
1	C	273/273 (100%)	-0.45	0 100 100	12, 40, 97, 122	0
All	All	819/819 (100%)	-0.34	0 100 100	4, 50, 112, 168	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.

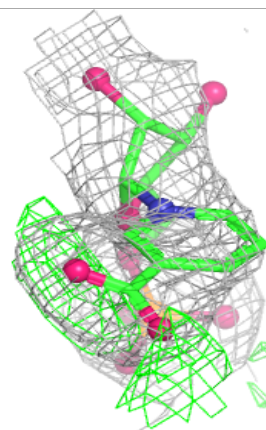
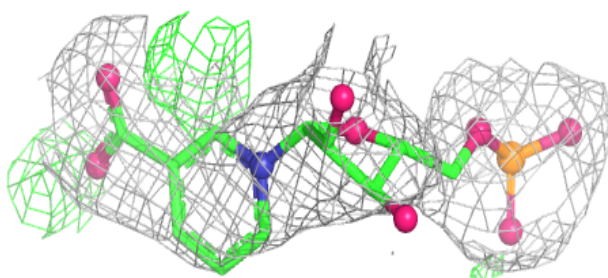
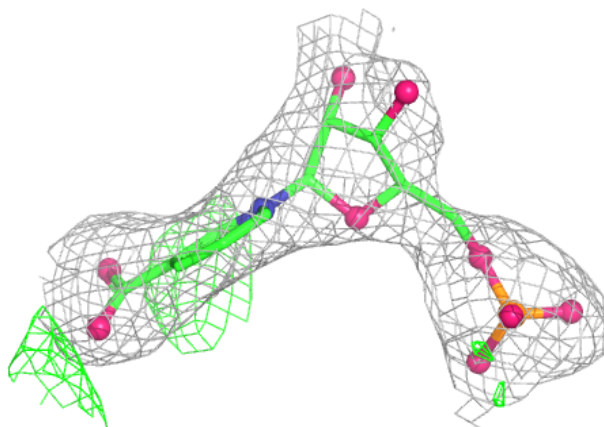
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NCN	C	1001	22/22	0.89	0.12	35,56,61,62	0
2	NCN	B	1003	22/22	0.93	0.12	36,44,52,55	0
2	NCN	A	1002	22/22	0.93	0.10	46,53,54,54	0

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.

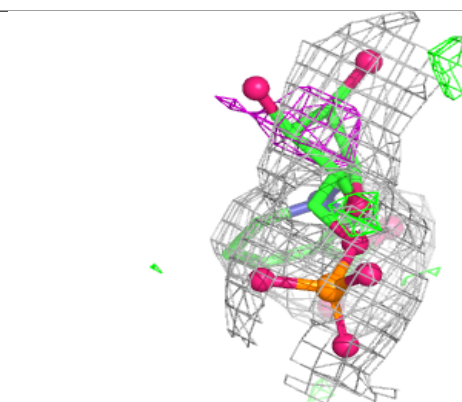
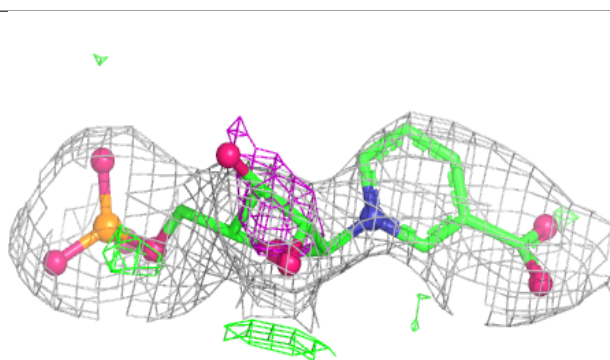
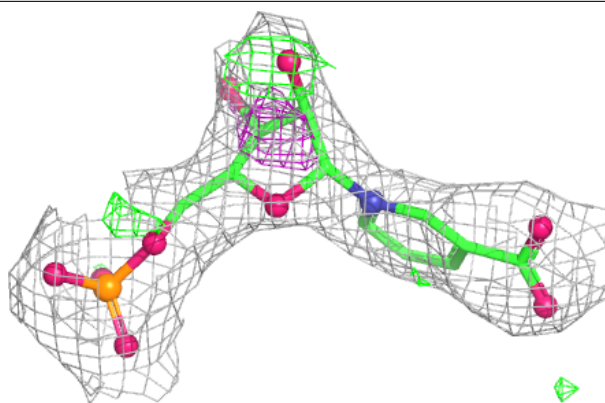
Electron density around NCN C 1001:

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

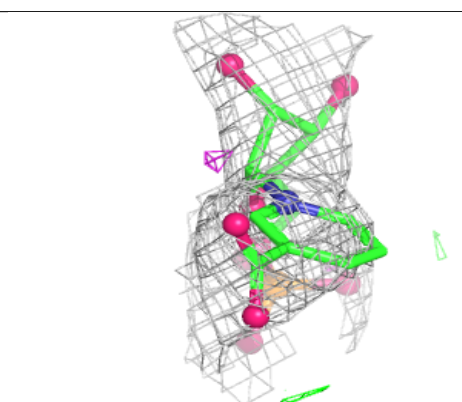
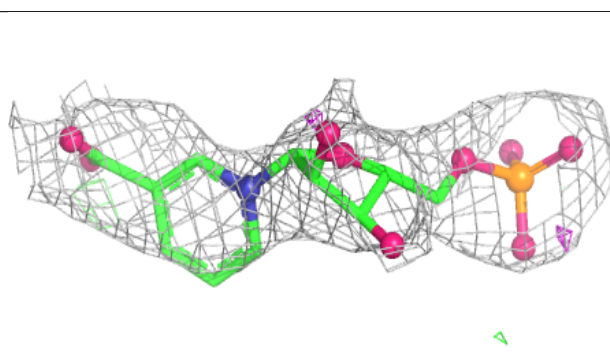
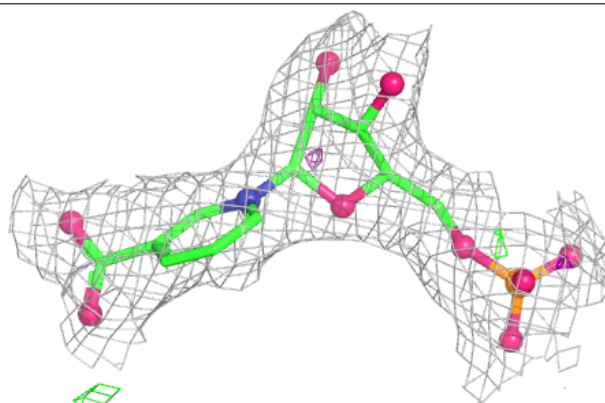


Electron density around NCN B 1003:

$2mF_o-DF_c$ (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.