



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:56 am BST

PDB ID : 3FTQ
Title : Crystal structure of Septin 2 in complex with GppNHp and Mg2+
Authors : Sirajuddin, M.; Wittinghofer, A.
Deposited on : 2009-01-13
Resolution : 2.90 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

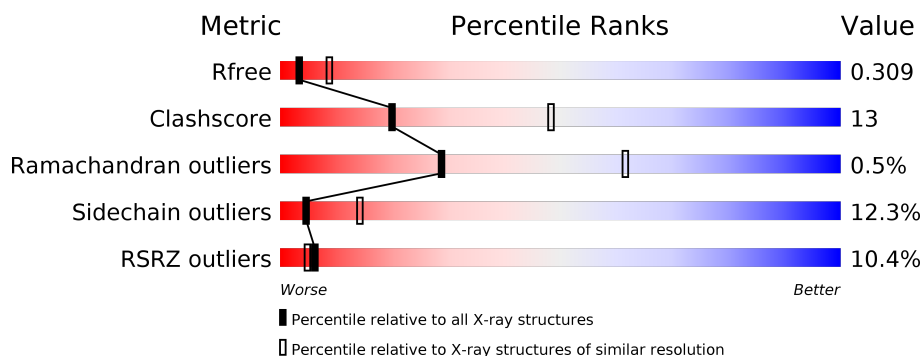
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	274	<div> <div>9%</div> <div>61% 25% 6% • 7%</div> </div>
1	B	274	<div> <div>8%</div> <div>62% 24% 5% • 8%</div> </div>
1	C	274	<div> <div>11%</div> <div>66% 21% 5% 9%</div> </div>
1	D	274	<div> <div>10%</div> <div>56% 26% 7% 11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8382 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 Septin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2070	1316	363	383	8			
1	B	252	Total	C	N	O	S	0	0	0
			2059	1314	358	379	8			
1	C	250	Total	C	N	O	S	0	0	0
			2045	1303	357	377	8			
1	D	243	Total	C	N	O	S	0	0	0
			1973	1261	342	362	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	D	1	Total 32	C 10	N 6	O 13	P 3	0	0

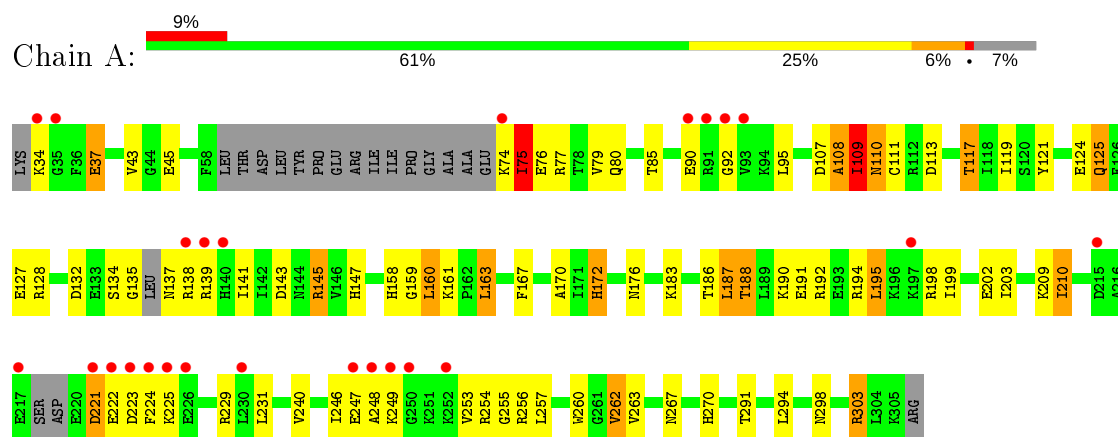
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	B	31	Total O 31 31	0	0
4	C	23	Total O 23 23	0	0
4	D	16	Total O 16 16	0	0

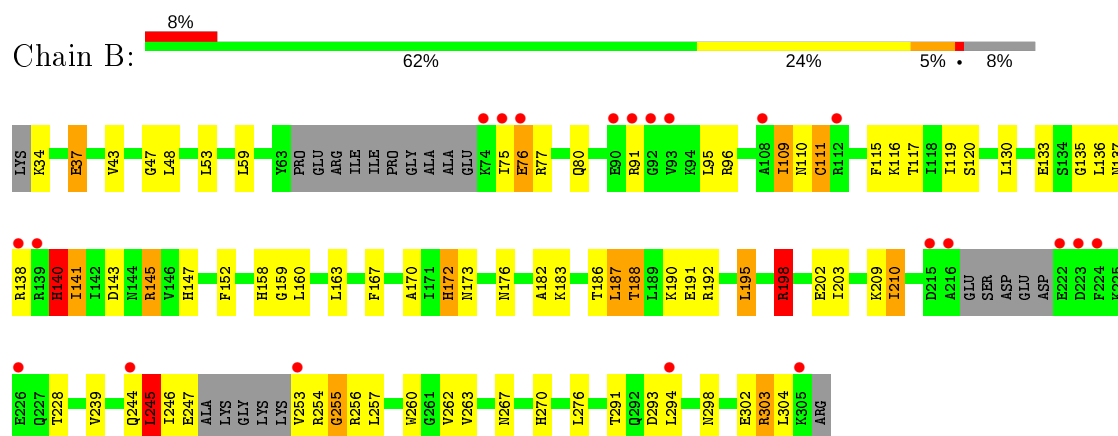
3 Residue-property plots [i](#)

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.

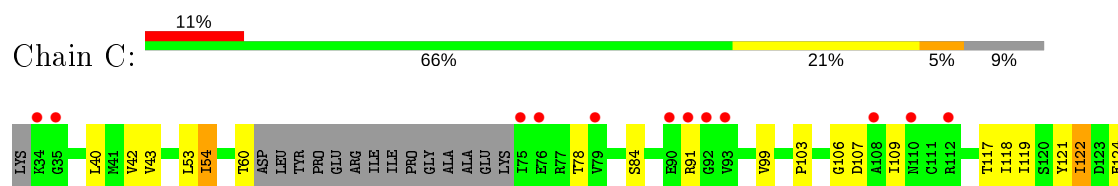
• Molecule 1: Septin-2

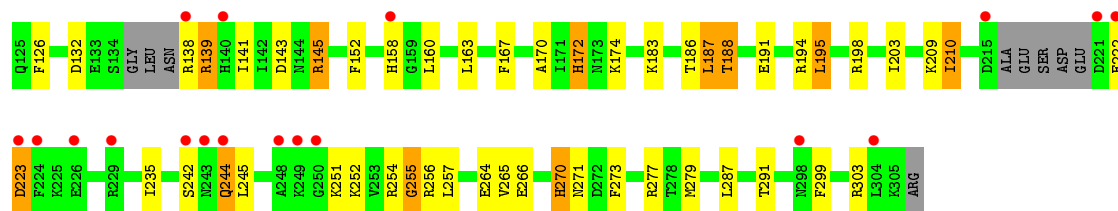


• Molecule 1: Septin-2

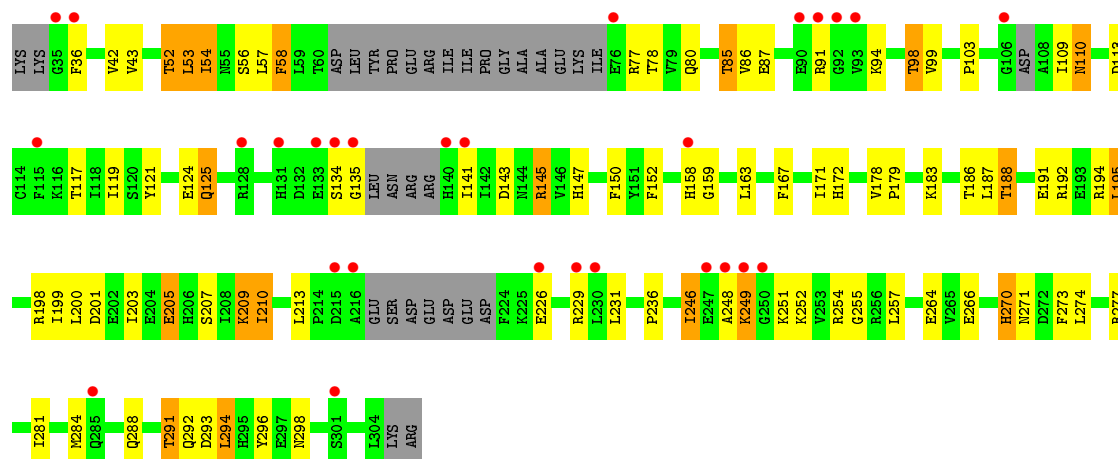


• Molecule 1: Septin-2





● Molecule 1: Septin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.98Å 118.44Å 190.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.90 19.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-2.90) 99.7 (19.96-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.247 , 0.290 0.265 , 0.309	Depositor DCC
R_{free} test set	1689 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8382	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/2106	0.78	13/2831 (0.5%)
1	B	0.46	1/2096 (0.0%)	0.84	11/2823 (0.4%)
1	C	0.44	0/2081	0.71	4/2799 (0.1%)
1	D	0.43	0/2008	0.70	8/2702 (0.3%)
All	All	0.44	1/8291 (0.0%)	0.76	36/11155 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	ARG	CZ-NH2	5.01	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	ASN	N-CA-CB	12.04	132.28	110.60
1	B	109	ILE	CB-CA-C	10.39	132.38	111.60
1	C	106	GLY	N-CA-C	9.70	137.35	113.10
1	B	140	HIS	CB-CA-C	9.39	129.18	110.40
1	C	107	ASP	N-CA-CB	9.14	127.05	110.60
1	A	249	LYS	N-CA-C	8.94	135.14	111.00
1	B	140	HIS	N-CA-C	-8.78	87.29	111.00
1	B	198	ARG	NH1-CZ-NH2	-8.59	109.96	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLY	N-CA-C	-8.00	93.11	113.10
1	A	221	ASP	CB-CA-C	-7.22	95.96	110.40
1	B	141	ILE	N-CA-C	-7.07	91.91	111.00
1	D	159	GLY	N-CA-C	-6.90	95.84	113.10
1	B	141	ILE	N-CA-CB	6.71	126.22	110.80
1	D	251	LYS	N-CA-CB	6.59	122.47	110.60
1	D	158	HIS	CB-CA-C	-6.51	97.39	110.40
1	B	109	ILE	N-CA-C	-6.42	93.65	111.00
1	B	245	LEU	CB-CA-C	-6.39	98.05	110.20
1	D	294	LEU	N-CA-C	6.30	128.00	111.00
1	A	76	GLU	N-CA-C	6.26	127.89	111.00
1	A	109	ILE	N-CA-CB	5.96	124.50	110.80
1	D	291	THR	CB-CA-C	5.71	127.02	111.60
1	B	159	GLY	N-CA-C	-5.71	98.83	113.10
1	A	108	ALA	CB-CA-C	-5.70	101.56	110.10
1	A	222	GLU	N-CA-C	5.46	125.73	111.00
1	D	246	ILE	CB-CA-C	5.42	122.43	111.60
1	A	248	ALA	N-CA-CB	5.36	117.61	110.10
1	C	109	ILE	CB-CA-C	5.32	122.24	111.60
1	A	249	LYS	CB-CA-C	-5.30	99.79	110.40
1	A	253	VAL	CB-CA-C	-5.27	101.38	111.40
1	A	75	ILE	N-CA-C	5.27	125.23	111.00
1	D	209	LYS	CD-CE-NZ	5.24	123.76	111.70
1	A	223	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	223	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	293	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	293	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	247	GLU	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	ARG	Sidechain

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	2070	0	2079	60	0
1	B	2059	0	2069	50	0
1	C	2045	0	2062	46	0
1	D	1973	0	1988	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	13	0	0
3	B	32	0	13	0	0
3	C	32	0	13	1	0
3	D	32	0	13	3	0
4	A	33	0	0	1	0
4	B	31	0	0	0	0
4	C	23	0	0	1	0
4	D	16	0	0	0	0
All	All	8382	0	8250	208	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 13.

All (208) 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:110:ASN:C	1:D:110:ASN:HD22	1.66	0.99
1:A:110:ASN:C	1:A:110:ASN:HD22	1.63	0.99
1:C:54:ILE:HG13	1:C:99:VAL:HG11	1.44	0.98
1:C:172:HIS:HD2	1:C:209:LYS:H	1.11	0.97
1:B:75:ILE:O	1:B:75:ILE:HG22	1.65	0.96
1:A:303:ARG:HH11	1:A:303:ARG:HG2	1.31	0.94
1:A:270:HIS:CE1	1:B:260:TRP:HB3	2.03	0.94
1:A:270:HIS:HE1	1:B:260:TRP:HB3	1.33	0.90
1:C:122:ILE:HD11	1:C:174:LYS:HB3	1.53	0.89
1:A:260:TRP:HB3	1:B:270:HIS:CE1	2.08	0.89
1:A:172:HIS:HD2	1:A:209:LYS:H	1.15	0.88
1:B:172:HIS:HD2	1:B:209:LYS:H	1.20	0.88
1:A:260:TRP:HB3	1:B:270:HIS:HE1	1.38	0.88
1:C:264:GLU:H	1:C:270:HIS:HD2	1.25	0.85
1:A:75:ILE:HG23	1:A:75:ILE:O	1.75	0.83
1:D:194:ARG:O	1:D:198:ARG:HG2	1.80	0.82
1:D:172:HIS:CD2	1:D:209:LYS:HB2	2.16	0.81
1:D:172:HIS:HD2	1:D:209:LYS:HB2	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:HIS:O	1:B:198:ARG:HD2	1.82	0.80
1:D:42:VAL:HG21	1:D:54:ILE:HD13	1.62	0.78
1:B:267:ASN:CG	1:B:270:HIS:HD2	1.87	0.78
1:C:54:ILE:HG13	1:C:99:VAL:CG1	2.14	0.77
1:B:183:LYS:O	1:B:186:THR:HG23	1.85	0.76
1:B:256:ARG:HB2	1:B:263:VAL:HB	1.68	0.76
1:A:303:ARG:HG2	1:A:303:ARG:NH1	1.95	0.76
1:C:139:ARG:CG	1:C:139:ARG:HH11	1.97	0.75
1:A:256:ARG:HB2	1:A:263:VAL:HB	1.68	0.75
1:D:42:VAL:HG21	1:D:54:ILE:CD1	2.18	0.74
1:D:147:HIS:CD2	1:D:291:THR:HG21	2.22	0.74
1:D:110:ASN:ND2	1:D:110:ASN:C	2.40	0.74
1:D:147:HIS:HD2	1:D:291:THR:HG21	1.51	0.74
1:A:125:GLN:HE21	1:A:125:GLN:HA	1.53	0.73
3:C:372:GNP:O2A	4:C:318:HOH:O	2.05	0.73
1:C:122:ILE:HD11	1:C:174:LYS:CB	2.17	0.72
1:A:267:ASN:CG	1:A:270:HIS:HD2	1.93	0.72
1:A:135:GLY:O	1:A:137:ASN:N	2.23	0.72
1:A:158:HIS:O	1:A:198:ARG:HD3	1.89	0.72
1:A:110:ASN:C	1:A:110:ASN:ND2	2.39	0.71
1:B:75:ILE:O	1:B:75:ILE:CG2	2.39	0.69
1:A:221:ASP:O	1:A:225:LYS:HG3	1.93	0.68
1:A:303:ARG:HH11	1:A:303:ARG:CG	2.03	0.68
1:C:203:ILE:HD13	1:C:210:ILE:HD12	1.75	0.68
1:C:139:ARG:HG2	1:C:139:ARG:HH11	1.57	0.67
1:D:56:SER:HA	1:D:254:ARG:NH1	2.10	0.67
1:B:188:THR:HG22	1:B:191:GLU:H	1.59	0.67
1:A:194:ARG:O	1:A:198:ARG:HG3	1.94	0.66
1:A:294:LEU:O	1:A:298:ASN:ND2	2.29	0.66
1:D:54:ILE:HG13	1:D:99:VAL:HG11	1.76	0.65
1:D:183:LYS:O	1:D:186:THR:HG23	1.96	0.65
1:B:111:CYS:SG	1:B:115:PHE:CE1	2.89	0.65
1:D:53:LEU:HD22	1:D:152:PHE:HZ	1.60	0.65
1:A:188:THR:HG22	1:A:191:GLU:H	1.61	0.65
1:B:203:ILE:HD13	1:B:210:ILE:HD12	1.79	0.65
1:A:183:LYS:O	1:A:186:THR:HG23	1.96	0.65
1:A:203:ILE:HD13	1:A:210:ILE:HD12	1.79	0.64
1:A:125:GLN:HE21	1:A:125:GLN:CA	2.11	0.64
1:A:172:HIS:CD2	1:A:209:LYS:H	2.07	0.64
1:D:264:GLU:H	1:D:270:HIS:HD2	1.46	0.64
1:C:53:LEU:HD22	1:C:152:PHE:HZ	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:HIS:O	1:C:198:ARG:HD3	1.98	0.63
1:C:194:ARG:O	1:C:198:ARG:HG3	1.98	0.63
1:C:172:HIS:CD2	1:C:209:LYS:H	2.03	0.63
1:D:125:GLN:HE21	1:D:125:GLN:HA	1.62	0.62
1:A:45:GLU:OE1	1:A:161:LYS:NZ	2.33	0.62
1:C:60:THR:HG22	1:C:254:ARG:HH22	1.65	0.62
1:A:147:HIS:HA	1:A:291:THR:HG21	1.81	0.61
1:C:244:GLN:H	1:C:244:GLN:HE21	1.47	0.61
1:B:303:ARG:HG3	1:B:304:LEU:N	2.16	0.61
1:C:139:ARG:NH1	1:C:139:ARG:HG2	2.12	0.61
1:B:147:HIS:HA	1:B:291:THR:HG21	1.81	0.61
1:C:42:VAL:HG21	1:C:54:ILE:HD13	1.83	0.60
1:D:85:THR:HG23	1:D:98:THR:HB	1.82	0.60
1:A:34:LYS:HB3	1:A:92:GLY:O	2.02	0.60
1:B:172:HIS:CD2	1:B:209:LYS:H	2.11	0.60
1:D:56:SER:HA	1:D:254:ARG:HH12	1.66	0.59
1:C:188:THR:HG22	1:C:191:GLU:H	1.67	0.59
1:D:52:THR:HG23	3:D:372:GNP:O1A	2.02	0.59
1:B:244:GLN:O	1:B:255:GLY:HA3	2.03	0.58
1:C:242:SER:OG	1:C:256:ARG:HG3	2.03	0.58
1:D:203:ILE:HD13	1:D:210:ILE:HD12	1.84	0.58
1:C:78:THR:O	1:C:103:PRO:HB3	2.04	0.57
1:D:125:GLN:HE21	1:D:125:GLN:CA	2.17	0.57
1:A:107:ASP:O	1:A:108:ALA:HB3	2.05	0.56
1:B:37:GLU:HG3	1:B:143:ASP:HB3	1.88	0.56
1:D:172:HIS:CD2	1:D:209:LYS:H	2.24	0.55
1:A:74:LYS:O	1:A:75:ILE:HG22	2.07	0.55
1:C:244:GLN:H	1:C:244:GLN:NE2	2.03	0.55
1:C:42:VAL:HG21	1:C:54:ILE:CD1	2.36	0.55
1:C:183:LYS:O	1:C:186:THR:HG23	2.06	0.55
1:A:37:GLU:HG3	1:A:143:ASP:HB3	1.89	0.54
1:A:267:ASN:CB	1:A:270:HIS:HD2	2.20	0.54
1:B:173:ASN:HD21	1:B:209:LYS:NZ	2.06	0.54
1:A:125:GLN:NE2	1:A:125:GLN:HA	2.22	0.54
1:D:54:ILE:HG13	1:D:99:VAL:CG1	2.36	0.53
1:C:132:ASP:HB3	1:C:141:ILE:HG21	1.91	0.53
1:C:264:GLU:HG3	1:C:270:HIS:CD2	2.44	0.52
1:B:116:LYS:O	1:B:120:SER:HB2	2.09	0.52
1:C:287:LEU:O	1:C:291:THR:OG1	2.26	0.52
1:D:188:THR:HG22	1:D:191:GLU:H	1.74	0.52
1:B:111:CYS:SG	1:B:163:LEU:HD22	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:HG2	1:B:77:ARG:N	2.25	0.52
1:D:179:PRO:HG2	1:D:236:PRO:HB3	1.92	0.52
1:A:132:ASP:O	1:A:138:ARG:HB2	2.10	0.51
1:C:254:ARG:O	1:C:265:VAL:N	2.43	0.51
1:D:87:GLU:OE2	1:D:94:LYS:HE2	2.11	0.51
1:A:172:HIS:CD2	1:A:209:LYS:HB2	2.46	0.51
1:B:119:ILE:HD11	1:B:170:ALA:HB1	1.92	0.51
1:D:172:HIS:HD2	1:D:209:LYS:H	1.58	0.51
1:D:246:ILE:O	1:D:252:LYS:HA	2.11	0.50
1:A:246:ILE:HD11	1:A:262:VAL:HG23	1.93	0.50
1:D:294:LEU:O	1:D:294:LEU:HD12	2.12	0.50
1:A:267:ASN:ND2	1:A:270:HIS:HD2	2.10	0.49
1:C:251:LYS:HG2	1:C:252:LYS:H	1.76	0.49
1:A:158:HIS:CD2	1:A:202:GLU:OE2	2.65	0.49
1:B:190:LYS:HD2	1:B:190:LYS:H	1.77	0.49
1:C:251:LYS:HG2	1:C:252:LYS:N	2.27	0.49
1:B:143:ASP:OD2	1:B:145:ARG:HD3	2.12	0.49
1:B:267:ASN:ND2	1:B:270:HIS:HD2	2.09	0.49
1:B:187:LEU:HD21	1:B:195:LEU:HD12	1.93	0.49
1:D:125:GLN:NE2	1:D:125:GLN:HA	2.28	0.49
1:C:256:ARG:NH2	1:D:191:GLU:OE2	2.46	0.49
1:D:248:ALA:O	1:D:249:LYS:HG3	2.13	0.48
1:A:113:ASP:O	1:A:117:THR:HG22	2.13	0.48
1:B:158:HIS:HE1	1:B:160:LEU:O	1.95	0.48
1:A:270:HIS:HD1	1:B:260:TRP:HE3	1.61	0.48
1:D:54:ILE:HD12	1:D:54:ILE:HA	1.65	0.48
1:A:77:ARG:NH2	1:A:107:ASP:O	2.46	0.48
1:D:271:ASN:ND2	1:D:273:PHE:HB2	2.29	0.48
1:C:186:THR:HG22	1:D:186:THR:HB	1.95	0.48
1:D:57:LEU:HA	1:D:273:PHE:HZ	1.78	0.48
1:B:133:GLU:HA	1:B:138:ARG:HG2	1.96	0.47
1:D:294:LEU:O	1:D:298:ASN:HB2	2.14	0.47
1:D:121:TYR:O	1:D:125:GLN:HG2	2.15	0.47
1:B:135:GLY:HA3	1:B:136:LEU:HA	1.56	0.47
1:A:125:GLN:NE2	1:A:128:ARG:HD3	2.30	0.47
1:D:78:THR:O	1:D:103:PRO:HB3	2.14	0.47
1:D:119:ILE:HG12	1:D:171:ILE:HG22	1.97	0.47
1:A:160:LEU:HD11	1:A:199:ILE:HG23	1.97	0.47
1:B:267:ASN:ND2	1:B:270:HIS:CD2	2.82	0.47
1:C:271:ASN:HD21	1:C:273:PHE:HB2	1.80	0.47
1:B:267:ASN:CG	1:B:270:HIS:CD2	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD21	1:A:195:LEU:HD12	1.96	0.46
1:A:267:ASN:HB3	1:A:270:HIS:CD2	2.50	0.46
1:B:192:ARG:NH2	1:B:270:HIS:O	2.39	0.46
1:A:119:ILE:HD11	1:A:170:ALA:HB1	1.96	0.46
1:A:191:GLU:OE2	1:B:256:ARG:NH2	2.48	0.46
1:D:77:ARG:HD2	3:D:372:GNP:O3G	2.16	0.46
1:D:143:ASP:OD2	1:D:145:ARG:HD3	2.15	0.46
1:D:150:PHE:HD1	1:D:178:VAL:HB	1.81	0.45
1:D:226:GLU:HG2	1:D:229:ARG:HH12	1.81	0.45
1:A:190:LYS:H	1:A:190:LYS:HD2	1.81	0.44
1:B:143:ASP:OD1	1:B:145:ARG:NH2	2.50	0.44
1:C:264:GLU:H	1:C:270:HIS:CD2	2.17	0.44
1:B:160:LEU:HD23	1:B:202:GLU:HB2	1.98	0.44
1:A:267:ASN:ND2	1:A:270:HIS:CD2	2.85	0.44
1:A:192:ARG:NH2	1:A:270:HIS:O	2.37	0.44
1:B:47:GLY:HA2	1:B:77:ARG:HH12	1.82	0.44
1:B:245:LEU:HA	1:B:254:ARG:HA	2.00	0.44
1:A:121:TYR:O	1:A:125:GLN:HG2	2.18	0.44
1:C:54:ILE:HD12	1:C:54:ILE:HA	1.68	0.44
1:C:118:ILE:O	1:C:122:ILE:HG23	2.17	0.43
1:B:34:LYS:HB2	1:B:140:HIS:CE1	2.53	0.43
1:C:222:GLU:HG3	1:C:223:ASP:H	1.84	0.43
1:D:266:GLU:HG2	1:D:274:LEU:HD21	2.00	0.43
1:B:294:LEU:O	1:B:298:ASN:ND2	2.52	0.43
1:D:201:ASP:O	1:D:205:GLU:HB2	2.18	0.43
1:C:187:LEU:HD21	1:C:195:LEU:HD12	1.99	0.43
1:B:176:ASN:ND2	1:B:291:THR:HG23	2.34	0.43
1:A:267:ASN:HB3	1:A:270:HIS:HD2	1.84	0.42
1:B:53:LEU:HD22	1:B:152:PHE:HZ	1.84	0.42
1:D:195:LEU:HD22	1:D:199:ILE:HG13	2.00	0.42
1:D:213:LEU:HD21	1:D:231:LEU:HD23	2.01	0.42
1:A:143:ASP:OD2	1:A:145:ARG:HD3	2.18	0.42
1:A:176:ASN:ND2	1:A:291:THR:HG23	2.33	0.42
1:C:139:ARG:HG3	1:C:139:ARG:HH11	1.80	0.42
1:D:147:HIS:HD2	1:D:291:THR:CG2	2.25	0.42
1:A:240:VAL:HG11	1:A:263:VAL:HG11	2.01	0.42
1:B:143:ASP:CG	1:B:145:ARG:HH21	2.22	0.42
1:C:143:ASP:OD2	1:C:145:ARG:HD3	2.18	0.42
1:C:191:GLU:OE2	3:D:372:GNP:O2'	2.28	0.42
1:A:108:ALA:O	1:A:109:ILE:HG12	2.19	0.42
1:D:113:ASP:O	1:D:117:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:GLU:HG3	1:D:270:HIS:CD2	2.55	0.42
1:D:125:GLN:NE2	1:D:125:GLN:CA	2.83	0.42
1:D:192:ARG:NH2	1:D:270:HIS:O	2.33	0.42
1:D:58:PHE:CE2	1:D:86:VAL:HG23	2.54	0.42
1:D:284:MET:O	1:D:288:GLN:HB2	2.20	0.42
1:A:111:CYS:HB2	1:A:163:LEU:HD12	2.02	0.42
1:B:137:ASN:HD22	1:B:137:ASN:HA	1.66	0.42
1:B:138:ARG:NE	1:B:141:ILE:HD11	2.35	0.42
1:C:119:ILE:HD11	1:C:170:ALA:HB1	2.02	0.42
1:C:254:ARG:HA	1:C:255:GLY:HA3	1.78	0.42
1:A:127:GLU:OE1	1:A:303:ARG:HD2	2.21	0.41
1:B:239:VAL:HG11	1:B:276:LEU:HD22	2.01	0.41
1:D:134:SER:HA	1:D:135:GLY:HA2	1.60	0.41
1:C:121:TYR:O	1:C:124:GLU:HB3	2.20	0.41
1:C:126:PHE:HB3	1:C:299:PHE:CD2	2.55	0.41
1:C:264:GLU:CG	1:C:270:HIS:CD2	3.02	0.41
1:A:160:LEU:CD1	1:A:199:ILE:HG23	2.50	0.41
1:D:277:ARG:O	1:D:281:ILE:HG12	2.20	0.41
1:D:292:GLN:HA	1:D:296:TYR:HB3	2.02	0.41
1:A:138:ARG:O	1:A:141:ILE:HG13	2.20	0.41
1:C:172:HIS:CD2	1:C:209:LYS:HB2	2.56	0.41
1:D:36:PHE:CZ	1:D:288:GLN:NE2	2.77	0.41
1:B:48:LEU:O	1:B:182:ALA:HB1	2.21	0.40
1:A:77:ARG:HG3	4:A:310:HOH:O	2.21	0.40
1:B:80:GLN:HE21	1:B:80:GLN:HB2	1.53	0.40
1:D:172:HIS:CD2	1:D:209:LYS:HD3	2.57	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	246/274 (90%)	240 (98%)	5 (2%)	1 (0%)	34	66
1	B	244/274 (89%)	238 (98%)	4 (2%)	2 (1%)	19	51
1	C	242/274 (88%)	238 (98%)	3 (1%)	1 (0%)	34	66
1	D	233/274 (85%)	225 (97%)	7 (3%)	1 (0%)	34	66
All	All	965/1096 (88%)	941 (98%)	19 (2%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	ILE
1	A	255	GLY
1	C	255	GLY
1	B	255	GLY
1	D	255	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/248 (93%)	199 (86%)	31 (14%)	4	11
1	B	230/248 (93%)	203 (88%)	27 (12%)	5	16
1	C	229/248 (92%)	202 (88%)	27 (12%)	5	16
1	D	220/248 (89%)	193 (88%)	27 (12%)	4	14
All	All	909/992 (92%)	797 (88%)	112 (12%)	4	14

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	43	VAL
1	A	75	ILE
1	A	79	VAL
1	A	80	GLN
1	A	85	THR

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Mol	Chain	Res	Type
1	A	90	GLU
1	A	95	LEU
1	A	109	ILE
1	A	110	ASN
1	A	117	THR
1	A	124	GLU
1	A	125	GLN
1	A	134	SER
1	A	139	ARG
1	A	145	ARG
1	A	160	LEU
1	A	163	LEU
1	A	167	PHE
1	A	172	HIS
1	A	187	LEU
1	A	188	THR
1	A	195	LEU
1	A	210	ILE
1	A	224	PHE
1	A	229	ARG
1	A	231	LEU
1	A	254	ARG
1	A	257	LEU
1	A	262	VAL
1	A	303	ARG
1	B	37	GLU
1	B	43	VAL
1	B	59	LEU
1	B	76	GLU
1	B	91	ARG
1	B	95	LEU
1	B	96	ARG
1	B	111	CYS
1	B	117	THR
1	B	130	LEU
1	B	140	HIS
1	B	145	ARG
1	B	167	PHE
1	B	172	HIS
1	B	187	LEU
1	B	188	THR
1	B	195	LEU

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Mol	Chain	Res	Type
1	B	210	ILE
1	B	228	THR
1	B	245	LEU
1	B	246	ILE
1	B	247	GLU
1	B	253	VAL
1	B	257	LEU
1	B	262	VAL
1	B	302	GLU
1	B	303	ARG
1	C	40	LEU
1	C	43	VAL
1	C	54	ILE
1	C	84	SER
1	C	91	ARG
1	C	117	THR
1	C	122	ILE
1	C	138	ARG
1	C	139	ARG
1	C	145	ARG
1	C	160	LEU
1	C	163	LEU
1	C	167	PHE
1	C	172	HIS
1	C	187	LEU
1	C	188	THR
1	C	195	LEU
1	C	210	ILE
1	C	235	ILE
1	C	244	GLN
1	C	245	LEU
1	C	257	LEU
1	C	266	GLU
1	C	270	HIS
1	C	277	ARG
1	C	279	MET
1	C	303	ARG
1	D	43	VAL
1	D	52	THR
1	D	53	LEU
1	D	54	ILE
1	D	58	PHE

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Mol	Chain	Res	Type
1	D	80	GLN
1	D	85	THR
1	D	91	ARG
1	D	98	THR
1	D	109	ILE
1	D	110	ASN
1	D	124	GLU
1	D	125	GLN
1	D	141	ILE
1	D	145	ARG
1	D	163	LEU
1	D	167	PHE
1	D	187	LEU
1	D	188	THR
1	D	195	LEU
1	D	200	LEU
1	D	205	GLU
1	D	207	SER
1	D	210	ILE
1	D	249	LYS
1	D	257	LEU
1	D	270	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	125	GLN
1	A	131	HIS
1	A	172	HIS
1	A	270	HIS
1	A	283	HIS
1	A	298	ASN
1	B	80	GLN
1	B	137	ASN
1	B	158	HIS
1	B	172	HIS
1	B	173	ASN
1	B	270	HIS
1	C	172	HIS
1	C	244	GLN
1	C	270	HIS

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Mol	Chain	Res	Type
1	C	271	ASN
1	C	292	GLN
1	D	80	GLN
1	D	110	ASN
1	D	125	GLN
1	D	172	HIS
1	D	270	HIS
1	D	271	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	GNP	B	372	2	28,34,34	2.54	8 (28%)	30,54,54	2.26	9 (30%)
3	GNP	C	372	2	28,34,34	2.50	9 (32%)	30,54,54	2.14	8 (26%)
3	GNP	A	372	2	28,34,34	2.60	9 (32%)	30,54,54	2.24	8 (26%)
3	GNP	D	372	2	28,34,34	2.63	9 (32%)	30,54,54	2.19	7 (23%)

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	GNP	B	372	2	-	12/17/38/38	0/3/3/3
3	GNP	C	372	2	-	4/17/38/38	0/3/3/3
3	GNP	A	372	2	-	7/17/38/38	0/3/3/3
3	GNP	D	372	2	-	5/17/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	372	GNP	C4-N9	-7.70	1.37	1.47
3	A	372	GNP	C5-C6	-7.69	1.39	1.52
3	A	372	GNP	C4-N9	-7.20	1.38	1.47
3	B	372	GNP	C4-N9	-7.10	1.38	1.47
3	C	372	GNP	C5-C6	-7.10	1.40	1.52
3	B	372	GNP	C5-C6	-7.07	1.40	1.52
3	D	372	GNP	C5-C6	-7.01	1.40	1.52
3	C	372	GNP	C4-N9	-6.36	1.39	1.47
3	D	372	GNP	C6-N1	4.06	1.39	1.33
3	B	372	GNP	C6-N1	3.93	1.39	1.33
3	D	372	GNP	PB-O3A	-3.86	1.54	1.59
3	C	372	GNP	PB-O3A	-3.85	1.54	1.59
3	C	372	GNP	C6-N1	3.80	1.39	1.33
3	A	372	GNP	C6-N1	3.50	1.39	1.33
3	B	372	GNP	PB-O3A	-3.44	1.54	1.59
3	C	372	GNP	PG-O1G	3.43	1.51	1.46
3	A	372	GNP	PG-O1G	3.35	1.51	1.46
3	B	372	GNP	PG-O1G	3.34	1.51	1.46
3	A	372	GNP	PB-O3A	-3.34	1.54	1.59
3	C	372	GNP	PB-O2B	-3.09	1.48	1.56
3	D	372	GNP	PG-O1G	3.03	1.51	1.46
3	A	372	GNP	PB-O2B	-3.03	1.48	1.56
3	B	372	GNP	PB-O2B	-3.00	1.48	1.56
3	D	372	GNP	PB-O2B	-3.00	1.48	1.56
3	C	372	GNP	C5-C4	-2.51	1.37	1.53
3	D	372	GNP	C5-C4	-2.39	1.38	1.53
3	A	372	GNP	C5-C4	-2.39	1.38	1.53
3	B	372	GNP	C5-C4	-2.38	1.38	1.53
3	D	372	GNP	PG-O3G	-2.18	1.50	1.56
3	B	372	GNP	C8-N9	-2.18	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	372	GNP	C8-N9	-2.17	1.38	1.45
3	A	372	GNP	C8-N9	-2.17	1.38	1.45
3	C	372	GNP	PG-O2G	-2.16	1.50	1.56
3	A	372	GNP	PB-O1B	2.09	1.49	1.46
3	D	372	GNP	C8-N9	-2.01	1.38	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	372	GNP	C4-C5-N7	7.56	112.48	102.46
3	D	372	GNP	C4-C5-N7	7.40	112.27	102.46
3	C	372	GNP	C4-C5-N7	7.05	111.80	102.46
3	B	372	GNP	C4-C5-N7	7.00	111.75	102.46
3	A	372	GNP	C5-C6-N1	-4.93	112.11	118.19
3	D	372	GNP	C5-C6-N1	-4.55	112.58	118.19
3	B	372	GNP	C5-C6-N1	-4.43	112.73	118.19
3	C	372	GNP	C5-C6-N1	-3.86	113.43	118.19
3	B	372	GNP	O6-C6-C5	3.78	127.57	119.86
3	B	372	GNP	O3G-PG-O1G	-3.74	104.05	113.45
3	D	372	GNP	O3G-PG-O1G	-3.68	104.20	113.45
3	A	372	GNP	O6-C6-C5	3.62	127.25	119.86
3	C	372	GNP	O6-C6-C5	3.53	127.06	119.86
3	A	372	GNP	O3G-PG-O1G	-3.52	104.61	113.45
3	D	372	GNP	O6-C6-C5	3.48	126.97	119.86
3	B	372	GNP	O3G-PG-O2G	3.47	116.89	107.64
3	C	372	GNP	O2B-PB-O1B	3.42	117.10	109.92
3	D	372	GNP	O2B-PB-O1B	3.35	116.94	109.92
3	C	372	GNP	O3G-PG-O1G	-3.20	105.42	113.45
3	C	372	GNP	O3G-PG-O2G	3.10	115.89	107.64
3	B	372	GNP	O4'-C1'-N9	-3.10	104.44	109.04
3	A	372	GNP	O2B-PB-O1B	2.84	115.88	109.92
3	B	372	GNP	O2B-PB-O1B	2.71	115.61	109.92
3	A	372	GNP	O1G-PG-N3B	-2.68	107.82	111.77
3	D	372	GNP	O3G-PG-O2G	2.39	114.00	107.64
3	C	372	GNP	O6-C6-N1	-2.37	119.51	122.69
3	B	372	GNP	PA-O3A-PB	-2.36	124.30	132.62
3	A	372	GNP	O3G-PG-O2G	2.31	113.80	107.64
3	B	372	GNP	O6-C6-N1	-2.23	119.70	122.69
3	D	372	GNP	O1G-PG-N3B	-2.22	108.50	111.77
3	C	372	GNP	O4'-C1'-N9	-2.10	105.92	109.04
3	A	372	GNP	PA-O3A-PB	-2.02	125.51	132.62

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	372	GNP	PB-N3B-PG-O1G
3	D	372	GNP	PG-N3B-PB-O1B
3	D	372	GNP	PA-O3A-PB-O1B
3	D	372	GNP	PA-O3A-PB-O2B
3	D	372	GNP	C2'-C1'-N9-C4
3	B	372	GNP	PB-N3B-PG-O1G
3	B	372	GNP	PG-N3B-PB-O1B
3	B	372	GNP	PG-N3B-PB-O3A
3	B	372	GNP	PA-O3A-PB-O1B
3	B	372	GNP	C5'-O5'-PA-O3A
3	B	372	GNP	C2'-C1'-N9-C8
3	B	372	GNP	C2'-C1'-N9-C4
3	C	372	GNP	PB-N3B-PG-O1G
3	C	372	GNP	PG-N3B-PB-O1B
3	C	372	GNP	C2'-C1'-N9-C4
3	A	372	GNP	PB-N3B-PG-O1G
3	A	372	GNP	PG-N3B-PB-O1B
3	A	372	GNP	PA-O3A-PB-O1B
3	A	372	GNP	C2'-C1'-N9-C8
3	A	372	GNP	C2'-C1'-N9-C4
3	B	372	GNP	C3'-C4'-C5'-O5'
3	B	372	GNP	O4'-C4'-C5'-O5'
3	B	372	GNP	C5'-O5'-PA-O1A
3	B	372	GNP	C5'-O5'-PA-O2A
3	A	372	GNP	PG-N3B-PB-O3A
3	B	372	GNP	PA-O3A-PB-O2B
3	A	372	GNP	PA-O3A-PB-O2B
3	C	372	GNP	O4'-C4'-C5'-O5'

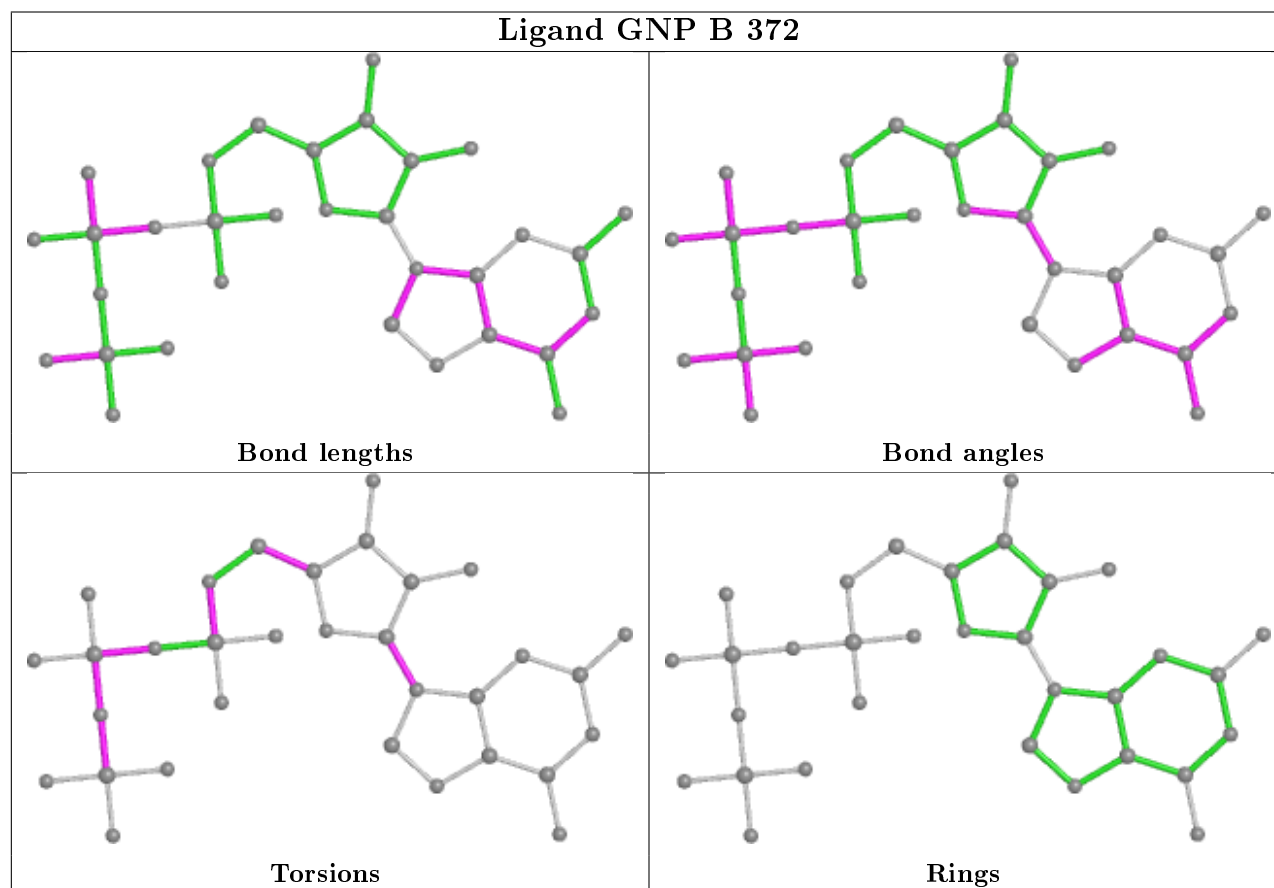
There are no ring outliers.

2 monomers are involved in 4 short contacts:

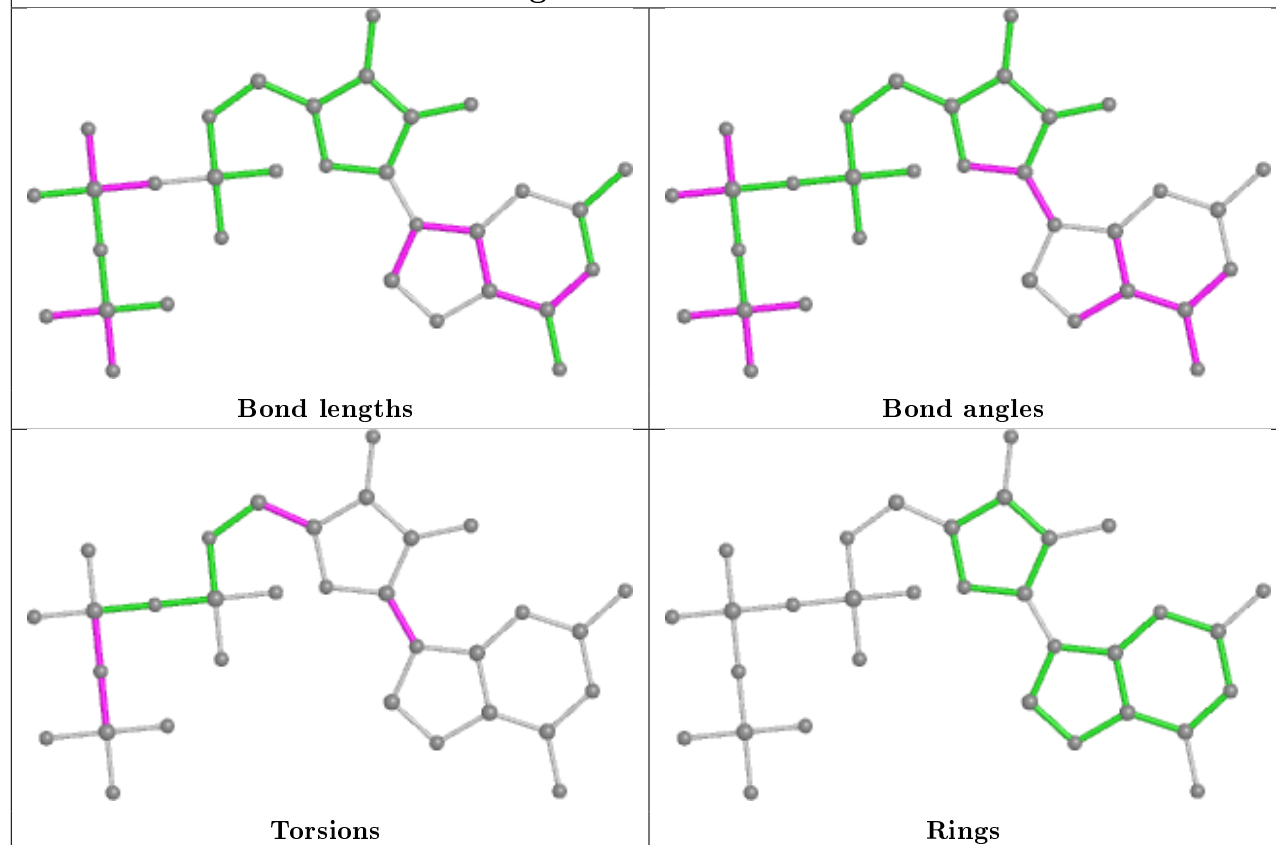
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	372	GNP	1	0
3	D	372	GNP	3	0

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

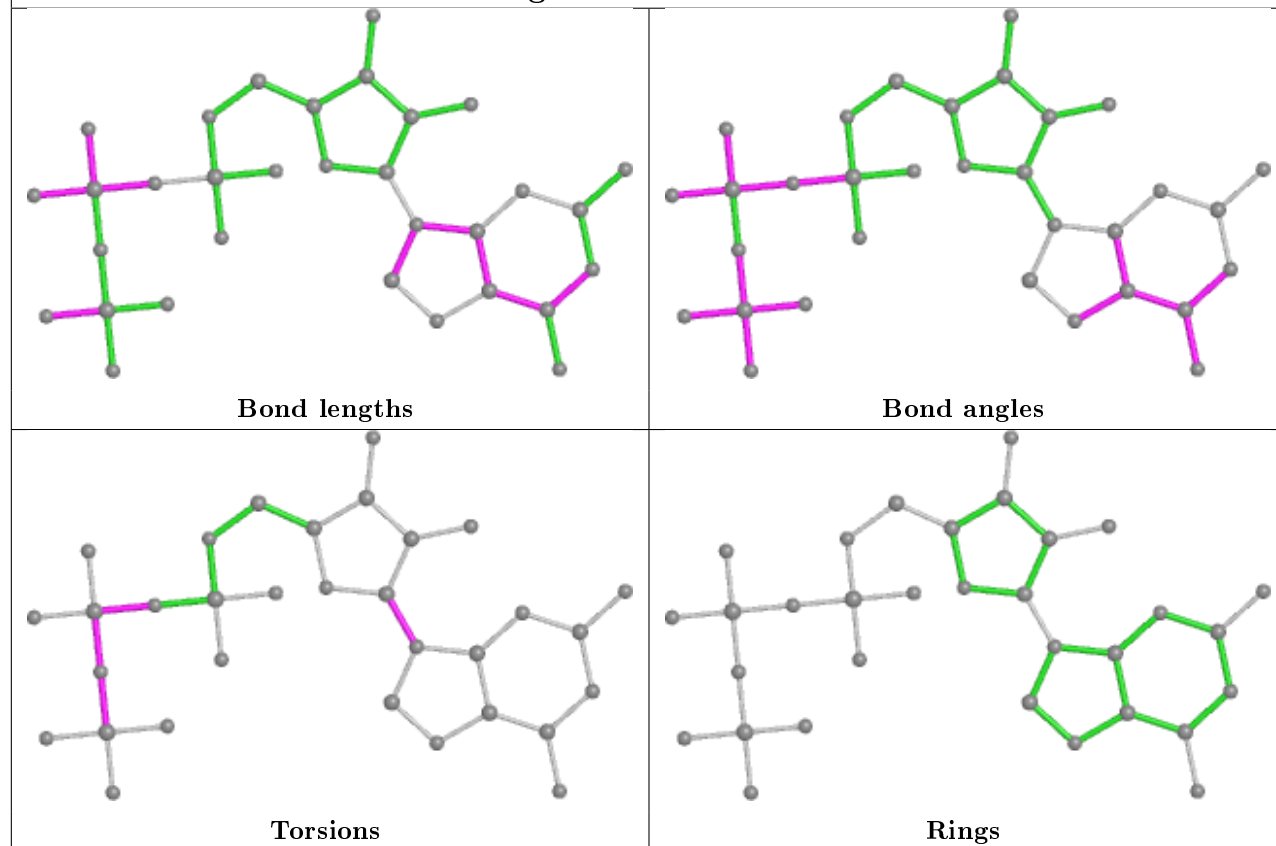
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

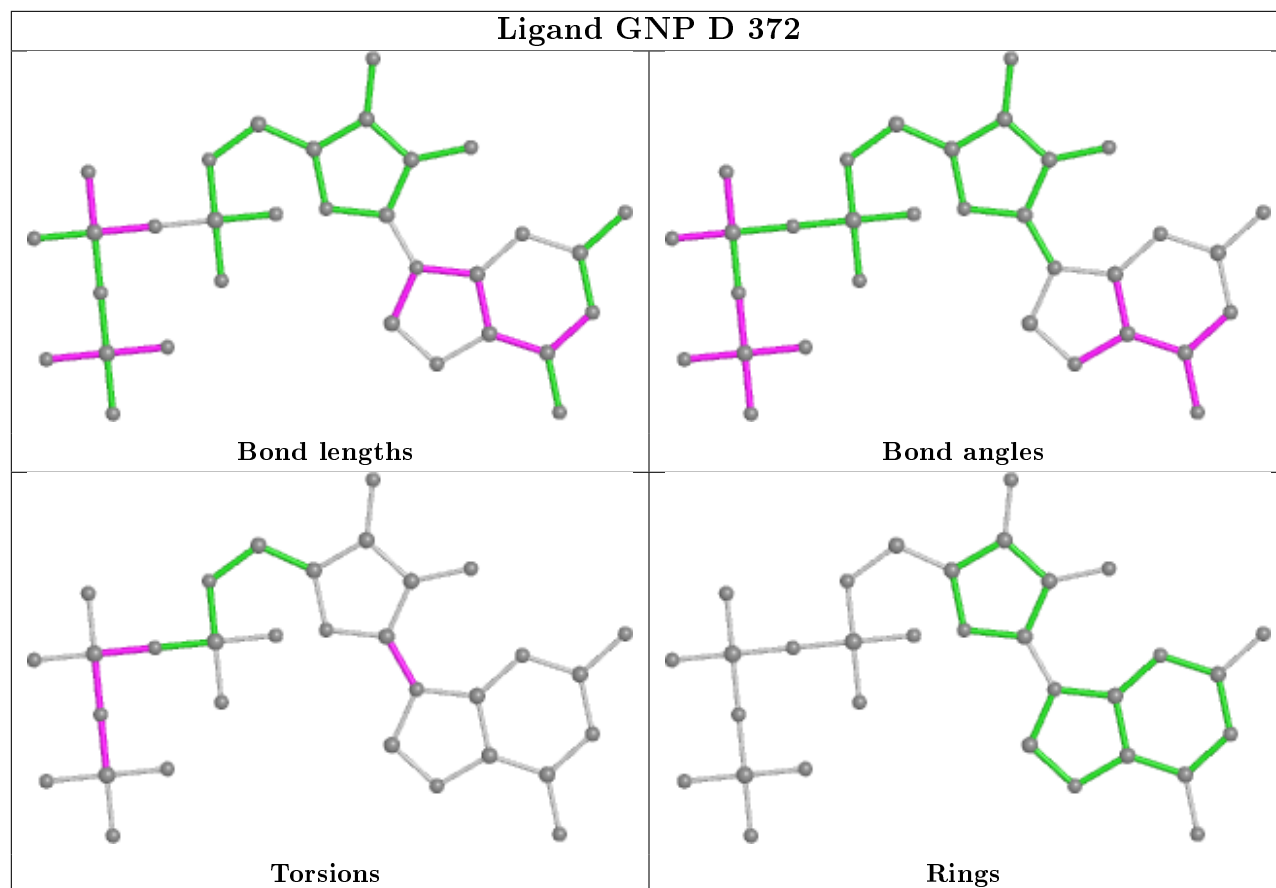


Ligand GNP C 372



Ligand GNP A 372





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, 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	254/274 (92%)	0.45	25 (9%) 7 5	15, 29, 46, 60	0
1	B	252/274 (91%)	0.49	21 (8%) 11 8	13, 28, 46, 58	0
1	C	250/274 (91%)	0.54	30 (12%) 4 3	15, 30, 51, 60	0
1	D	243/274 (88%)	0.57	28 (11%) 4 3	13, 32, 51, 57	0
All	All	999/1096 (91%)	0.51	104 (10%) 6 5	13, 30, 49, 60	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	GLY	6.8
1	C	249	LYS	6.4
1	D	140	HIS	6.0
1	C	223	ASP	5.6
1	A	249	LYS	5.0
1	B	226	GLU	4.7
1	C	75	ILE	4.6
1	C	222	GLU	4.6
1	B	223	ASP	4.4
1	C	92	GLY	4.4
1	B	93	VAL	4.4
1	C	250	GLY	4.3
1	B	253	VAL	4.2
1	B	91	ARG	4.1
1	D	91	ARG	4.1
1	B	305	LYS	4.1
1	D	226	GLU	4.1
1	A	250	GLY	4.0
1	D	249	LYS	4.0
1	D	35	GLY	4.0
1	C	34	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	247	GLU	3.7
1	A	215	ASP	3.6
1	B	75	ILE	3.5
1	D	134	SER	3.4
1	A	34	LYS	3.4
1	A	222	GLU	3.4
1	A	91	ARG	3.3
1	A	252	LYS	3.3
1	C	243	ASN	3.3
1	D	216	ALA	3.3
1	B	216	ALA	3.3
1	B	112	ARG	3.3
1	A	221	ASP	3.2
1	C	35	GLY	3.2
1	D	128	ARG	3.2
1	C	91	ARG	3.2
1	C	221	ASP	3.2
1	D	141	ILE	3.1
1	A	223	ASP	3.1
1	D	285	GLN	3.1
1	B	138	ARG	3.0
1	A	138	ARG	3.0
1	B	139	ARG	3.0
1	D	131	HIS	3.0
1	C	93	VAL	3.0
1	C	229	ARG	2.9
1	D	158	HIS	2.9
1	D	215	ASP	2.9
1	A	224	PHE	2.9
1	D	92	GLY	2.9
1	C	108	ALA	2.8
1	A	217	GLU	2.8
1	B	90	GLU	2.7
1	D	76	GLU	2.7
1	A	92	GLY	2.7
1	B	222	GLU	2.7
1	C	226	GLU	2.7
1	D	133	GLU	2.7
1	B	76	GLU	2.6
1	D	93	VAL	2.6
1	B	74	LYS	2.6
1	A	248	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	244	GLN	2.6
1	C	298	ASN	2.5
1	D	115	PHE	2.5
1	D	135	GLY	2.5
1	D	250	GLY	2.5
1	C	158	HIS	2.5
1	A	93	VAL	2.5
1	A	197	LYS	2.5
1	D	106	GLY	2.5
1	C	248	ALA	2.5
1	C	76	GLU	2.4
1	C	112	ARG	2.4
1	A	74	LYS	2.4
1	A	139	ARG	2.4
1	A	35	GLY	2.4
1	B	215	ASP	2.4
1	D	229	ARG	2.4
1	C	90	GLU	2.4
1	C	138	ARG	2.3
1	D	230	LEU	2.3
1	D	90	GLU	2.3
1	C	215	ASP	2.3
1	A	230	LEU	2.3
1	A	140	HIS	2.2
1	B	108	ALA	2.2
1	C	110	ASN	2.2
1	C	140	HIS	2.2
1	D	36	PHE	2.2
1	C	242	SER	2.2
1	C	79	VAL	2.1
1	A	247	GLU	2.1
1	D	301	SER	2.1
1	A	225	LYS	2.1
1	B	244	GLN	2.1
1	C	304	LEU	2.1
1	A	90	GLU	2.1
1	D	248	ALA	2.1
1	A	226	GLU	2.1
1	B	294	LEU	2.1
1	B	224	PHE	2.0
1	C	224	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

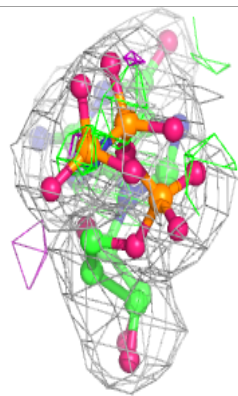
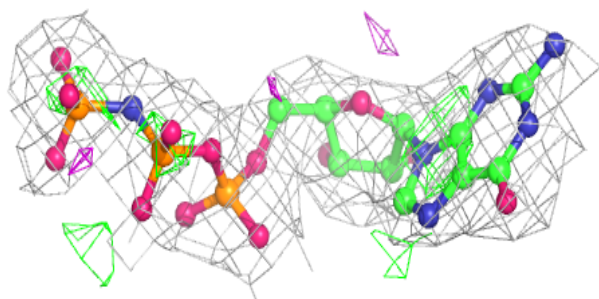
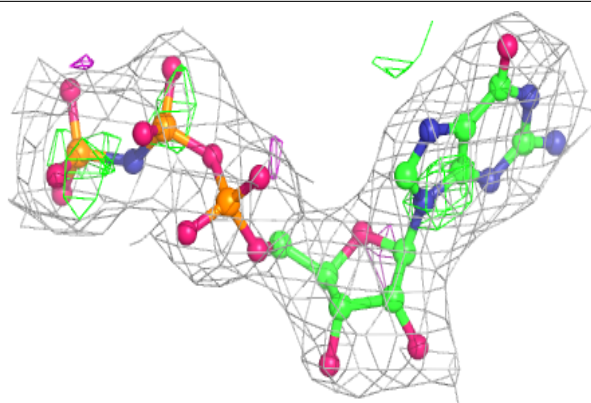
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	C	371	1/1	0.86	0.14	42,42,42,42	0
2	MG	A	371	1/1	0.90	0.13	28,28,28,28	0
2	MG	D	371	1/1	0.93	0.14	36,36,36,36	0
2	MG	B	371	1/1	0.96	0.25	29,29,29,29	0
3	GNP	B	372	32/32	0.97	0.22	28,32,36,37	0
3	GNP	C	372	32/32	0.97	0.20	37,38,40,40	0
3	GNP	A	372	32/32	0.97	0.20	27,28,29,29	0
3	GNP	D	372	32/32	0.97	0.20	29,32,33,34	0

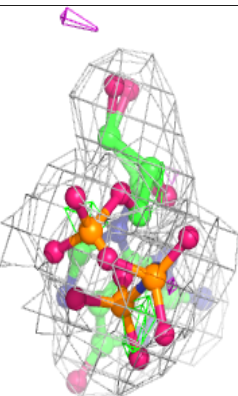
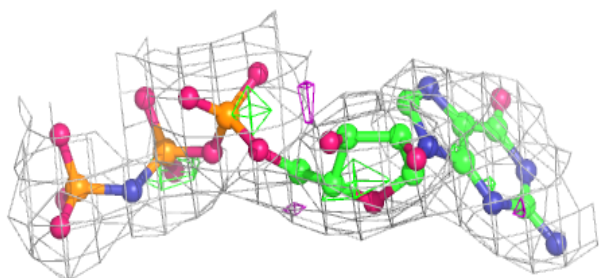
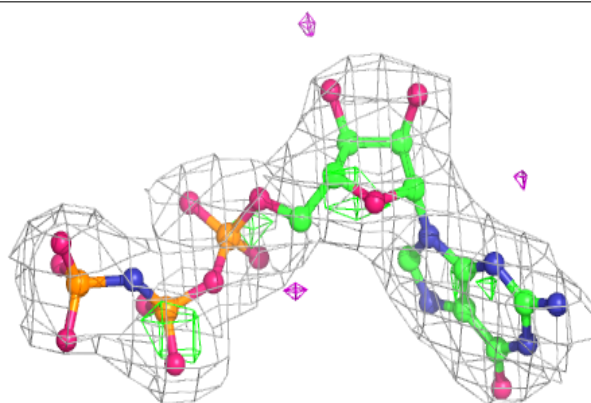
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP B 372:

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

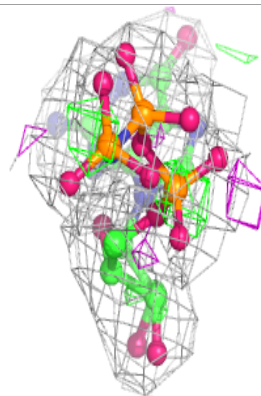
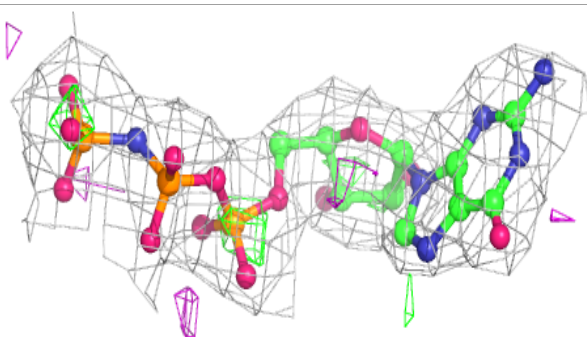
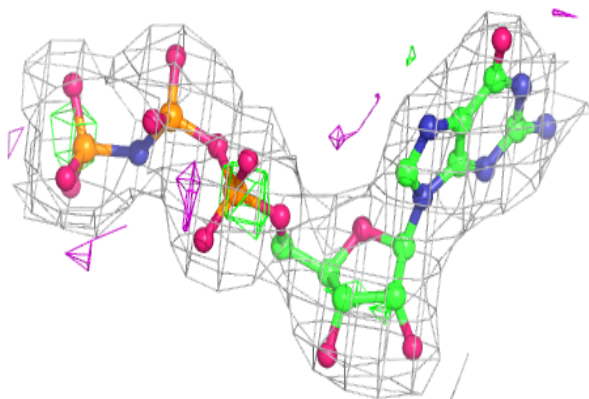
**Electron density around GNP C 372:**

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

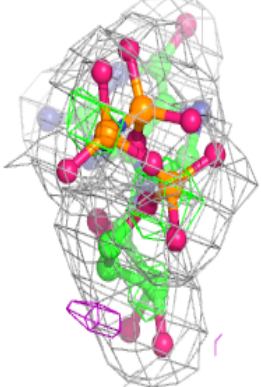
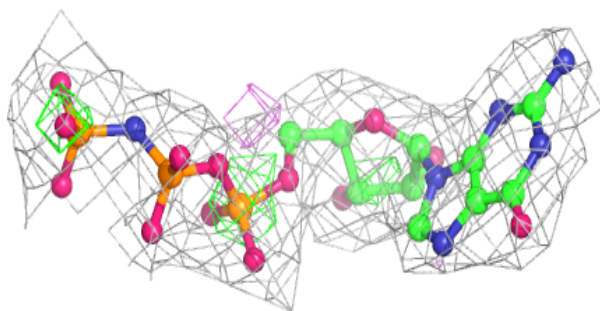
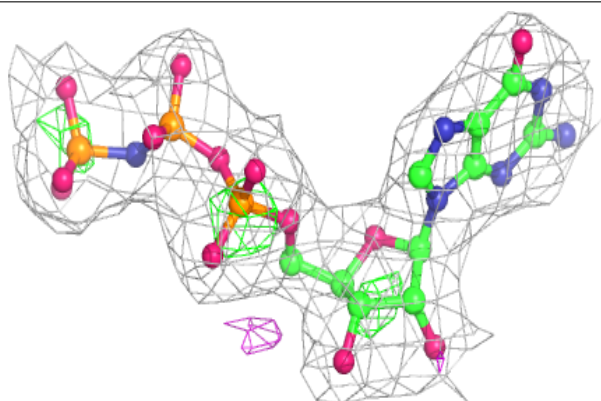


Electron density around GNP A 372:

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

**Electron density around GNP D 372:**

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



6.5 Other polymers

There are no such residues in this entry.