



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:51 AM UTC

PDB ID : 1JPN / pdb_00001jpn
Title : GMPPNP Complex of SRP GTPase NG Domain
Authors : Padmanabhan, S.; Freymann, D.M.
Deposited on : 2001-08-02
Resolution : 1.90 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 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

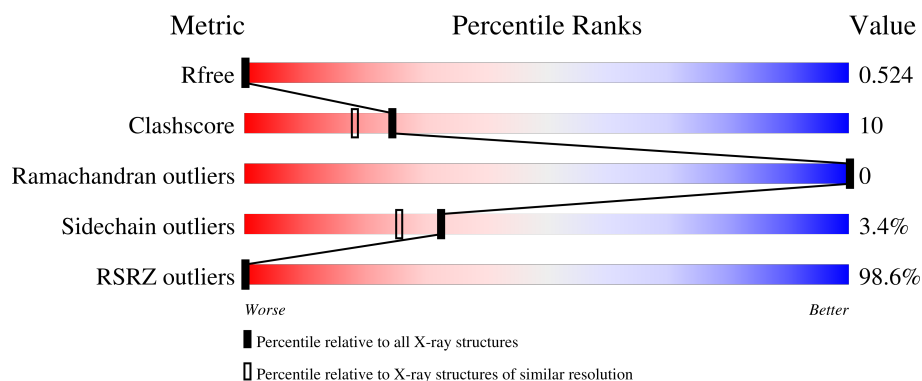
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 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	296	98% 80%19%.
1	B	296	99% 77%22%.

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	A	952	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5117 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.

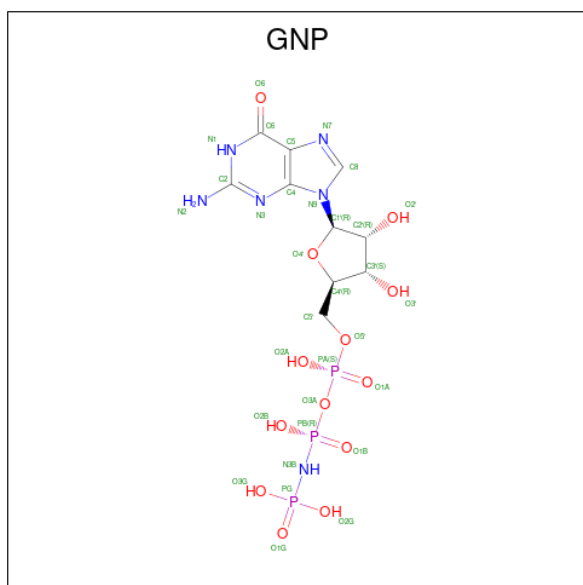
- Molecule 1 is a protein called SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	295	Total	C	N	O	S	0	6	0
			2318	1454	423	434	7			
1	A	296	Total	C	N	O	S	0	1	0
			2286	1435	416	428	7			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

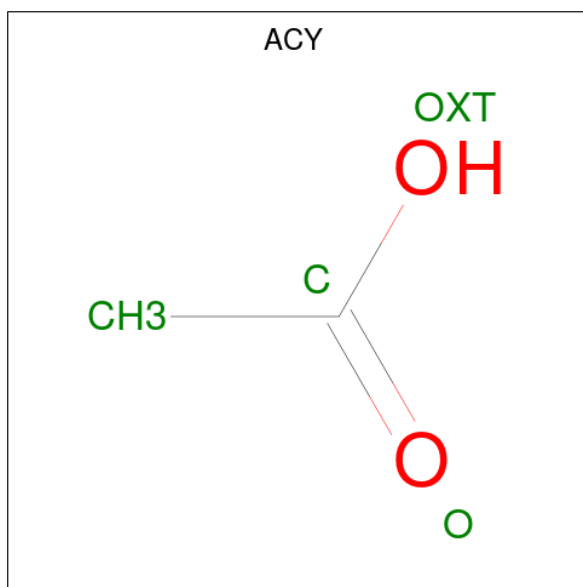
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

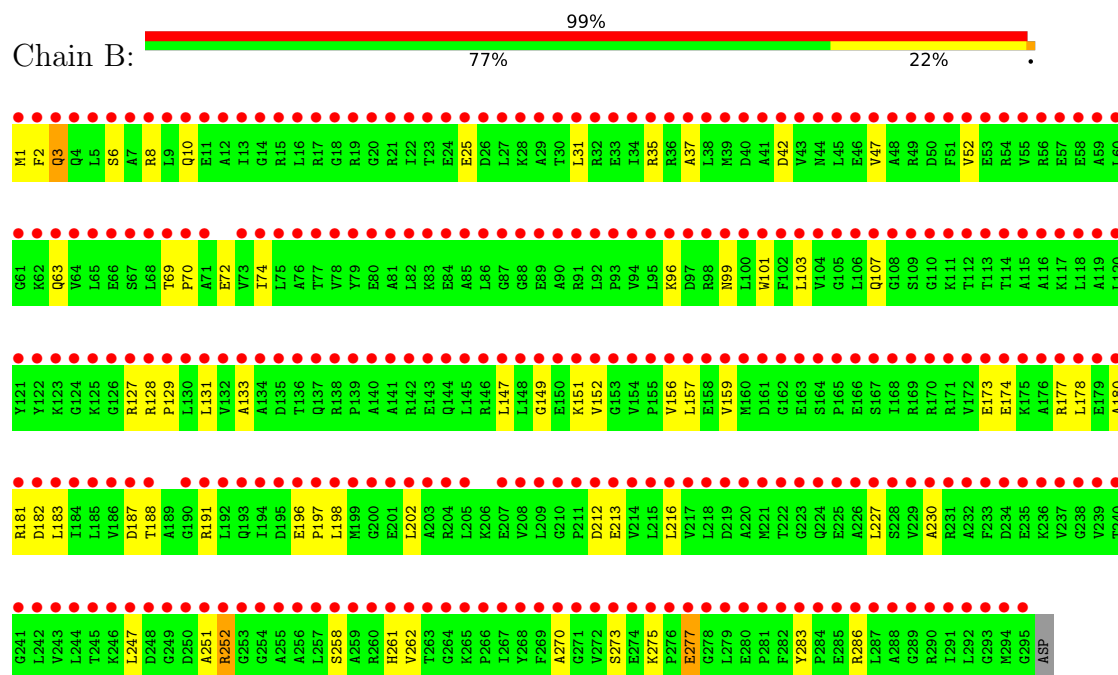
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	180	Total	O	0	0
			180	180		
5	A	251	Total	O	0	0
			251	251		

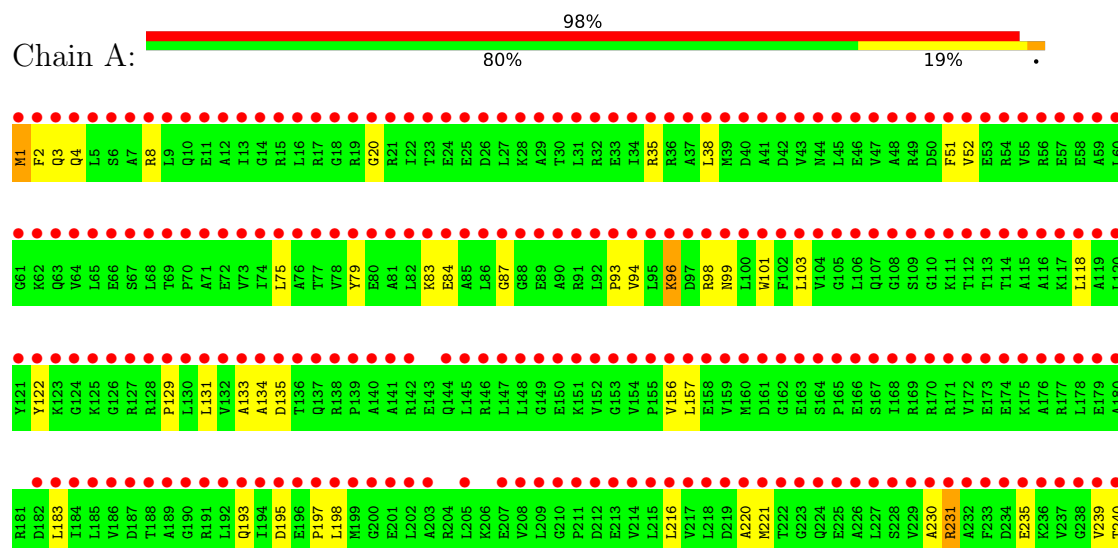
3 Residue-property plots

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: SIGNAL RECOGNITION PARTICLE PROTEIN



• Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN



G241	L242	V243	L244	T245	K246	L247	E248	D249	D250	A251	R252	G253	G254	A255	A256	L257	S258	A259	R260	R261	V262	T263	Q264	K265	P266	I267	Y268	F269	A270	G271	V272	S273	E274	K275	P276	F277	G278	L279	E280	P281	F282	Y283	P284	E285	R286	L287	A288	G289	R290	I291	L292	G293	M294	Q295	D296
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.81Å 54.53Å 99.08Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 15.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.90) 22.7 (15.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.241 0.521 , 0.524	Depositor DCC
R_{free} test set	4875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.35 , 736.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.03	EDS
Total number of atoms	5117	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: ACY, GNP, CA

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	0.30	0/2311	0.75	2/3112 (0.1%)
1	B	0.29	0/2343	0.76	1/3155 (0.0%)
All	All	0.29	0/4654	0.75	3/6267 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	VAL	N-CA-C	6.99	117.10	110.53
1	A	262	VAL	N-CA-C	6.14	116.78	110.82
1	A	134	ALA	N-CA-C	5.21	119.27	113.02

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	2286	0	2385	40	0
1	B	2318	0	2416	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	13	0	0
3	B	32	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	6	3	0
4	B	8	0	6	1	0
5	A	251	0	0	4	3
5	B	180	0	0	2	3
All	All	5117	0	4839	94	4

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 10.

All (94) 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:B:96:LYS:H	1:B:99:ASN:HD21	1.06	0.93
1:A:96:LYS:H	1:A:99:ASN:HD21	1.13	0.92
1:B:35:ARG:HB2	1:B:52[A]:VAL:HG21	1.68	0.76
1:B:69:THR:HB	1:B:72:GLU:HG3	1.69	0.73
1:A:1:MET:HA	1:A:3:GLN:HE22	1.51	0.73
1:B:96:LYS:H	1:B:99:ASN:ND2	1.85	0.71
1:B:96:LYS:N	1:B:99:ASN:HD21	1.86	0.70
1:B:283:TYR:HB3	1:B:286:ARG:HG3	1.73	0.68
1:A:231:ARG:O	1:A:235:GLU:HG2	1.94	0.68
1:B:247:LEU:HD12	1:B:270:ALA:HB1	1.76	0.67
1:B:128:ARG:NH1	1:B:180:ALA:HB3	2.11	0.66
1:A:20:GLY:HA2	5:A:1476:HOH:O	1.96	0.64
1:A:247:LEU:HD12	1:A:270:ALA:HB1	1.80	0.63
1:B:1:MET:H1	1:B:3:GLN:HE22	1.47	0.61
1:B:275:LYS:HG3	1:B:277:GLU:HG2	1.83	0.60
1:A:1:MET:HE3	1:A:253:GLY:HA2	1.82	0.60
1:B:283:TYR:CB	1:B:286:ARG:HG3	2.32	0.59
1:B:227:LEU:HD11	1:B:258:SER:HB2	1.85	0.58
1:B:273:SER:OG	1:B:275:LYS:HG2	2.04	0.58
1:A:195:ASP:HB3	1:A:198:LEU:HB3	1.84	0.58
1:B:128:ARG:HH12	1:B:180:ALA:HB3	1.69	0.58
1:A:272:VAL:HG22	1:A:278:GLY:O	2.05	0.57
1:A:1:MET:HG2	1:A:247:LEU:O	2.04	0.57
1:B:174:GLU:HG3	1:B:177:ARG:HH22	1.69	0.57
1:A:1:MET:SD	1:A:251:ALA:HB3	2.45	0.56
1:B:1:MET:N	1:B:3:GLN:HE22	2.04	0.55
1:A:1:MET:HA	1:A:3:GLN:NE2	2.19	0.55
1:A:35:ARG:HB2	1:A:52:VAL:HG21	1.88	0.54
1:B:42:ASP:HB2	1:B:252:ARG:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLU:HB3	1:B:197:PRO:HD3	1.89	0.54
1:A:290:ARG:HG3	1:A:291:ILE:N	2.23	0.53
1:B:8[A]:ARG:HG2	1:B:37:ALA:HB2	1.90	0.53
1:A:216:LEU:CD2	1:A:230:ALA:HA	2.39	0.53
1:B:25:GLU:HB2	5:B:1334:HOH:O	2.08	0.53
1:A:133:ALA:HB1	4:A:952:ACY:H2	1.90	0.52
1:A:87:GLY:HA2	1:A:260:ARG:HD2	1.91	0.52
1:B:191:ARG:HG2	1:B:198:LEU:HD13	1.91	0.51
1:B:47:VAL:HG22	1:B:261:HIS:CG	2.45	0.51
1:B:31:LEU:HD22	1:B:52[A]:VAL:HG13	1.92	0.51
1:B:42:ASP:HB2	1:B:252:ARG:HH11	1.76	0.50
1:B:216:LEU:CD2	1:B:230:ALA:HA	2.42	0.49
1:B:273:SER:OG	1:B:275:LYS:HE3	2.13	0.48
1:B:31:LEU:HB3	1:B:52[B]:VAL:CG2	2.43	0.48
1:B:216:LEU:HD21	1:B:230:ALA:HA	1.97	0.47
1:A:195:ASP:CG	1:A:197:PRO:HD2	2.39	0.47
1:A:38:LEU:HD11	1:A:51:PHE:CD1	2.50	0.47
1:A:118:LEU:HD22	1:A:122:TYR:HE2	1.80	0.47
1:A:216:LEU:HD21	1:A:230:ALA:HA	1.96	0.47
1:B:35:ARG:HG2	1:B:35:ARG:HH11	1.80	0.47
1:B:127:ARG:HH21	1:B:182:ASP:HB2	1.79	0.47
1:B:129:PRO:HA	1:B:183:LEU:O	2.16	0.46
1:B:131:LEU:HB2	1:B:156:VAL:HG22	1.97	0.46
1:A:129:PRO:HA	1:A:183:LEU:O	2.16	0.46
1:A:84:GLU:HG3	5:A:1452:HOH:O	2.15	0.45
1:B:133:ALA:O	1:B:159:VAL:HG22	2.17	0.45
1:B:1:MET:O	1:B:2:PHE:HB2	2.17	0.45
1:B:174:GLU:O	1:B:178:LEU:HG	2.17	0.45
1:A:193:GLN:HG2	5:A:1443:HOH:O	2.16	0.45
1:B:149:GLY:O	1:B:152:VAL:HG22	2.17	0.44
1:A:275:LYS:HB2	1:A:276:PRO:HD2	1.99	0.44
1:A:273:SER:OG	1:A:275:LYS:HG2	2.17	0.44
1:B:107:GLN:HA	3:B:910:GNP:O2G	2.17	0.44
1:B:128:ARG:NH2	1:B:181:ARG:HH21	2.15	0.44
1:B:188:THR:HB	1:B:202:LEU:HD21	2.00	0.44
1:A:93:PRO:HB2	1:A:101:TRP:CH2	2.53	0.44
1:A:135:ASP:HB2	4:A:952:ACY:H1	1.99	0.43
1:B:273:SER:HG	1:B:275:LYS:HE3	1.82	0.43
1:A:1:MET:HE3	1:A:253:GLY:CA	2.47	0.43
1:A:1:MET:HE1	1:A:220:ALA:HB1	2.00	0.43
1:A:1:MET:O	1:A:2:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HB2	1:A:156:VAL:HG22	1.99	0.43
1:B:6[B]:SER:O	1:B:10:GLN:HG3	2.18	0.43
1:A:157:LEU:C	1:A:157:LEU:HD23	2.44	0.43
1:B:101:TRP:CD1	1:B:213:GLU:HB2	2.54	0.43
1:B:157:LEU:C	1:B:157:LEU:HD23	2.44	0.43
1:A:135:ASP:CB	4:A:952:ACY:H1	2.49	0.43
1:B:1:MET:N	1:B:3:GLN:NE2	2.66	0.42
1:B:2:PHE:HE1	1:B:247:LEU:HD22	1.85	0.42
1:B:6[A]:SER:O	1:B:10:GLN:HG3	2.19	0.42
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.91	0.42
1:A:94:VAL:HG23	5:A:1252:HOH:O	2.20	0.42
1:B:187:ASP:OD2	4:B:950:ACY:H2	2.19	0.42
1:A:75:LEU:HD12	1:A:292:LEU:HD13	2.01	0.42
1:A:8:ARG:HA	1:A:8:ARG:HD3	1.87	0.42
1:A:239:VAL:HG12	1:A:240:THR:N	2.35	0.42
1:B:1:MET:HG3	1:B:251:ALA:O	2.20	0.41
1:B:70:PRO:O	1:B:74:ILE:HG12	2.20	0.41
1:B:1:MET:HG2	1:B:2:PHE:CD1	2.55	0.41
1:A:221:MET:SD	1:A:249:GLY:HA3	2.61	0.41
1:B:31:LEU:HB3	1:B:52[A]:VAL:CG1	2.49	0.41
1:B:261:HIS:HB2	5:B:1266:HOH:O	2.20	0.41
1:A:79:TYR:OH	1:A:285:GLU:HG3	2.21	0.41
1:B:147:LEU:O	1:B:151:LYS:HB2	2.21	0.41
1:A:3:GLN:HE21	1:A:3:GLN:HB2	1.76	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1121:HOH:O	5:B:1407:HOH:O[2_656]	1.93	0.27
5:B:1299:HOH:O	5:A:1385:HOH:O[3_445]	2.02	0.18
5:A:1180:HOH:O	5:A:1321:HOH:O[2_655]	2.04	0.16
5:B:1158:HOH:O	5:A:1050:HOH:O[4_546]	2.11	0.09

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	295/296 (100%)	289 (98%)	6 (2%)	0	100	100
1	B	299/296 (101%)	295 (99%)	4 (1%)	0	100	100
All	All	594/592 (100%)	584 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	235/234 (100%)	226 (96%)	9 (4%)	29	21
1	B	239/234 (102%)	232 (97%)	7 (3%)	37	31
All	All	474/468 (101%)	458 (97%)	16 (3%)	32	25

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	63	GLN
1	B	103	LEU
1	B	173	GLU
1	B	212	ASP
1	B	252	ARG
1	B	277	GLU
1	A	1	MET
1	A	4	GLN
1	A	83	LYS
1	A	96	LYS
1	A	98	ARG
1	A	103	LEU
1	A	231	ARG

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Mol	Chain	Res	Type
1	A	273	SER
1	A	290	ARG

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

Mol	Chain	Res	Type
1	B	3	GLN
1	B	99	ASN
1	B	144	GLN
1	B	193	GLN
1	B	261	HIS
1	A	10	GLN
1	A	44	ASN
1	A	99	ASN
1	A	107	GLN
1	A	224	GLN
1	A	261	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
4	ACY	A	952	-	3,3,3	1.32	0	3,3,3	1.32	0
3	GNP	B	910	-	34,34,34	1.48	8 (23%)	47,54,54	1.06	4 (8%)
4	ACY	B	951	-	3,3,3	1.45	0	3,3,3	1.26	0
3	GNP	A	911	-	34,34,34	1.49	7 (20%)	47,54,54	1.03	3 (6%)
4	ACY	B	950	-	3,3,3	1.46	0	3,3,3	1.25	0
4	ACY	A	953	-	3,3,3	1.42	0	3,3,3	1.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	A	911	-	-	1/18/38/38	0/3/3/3
3	GNP	B	910	-	-	2/18/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	911	GNP	PB-N3B	3.19	1.71	1.63
3	A	911	GNP	PG-N3B	3.12	1.71	1.63
3	B	910	GNP	PB-N3B	2.96	1.71	1.63
3	B	910	GNP	PG-N3B	2.94	1.71	1.63
3	B	910	GNP	PB-O1B	2.88	1.50	1.46
3	A	911	GNP	PB-O1B	2.86	1.50	1.46
3	A	911	GNP	PG-O1G	2.62	1.50	1.46
3	B	910	GNP	PG-O1G	2.56	1.50	1.46
3	B	910	GNP	PG-O2G	-2.54	1.50	1.56
3	A	911	GNP	PG-O3G	-2.52	1.50	1.56
3	B	910	GNP	PB-O2B	-2.41	1.50	1.56
3	A	911	GNP	PG-O2G	-2.40	1.50	1.56
3	A	911	GNP	PB-O2B	-2.38	1.50	1.56
3	B	910	GNP	PG-O3G	-2.34	1.50	1.56
3	B	910	GNP	C4-N3	2.05	1.38	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	911	GNP	O2B-PB-O1B	4.19	118.85	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	910	GNP	O2B-PB-O1B	4.18	118.83	109.87
3	B	910	GNP	O1G-PG-N3B	-2.25	108.46	111.77
3	A	911	GNP	O3A-PB-N3B	-2.15	100.64	106.59
3	A	911	GNP	O1B-PB-N3B	-2.14	108.62	111.77
3	B	910	GNP	O1B-PB-N3B	-2.11	108.66	111.77
3	B	910	GNP	O3A-PB-N3B	-2.04	100.94	106.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	910	GNP	PB-N3B-PG-O1G
3	A	911	GNP	PG-N3B-PB-O1B
3	B	910	GNP	PB-O3A-PA-O1A

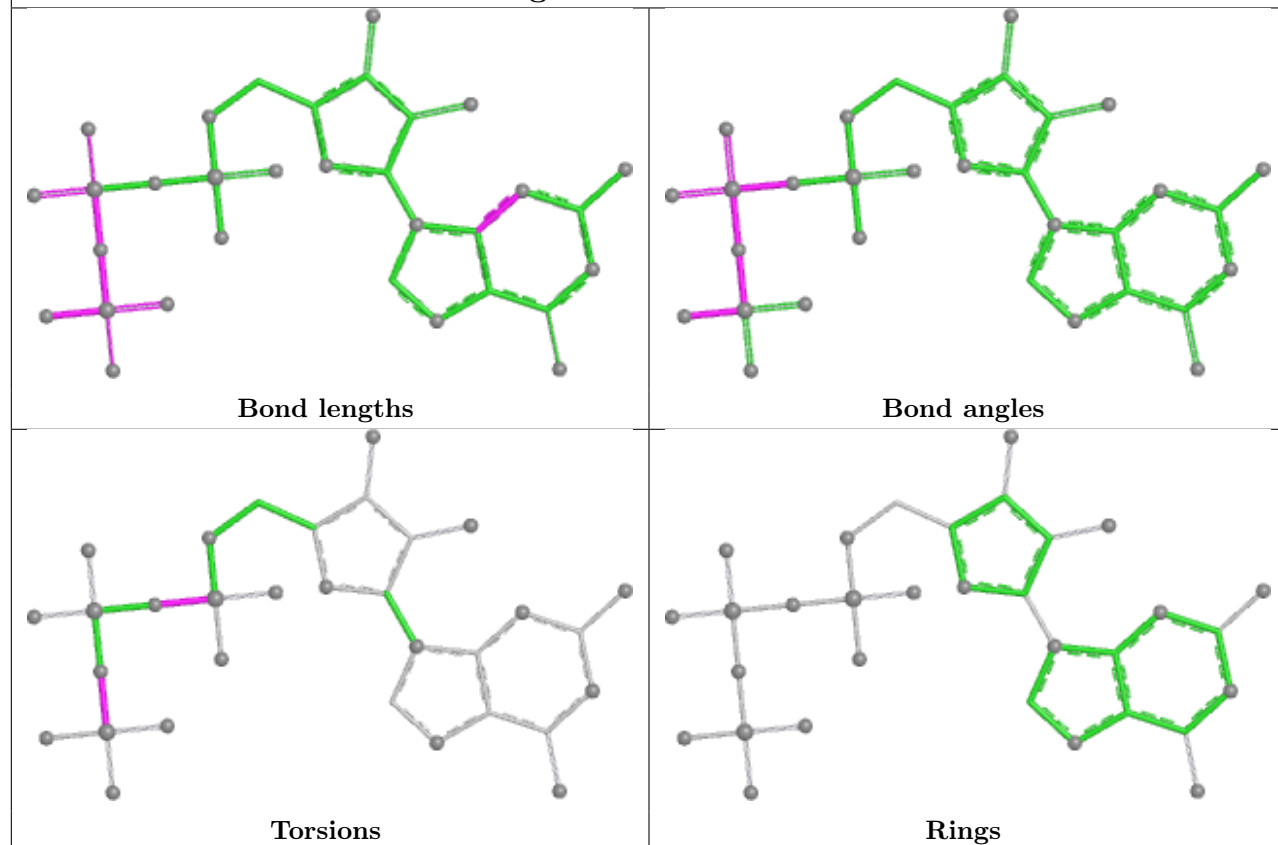
There are no ring outliers.

3 monomers are involved in 5 short contacts:

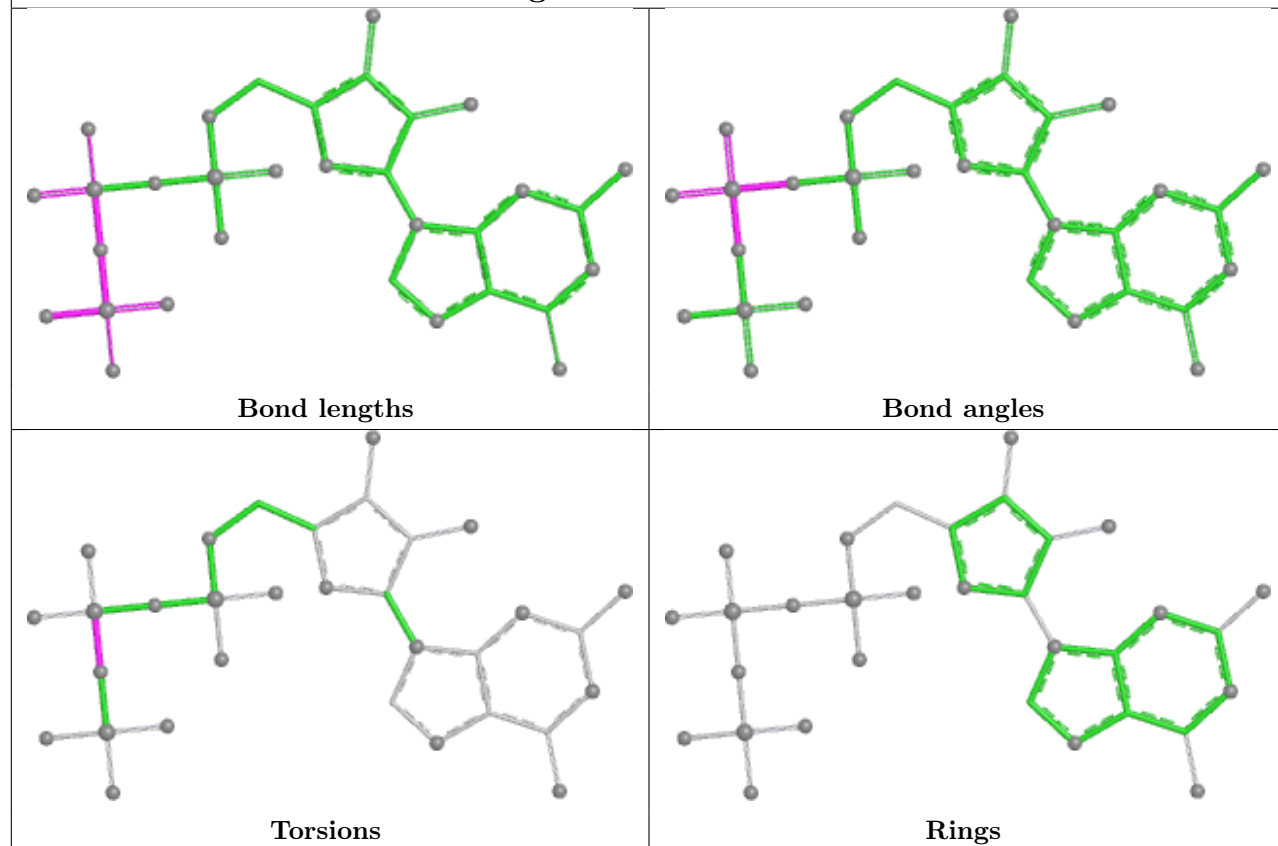
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	952	ACY	3	0
3	B	910	GNP	1	0
4	B	950	ACY	1	0

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 B 910



Ligand GNP A 911



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	296/296 (100%)	4.73	291 (98%) 0 0	8, 17, 37, 63	1 (0%)
1	B	295/296 (99%)	4.78	292 (98%) 0 0	8, 20, 43, 65	6 (2%)
All	All	591/592 (99%)	4.75	583 (98%) 0 0	8, 18, 42, 65	7 (1%)

All (583) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	GLY	12.0
1	B	172	VAL	10.9
1	A	245	THR	10.3
1	B	267	ILE	9.8
1	B	69	THR	9.4
1	B	194	ILE	9.3
1	A	74	ILE	9.3
1	A	259	ALA	9.1
1	A	110	GLY	9.0
1	B	230	ALA	9.0
1	B	283	TYR	9.0
1	B	102	PHE	8.9
1	A	122	TYR	8.9
1	A	278	GLY	8.6
1	B	268	TYR	8.5
1	A	12	ALA	8.5
1	B	61	GLY	8.4
1	B	240	THR	8.4
1	A	230	ALA	8.3
1	B	7	ALA	8.2
1	B	82	LEU	8.2
1	B	228	SER	8.1
1	A	271	GLY	8.1
1	B	247	LEU	8.1

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Mol	Chain	Res	Type	RSRZ
1	B	31	LEU	8.0
1	B	68	LEU	7.9
1	B	95	LEU	7.9
1	A	214	VAL	7.8
1	A	247	LEU	7.8
1	A	73	VAL	7.8
1	A	272	VAL	7.8
1	B	151	LYS	7.8
1	A	255	ALA	7.7
1	A	256	ALA	7.7
1	A	193	GLN	7.7
1	A	147	LEU	7.7
1	B	295	GLY	7.7
1	A	19	ARG	7.6
1	B	59	ALA	7.6
1	B	41	ALA	7.6
1	B	64	VAL	7.6
1	A	47	VAL	7.4
1	A	253	GLY	7.4
1	A	38	LEU	7.3
1	A	87	GLY	7.3
1	B	243	VAL	7.3
1	B	251	ALA	7.3
1	B	272	VAL	7.2
1	A	227	LEU	7.2
1	A	94	VAL	7.2
1	A	184	ILE	7.2
1	A	118	LEU	7.1
1	A	282	PHE	7.1
1	A	209	LEU	7.1
1	A	115	ALA	7.1
1	B	258	SER	7.0
1	A	217	VAL	7.0
1	A	294	MET	7.0
1	A	79	TYR	7.0
1	B	200	GLY	6.9
1	A	51	PHE	6.9
1	A	102	PHE	6.9
1	A	222	THR	6.9
1	A	203	ALA	6.9
1	A	53	GLU	6.9
1	A	187	ASP	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	6.9
1	A	2	PHE	6.9
1	A	121	TYR	6.9
1	A	136	THR	6.8
1	B	235	GLU	6.8
1	A	258	SER	6.7
1	B	101	TRP	6.7
1	B	195	ASP	6.7
1	B	88	GLY	6.7
1	A	42	ASP	6.7
1	B	22	ILE	6.7
1	B	87	GLY	6.7
1	A	31	LEU	6.7
1	A	75	LEU	6.6
1	A	229	VAL	6.6
1	A	16	LEU	6.6
1	A	69	THR	6.6
1	B	259	ALA	6.6
1	A	48	ALA	6.6
1	B	27	LEU	6.6
1	B	136	THR	6.5
1	B	90	ALA	6.5
1	B	209	LEU	6.5
1	B	238	GLY	6.5
1	B	86	LEU	6.5
1	B	100	LEU	6.4
1	B	222	THR	6.4
1	A	154	VAL	6.4
1	B	256	ALA	6.4
1	A	254	GLY	6.3
1	A	27	LEU	6.3
1	B	110	GLY	6.3
1	B	289	GLY	6.3
1	B	188	THR	6.3
1	B	277	GLU	6.3
1	B	140	ALA	6.3
1	A	26	ASP	6.2
1	A	260	ARG	6.2
1	B	279	LEU	6.2
1	A	149	GLY	6.2
1	A	7	ALA	6.2
1	B	65	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	155	PRO	6.2
1	B	217	VAL	6.2
1	B	16	LEU	6.1
1	A	86	LEU	6.1
1	B	278	GLY	6.1
1	A	6	SER	6.1
1	A	4	GLN	6.1
1	B	48	ALA	6.1
1	A	81	ALA	6.1
1	B	164	SER	6.1
1	A	103	LEU	6.1
1	A	186	VAL	6.0
1	B	142	ARG	6.0
1	B	191	ARG	6.0
1	A	98	ARG	6.0
1	B	37	ALA	5.9
1	A	248	ASP	5.9
1	B	15	ARG	5.9
1	B	250	ASP	5.9
1	A	252	ARG	5.9
1	A	194	ILE	5.9
1	A	50	ASP	5.9
1	B	192	LEU	5.9
1	A	29	ALA	5.8
1	B	1	MET	5.8
1	A	70	PRO	5.8
1	B	60	LEU	5.8
1	A	164	SER	5.8
1	B	163	GLU	5.8
1	B	186	VAL	5.8
1	A	243	VAL	5.8
1	A	106	LEU	5.8
1	A	244	LEU	5.8
1	B	112	THR	5.8
1	B	152	VAL	5.8
1	A	198	LEU	5.8
1	A	152	VAL	5.7
1	B	216	LEU	5.7
1	A	9	LEU	5.7
1	A	95	LEU	5.7
1	A	279	LEU	5.7
1	B	165	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.7
1	A	263	THR	5.7
1	A	257	LEU	5.7
1	A	107	GLN	5.7
1	A	291	ILE	5.7
1	B	212	ASP	5.7
1	B	52[A]	VAL	5.7
1	B	84	GLU	5.7
1	B	229	VAL	5.6
1	B	239	VAL	5.6
1	A	119	ALA	5.6
1	B	19	ARG	5.6
1	B	18	GLY	5.6
1	B	282	PHE	5.6
1	A	109	SER	5.6
1	A	23	THR	5.6
1	A	251	ALA	5.5
1	A	8	ARG	5.5
1	A	233	PHE	5.5
1	A	242	LEU	5.5
1	B	47	VAL	5.5
1	B	70	PRO	5.5
1	A	77	THR	5.5
1	A	250	ASP	5.5
1	B	92	LEU	5.5
1	A	155	PRO	5.5
1	B	115	ALA	5.5
1	B	66	GLU	5.5
1	B	130	LEU	5.4
1	A	273	SER	5.4
1	B	137	GLN	5.4
1	B	227	LEU	5.4
1	B	246	LYS	5.4
1	B	5	LEU	5.4
1	A	120	LEU	5.4
1	B	91	ARG	5.4
1	A	138	ARG	5.4
1	A	139	PRO	5.4
1	A	281	PRO	5.4
1	B	249	GLY	5.4
1	B	244	LEU	5.4
1	B	273	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	55	VAL	5.3
1	A	234	ASP	5.3
1	B	131	LEU	5.3
1	B	205	LEU	5.3
1	A	168	ILE	5.3
1	A	268	TYR	5.3
1	B	51	PHE	5.3
1	B	287	LEU	5.3
1	B	270	ALA	5.3
1	A	88	GLY	5.3
1	B	266	PRO	5.3
1	A	101	TRP	5.3
1	A	286	ARG	5.3
1	A	172	VAL	5.2
1	B	109	SER	5.2
1	A	145	LEU	5.2
1	A	100	LEU	5.2
1	B	207	GLU	5.2
1	B	198	LEU	5.2
1	A	269	PHE	5.2
1	B	39[A]	MET	5.2
1	A	249	GLY	5.2
1	B	219	ASP	5.1
1	B	221	MET	5.1
1	B	269	PHE	5.1
1	B	93	PRO	5.1
1	A	276	PRO	5.1
1	A	188	THR	5.1
1	A	220	ALA	5.1
1	B	20	GLY	5.1
1	A	111	LYS	5.1
1	B	29	ALA	5.1
1	A	219	ASP	5.1
1	B	124	GLY	5.0
1	A	180	ALA	5.0
1	B	178	LEU	5.0
1	B	294	MET	5.0
1	A	133	ALA	5.0
1	B	262	VAL	5.0
1	A	156	VAL	5.0
1	A	57	GLU	5.0
1	A	34	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	4.9
1	B	2	PHE	4.9
1	A	237	VAL	4.9
1	A	280	GLU	4.9
1	B	145	LEU	4.9
1	A	93	PRO	4.9
1	B	171	ARG	4.9
1	A	210	GLY	4.9
1	B	116	ALA	4.9
1	A	141	ALA	4.9
1	B	253	GLY	4.9
1	A	293	GLY	4.9
1	B	156	VAL	4.9
1	A	64	VAL	4.9
1	B	76	ALA	4.9
1	B	187	ASP	4.8
1	B	118	LEU	4.8
1	A	43	VAL	4.8
1	B	85	ALA	4.8
1	B	255	ALA	4.8
1	B	9	LEU	4.8
1	A	160[A]	MET	4.8
1	A	270	ALA	4.8
1	B	276	PRO	4.8
1	A	99	ASN	4.8
1	B	46	GLU	4.8
1	A	235	GLU	4.8
1	A	262	VAL	4.8
1	A	185	LEU	4.8
1	B	176	ALA	4.7
1	B	180	ALA	4.7
1	A	76	ALA	4.7
1	A	28	LYS	4.7
1	B	77	THR	4.7
1	B	144	GLN	4.7
1	B	292	LEU	4.7
1	A	148	LEU	4.7
1	B	122	TYR	4.7
1	A	84	GLU	4.7
1	B	13	ILE	4.7
1	B	202	LEU	4.7
1	A	45	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	79	TYR	4.7
1	B	78	VAL	4.7
1	A	52	VAL	4.7
1	A	264	GLY	4.7
1	B	146	ARG	4.7
1	A	140	ALA	4.6
1	B	193	GLN	4.6
1	B	32	ARG	4.6
1	B	160	MET	4.6
1	B	113[A]	THR	4.6
1	B	54	ARG	4.6
1	A	239	VAL	4.6
1	B	208	VAL	4.5
1	B	185	LEU	4.5
1	B	291	ILE	4.5
1	A	182	ASP	4.5
1	B	154	VAL	4.5
1	B	45	LEU	4.5
1	B	135	ASP	4.5
1	B	261	HIS	4.5
1	B	50	ASP	4.5
1	B	237	VAL	4.5
1	A	192	LEU	4.5
1	B	264	GLY	4.5
1	A	266	PRO	4.5
1	B	25	GLU	4.5
1	B	226	ALA	4.4
1	A	59	ALA	4.4
1	B	218	LEU	4.4
1	A	82	LEU	4.4
1	B	177	ARG	4.4
1	A	97	ASP	4.4
1	B	173	GLU	4.4
1	A	267	ILE	4.4
1	B	114	THR	4.4
1	A	228	SER	4.3
1	B	73	VAL	4.3
1	B	74	ILE	4.3
1	A	116	ALA	4.3
1	B	108	GLY	4.3
1	B	153	GLY	4.3
1	B	211	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	33	GLU	4.3
1	B	141	ALA	4.3
1	B	149	GLY	4.3
1	A	167	SER	4.3
1	B	120	LEU	4.3
1	A	236	LYS	4.3
1	B	220	ALA	4.3
1	B	26	ASP	4.3
1	B	99	ASN	4.3
1	B	139	PRO	4.3
1	A	287	LEU	4.2
1	A	134	ALA	4.2
1	A	24	GLU	4.2
1	A	35	ARG	4.2
1	B	245	THR	4.2
1	B	242	LEU	4.2
1	A	183	LEU	4.2
1	B	196	GLU	4.2
1	B	254	GLY	4.2
1	B	134	ALA	4.2
1	A	83	LYS	4.2
1	A	284	PRO	4.2
1	A	112	THR	4.2
1	B	280	GLU	4.2
1	A	201	GLU	4.2
1	A	213	GLU	4.2
1	B	232	ALA	4.2
1	A	221	MET	4.2
1	A	129	PRO	4.2
1	B	4	GLN	4.1
1	B	43	VAL	4.1
1	A	241	GLY	4.1
1	B	63	GLN	4.1
1	A	41	ALA	4.1
1	A	96	LYS	4.1
1	A	226	ALA	4.1
1	A	58	GLU	4.1
1	A	80	GLU	4.1
1	B	23	THR	4.1
1	A	127	ARG	4.1
1	A	20	GLY	4.1
1	A	46	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	231	ARG	4.1
1	A	246	LYS	4.1
1	A	275	LYS	4.1
1	B	236	LYS	4.1
1	A	44	ASN	4.1
1	B	215	LEU	4.1
1	A	37	ALA	4.0
1	A	290	ARG	4.0
1	A	240	THR	4.0
1	B	53	GLU	4.0
1	A	200	GLY	4.0
1	A	137	GLN	4.0
1	A	212	ASP	4.0
1	B	129	PRO	4.0
1	A	283	TYR	4.0
1	B	203	ALA	4.0
1	A	159	VAL	4.0
1	A	288	ALA	4.0
1	B	197	PRO	4.0
1	A	175	LYS	4.0
1	A	292	LEU	4.0
1	B	284	PRO	4.0
1	A	208	VAL	4.0
1	B	126	GLY	3.9
1	B	190	GLY	3.9
1	A	65	LEU	3.9
1	A	68	LEU	3.9
1	B	94	VAL	3.9
1	B	12	ALA	3.9
1	B	3	GLN	3.9
1	A	67	SER	3.9
1	B	11	GLU	3.9
1	A	158	GLU	3.9
1	A	114	THR	3.9
1	B	161	ASP	3.9
1	B	199	MET	3.9
1	A	225	GLU	3.8
1	B	147	LEU	3.8
1	B	175	LYS	3.8
1	B	36	ARG	3.8
1	A	33	GLU	3.8
1	A	130	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	42	ASP	3.8
1	A	15	ARG	3.8
1	A	13	ILE	3.8
1	A	104	VAL	3.8
1	A	117	LYS	3.8
1	A	151	LYS	3.8
1	B	290	ARG	3.8
1	B	210	GLY	3.8
1	B	223	GLY	3.8
1	A	61	GLY	3.8
1	A	215	LEU	3.8
1	B	263	THR	3.8
1	B	58	GLU	3.8
1	A	32	ARG	3.8
1	B	182	ASP	3.7
1	A	153	GLY	3.7
1	B	183	LEU	3.7
1	A	157	LEU	3.7
1	B	275	LYS	3.7
1	A	170	ARG	3.7
1	A	39	MET	3.7
1	A	207	GLU	3.7
1	B	56	ARG	3.7
1	B	127	ARG	3.7
1	A	231	ARG	3.7
1	B	159	VAL	3.7
1	B	96	LYS	3.7
1	B	123	LYS	3.7
1	B	252	ARG	3.7
1	A	54	ARG	3.7
1	A	90	ALA	3.7
1	B	57	GLU	3.7
1	B	80[A]	GLU	3.7
1	B	97	ASP	3.7
1	A	11	GLU	3.7
1	A	126	GLY	3.7
1	B	71	ALA	3.6
1	B	103	LEU	3.6
1	A	205	LEU	3.6
1	B	168	ILE	3.6
1	B	148	LEU	3.6
1	A	202	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	135	ASP	3.6
1	B	138	ARG	3.6
1	A	105	GLY	3.5
1	B	125	LYS	3.5
1	A	25	GLU	3.5
1	B	241	GLY	3.5
1	B	184	ILE	3.5
1	B	44	ASN	3.5
1	B	225	GLU	3.5
1	B	106	LEU	3.5
1	A	218	LEU	3.5
1	B	117	LYS	3.5
1	B	17	ARG	3.4
1	B	62	LYS	3.4
1	A	165	PRO	3.4
1	B	121	TYR	3.4
1	B	170	ARG	3.4
1	A	128	ARG	3.4
1	B	34	ILE	3.4
1	A	22	ILE	3.4
1	A	261	HIS	3.4
1	B	55	VAL	3.4
1	B	14	GLY	3.4
1	B	162	GLY	3.4
1	A	60	LEU	3.4
1	A	216	LEU	3.4
1	B	281	PRO	3.4
1	B	98	ARG	3.4
1	B	265	LYS	3.4
1	A	265	LYS	3.4
1	A	124	GLY	3.4
1	A	91	ARG	3.4
1	B	213	GLU	3.3
1	A	296	ASP	3.3
1	B	169	ARG	3.3
1	A	56	ARG	3.3
1	A	171	ARG	3.3
1	A	150	GLU	3.3
1	B	40	ASP	3.3
1	B	260	ARG	3.3
1	B	166	GLU	3.3
1	B	179	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	30	THR	3.3
1	B	107	GLN	3.3
1	A	211	PRO	3.3
1	B	181	ARG	3.3
1	B	67	SER	3.3
1	B	274	GLU	3.3
1	A	166	GLU	3.3
1	A	199	MET	3.3
1	B	288	ALA	3.3
1	B	30	THR	3.3
1	A	274	GLU	3.2
1	A	62	LYS	3.2
1	B	133	ALA	3.2
1	A	40	ASP	3.2
1	A	169	ARG	3.2
1	B	21	ARG	3.2
1	A	72	GLU	3.2
1	B	6[A]	SER	3.2
1	A	92	LEU	3.1
1	A	277	GLU	3.1
1	B	132	VAL	3.1
1	A	174	GLU	3.1
1	A	285	GLU	3.1
1	A	238	GLY	3.1
1	A	163	GLU	3.1
1	B	248	ASP	3.1
1	A	21	ARG	3.1
1	A	14	GLY	3.1
1	B	111	LYS	3.0
1	B	174	GLU	3.0
1	A	232	ALA	3.0
1	A	223	GLY	3.0
1	B	38	LEU	3.0
1	A	178	LEU	3.0
1	B	257	LEU	2.9
1	B	150	GLU	2.9
1	A	146	ARG	2.9
1	A	195	ASP	2.9
1	A	18	GLY	2.9
1	B	233	PHE	2.9
1	A	36	ARG	2.9
1	B	104	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	113	THR	2.9
1	A	176	ALA	2.9
1	A	177	ARG	2.8
1	B	81	ALA	2.8
1	B	285	GLU	2.8
1	A	89	GLU	2.8
1	A	161	ASP	2.8
1	B	105	GLY	2.8
1	B	24	GLU	2.8
1	A	196	GLU	2.8
1	B	89	GLU	2.7
1	A	71	ALA	2.7
1	B	293	GLY	2.7
1	B	35	ARG	2.7
1	A	125	LYS	2.7
1	A	108	GLY	2.7
1	B	286	ARG	2.7
1	A	197	PRO	2.7
1	B	158	GLU	2.7
1	B	224	GLN	2.6
1	A	63	GLN	2.6
1	A	66	GLU	2.6
1	A	224	GLN	2.6
1	A	132	VAL	2.6
1	A	179	GLU	2.6
1	B	167	SER	2.6
1	A	142	ARG	2.6
1	B	143	GLU	2.6
1	A	123	LYS	2.6
1	A	144	GLN	2.5
1	A	17	ARG	2.5
1	A	49	ARG	2.5
1	B	28	LYS	2.5
1	B	234	ASP	2.5
1	B	128	ARG	2.4
1	A	190	GLY	2.4
1	A	3	GLN	2.4
1	A	10	GLN	2.4
1	B	214	VAL	2.3
1	B	157	LEU	2.3
1	B	201	GLU	2.3
1	A	173	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	10	GLN	2.3
1	A	85	ALA	2.3
1	B	8[A]	ARG	2.2
1	B	49	ARG	2.2
1	A	131	LEU	2.2
1	B	119	ALA	2.2
1	A	189	ALA	2.2
1	A	191	ARG	2.2
1	A	78	VAL	2.1
1	A	162	GLY	2.1
1	B	83	LYS	2.1
1	B	204	ARG	2.1
1	A	289	GLY	2.1

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.

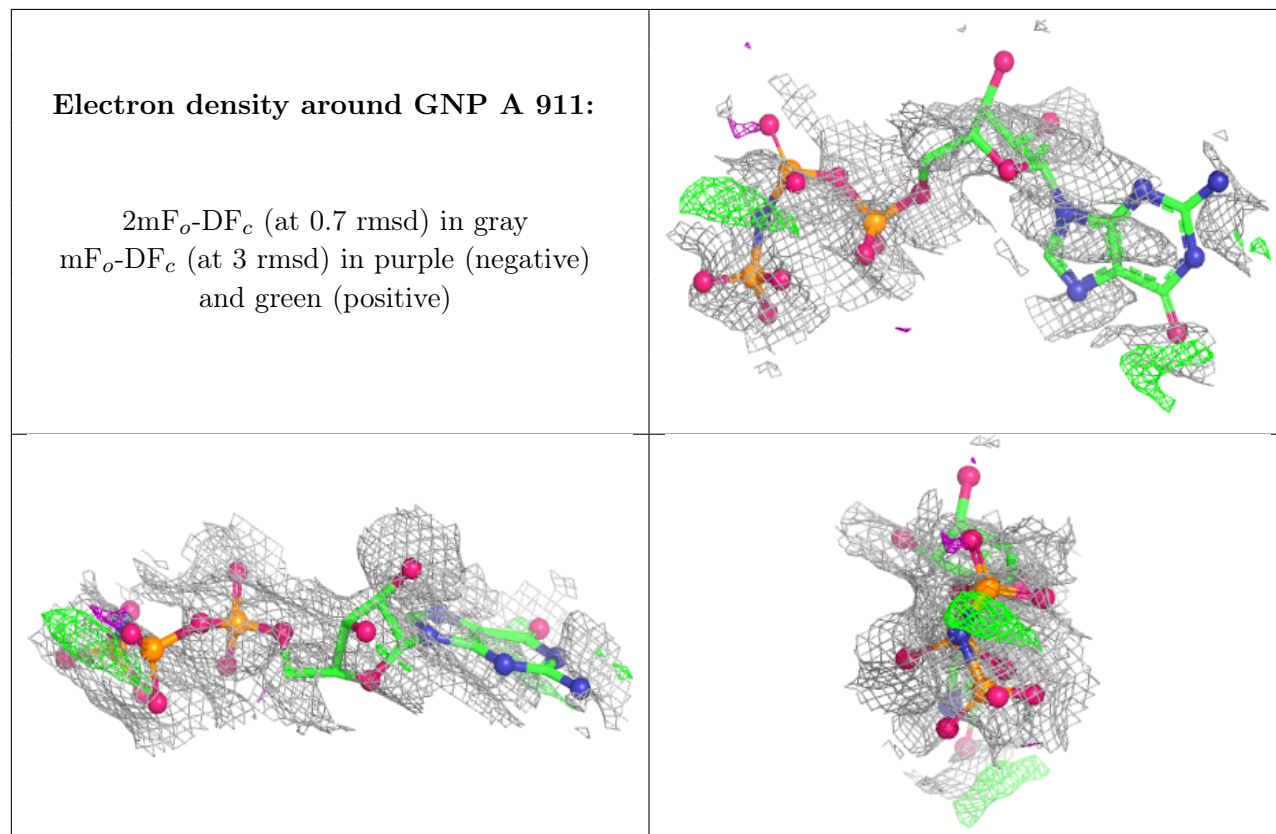
6.4 Ligands [i](#)

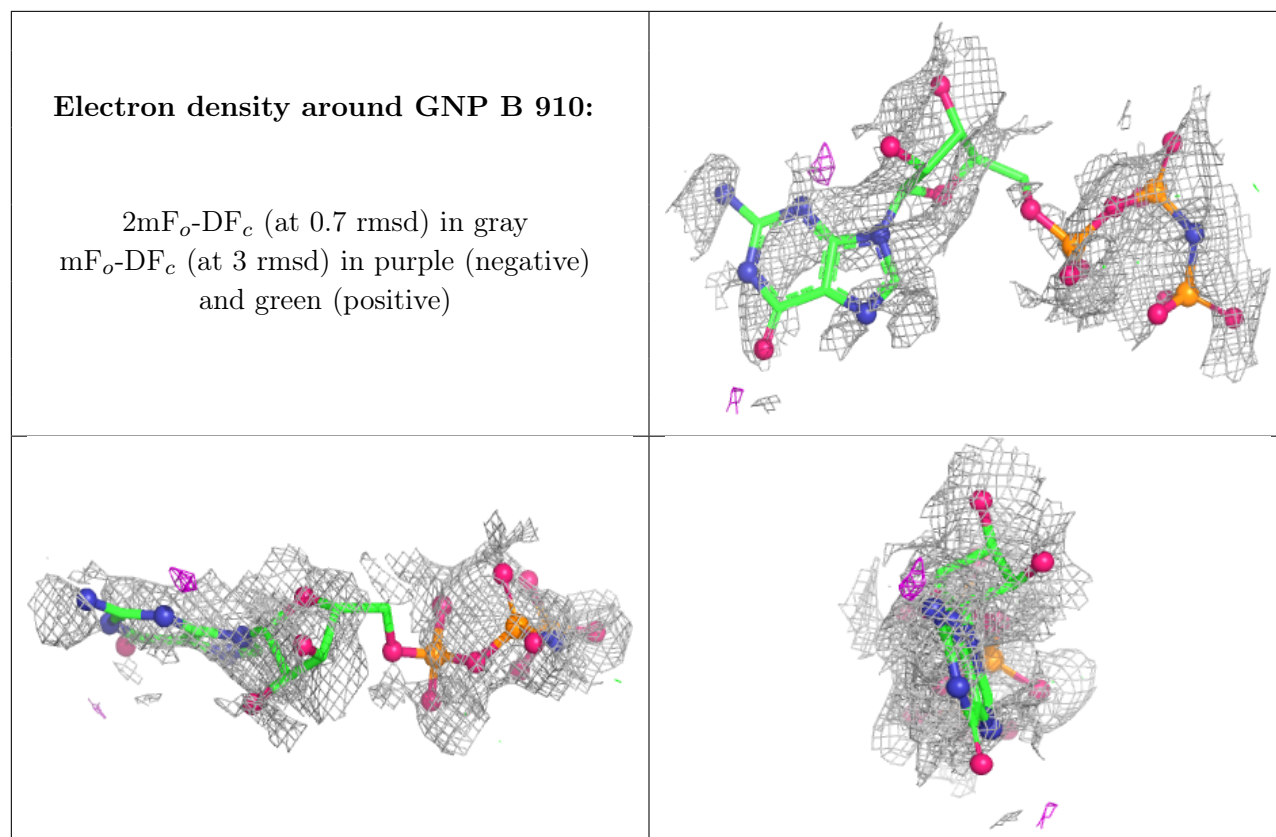
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACY	B	951	4/4	-0.04	0.36	44,45,46,47	0
4	ACY	A	953	4/4	0.07	0.30	62,64,64,65	0
2	CA	A	901	1/1	0.16	0.35	37,37,37,37	0
4	ACY	A	952	4/4	0.18	0.40	90,90,91,92	0
3	GNP	A	911	32/32	0.35	0.30	20,31,48,50	0
4	ACY	B	950	4/4	0.45	0.29	41,42,43,44	0
3	GNP	B	910	32/32	0.53	0.29	23,51,71,71	0
2	CA	B	900	1/1	0.69	0.17	16,16,16,16	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.