



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 11:04 AM EDT

PDB ID : 1ZC4  
Title : Crystal structure of the Ral-binding domain of Exo84 in complex with the active RalA  
Authors : Jin, R.; Junutula, J.R.; Matern, H.T.; Ervin, K.E.; Scheller, R.H.; Brunger, A.T.  
Deposited on : 2005-04-10  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

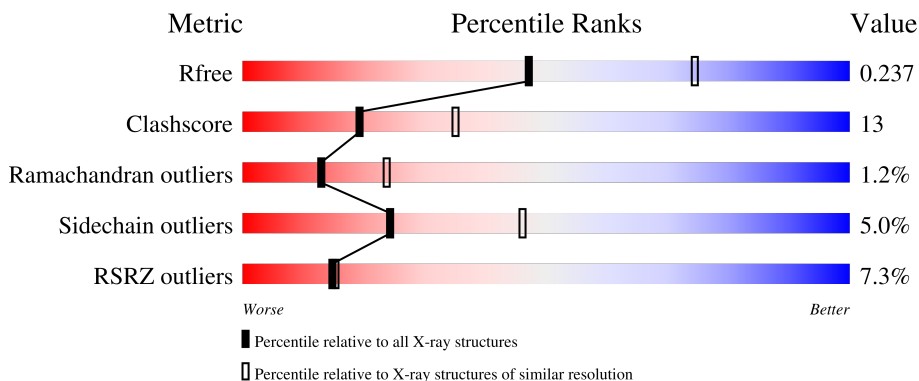
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	175	 3% 74% 23% ..
1	C	175	 3% 78% 19% ..
2	B	120	 12% 69% 22% .. 6%
2	D	120	 14% 59% 28% 5% 6%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4895 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 Ras-related protein Ral-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1388	871	233	278	6	0	0	0
1	C	173	1388	871	233	278	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	LEU	GLN	engineered mutation	UNP P11233
C	72	LEU	GLN	engineered mutation	UNP P11233

- Molecule 2 is a protein called exocyst complex protein Exo84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	113	950	605	171	167	7	7	0	0
2	D	113	950	605	171	167	7	7	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

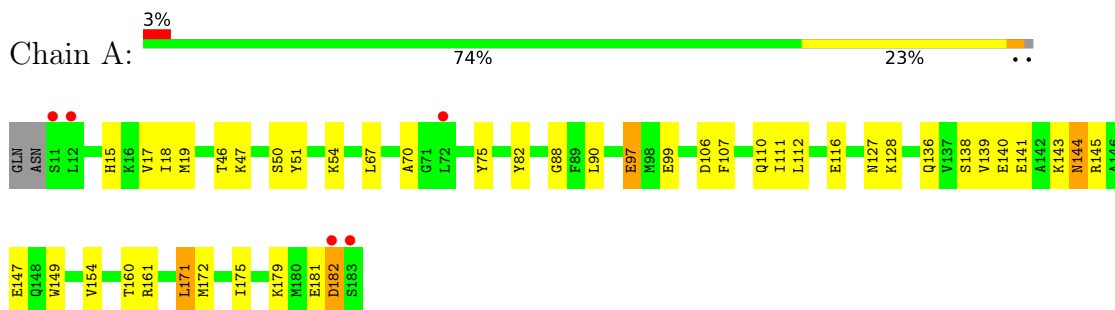
- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



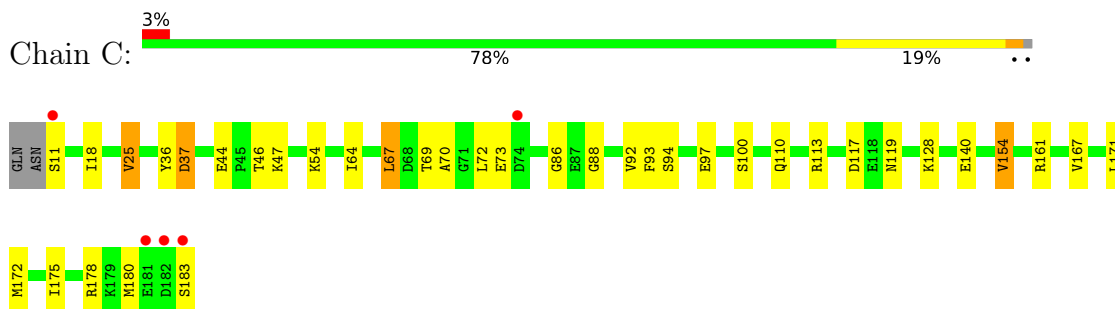
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

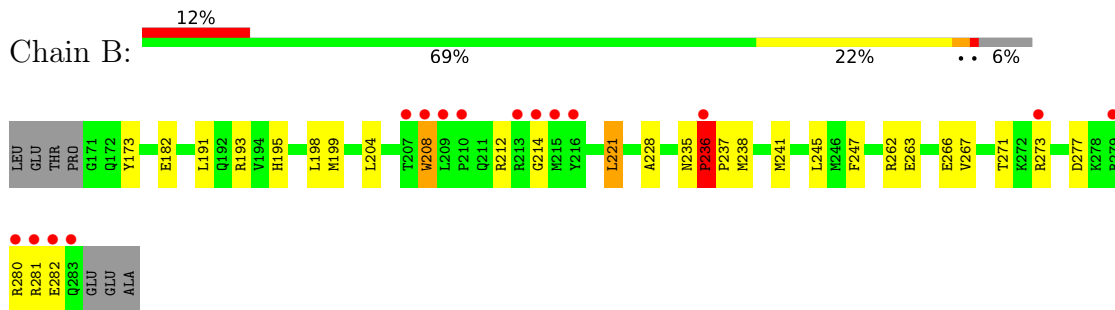
- Molecule 1: Ras-related protein Ral-A



- Molecule 1: Ras-related protein Ral-A

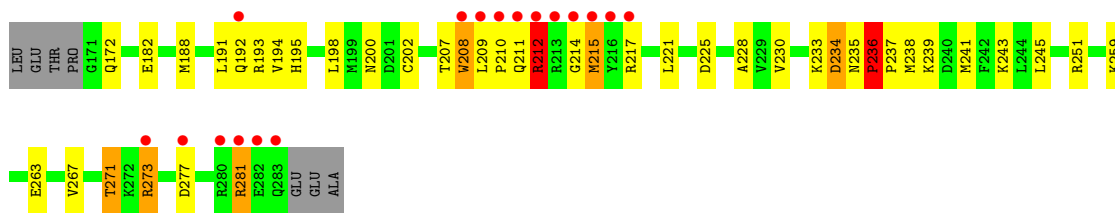


- Molecule 2: exocyst complex protein Exo84



- Molecule 2: exocyst complex protein Exo84





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.91Å 113.39Å 70.68Å 90.00° 102.77° 90.00°	Depositor
Resolution (Å)	43.79 – 2.50 46.97 – 2.48	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.79-2.50) 96.2 (46.97-2.48)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.48Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.208 , 0.248 0.197 , 0.237	Depositor DCC
$R_{free}$ test set	5389 reflections (9.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtrriage
Anisotropy	0.379	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/1408	0.58	0/1892
1	C	0.40	0/1408	0.60	0/1892
2	B	0.40	0/970	0.62	0/1306
2	D	0.40	0/970	0.61	0/1306
All	All	0.40	0/4756	0.60	0/6396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1388	0	1351	33	0
1	C	1388	0	1351	28	0
2	B	950	0	952	23	0
2	D	950	0	952	42	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	32	0	13	0	0
4	C	32	0	13	0	0
5	A	44	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	31	0	0	2	0
5	C	50	0	0	4	0
5	D	28	0	0	3	0
All	All	4895	0	4632	120	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 (120) 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)
2:D:267:VAL:O	2:D:271:THR:HG23	1.68	0.94
2:D:281:ARG:HH11	2:D:281:ARG:HB2	1.30	0.93
2:B:267:VAL:O	2:B:271:THR:HG22	1.79	0.83
1:A:138:SER:OG	1:A:141:GLU:HG3	1.80	0.81
1:C:64:ILE:HB	1:C:172:MET:HE1	1.67	0.76
1:C:25:VAL:HG21	1:C:93:PHE:HA	1.68	0.76
2:D:228:ALA:HB3	2:D:245:LEU:HB2	1.70	0.73
2:D:192:GLN:HE22	2:D:209:LEU:HA	1.52	0.72
1:C:44:GLU:O	1:C:44:GLU:HG2	1.89	0.72
2:D:188:MET:HE2	2:D:238:MET:HG2	1.69	0.72
2:B:173:TYR:HA	2:D:221:LEU:HD23	1.72	0.71
1:A:46:THR:O	1:A:70:ALA:HB2	1.90	0.70
2:B:238:MET:HB2	2:B:241:MET:CE	2.23	0.68
1:C:140:GLU:HG3	5:C:533:HOH:O	1.93	0.67
2:D:238:MET:HB3	2:D:241:MET:HE2	1.80	0.63
1:C:64:ILE:HB	1:C:172:MET:CE	2.29	0.63
2:D:281:ARG:HH11	2:D:281:ARG:CB	2.08	0.63
1:C:72:LEU:HD23	1:C:73:GLU:N	2.14	0.62
1:A:97:GLU:OE1	1:A:99:GLU:HB2	2.00	0.62
1:C:183:SER:HB2	5:C:519:HOH:O	2.00	0.62
2:D:193:ARG:HG3	5:D:57:HOH:O	2.00	0.61
1:A:175:ILE:HG22	1:A:179:LYS:HE3	1.82	0.61
2:D:202:CYS:SG	2:D:221:LEU:HD11	2.41	0.61
1:A:182:ASP:HA	5:A:422:HOH:O	2.02	0.60
2:B:263:GLU:O	2:B:267:VAL:HG22	2.01	0.60
1:A:143:LYS:O	1:A:147:GLU:HG2	2.02	0.60
2:B:208:TRP:N	2:B:208:TRP:CD1	2.69	0.60
2:D:238:MET:HB3	2:D:241:MET:CE	2.33	0.59
2:B:262:ARG:O	2:B:266:GLU:HG3	2.02	0.58
1:A:106:ASP:O	1:A:110:GLN:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:O	1:A:179:LYS:HG3	2.04	0.57
2:B:238:MET:HB2	2:B:241:MET:SD	2.43	0.57
1:C:117:ASP:OD2	1:C:178:ARG:NH1	2.37	0.57
1:A:107:PHE:O	1:A:111:ILE:HG13	2.04	0.57
5:B:34:HOH:O	1:C:47:LYS:HD2	2.04	0.57
1:A:54:LYS:HB2	1:A:54:LYS:NZ	2.21	0.56
1:C:25:VAL:HG22	1:C:94:SER:N	2.21	0.56
2:D:195:HIS:HB2	5:D:36:HOH:O	2.05	0.56
2:D:217:ARG:HH11	2:D:217:ARG:HB3	1.71	0.55
2:D:236:PRO:HB2	2:D:237:PRO:CD	2.36	0.55
1:A:17:VAL:HG22	1:A:171:LEU:HD13	1.89	0.55
2:B:277:ASP:HB3	2:B:281:ARG:NH2	2.22	0.55
2:B:193:ARG:HH21	2:B:208:TRP:HH2	1.54	0.54
1:C:110:GLN:HG2	1:C:113:ARG:HH12	1.72	0.54
2:D:208:TRP:CD1	2:D:208:TRP:N	2.76	0.54
2:B:182:GLU:HG2	2:B:191:LEU:HD12	1.89	0.54
1:A:139:VAL:CG1	1:A:143:LYS:HE3	2.38	0.54
1:A:51:TYR:CE1	2:D:233:LYS:HG3	2.43	0.54
2:D:188:MET:SD	2:D:238:MET:SD	3.07	0.53
2:D:172:GLN:HA	2:D:200:ASN:ND2	2.24	0.53
2:B:238:MET:HB2	2:B:241:MET:HE2	1.90	0.53
1:C:25:VAL:HG13	1:C:92:VAL:HG12	1.92	0.52
1:A:175:ILE:CG2	1:A:179:LYS:HE3	2.39	0.52
2:B:236:PRO:HB2	2:B:237:PRO:CD	2.40	0.51
2:D:188:MET:HE1	2:D:241:MET:SD	2.51	0.51
2:B:247:PHE:C	2:B:247:PHE:CD1	2.84	0.51
1:C:25:VAL:CG2	1:C:93:PHE:HA	2.40	0.50
2:D:210:PRO:HG3	2:D:215:MET:SD	2.51	0.50
1:A:19:MET:SD	1:A:90:LEU:HD12	2.51	0.50
2:B:173:TYR:CA	2:D:221:LEU:HD23	2.41	0.50
1:A:144:ASN:HD22	1:A:144:ASN:N	2.09	0.50
1:A:145:ARG:HD3	1:A:149:TRP:CH2	2.46	0.50
2:B:228:ALA:HB3	2:B:245:LEU:HB2	1.94	0.50
2:D:217:ARG:HB3	2:D:217:ARG:NH1	2.27	0.49
2:B:235:ASN:O	2:B:237:PRO:HD2	2.13	0.49
1:A:88:GLY:HA3	1:A:175:ILE:HD11	1.95	0.49
2:B:193:ARG:NH2	2:B:208:TRP:HH2	2.11	0.49
1:C:46:THR:O	1:C:70:ALA:HB2	2.13	0.49
1:C:154:VAL:HG11	1:C:167:VAL:HG12	1.96	0.48
2:D:182:GLU:HG2	2:D:191:LEU:HD12	1.96	0.48
2:D:188:MET:CE	2:D:238:MET:HG2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:238:MET:CG	2:D:241:MET:HE1	2.44	0.47
1:A:140:GLU:O	1:A:144:ASN:ND2	2.48	0.47
2:D:234:ASP:OD2	2:D:239:LYS:HG3	2.14	0.47
2:D:273:ARG:HD3	2:D:273:ARG:C	2.35	0.47
1:A:160:THR:O	1:A:161:ARG:HB2	2.14	0.47
1:A:15:HIS:HD2	1:A:172:MET:HE2	1.80	0.46
2:D:243:LYS:HG3	2:D:251:ARG:O	2.16	0.46
2:B:212:ARG:HA	2:B:212:ARG:HD2	1.82	0.46
1:C:67:LEU:HD22	1:C:69:THR:HG23	1.97	0.46
2:D:238:MET:SD	2:D:241:MET:HE1	2.56	0.46
1:A:75:TYR:CE2	2:D:225:ASP:HB2	2.51	0.46
1:C:18:ILE:HD12	1:C:67:LEU:HD12	1.97	0.45
2:D:194:VAL:HG12	2:D:207:THR:HG23	1.99	0.45
2:D:277:ASP:O	2:D:281:ARG:HD3	2.16	0.45
1:A:47:LYS:HE2	5:A:442:HOH:O	2.17	0.44
1:C:88:GLY:HA3	1:C:175:ILE:HD11	2.00	0.44
1:A:15:HIS:HD2	1:A:172:MET:CE	2.30	0.44
1:C:97:GLU:OE2	1:C:100:SER:HB3	2.18	0.43
1:C:94:SER:OG	1:C:128:LYS:HD2	2.18	0.43
2:D:211:GLN:O	2:D:212:ARG:C	2.55	0.43
2:B:195:HIS:HB2	5:B:17:HOH:O	2.19	0.43
1:A:139:VAL:HG12	1:A:143:LYS:HE3	2.00	0.43
1:C:54:LYS:HE2	1:C:54:LYS:HB3	1.75	0.43
1:C:18:ILE:CG1	1:C:86:GLY:HA3	2.49	0.43
1:A:50:SER:HB2	2:D:230:VAL:HG11	2.00	0.43
1:A:181:GLU:HG3	1:A:182:ASP:OD2	2.18	0.42
1:C:47:LYS:HE2	5:C:503:HOH:O	2.19	0.42
2:B:221:LEU:HD23	2:B:221:LEU:HA	1.84	0.42
2:B:280:ARG:C	2:B:282:GLU:H	2.22	0.42
1:A:82:TYR:CE1	2:D:228:ALA:HB1	2.55	0.42
2:D:209:LEU:C	2:D:209:LEU:HD23	2.40	0.42
1:C:180:MET:HA	1:C:180:MET:CE	2.50	0.41
1:A:127:ASN:ND2	1:A:128:LYS:H	2.18	0.41
2:B:235:ASN:O	2:B:237:PRO:CD	2.68	0.41
2:B:236:PRO:C	2:B:238:MET:H	2.23	0.41
2:D:259:LYS:O	2:D:263:GLU:HG3	2.20	0.41
1:C:11:SER:HB3	5:C:514:HOH:O	2.20	0.41
2:D:217:ARG:NH1	2:D:217:ARG:CB	2.82	0.41
2:D:235:ASN:O	2:D:237:PRO:HD2	2.20	0.41
1:C:36:TYR:O	1:C:37:ASP:HB2	2.21	0.41
1:A:18:ILE:HD12	1:A:67:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:O	1:A:116:GLU:N	2.50	0.41
1:A:127:ASN:CG	1:A:128:LYS:H	2.24	0.41
1:C:117:ASP:OD1	1:C:119:ASN:N	2.54	0.41
2:D:212:ARG:HG2	2:D:212:ARG:HH11	1.85	0.41
1:C:161:ARG:HH11	1:C:161:ARG:HG3	1.86	0.41
2:D:239:LYS:O	2:D:241:MET:HG3	2.21	0.41
1:A:47:LYS:HD2	5:D:29:HOH:O	2.20	0.40
2:D:192:GLN:NE2	2:D:209:LEU:HA	2.28	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	171/175 (98%)	162 (95%)	8 (5%)	1 (1%)	25	43
1	C	171/175 (98%)	166 (97%)	5 (3%)	0	100	100
2	B	111/120 (92%)	99 (89%)	10 (9%)	2 (2%)	8	14
2	D	111/120 (92%)	100 (90%)	7 (6%)	4 (4%)	3	4
All	All	564/590 (96%)	527 (93%)	30 (5%)	7 (1%)	13	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	236	PRO
2	D	236	PRO
2	D	215	MET
2	D	214	GLY
1	A	182	ASP
2	D	212	ARG
2	B	214	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	150/152 (99%)	145 (97%)	5 (3%)	38	64
1	C	150/152 (99%)	145 (97%)	5 (3%)	38	64
2	B	101/107 (94%)	94 (93%)	7 (7%)	15	30
2	D	101/107 (94%)	93 (92%)	8 (8%)	12	24
All	All	502/518 (97%)	477 (95%)	25 (5%)	24	46

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	136	GLN
1	A	144	ASN
1	A	154	VAL
1	A	171	LEU
2	B	198	LEU
2	B	199	MET
2	B	204	LEU
2	B	208	TRP
2	B	221	LEU
2	B	236	PRO
2	B	273	ARG
1	C	25	VAL
1	C	37	ASP
1	C	67	LEU
1	C	154	VAL
1	C	171	LEU
2	D	198	LEU
2	D	208	TRP
2	D	212	ARG
2	D	234	ASP
2	D	236	PRO
2	D	271	THR
2	D	273	ARG
2	D	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	144	ASN
1	C	127	ASN
1	C	144	ASN
2	D	211	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GNP	A	400	3	28,34,34	2.48	9 (32%)	30,54,54	2.34	6 (20%)
4	GNP	C	500	3	28,34,34	2.44	8 (28%)	30,54,54	2.27	6 (20%)

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
4	GNP	A	400	3	-	4/17/38/38	0/3/3/3
4	GNP	C	500	3	-	6/17/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	GNP	C4-N9	-7.47	1.37	1.47
4	C	500	GNP	C4-N9	-7.39	1.37	1.47
4	A	400	GNP	C6-N1	6.29	1.43	1.33
4	C	500	GNP	C6-N1	5.82	1.42	1.33
4	C	500	GNP	C5-C6	-5.06	1.44	1.52
4	A	400	GNP	C5-C6	-4.83	1.44	1.52
4	A	400	GNP	PG-O1G	3.14	1.51	1.46
4	C	500	GNP	PG-O1G	3.11	1.51	1.46
4	C	500	GNP	PG-N3B	2.71	1.70	1.63
4	A	400	GNP	PG-N3B	2.68	1.70	1.63
4	C	500	GNP	PG-O3G	-2.64	1.49	1.56
4	C	500	GNP	C5-C4	-2.54	1.37	1.53
4	A	400	GNP	PG-O3G	-2.47	1.50	1.56
4	A	400	GNP	C5-C4	-2.46	1.37	1.53
4	C	500	GNP	C8-N9	-2.33	1.37	1.45
4	A	400	GNP	C8-N9	-2.15	1.38	1.45
4	A	400	GNP	PB-O3A	2.05	1.61	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	GNP	C4-C5-N7	7.12	111.90	102.46
4	C	500	GNP	C4-C5-N7	7.01	111.75	102.46
4	A	400	GNP	C5-C6-N1	-5.26	111.70	118.19
4	C	500	GNP	C5-C6-N1	-5.16	111.82	118.19
4	A	400	GNP	O6-C6-C5	4.88	129.81	119.86
4	C	500	GNP	O6-C6-C5	4.88	129.81	119.86
4	A	400	GNP	O1G-PG-N3B	-3.91	106.02	111.77
4	C	500	GNP	O1G-PG-N3B	-3.23	107.01	111.77
4	C	500	GNP	O6-C6-N1	-3.22	118.37	122.69
4	A	400	GNP	O6-C6-N1	-3.13	118.48	122.69
4	A	400	GNP	O2B-PB-O1B	2.31	114.76	109.92
4	C	500	GNP	O2B-PB-O1B	2.30	114.73	109.92

There are no chirality outliers.

All (10) torsion outliers are listed below:

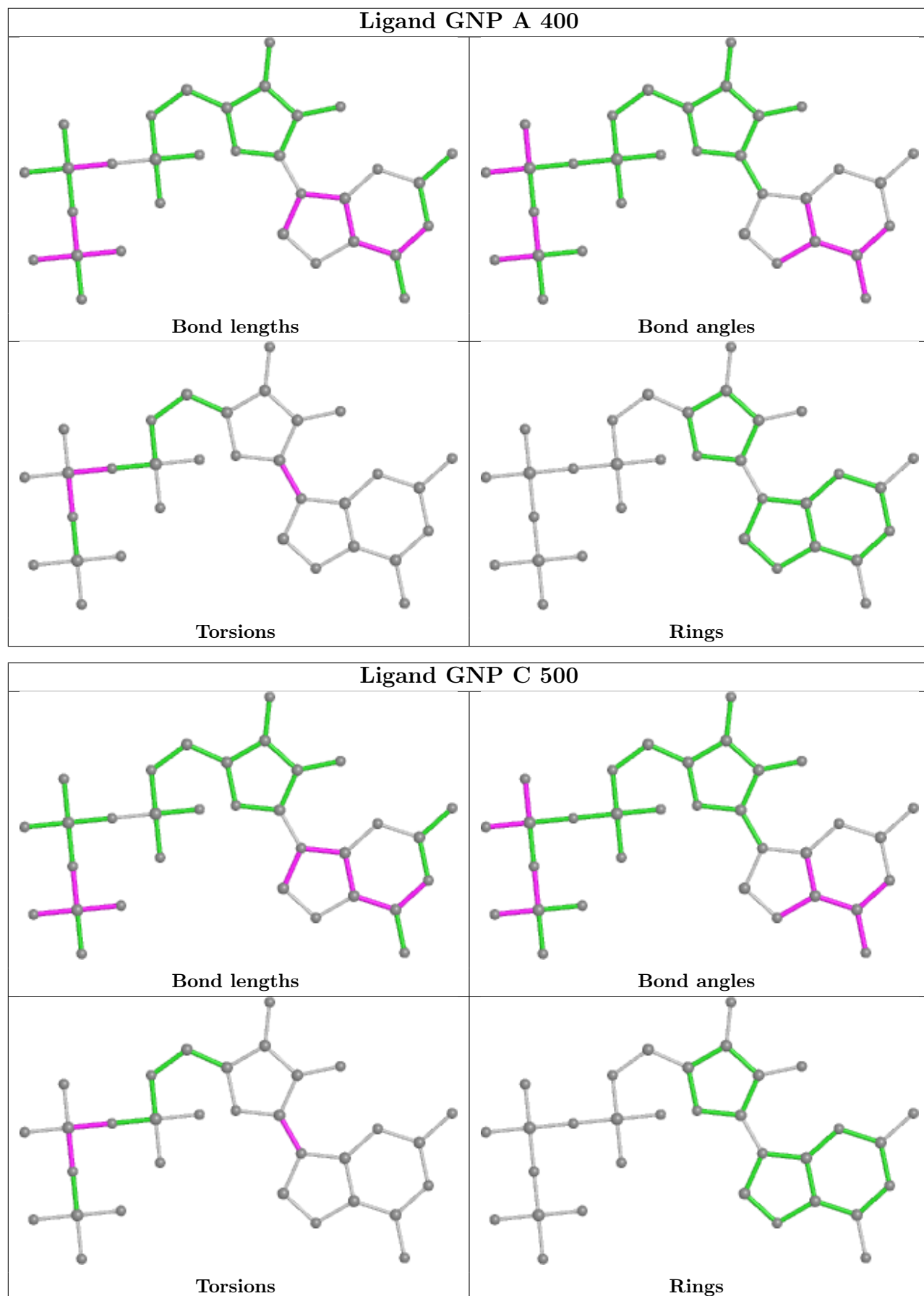
Mol	Chain	Res	Type	Atoms
4	A	400	GNP	PG-N3B-PB-O1B
4	A	400	GNP	PA-O3A-PB-O1B
4	A	400	GNP	PA-O3A-PB-O2B
4	A	400	GNP	C2'-C1'-N9-C4
4	C	500	GNP	PG-N3B-PB-O1B
4	C	500	GNP	PG-N3B-PB-O3A
4	C	500	GNP	PA-O3A-PB-O1B
4	C	500	GNP	PA-O3A-PB-O2B
4	C	500	GNP	O4'-C1'-N9-C4
4	C	500	GNP	C2'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	173/175 (98%)	0.13	5 (2%) 51 55	22, 39, 70, 102	0
1	C	173/175 (98%)	0.09	5 (2%) 51 55	19, 34, 64, 93	0
2	B	113/120 (94%)	0.43	15 (13%) 3 2	21, 35, 100, 109	1 (0%)
2	D	113/120 (94%)	0.47	17 (15%) 2 2	21, 37, 101, 113	1 (0%)
All	All	572/590 (96%)	0.25	42 (7%) 15 15	19, 37, 87, 113	2 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	283	GLN	5.3
2	B	214	GLY	5.2
2	B	283	GLN	4.8
2	D	216	TYR	4.5
2	D	209	LEU	4.4
2	B	210	PRO	4.3
2	D	210	PRO	4.3
2	B	216	TYR	4.1
2	B	215	MET	4.1
2	B	280	ARG	4.0
1	A	11	SER	3.8
1	C	183	SER	3.8
2	D	214	GLY	3.8
2	B	209	LEU	3.8
2	B	207	THR	3.6
2	D	213	ARG	3.5
1	A	12	LEU	3.4
2	D	215	MET	3.4
2	D	280	ARG	3.3
1	A	72	LEU	3.3
2	B	282	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	74	ASP	3.2
2	D	217	ARG	3.2
2	D	282	GLU	3.1
1	A	183	SER	3.1
2	B	213	ARG	3.0
2	D	277	ASP	2.8
2	B	279	ARG	2.7
2	B	208	TRP	2.7
2	D	281	ARG	2.6
2	B	281	ARG	2.6
1	C	181	GLU	2.6
2	D	208	TRP	2.5
1	C	11	SER	2.4
1	C	182	ASP	2.3
2	D	212	ARG	2.2
2	D	192	GLN	2.2
1	A	182	ASP	2.1
2	D	211	GLN	2.1
2	D	273	ARG	2.1
2	B	273	ARG	2.0
2	B	236	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

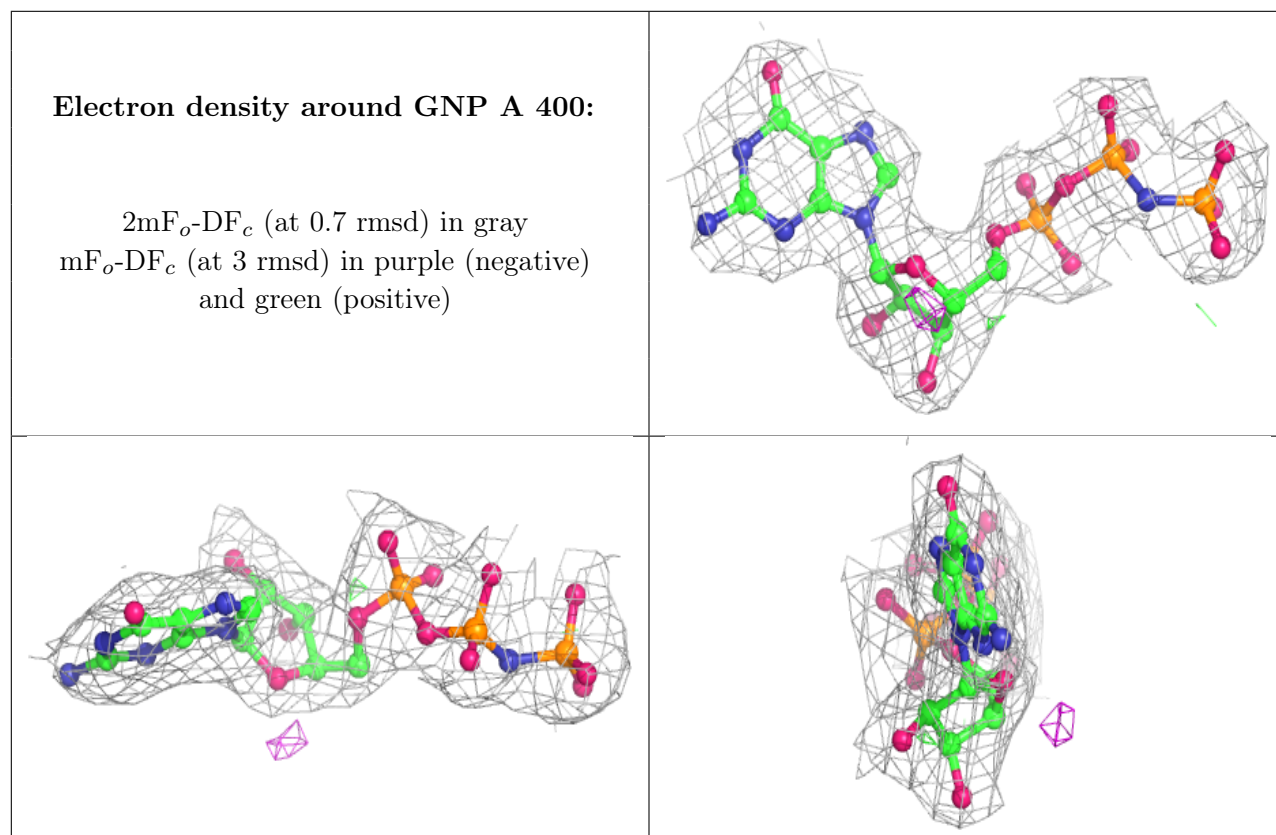
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	200	1/1	0.95	0.09	35,35,35,35	0
3	MG	C	300	1/1	0.97	0.06	27,27,27,27	0

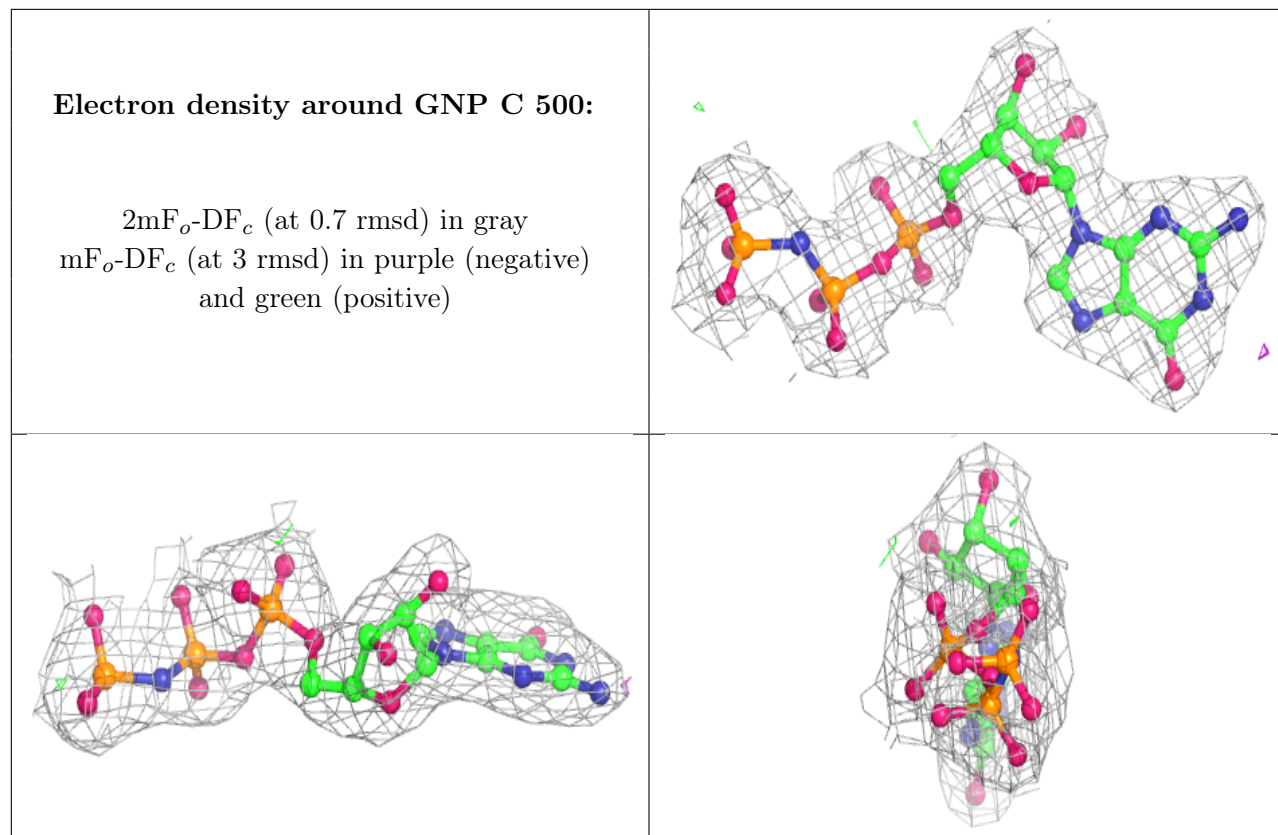
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GNP	A	400	32/32	0.98	0.12	31,40,43,43	0
4	GNP	C	500	32/32	0.99	0.13	27,33,37,37	0

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.