



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:58 PM EDT

PDB ID : 1N7G / pdb_00001n7g
Title : Crystal Structure of the GDP-mannose 4,6-dehydratase ternary complex with NADPH and GDP-rhamnose.
Authors : Mulichak, A.M.; Bonin, C.P.; Reiter, W.-D.; Garavito, R.M.
Deposited on : 2002-11-14
Resolution : 2.20 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

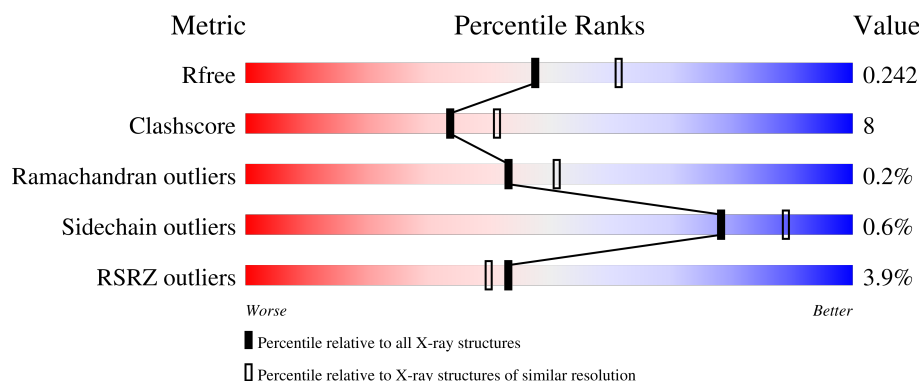
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	381	0% 71% 16% • 13%
1	B	381	2% 69% 19% • 12%
1	C	381	2% 72% 15% • 12%
1	D	381	9% 70% 12% • 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11034 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 GDP-D-mannose-4,6-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2625	1675	453	488	9			
1	B	336	Total	C	N	O	S	0	0	0
			2626	1676	451	490	9			
1	C	334	Total	C	N	O	S	0	0	0
			2620	1672	449	490	9			
1	D	313	Total	C	N	O	S	0	0	0
			2382	1514	414	446	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	LEU	-	expression tag	UNP P93031
A	375	GLU	-	expression tag	UNP P93031
A	376	HIS	-	expression tag	UNP P93031
A	377	HIS	-	expression tag	UNP P93031
A	378	HIS	-	expression tag	UNP P93031
A	379	HIS	-	expression tag	UNP P93031
A	380	HIS	-	expression tag	UNP P93031
A	381	HIS	-	expression tag	UNP P93031
B	374	LEU	-	expression tag	UNP P93031
B	375	GLU	-	expression tag	UNP P93031
B	376	HIS	-	expression tag	UNP P93031
B	377	HIS	-	expression tag	UNP P93031
B	378	HIS	-	expression tag	UNP P93031
B	379	HIS	-	expression tag	UNP P93031
B	380	HIS	-	expression tag	UNP P93031
B	381	HIS	-	expression tag	UNP P93031
C	374	LEU	-	expression tag	UNP P93031
C	375	GLU	-	expression tag	UNP P93031
C	376	HIS	-	expression tag	UNP P93031
C	377	HIS	-	expression tag	UNP P93031
C	378	HIS	-	expression tag	UNP P93031

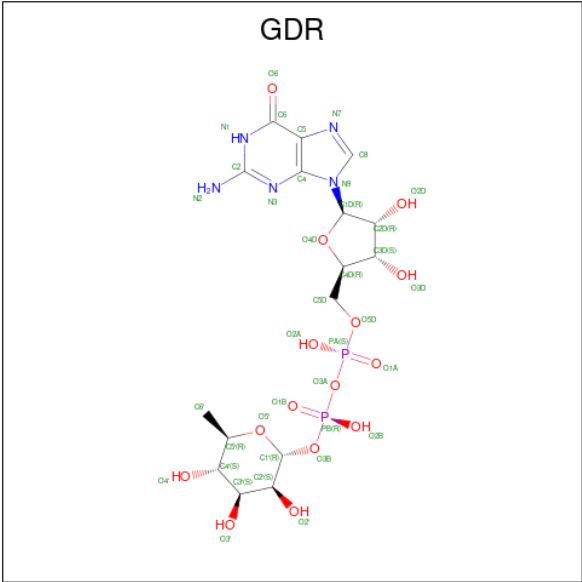
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Chain	Residue	Modelled	Actual	Comment	Reference
C	379	HIS	-	expression tag	UNP P93031
C	380	HIS	-	expression tag	UNP P93031
C	381	HIS	-	expression tag	UNP P93031
D	374	LEU	-	expression tag	UNP P93031
D	375	GLU	-	expression tag	UNP P93031
D	376	HIS	-	expression tag	UNP P93031
D	377	HIS	-	expression tag	UNP P93031
D	378	HIS	-	expression tag	UNP P93031
D	379	HIS	-	expression tag	UNP P93031
D	380	HIS	-	expression tag	UNP P93031
D	381	HIS	-	expression tag	UNP P93031

- # NDP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

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- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	A	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	A	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

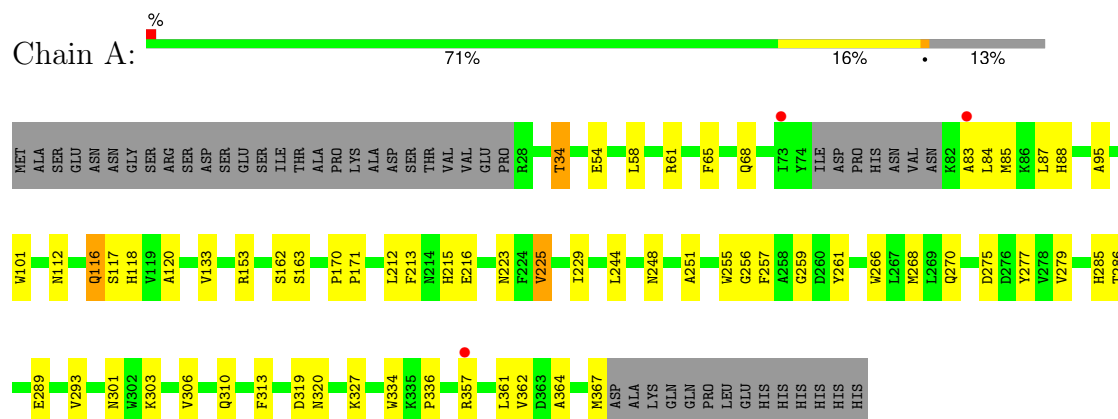
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	109	Total	O	0	0
			109	109		
4	C	130	Total	O	0	0
			130	130		
4	D	96	Total	O	0	0
			96	96		

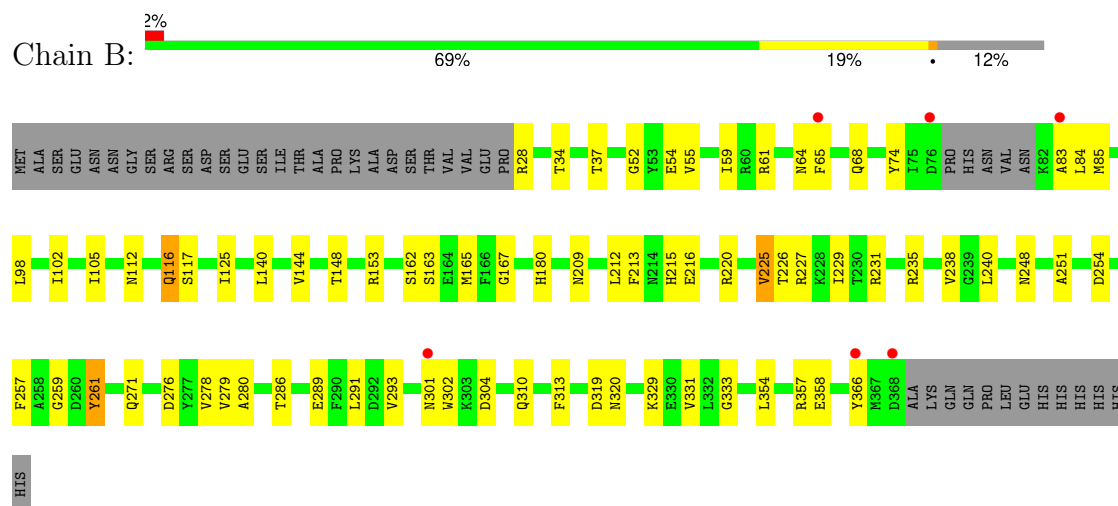
3 Residue-property plots [i](#)

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.

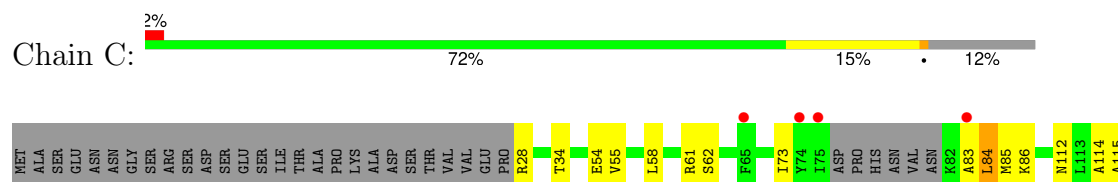
• Molecule 1: GDP-D-mannose-4,6-dehydratase

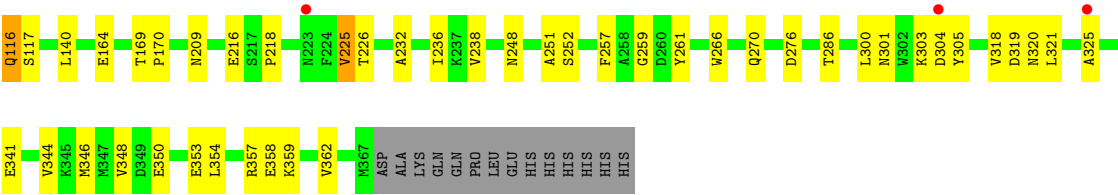


• Molecule 1: GDP-D-mannose-4,6-dehydratase

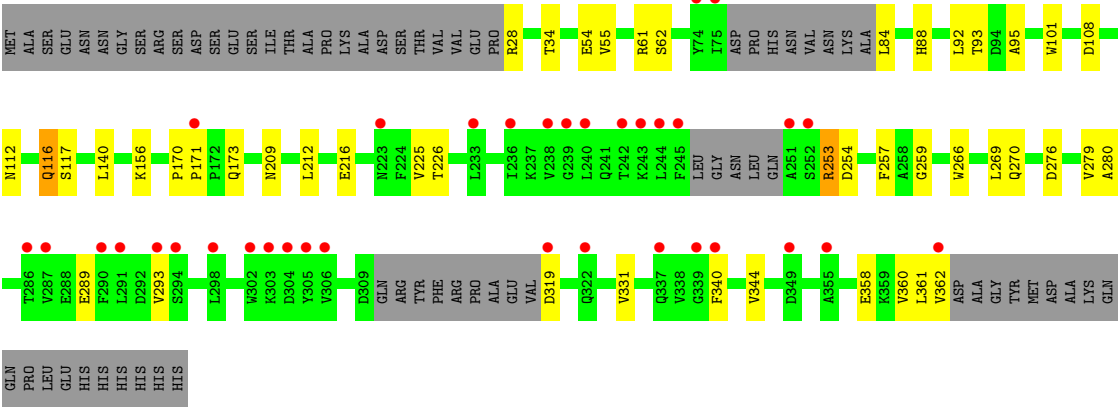


• Molecule 1: GDP-D-mannose-4,6-dehydratase





● Molecule 1: GDP-D-mannose-4,6-dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.18Å 119.01Å 118.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 87.8 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.247 0.195 , 0.242	Depositor DCC
R_{free} test set	3775 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.989	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.015 for -k,-h,l 0.015 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11034	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/2688	0.90	10/3648 (0.3%)
1	B	0.35	0/2689	0.89	9/3653 (0.2%)
1	C	0.36	0/2683	0.90	9/3644 (0.2%)
1	D	0.35	0/2434	0.88	7/3306 (0.2%)
All	All	0.36	0/10494	0.89	35/14251 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	GLN	N-CA-C	-8.55	92.93	107.99
1	C	319	ASP	N-CA-C	8.53	120.50	111.03
1	B	319	ASP	N-CA-C	8.24	120.18	111.03
1	A	319	ASP	N-CA-C	8.21	120.01	111.14
1	A	116	GLN	N-CA-C	-8.16	92.64	107.98
1	D	116	GLN	N-CA-C	-7.98	93.95	107.99
1	B	225	VAL	N-CA-C	7.87	118.63	110.36
1	A	225	VAL	N-CA-C	7.75	118.50	110.36
1	C	225	VAL	N-CA-C	7.60	119.28	110.62
1	A	54	GLU	N-CA-C	-7.48	96.54	108.73
1	C	116	GLN	N-CA-C	-7.39	94.09	107.98
1	C	117	SER	N-CA-C	6.76	121.36	113.18
1	B	54	GLU	N-CA-C	-6.45	98.22	108.73
1	D	117	SER	N-CA-C	6.42	120.73	113.02
1	D	55	VAL	N-CA-C	6.32	117.02	108.17
1	A	261	TYR	N-CA-C	6.26	118.11	111.28
1	B	117	SER	N-CA-C	6.21	120.86	113.16
1	C	54	GLU	N-CA-C	-5.90	98.11	108.20
1	D	253	ARG	N-CA-C	5.85	118.07	109.24
1	B	55	VAL	N-CA-C	5.71	116.53	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	331	VAL	N-CA-C	5.66	115.85	110.53
1	D	54	GLU	N-CA-C	-5.64	99.54	108.73
1	A	117	SER	N-CA-C	5.62	120.13	113.16
1	C	84	LEU	N-CA-C	-5.60	106.11	113.17
1	A	170	PRO	N-CA-C	5.51	115.76	110.47
1	A	34	THR	N-CA-C	-5.49	101.59	110.32
1	C	170	PRO	N-CA-C	5.42	115.67	110.47
1	B	261	TYR	N-CA-C	5.41	117.17	111.28
1	A	133	VAL	N-CA-C	5.17	115.94	110.72
1	B	105	ILE	N-CA-C	5.16	116.63	111.00
1	D	108	ASP	N-CA-C	-5.10	106.74	113.12
1	A	255	TRP	N-CA-C	5.09	117.03	108.73
1	B	320	ASN	N-CA-C	5.08	116.60	107.80
1	C	169	THR	CA-C-N	5.02	123.33	119.66
1	C	169	THR	C-N-CA	5.02	123.33	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2625	0	2532	37	0
1	B	2626	0	2510	49	0
1	C	2620	0	2510	35	0
1	D	2382	0	2239	26	0
2	A	48	0	26	4	0
2	B	48	0	26	6	0
2	C	48	0	26	5	0
2	D	48	0	26	1	0
3	A	114	0	69	17	0
4	A	140	0	0	4	0
4	B	109	0	0	0	0
4	C	130	0	0	3	0
4	D	96	0	0	2	0
All	All	11034	0	9964	157	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 8.

All (157) 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:A:701:NDP:H41N	3:A:801:GDR:HC62	1.41	1.02
3:A:802:GDR:HC62	2:B:702:NDP:H41N	1.44	0.97
3:A:803:GDR:HC62	2:C:703:NDP:H41N	1.52	0.90
1:B:231:ARG:HG3	1:B:235:ARG:HH12	1.46	0.80
1:B:215:HIS:CE1	2:B:702:NDP:H42N	2.17	0.79
1:A:171:PRO:HG3	1:A:320:ASN:ND2	1.98	0.78
1:B:28:ARG:HD2	1:B:52:GLY:O	1.84	0.78
1:C:320:ASN:HD22	1:C:321:LEU:N	1.85	0.75
3:A:802:GDR:HC4'	2:B:702:NDP:C3N	2.18	0.72
2:A:701:NDP:C3N	3:A:801:GDR:HC4'	2.22	0.69
3:A:803:GDR:C6'	2:C:703:NDP:H41N	2.23	0.68
1:C:320:ASN:HD22	1:C:320:ASN:C	2.03	0.67
1:B:65:PHE:CE2	1:B:68:GLN:HG3	2.31	0.66
1:B:231:ARG:HG3	1:B:235:ARG:NH1	2.12	0.64
1:D:171:PRO:HG3	1:D:173:GLN:HE22	1.62	0.63
2:A:701:NDP:H41N	3:A:801:GDR:C6'	2.25	0.63
1:A:215:HIS:CE1	2:A:701:NDP:H42N	2.34	0.62
1:B:286:THR:OG1	1:B:289:GLU:HG3	2.01	0.61
1:D:289:GLU:O	1:D:293:VAL:HG23	2.00	0.60
1:B:64:ASN:HB2	4:D:779:HOH:O	2.01	0.59
3:A:801:GDR:HC61	4:A:922:HOH:O	2.02	0.58
3:A:803:GDR:HC4'	2:C:703:NDP:C3N	2.33	0.58
1:C:344:VAL:O	1:C:348:VAL:HG23	2.05	0.57
1:C:266:TRP:O	1:C:270:GLN:HG2	2.05	0.57
1:D:28:ARG:NH1	1:D:84:LEU:HD21	2.20	0.56
1:A:361:LEU:HD12	1:A:367:MET:HE3	1.88	0.56
1:B:28:ARG:NH2	1:B:84:LEU:HD21	2.21	0.55
1:C:164:GLU:OE2	1:C:318:VAL:HG21	2.07	0.55
1:C:358:GLU:O	1:C:362:VAL:HG23	2.07	0.55
1:B:366:TYR:CE1	1:D:360:VAL:HG21	2.41	0.55
1:C:216:GLU:HG3	1:C:226:THR:HG21	1.89	0.54
1:C:209:ASN:HB2	1:C:276:ASP:OD1	2.08	0.53
1:D:216:GLU:HG3	1:D:226:THR:HG21	1.89	0.53
1:A:61:ARG:C	1:A:61:ARG:HD3	2.33	0.53
1:B:301:ASN:HB3	1:B:304:ASP:OD2	2.08	0.53
1:D:254:ASP:OD1	1:D:280:ALA:HB1	2.10	0.52
1:A:88:HIS:HB3	1:A:101:TRP:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLU:O	1:B:293:VAL:HG23	2.09	0.52
1:C:325:ALA:HA	4:C:783:HOH:O	2.08	0.52
1:C:55:VAL:O	1:C:85:MET:HA	2.09	0.52
1:B:215:HIS:HE1	2:B:702:NDP:H42N	1.73	0.51
1:A:266:TRP:O	1:A:270:GLN:HG2	2.11	0.51
1:C:61:ARG:HD3	1:C:61:ARG:C	2.36	0.51
1:C:248:ASN:HD22	1:C:251:ALA:HB2	1.76	0.51
1:A:285:HIS:HD2	4:A:934:HOH:O	1.93	0.50
1:C:257:PHE:CE2	1:C:259:GLY:HA3	2.46	0.50
1:D:257:PHE:CE2	1:D:259:GLY:HA3	2.47	0.50
1:B:238:VAL:HG23	1:B:240:LEU:HG	1.94	0.49
1:D:266:TRP:O	1:D:270:GLN:HG2	2.13	0.49
1:B:248:ASN:ND2	1:B:251:ALA:HB2	2.28	0.48
1:B:254:ASP:OD1	1:B:280:ALA:HB1	2.13	0.48
3:A:803:GDR:HC4'	2:C:703:NDP:H41N	1.95	0.48
1:D:61:ARG:HD3	1:D:62:SER:N	2.29	0.48
1:C:225:VAL:HG13	1:C:226:THR:N	2.28	0.48
1:D:61:ARG:HD3	1:D:61:ARG:C	2.38	0.48
1:B:231:ARG:CG	1:B:235:ARG:HH12	2.23	0.48
1:C:303:LYS:HE3	4:C:754:HOH:O	2.12	0.48
1:D:212:LEU:O	2:D:704:NDP:H5N	2.13	0.48
1:B:34:THR:OG1	1:B:112:ASN:HA	2.13	0.48
1:C:114:ALA:O	1:C:115:ALA:HB2	2.14	0.48
1:B:271:GLN:HE21	1:B:331:VAL:HG12	1.78	0.48
1:B:209:ASN:HB2	1:B:276:ASP:OD1	2.14	0.48
3:A:803:GDR:H8	1:C:248:ASN:O	2.14	0.47
1:C:34:THR:HG22	1:C:58:LEU:HD12	1.96	0.47
1:A:95:ALA:HB3	1:D:95:ALA:HB3	1.97	0.47
1:A:357:ARG:O	1:A:361:LEU:HG	2.14	0.47
1:D:93:THR:HG21	4:D:776:HOH:O	2.15	0.47
1:A:225:VAL:O	1:A:229:ILE:HG13	2.14	0.47
1:A:257:PHE:CE2	1:A:259:GLY:HA3	2.50	0.47
1:A:289:GLU:O	1:A:293:VAL:HG23	2.15	0.47
1:C:232:ALA:O	1:C:236:ILE:HG13	2.15	0.47
1:B:235:ARG:HH11	1:B:235:ARG:HG3	1.80	0.46
1:C:300:LEU:HD22	1:C:305:TYR:OH	2.15	0.46
1:B:310:GLN:HA	1:B:313:PHE:CD2	2.51	0.46
1:A:225:VAL:HG12	3:A:801:GDR:O1A	2.16	0.46
1:B:310:GLN:HA	1:B:313:PHE:HD2	1.80	0.46
1:B:61:ARG:HD3	1:B:61:ARG:C	2.40	0.46
3:A:802:GDR:HC4'	2:B:702:NDP:C2N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:MET:O	1:C:350:GLU:HG2	2.16	0.46
1:D:225:VAL:HG13	1:D:226:THR:N	2.31	0.45
1:B:216:GLU:HG3	1:B:226:THR:HG21	1.98	0.45
1:A:275:ASP:OD1	1:A:327:LYS:NZ	2.48	0.45
1:B:261:TYR:CD1	1:B:261:TYR:N	2.85	0.45
1:D:212:LEU:HG	1:D:279:VAL:HB	1.98	0.45
3:A:802:GDR:C6'	2:B:702:NDP:H41N	2.30	0.45
1:B:257:PHE:CE2	1:B:259:GLY:HA3	2.51	0.45
1:D:34:THR:HG1	1:D:112:ASN:HA	1.82	0.45
1:D:112:ASN:HB2	1:D:140:LEU:HD23	1.99	0.45
1:A:34:THR:OG1	1:A:112:ASN:HA	2.18	0.44
1:A:286:THR:OG1	1:A:289:GLU:HG3	2.17	0.44
1:A:65:PHE:CD2	1:A:68:GLN:HG3	2.52	0.44
1:A:248:ASN:ND2	1:A:251:ALA:HB2	2.32	0.44
1:B:225:VAL:HG13	1:B:226:THR:N	2.32	0.44
1:B:125:ILE:HG13	1:B:125:ILE:O	2.18	0.44
1:B:231:ARG:CZ	1:B:235:ARG:HH22	2.30	0.44
1:D:156:LYS:HD3	1:D:269:LEU:O	2.18	0.44
1:B:213:PHE:CE1	1:B:278:VAL:HG13	2.52	0.44
1:B:231:ARG:NH2	1:B:235:ARG:HH22	2.16	0.44
1:D:88:HIS:HB3	1:D:101:TRP:CE2	2.52	0.44
1:B:329:LYS:O	1:B:333:GLY:HA2	2.18	0.44
1:C:83:ALA:HB1	1:C:86:LYS:NZ	2.32	0.44
1:B:162:SER:O	1:B:165:MET:HG3	2.18	0.44
1:A:118:HIS:CE1	1:A:120:ALA:HB3	2.53	0.44
1:A:301:ASN:OD1	1:A:303:LYS:HB2	2.18	0.44
1:A:248:ASN:O	3:A:801:GDR:H8	2.18	0.43
1:A:84:LEU:HD13	4:A:895:HOH:O	2.17	0.43
1:A:162:SER:OG	3:A:801:GDR:HC63	2.19	0.43
1:C:261:TYR:CD1	1:C:261:TYR:N	2.86	0.43
1:C:320:ASN:C	1:C:320:ASN:ND2	2.70	0.43
1:C:28:ARG:NH1	1:C:84:LEU:HD21	2.33	0.43
1:A:212:LEU:HG	1:A:279:VAL:HB	2.00	0.43
1:D:170:PRO:HA	1:D:171:PRO:HD3	1.84	0.43
1:D:209:ASN:HB2	1:D:276:ASP:OD1	2.19	0.43
1:D:92:LEU:HD21	1:D:112:ASN:HD21	1.83	0.43
1:B:261:TYR:N	1:B:261:TYR:HD1	2.16	0.43
1:B:291:LEU:HD13	1:B:302:TRP:CE3	2.54	0.43
1:B:354:LEU:O	1:B:358:GLU:HG3	2.19	0.43
1:C:112:ASN:HB2	1:C:140:LEU:HD23	2.00	0.43
1:C:73:ILE:O	1:C:73:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:VAL:HB	1:C:359:LYS:HD2	2.01	0.42
1:C:301:ASN:HB3	1:C:304:ASP:OD2	2.18	0.42
1:A:215:HIS:HA	1:A:256:GLY:O	2.19	0.42
1:B:153:ARG:HB3	1:B:153:ARG:CZ	2.50	0.42
1:A:163:SER:HB3	1:A:213:PHE:CD1	2.54	0.42
1:B:74:TYR:HD2	1:B:85:MET:HE2	1.84	0.42
1:B:98:LEU:O	1:B:102:ILE:HG13	2.20	0.42
1:A:361:LEU:CD1	1:A:367:MET:HE3	2.50	0.42
3:A:803:GDR:HC4'	2:C:703:NDP:C4N	2.50	0.42
1:C:341:GLU:HB3	4:C:813:HOH:O	2.18	0.42
1:C:218:PRO:CG	1:C:350:GLU:HG3	2.50	0.42
1:D:253:ARG:HH11	1:D:319:ASP:N	2.18	0.42
1:D:340:PHE:O	1:D:344:VAL:HG23	2.20	0.41
1:A:223:ASN:HB3	4:A:891:HOH:O	2.19	0.41
1:B:144:VAL:O	1:B:148:THR:HG23	2.20	0.41
1:A:310:GLN:HA	1:A:313:PHE:CD2	2.56	0.41
1:B:220:ARG:O	1:B:227:ARG:HG2	2.20	0.41
1:C:261:TYR:N	1:C:261:TYR:HD1	2.18	0.41
1:B:357:ARG:NH1	1:D:361:LEU:HD11	2.36	0.41
1:A:244:LEU:O	1:A:306:VAL:HA	2.21	0.41
1:B:37:THR:HG23	1:B:59:ILE:HG22	2.03	0.41
1:B:225:VAL:O	1:B:229:ILE:HG13	2.21	0.41
1:A:268:MET:HG2	1:A:277:TYR:CD1	2.56	0.41
1:B:231:ARG:NH1	1:B:235:ARG:NH1	2.68	0.41
1:D:358:GLU:O	1:D:362:VAL:HG23	2.21	0.41
1:A:65:PHE:CE2	1:A:68:GLN:HG3	2.56	0.40
1:C:61:ARG:HD3	1:C:62:SER:N	2.36	0.40
1:C:252:SER:HA	1:C:286:THR:HA	2.03	0.40
1:C:353:GLU:O	1:C:357:ARG:HG3	2.21	0.40
1:A:362:VAL:C	1:A:364:ALA:H	2.30	0.40
1:B:167:GLY:HA3	1:B:180:HIS:O	2.22	0.40
1:A:34:THR:HG22	1:A:58:LEU:HD12	2.04	0.40
1:A:85:MET:HE3	1:A:87:LEU:HD21	2.04	0.40
1:B:112:ASN:HB2	1:B:140:LEU:HD23	2.02	0.40
1:B:163:SER:HB3	1:B:213:PHE:CG	2.57	0.40
1:A:153:ARG:CZ	1:A:153:ARG:HB3	2.52	0.40
1:A:334:TRP:CZ3	1:A:336:PRO:HD3	2.57	0.40
1:B:212:LEU:HG	1:B:279:VAL:HB	2.03	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	329/381 (86%)	319 (97%)	9 (3%)	1 (0%)	36	42
1	B	332/381 (87%)	325 (98%)	6 (2%)	1 (0%)	36	42
1	C	330/381 (87%)	318 (96%)	12 (4%)	0	100	100
1	D	305/381 (80%)	295 (97%)	10 (3%)	0	100	100
All	All	1296/1524 (85%)	1257 (97%)	37 (3%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ALA
1	B	83	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/323 (84%)	268 (99%)	2 (1%)	76	87
1	B	267/323 (83%)	266 (100%)	1 (0%)	84	92
1	C	268/323 (83%)	266 (99%)	2 (1%)	76	87
1	D	235/323 (73%)	234 (100%)	1 (0%)	84	92
All	All	1040/1292 (80%)	1034 (99%)	6 (1%)	78	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	216	GLU
1	B	116	GLN
1	C	116	GLN
1	C	354	LEU
1	D	116	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	198	ASN
1	A	209	ASN
1	A	223	ASN
1	A	271	GLN
1	B	71	ASN
1	B	209	ASN
1	B	223	ASN
1	C	223	ASN
1	C	248	ASN
1	C	301	ASN
1	C	320	ASN
1	D	71	ASN
1	D	112	ASN
1	D	118	HIS
1	D	159	GLN
1	D	173	GLN
1	D	180	HIS
1	D	209	ASN
1	D	285	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDR	A	803	-	40,41,41	0.98	2 (5%)	61,64,64	0.51	0
2	NDP	B	702	-	51,52,52	1.86	6 (11%)	71,80,80	0.73	1 (1%)
2	NDP	A	701	-	51,52,52	1.83	6 (11%)	71,80,80	0.68	0
3	GDR	A	801	-	40,41,41	0.96	3 (7%)	61,64,64	0.49	0
3	GDR	A	802	-	40,41,41	1.01	3 (7%)	61,64,64	0.51	0
2	NDP	C	703	-	51,52,52	1.85	6 (11%)	71,80,80	0.71	1 (1%)
2	NDP	D	704	-	51,52,52	1.88	6 (11%)	71,80,80	0.73	1 (1%)

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	GDR	A	803	-	-	5/21/57/57	0/4/4/4
2	NDP	B	702	-	-	8/34/77/77	0/5/5/5
2	NDP	A	701	-	-	5/34/77/77	0/5/5/5
3	GDR	A	801	-	-	3/21/57/57	0/4/4/4
3	GDR	A	802	-	-	4/21/57/57	0/4/4/4
2	NDP	C	703	-	-	5/34/77/77	0/5/5/5
2	NDP	D	704	-	-	9/34/77/77	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	704	NDP	C4N-C3N	-7.75	1.35	1.50
2	B	702	NDP	C4N-C3N	-7.67	1.35	1.50
2	C	703	NDP	C4N-C3N	-7.62	1.35	1.50
2	A	701	NDP	C4N-C3N	-7.54	1.35	1.50
2	D	704	NDP	C7N-C3N	-6.31	1.35	1.48
2	B	702	NDP	C7N-C3N	-6.23	1.35	1.48
2	C	703	NDP	C7N-C3N	-6.17	1.35	1.48
2	A	701	NDP	C7N-C3N	-6.05	1.35	1.48
2	D	704	NDP	P2B-O2B	-5.44	1.50	1.59
2	A	701	NDP	P2B-O2B	-5.39	1.50	1.59
2	B	702	NDP	P2B-O2B	-5.39	1.50	1.59
2	C	703	NDP	P2B-O2B	-5.31	1.50	1.59
2	D	704	NDP	C4N-C5N	-4.43	1.37	1.49
2	B	702	NDP	C4N-C5N	-4.42	1.37	1.49
2	C	703	NDP	C4N-C5N	-4.36	1.37	1.49
2	A	701	NDP	C4N-C5N	-4.23	1.38	1.49
3	A	802	GDR	PB-O3A	3.91	1.63	1.59
3	A	803	GDR	PB-O3A	3.76	1.63	1.59
3	A	802	GDR	PA-O3A	3.69	1.63	1.59
3	A	801	GDR	PA-O3A	3.68	1.63	1.59
3	A	803	GDR	PA-O3A	3.62	1.63	1.59
3	A	801	GDR	PB-O3A	3.48	1.63	1.59
2	D	704	NDP	PA-O3	3.20	1.63	1.59
2	B	702	NDP	PN-O3	3.14	1.62	1.59
2	C	703	NDP	PA-O3	3.11	1.62	1.59
2	A	701	NDP	PN-O3	3.10	1.62	1.59
2	D	704	NDP	PN-O3	3.02	1.62	1.59
2	C	703	NDP	PN-O3	2.97	1.62	1.59
2	A	701	NDP	PA-O3	2.93	1.62	1.59
2	B	702	NDP	PA-O3	2.91	1.62	1.59
3	A	802	GDR	PB-O3B	-2.13	1.52	1.59
3	A	801	GDR	PB-O3B	-2.04	1.53	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	704	NDP	O4B-C1B-C2B	-2.79	101.78	106.59
2	B	702	NDP	O4B-C1B-C2B	-2.50	102.28	106.59
2	C	703	NDP	O4B-C1B-C2B	-2.38	102.50	106.59

There are no chirality outliers.

All (39) torsion outliers are listed below:

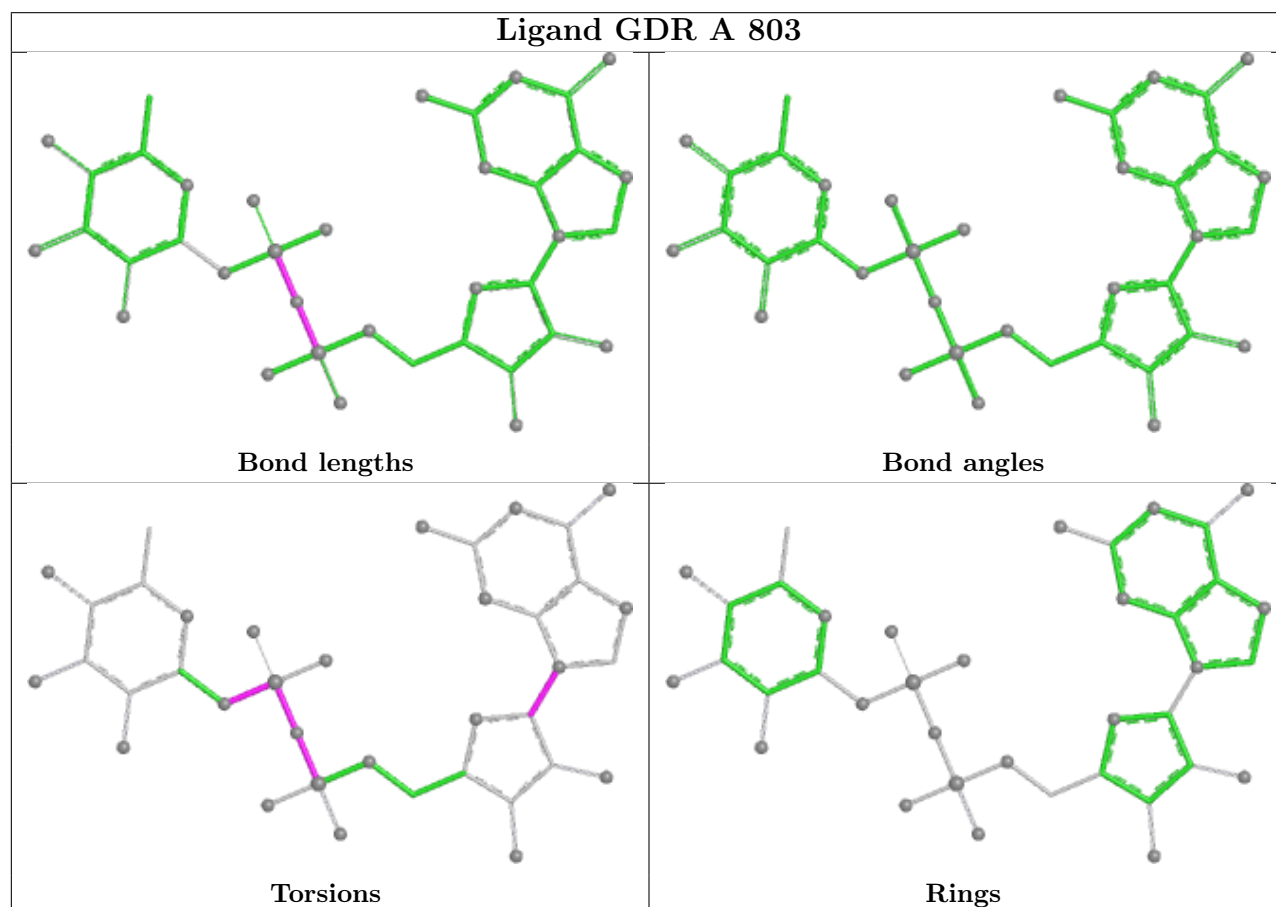
Mol	Chain	Res	Type	Atoms
3	A	801	GDR	C1'-O3B-PB-O3A
3	A	802	GDR	C1'-O3B-PB-O3A
3	A	803	GDR	C1'-O3B-PB-O3A
2	D	704	NDP	PN-O3-PA-O1A
2	C	703	NDP	C2D-C1D-N1N-C6N
2	D	704	NDP	C2D-C1D-N1N-C6N
3	A	801	GDR	PB-O3A-PA-O5D
3	A	802	GDR	PB-O3A-PA-O5D
3	A	803	GDR	PB-O3A-PA-O5D
2	C	703	NDP	C2D-C1D-N1N-C2N
2	C	703	NDP	O4D-C1D-N1N-C6N
2	D	704	NDP	O4D-C1D-N1N-C6N
2	B	702	NDP	C2D-C1D-N1N-C2N
2	C	703	NDP	O4D-C1D-N1N-C2N
2	B	702	NDP	O4D-C1D-N1N-C2N
2	B	702	NDP	O4D-C1D-N1N-C6N
2	A	701	NDP	C2D-C1D-N1N-C6N
2	B	702	NDP	C2D-C1D-N1N-C6N
2	D	704	NDP	O4D-C1D-N1N-C2N
2	D	704	NDP	C2D-C1D-N1N-C2N
2	D	704	NDP	PN-O3-PA-O2A
2	A	701	NDP	O4D-C1D-N1N-C2N
2	A	701	NDP	O4D-C1D-N1N-C6N
2	D	704	NDP	C2N-C3N-C7N-N7N
2	A	701	NDP	C2D-C1D-N1N-C2N
2	C	703	NDP	C2B-O2B-P2B-O1X
2	D	704	NDP	C2B-O2B-P2B-O1X
2	B	702	NDP	PN-O3-PA-O1A
3	A	803	GDR	PA-O3A-PB-O1B
3	A	802	GDR	C1'-O3B-PB-O1B
3	A	801	GDR	C2D-C1D-N9-C4
3	A	803	GDR	C2D-C1D-N9-C4
2	B	702	NDP	PN-O3-PA-O2A
3	A	803	GDR	PA-O3A-PB-O2B
2	B	702	NDP	O4B-C4B-C5B-O5B
2	A	701	NDP	C2B-O2B-P2B-O1X
2	B	702	NDP	C2B-O2B-P2B-O1X
2	D	704	NDP	O4B-C4B-C5B-O5B
3	A	802	GDR	C2D-C1D-N9-C4

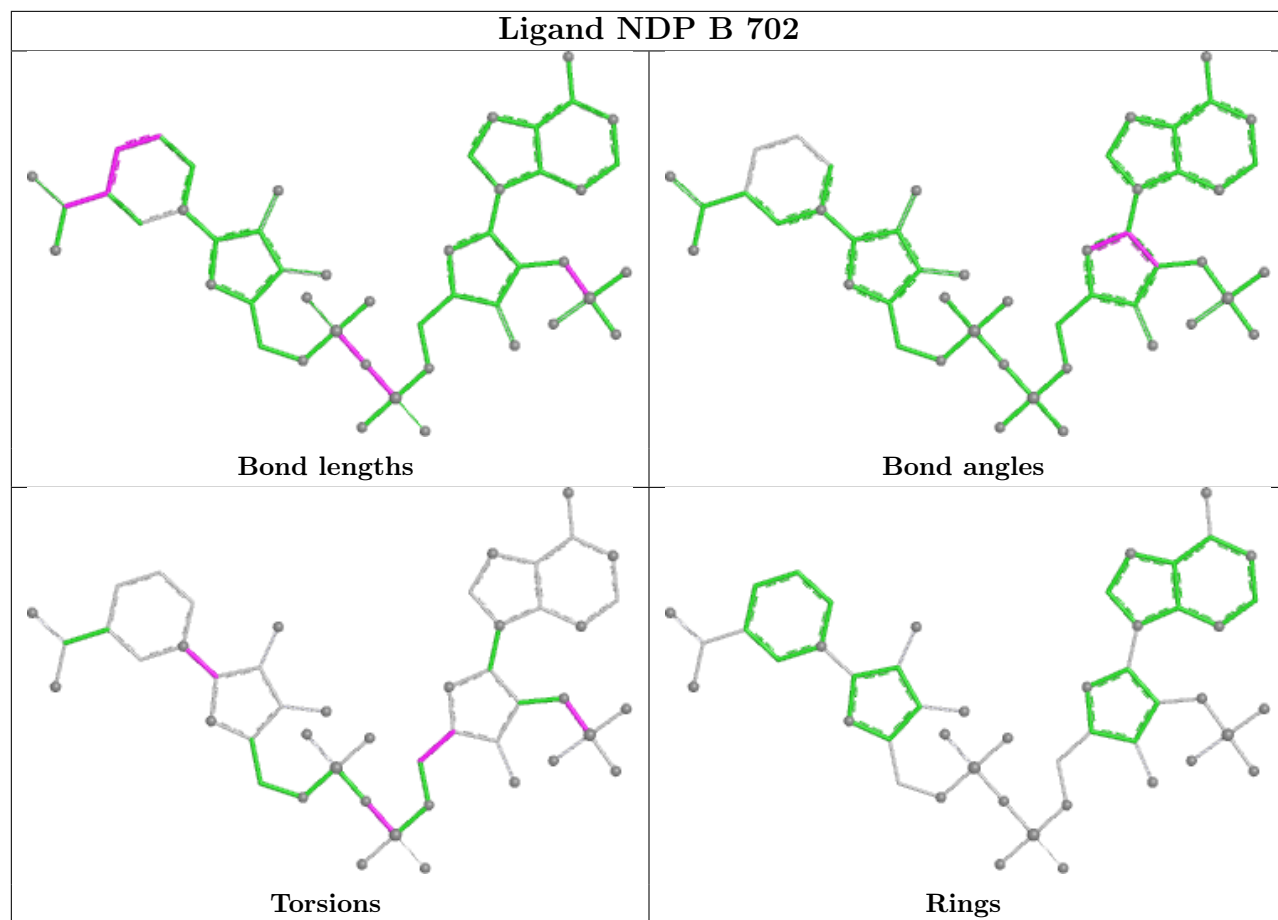
There are no ring outliers.

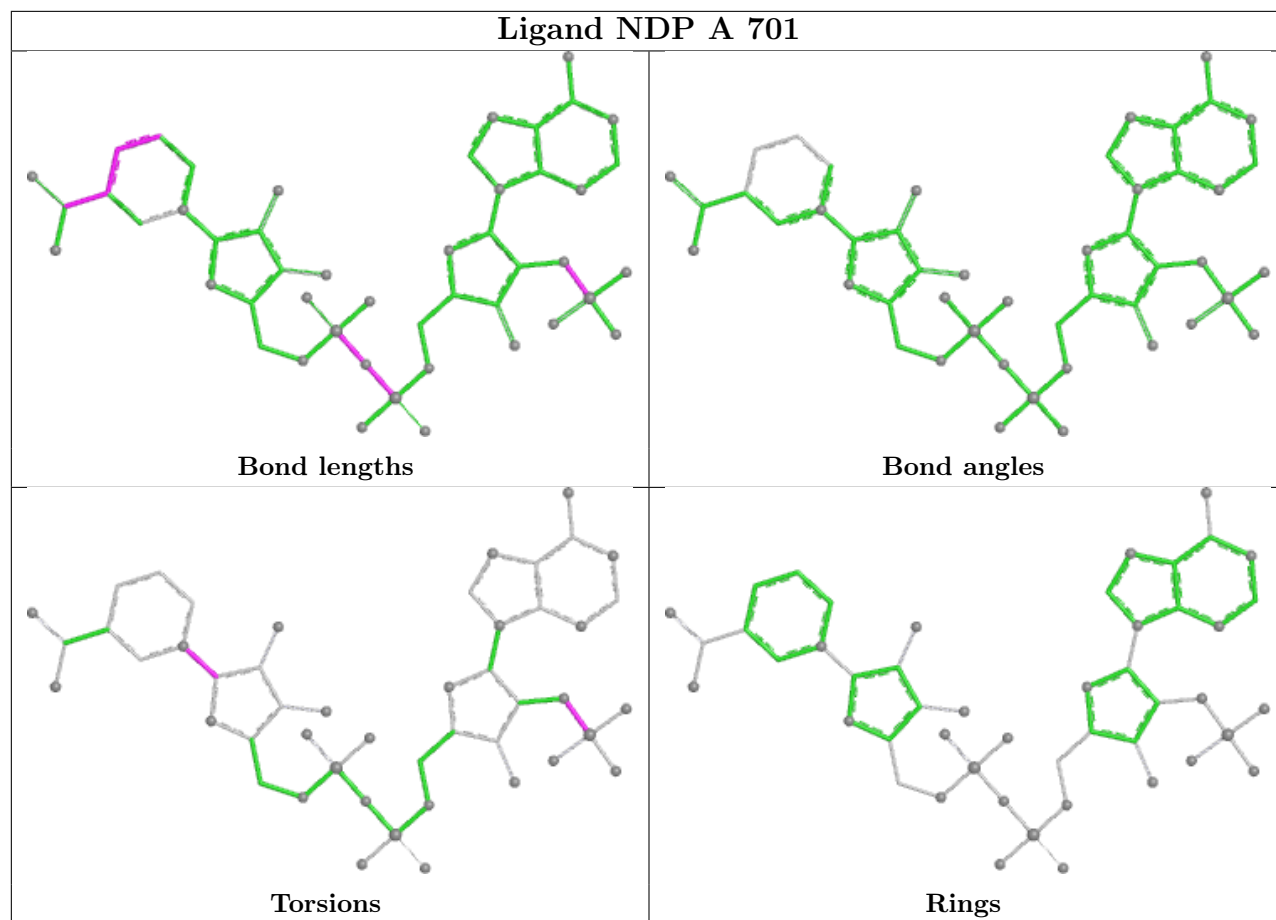
7 monomers are involved in 21 short contacts:

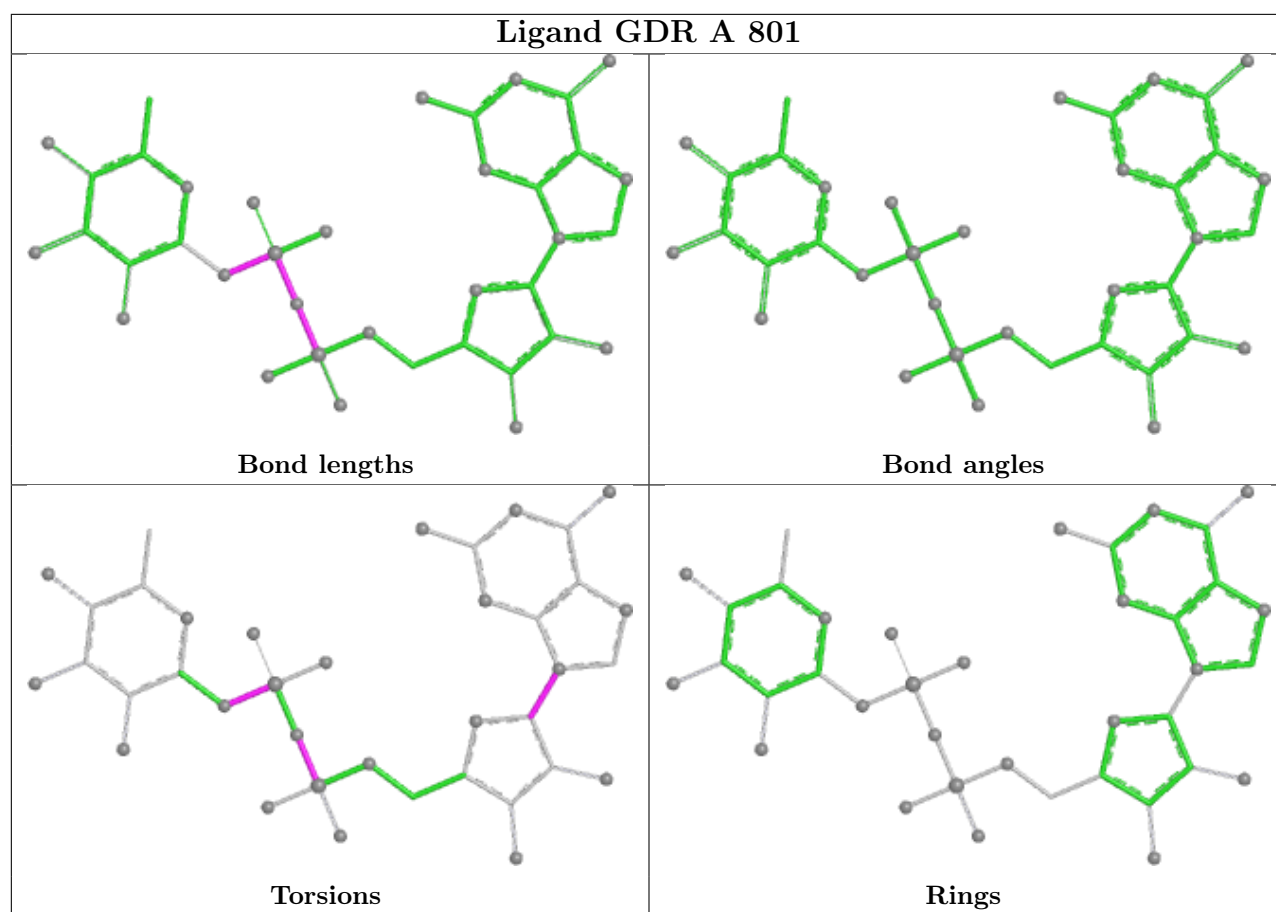
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	GDR	6	0
2	B	702	NDP	6	0
2	A	701	NDP	4	0
3	A	801	GDR	7	0
3	A	802	GDR	4	0
2	C	703	NDP	5	0
2	D	704	NDP	1	0

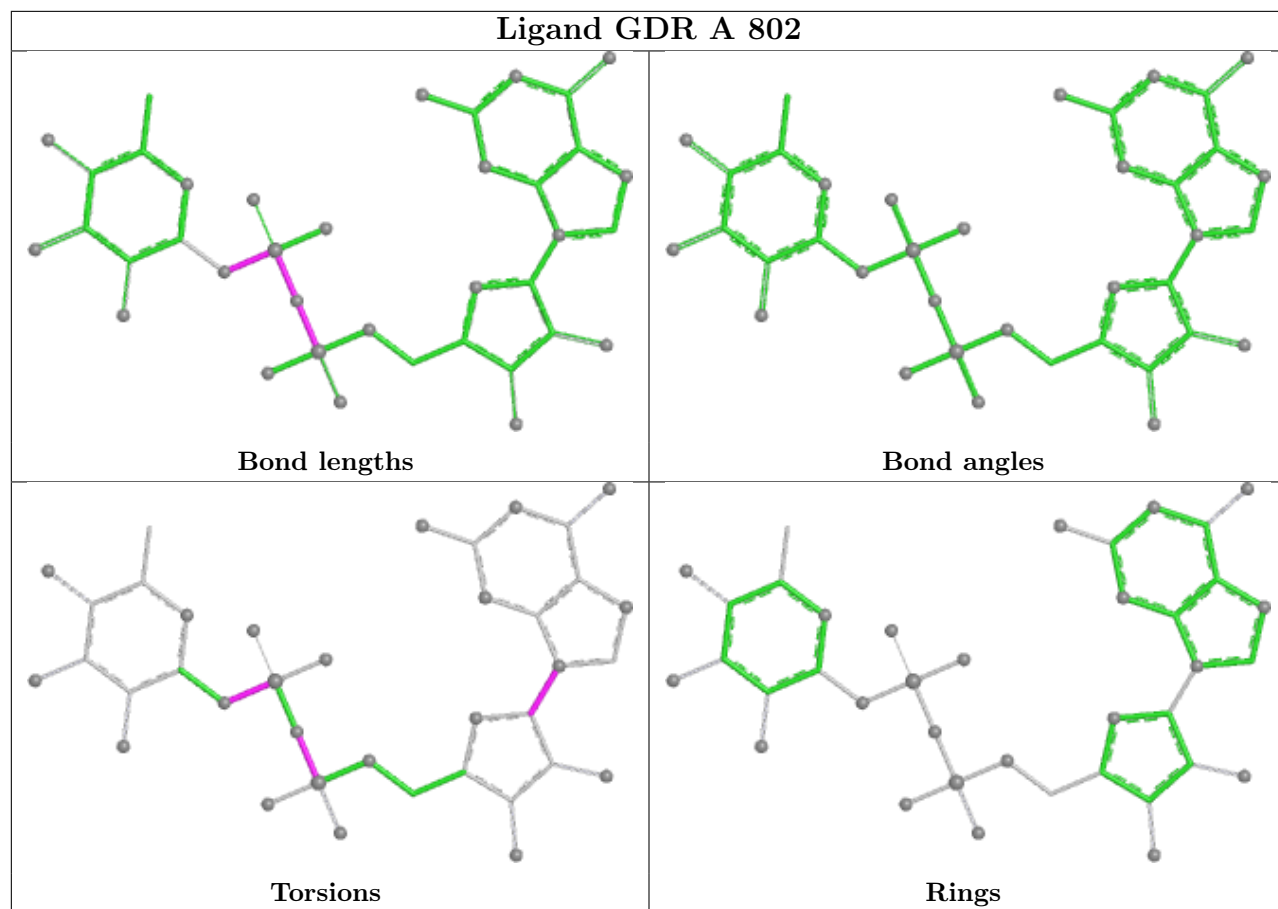
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

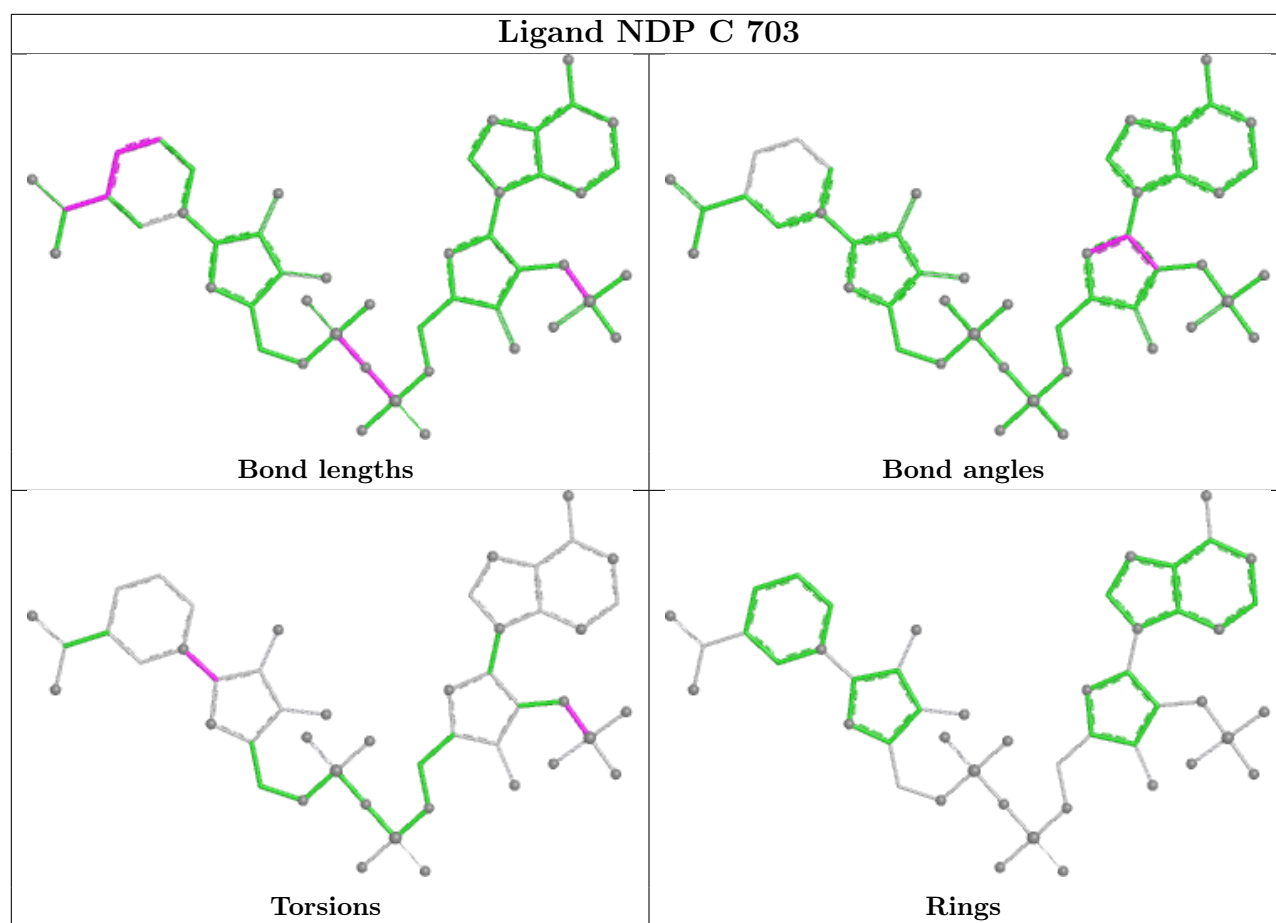


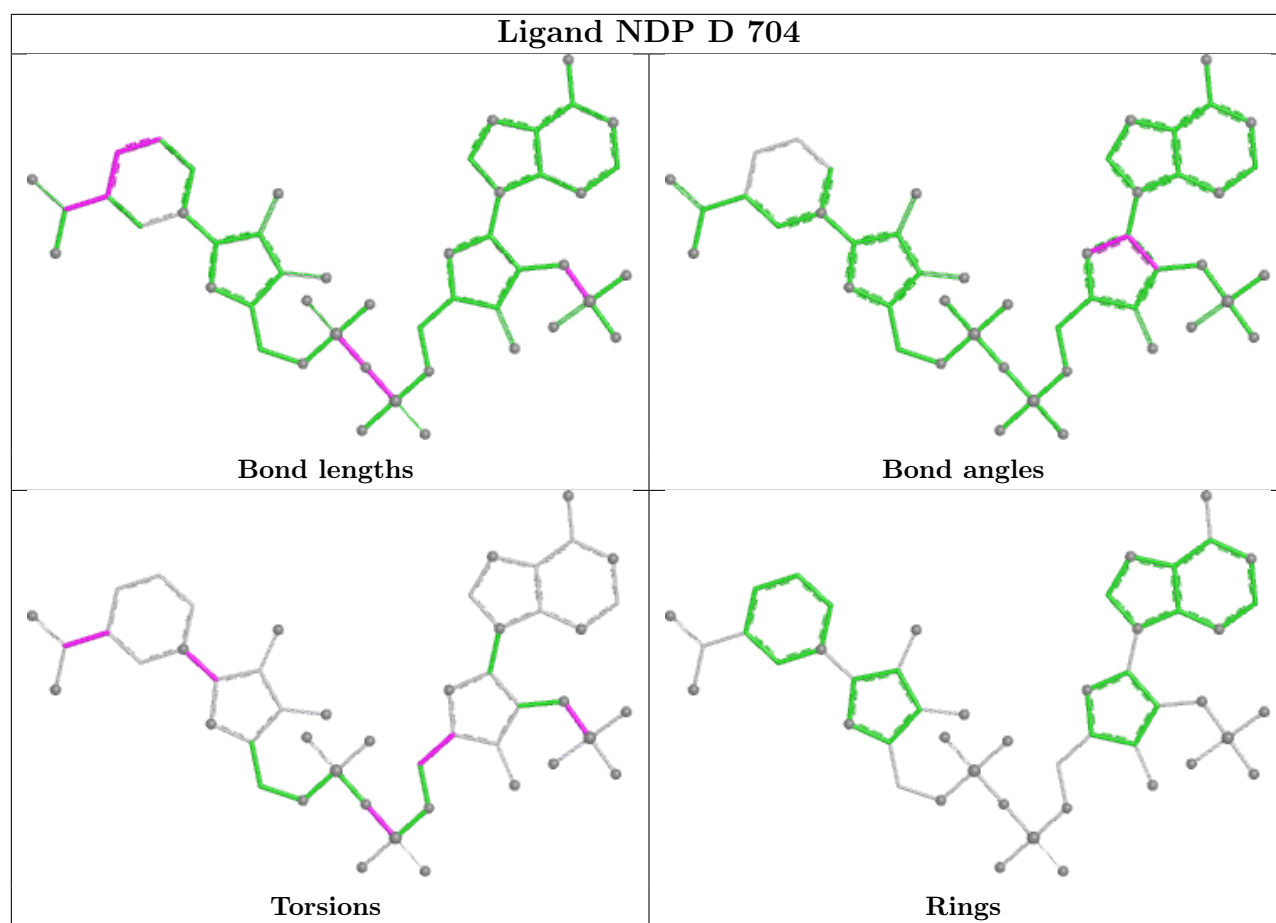












5.7 Other polymers [i](#)

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	333/381 (87%)	-0.08	3 (0%) 81 79	20, 32, 46, 60	0
1	B	336/381 (88%)	0.09	6 (1%) 67 64	22, 35, 48, 61	0
1	C	334/381 (87%)	0.24	7 (2%) 63 60	20, 36, 47, 54	0
1	D	313/381 (82%)	0.39	35 (11%) 10 8	22, 35, 54, 59	0
All	All	1316/1524 (86%)	0.16	51 (3%) 43 40	20, 34, 50, 61	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	TYR	4.6
1	D	252	SER	4.3
1	D	242	THR	4.3
1	D	340	PHE	4.0
1	D	294	SER	3.9
1	C	83	ALA	3.7
1	D	302	TRP	3.6
1	D	240	LEU	3.5
1	C	304	ASP	3.2
1	D	243	LYS	3.2
1	D	339	GLY	3.1
1	D	75	ILE	3.1
1	D	251	ALA	3.1
1	A	83	ALA	3.0
1	D	319	ASP	3.0
1	D	291	LEU	2.8
1	D	233	LEU	2.8
1	C	74	TYR	2.7
1	D	245	PHE	2.7
1	D	337	GLN	2.7
1	D	286	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	349	ASP	2.7
1	C	75	ILE	2.6
1	B	76	ASP	2.5
1	D	293	VAL	2.5
1	A	73	ILE	2.5
1	D	236	ILE	2.4
1	C	65	PHE	2.4
1	D	298	LEU	2.4
1	D	322	GLN	2.3
1	D	355	ALA	2.3
1	B	366	TYR	2.3
1	D	362	VAL	2.3
1	D	244	LEU	2.2
1	D	238	VAL	2.2
1	C	223	ASN	2.2
1	D	171	PRO	2.2
1	D	305	TYR	2.1
1	D	304	ASP	2.1
1	D	306	VAL	2.1
1	D	239	GLY	2.1
1	B	83	ALA	2.1
1	B	301	ASN	2.1
1	B	368	ASP	2.1
1	D	303	LYS	2.1
1	D	223	ASN	2.1
1	B	65	PHE	2.1
1	C	325	ALA	2.0
1	A	357	ARG	2.0
1	D	287	VAL	2.0
1	D	290	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

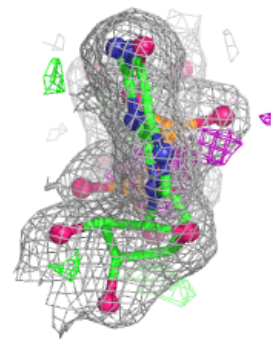
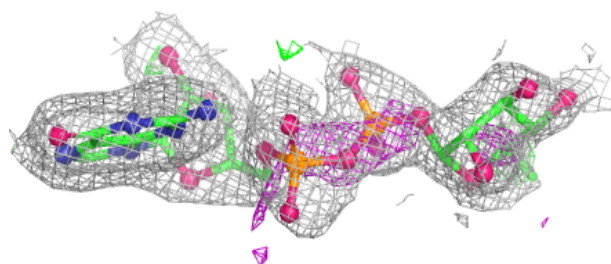
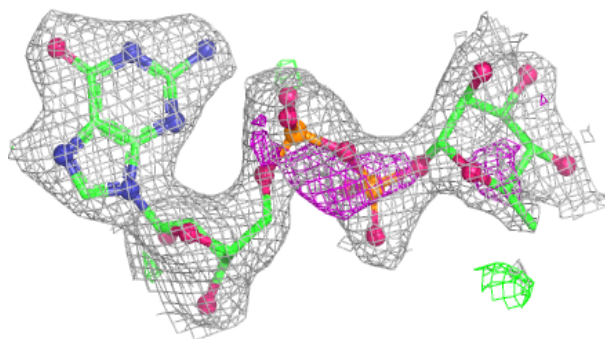
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	GDR	A	802	38/38	0.91	0.11	40,43,48,48	0
3	GDR	A	803	38/38	0.93	0.10	38,43,47,47	0
3	GDR	A	801	38/38	0.95	0.08	34,38,40,41	0
2	NDP	A	701	48/48	0.97	0.06	20,24,29,30	0
2	NDP	C	703	48/48	0.97	0.07	21,27,36,38	0
2	NDP	D	704	48/48	0.97	0.07	23,28,34,35	0
2	NDP	B	702	48/48	0.98	0.06	23,26,36,37	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.

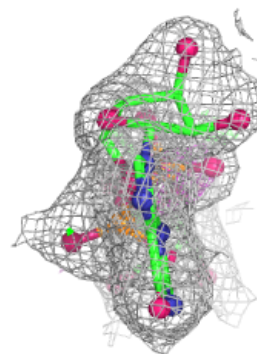
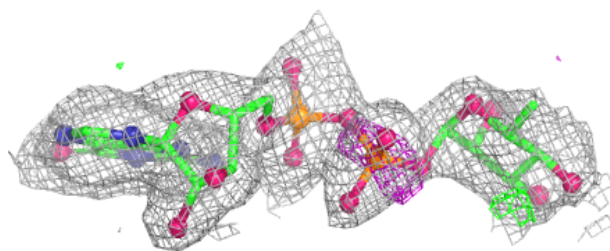
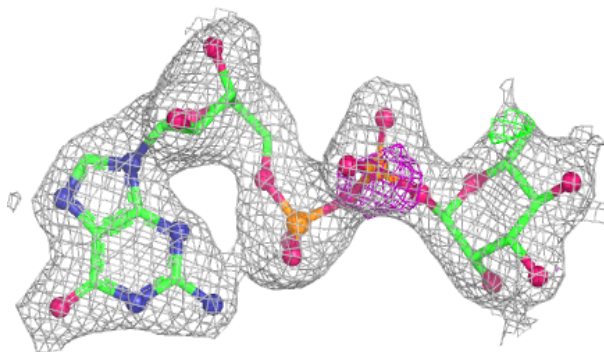
Electron density around GDR A 802:

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

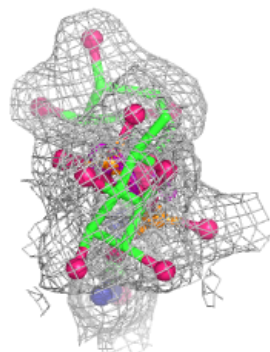
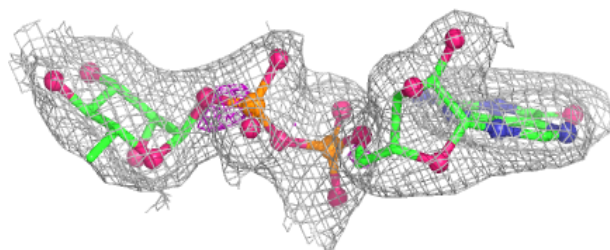
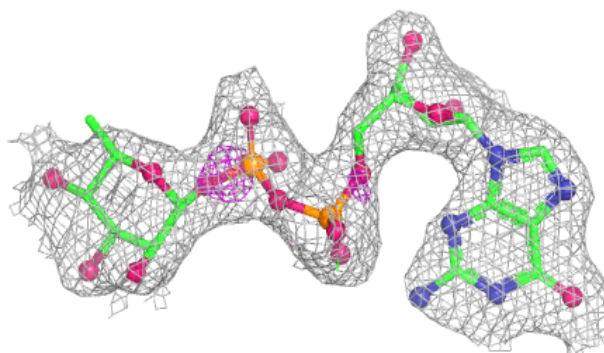


Electron density around GDR A 803:

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

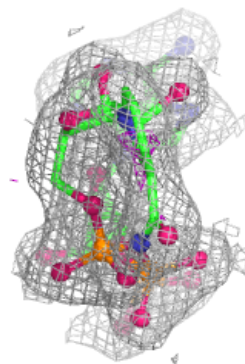
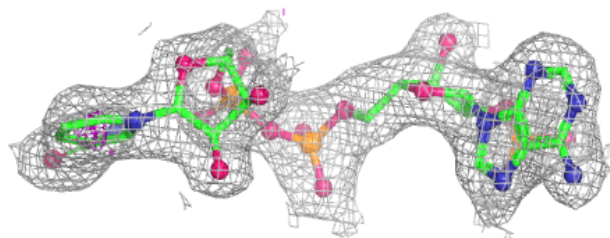
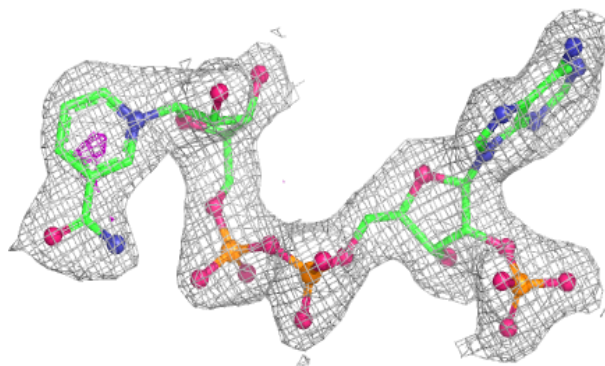
**Electron density around GDR A 801:**

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

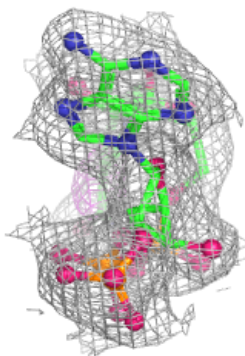
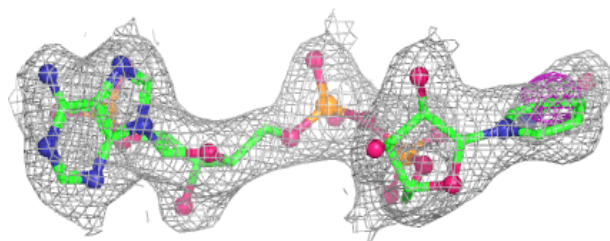
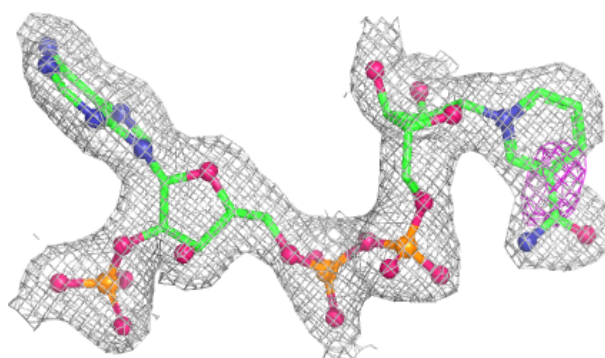


Electron density around NDP A 701:

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

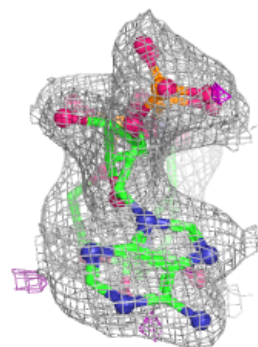
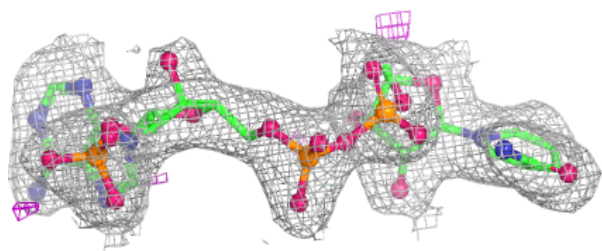
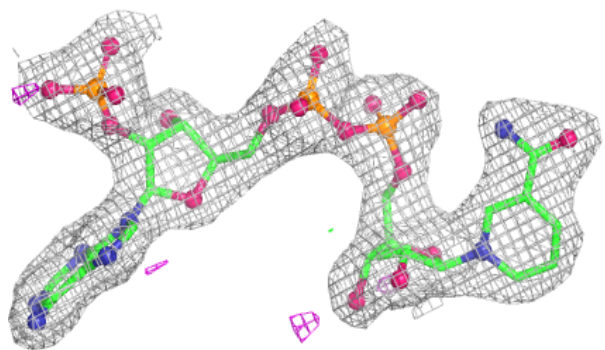
**Electron density around NDP C 703:**

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

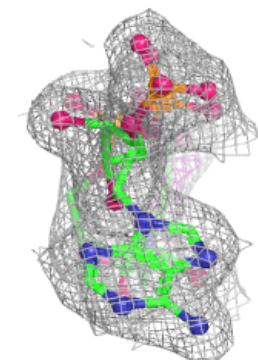
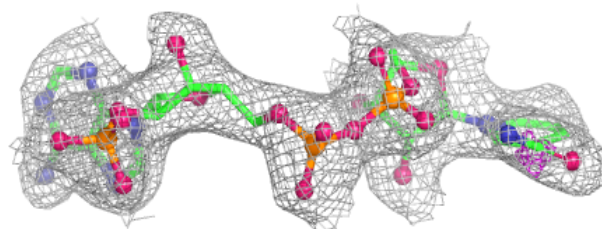
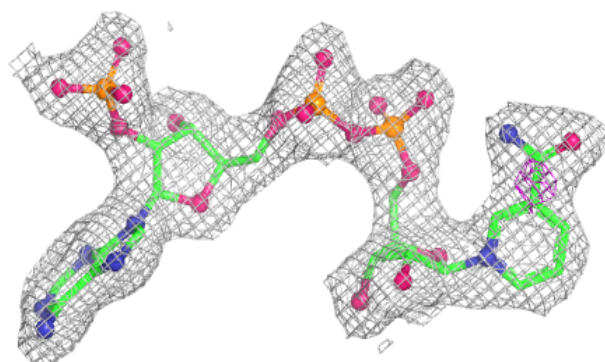


Electron density around NDP D 704:

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

**Electron density around NDP B 702:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.