



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:01 PM UTC

PDB ID : 3RAN / pdb_00003ran
Title : CANINE GDP-RAN Q69L MUTANT
Authors : Stewart, M.; Kent, H.M.; Mccoy, A.J.
Deposited on : 1998-10-19
Resolution : 2.15 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

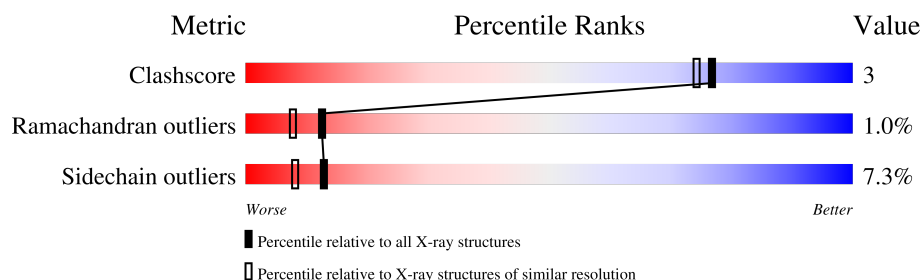
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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))
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	 62% 26% • • 7%
1	B	216	 65% 26% • 6%
1	C	216	 70% 21% • 6%
1	D	216	 66% 22% 6% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6829 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 PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	22	0	0
			1612	1045	278	283	6			
1	B	204	Total	C	N	O	S	39	0	0
			1635	1058	282	289	6			
1	C	203	Total	C	N	O	S	11	0	0
			1628	1054	281	287	6			
1	D	203	Total	C	N	O	S	48	0	0
			1628	1054	281	287	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LEU	GLN	engineered mutation	UNP P62825
B	69	LEU	GLN	engineered mutation	UNP P62825
C	69	LEU	GLN	engineered mutation	UNP P62825
D	69	LEU	GLN	engineered mutation	UNP P62825

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 4 is water.

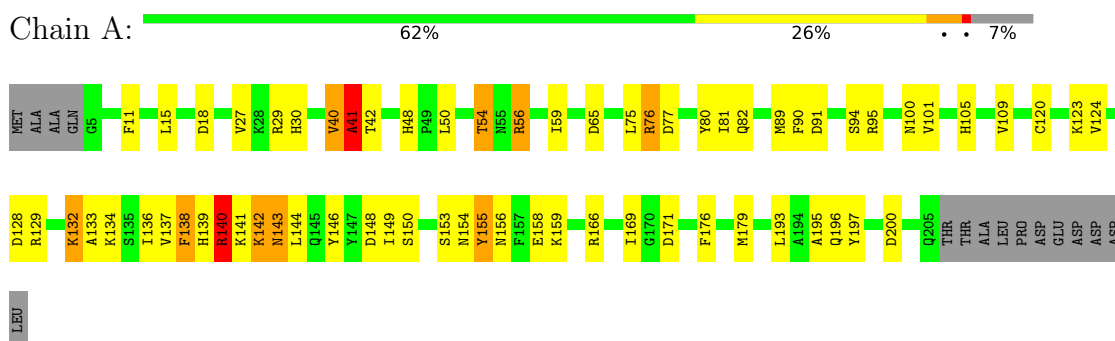
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	9	Total O 9 9	0	0
4	C	73	Total O 73 73	0	0
4	D	72	Total O 72 72	1	0

3 Residue-property plots

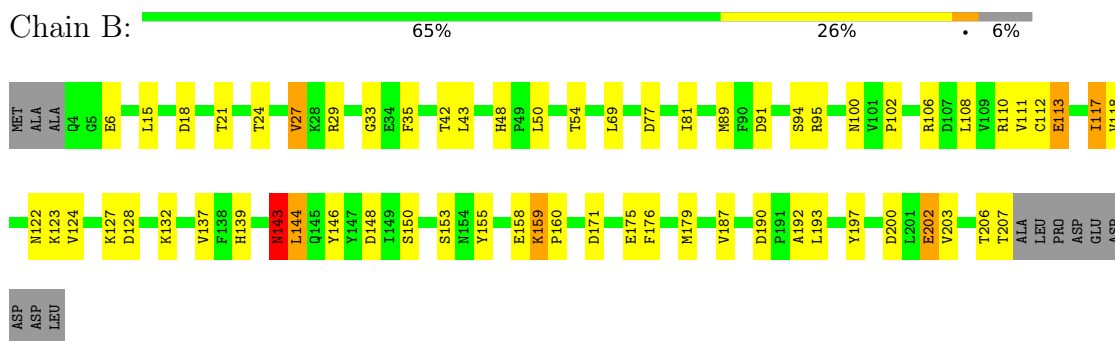
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

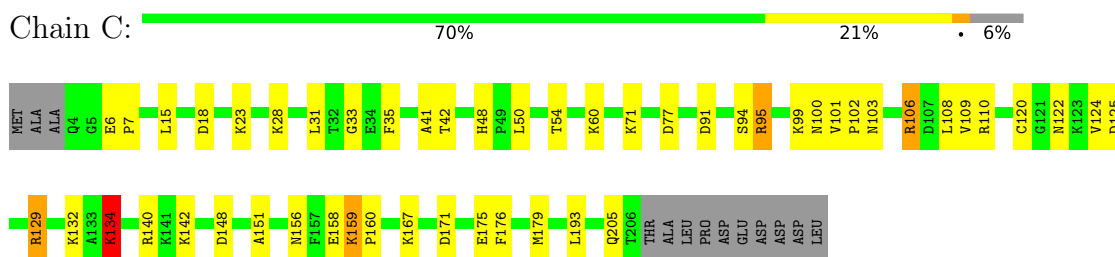
- Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)



- Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)

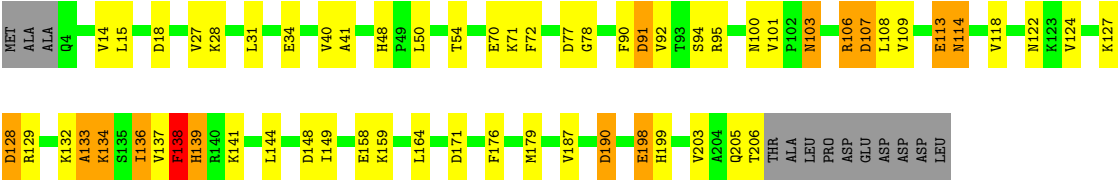


- Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)



- Molecule 1: PROTEIN (GTP-BINDING NUCLEAR PROTEIN RAN)

Chain D: 66% 22% 6% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.09Å 59.17Å 116.37Å 90.00° 100.68° 90.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	94.7 (6.00-2.15)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6829	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.81	1/1653 (0.1%)	2.15	78/2240 (3.5%)
1	B	0.79	0/1676	1.96	62/2272 (2.7%)
1	C	0.81	0/1669	2.01	47/2262 (2.1%)
1	D	0.85	4/1669 (0.2%)	2.04	61/2262 (2.7%)
All	All	0.81	5/6667 (0.1%)	2.04	248/9036 (2.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	2
1	D	0	3
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	PHE	N-CA	-7.00	1.37	1.46
1	D	141	LYS	C-N	7.00	1.43	1.33
1	A	138	PHE	N-CA	-6.74	1.37	1.46
1	D	141	LYS	C-O	-6.00	1.16	1.24
1	D	136	ILE	CA-C	-5.08	1.46	1.52

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	ARG	CD-NE-CZ	26.43	161.41	124.40
1	A	137	VAL	CA-C-N	22.39	164.29	121.54
1	A	137	VAL	C-N-CA	22.39	164.29	121.54
1	D	137	VAL	O-C-N	19.16	143.29	123.18
1	D	136	ILE	CA-C-N	-12.40	107.82	123.19
1	D	136	ILE	C-N-CA	-12.40	107.82	123.19
1	A	56	ARG	CD-NE-CZ	11.26	140.16	124.40
1	A	100	ASN	CA-C-N	10.84	130.83	120.43
1	A	100	ASN	C-N-CA	10.84	130.83	120.43
1	B	202	GLU	CA-C-N	10.32	138.10	120.86
1	B	202	GLU	C-N-CA	10.32	138.10	120.86
1	C	129	ARG	NE-CZ-NH2	9.95	128.16	119.20
1	D	103	ASN	CA-CB-CG	9.90	122.50	112.60
1	C	205	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	D	205	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	A	77	ASP	CA-C-N	9.79	132.38	120.14
1	A	77	ASP	C-N-CA	9.79	132.38	120.14
1	D	139	HIS	CA-CB-CG	-9.17	104.63	113.80
1	B	91	ASP	CA-CB-CG	9.14	121.74	112.60
1	B	100	ASN	CA-C-N	9.14	129.21	120.43
1	B	100	ASN	C-N-CA	9.14	129.21	120.43
1	D	122	ASN	CA-CB-CG	8.86	121.46	112.60
1	A	136	ILE	O-C-N	-8.82	113.59	122.14
1	A	195	ALA	CA-C-O	-8.80	111.48	120.90
1	C	100	ASN	CA-C-N	8.63	128.71	120.43
1	C	100	ASN	C-N-CA	8.63	128.71	120.43
1	A	148	ASP	CA-CB-CG	8.62	121.22	112.60
1	D	176	PHE	CA-CB-CG	8.54	122.33	113.80
1	D	100	ASN	CA-C-N	8.52	127.15	120.33
1	D	100	ASN	C-N-CA	8.52	127.15	120.33
1	D	113	GLU	CA-C-N	8.34	137.46	121.54
1	D	113	GLU	C-N-CA	8.34	137.46	121.54
1	C	77	ASP	CA-C-N	8.27	129.16	119.98
1	C	77	ASP	C-N-CA	8.27	129.16	119.98
1	D	139	HIS	N-CA-C	-8.03	103.50	113.38
1	A	42	THR	N-CA-C	7.85	121.96	112.38
1	D	199	HIS	CB-CA-C	-7.58	98.21	110.79
1	C	95	ARG	N-CA-C	7.54	119.50	111.28
1	B	128	ASP	CA-C-N	7.50	132.76	122.19
1	B	128	ASP	C-N-CA	7.50	132.76	122.19
1	D	95	ARG	CA-C-N	7.49	132.30	120.47
1	D	95	ARG	C-N-CA	7.49	132.30	120.47
1	C	91	ASP	CA-CB-CG	7.49	120.09	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	ALA	CA-C-N	7.38	131.89	120.82
1	D	133	ALA	C-N-CA	7.38	131.89	120.82
1	A	140	ARG	CA-C-N	7.36	135.59	121.54
1	A	140	ARG	C-N-CA	7.36	135.59	121.54
1	B	94	SER	CA-C-N	7.33	130.43	120.38
1	B	94	SER	C-N-CA	7.33	130.43	120.38
1	B	35	PHE	CA-CB-CG	7.31	121.11	113.80
1	C	122	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	D	187	VAL	N-CA-CB	7.17	122.57	112.52
1	D	138	PHE	CA-CB-CG	7.16	120.96	113.80
1	D	91	ASP	CA-CB-CG	7.05	119.65	112.60
1	C	35	PHE	CA-CB-CG	7.03	120.83	113.80
1	B	146	TYR	O-C-N	-7.02	114.98	123.19
1	A	94	SER	CA-C-N	6.96	129.61	120.28
1	A	94	SER	C-N-CA	6.96	129.61	120.28
1	C	108	LEU	CA-C-N	6.93	129.96	120.46
1	C	108	LEU	C-N-CA	6.93	129.96	120.46
1	D	27	VAL	CA-C-N	6.88	132.21	120.72
1	D	27	VAL	C-N-CA	6.88	132.21	120.72
1	B	95	ARG	CA-C-O	-6.84	113.24	120.63
1	C	48	HIS	CA-CB-CG	6.83	120.64	113.80
1	B	143	ASN	CA-C-N	6.72	132.19	122.44
1	B	143	ASN	C-N-CA	6.72	132.19	122.44
1	D	205	GLN	CG-CD-NE2	6.69	126.43	116.40
1	D	34	GLU	CA-C-N	6.65	129.19	120.28
1	D	34	GLU	C-N-CA	6.65	129.19	120.28
1	C	156	ASN	CA-C-N	6.64	129.48	120.38
1	C	156	ASN	C-N-CA	6.64	129.48	120.38
1	C	205	GLN	CG-CD-NE2	6.63	126.35	116.40
1	B	6	GLU	CG-CD-OE1	-6.61	103.20	118.40
1	A	132	LYS	CA-C-N	6.52	129.31	120.38
1	A	132	LYS	C-N-CA	6.52	129.31	120.38
1	D	199	HIS	CA-CB-CG	-6.50	107.30	113.80
1	D	94	SER	CA-C-N	6.42	129.20	120.54
1	D	94	SER	C-N-CA	6.42	129.20	120.54
1	B	148	ASP	CA-CB-CG	6.42	119.02	112.60
1	C	31	LEU	N-CA-C	6.41	118.26	111.28
1	C	94	SER	CA-C-N	6.38	128.83	120.28
1	C	94	SER	C-N-CA	6.38	128.83	120.28
1	A	95	ARG	N-CA-C	6.36	118.21	111.28
1	C	205	GLN	CA-C-N	6.36	133.15	121.70
1	C	205	GLN	C-N-CA	6.36	133.15	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASP	CA-C-N	6.31	128.03	120.14
1	B	77	ASP	C-N-CA	6.31	128.03	120.14
1	B	106	ARG	CD-NE-CZ	6.30	133.22	124.40
1	B	102	PRO	CA-C-N	6.29	128.71	120.28
1	B	102	PRO	C-N-CA	6.29	128.71	120.28
1	D	124	VAL	CA-C-N	6.28	131.35	120.68
1	D	124	VAL	C-N-CA	6.28	131.35	120.68
1	A	146	TYR	O-C-N	-6.25	115.88	123.19
1	B	29	ARG	CA-C-O	-6.23	113.94	120.55
1	B	122	ASN	CA-CB-CG	6.18	118.78	112.60
1	B	190	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	48	HIS	CA-CB-CG	6.16	119.96	113.80
1	A	101	VAL	CA-C-N	6.16	126.35	119.32
1	A	101	VAL	C-N-CA	6.16	126.35	119.32
1	A	18	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	176	PHE	CA-CB-CG	6.13	119.93	113.80
1	B	111	VAL	CB-CA-C	-6.10	105.44	111.30
1	A	150	SER	CA-C-N	6.03	128.36	120.28
1	A	150	SER	C-N-CA	6.03	128.36	120.28
1	D	18	ASP	CA-CB-CG	6.00	118.61	112.60
1	A	120	CYS	N-CA-C	5.99	118.66	108.90
1	D	92	VAL	N-CA-C	5.96	120.33	112.76
1	B	24	THR	CA-C-N	5.95	128.25	120.28
1	B	24	THR	C-N-CA	5.95	128.25	120.28
1	B	113	GLU	CB-CA-C	-5.95	109.73	116.63
1	D	48	HIS	CA-CB-CG	5.90	119.70	113.80
1	C	167	LYS	CA-C-O	-5.88	114.18	120.42
1	A	156	ASN	CA-CB-CG	5.85	118.45	112.60
1	C	171	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	124	VAL	CA-C-N	5.84	128.10	120.28
1	C	124	VAL	C-N-CA	5.84	128.10	120.28
1	D	101	VAL	CA-C-N	5.83	125.69	119.28
1	D	101	VAL	C-N-CA	5.83	125.69	119.28
1	A	30	HIS	CA-CB-CG	5.83	119.63	113.80
1	A	41	ALA	O-C-N	-5.82	114.85	122.59
1	A	129	ARG	CD-NE-CZ	5.82	132.55	124.40
1	A	137	VAL	O-C-N	-5.82	115.30	122.57
1	C	176	PHE	CA-CB-CG	5.82	119.62	113.80
1	B	48	HIS	CA-CB-CG	5.79	119.59	113.80
1	B	132	LYS	CA-C-N	5.79	128.31	120.38
1	B	132	LYS	C-N-CA	5.79	128.31	120.38
1	C	148	ASP	CA-CB-CG	5.78	118.38	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	TYR	O-C-N	-5.75	115.94	123.02
1	D	114	ASN	N-CA-C	5.74	123.02	110.80
1	A	105	HIS	CA-C-N	5.71	128.25	120.54
1	A	105	HIS	C-N-CA	5.71	128.25	120.54
1	D	31	LEU	N-CA-C	5.71	117.50	111.28
1	B	117	ILE	O-C-N	-5.71	117.00	123.10
1	C	23	LYS	CA-C-N	5.68	127.82	120.44
1	C	23	LYS	C-N-CA	5.68	127.82	120.44
1	A	156	ASN	CA-C-N	5.67	127.87	120.28
1	A	156	ASN	C-N-CA	5.67	127.87	120.28
1	D	171	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	198	GLU	CA-C-N	5.65	127.85	120.28
1	D	198	GLU	C-N-CA	5.65	127.85	120.28
1	D	91	ASP	O-C-N	-5.64	116.80	123.22
1	D	141	LYS	CA-C-N	-5.63	110.78	121.54
1	D	141	LYS	C-N-CA	-5.63	110.78	121.54
1	B	124	VAL	CA-C-N	5.63	130.25	120.68
1	B	124	VAL	C-N-CA	5.63	130.25	120.68
1	B	95	ARG	CA-C-N	5.62	129.53	120.30
1	B	95	ARG	C-N-CA	5.62	129.53	120.30
1	D	90	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	21	THR	CA-C-N	5.61	129.78	122.26
1	B	21	THR	C-N-CA	5.61	129.78	122.26
1	A	124	VAL	CA-C-N	5.59	130.19	120.68
1	A	124	VAL	C-N-CA	5.59	130.19	120.68
1	B	175	GLU	CA-CB-CG	5.59	125.28	114.10
1	A	200	ASP	N-CA-C	5.56	117.34	111.28
1	A	91	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	95	ARG	N-CA-C	5.53	117.75	111.11
1	D	122	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	D	28	LYS	O-C-N	-5.53	115.02	122.43
1	A	40	VAL	N-CA-CB	5.53	117.42	112.06
1	A	29	ARG	CA-C-O	-5.51	114.71	120.55
1	B	27	VAL	O-C-N	-5.47	116.34	121.87
1	A	154	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	197	TYR	N-CA-C	5.44	117.21	111.28
1	B	192	ALA	CA-C-N	5.42	127.54	120.28
1	B	192	ALA	C-N-CA	5.42	127.54	120.28
1	B	176	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	80	TYR	N-CA-C	5.41	119.05	112.23
1	B	200	ASP	CA-C-N	5.41	127.79	120.44
1	B	200	ASP	C-N-CA	5.41	127.79	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	ALA	N-CA-C	5.41	117.17	111.28
1	D	206	THR	CB-CA-C	-5.40	97.22	109.10
1	C	120	CYS	N-CA-C	5.39	117.68	108.90
1	A	128	ASP	CA-C-N	5.38	129.20	121.50
1	A	128	ASP	C-N-CA	5.38	129.20	121.50
1	A	11	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	196	GLN	CA-C-N	5.38	127.48	120.28
1	A	196	GLN	C-N-CA	5.38	127.48	120.28
1	B	33	GLY	CA-C-N	5.38	127.75	120.44
1	B	33	GLY	C-N-CA	5.38	127.75	120.44
1	C	122	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	133	ALA	N-CA-C	5.34	117.80	111.33
1	B	143	ASN	CA-C-O	5.34	127.37	121.39
1	B	153	SER	O-C-N	-5.34	115.78	122.24
1	C	151	ALA	N-CA-C	5.34	117.10	111.28
1	C	110	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	D	40	VAL	CA-C-N	5.33	127.43	120.28
1	D	40	VAL	C-N-CA	5.33	127.43	120.28
1	D	148	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	90	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	65	ASP	CA-C-N	-5.30	112.62	120.94
1	A	65	ASP	C-N-CA	-5.30	112.62	120.94
1	A	124	VAL	O-C-N	-5.28	115.97	122.57
1	A	149	ILE	CA-CB-CG2	5.26	119.45	110.50
1	C	125	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	140	ARG	O-C-N	-5.24	115.62	122.59
1	C	142	LYS	CA-C-N	5.24	131.48	123.47
1	C	142	LYS	C-N-CA	5.24	131.48	123.47
1	B	197	TYR	N-CA-C	5.23	116.98	111.28
1	A	197	TYR	CA-C-N	5.22	127.71	120.29
1	A	197	TYR	C-N-CA	5.22	127.71	120.29
1	A	133	ALA	CA-C-N	5.22	127.80	120.28
1	A	133	ALA	C-N-CA	5.22	127.80	120.28
1	A	171	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	143	ASN	CA-C-N	5.18	130.29	122.99
1	A	143	ASN	C-N-CA	5.18	130.29	122.99
1	B	143	ASN	N-CA-CB	5.18	119.12	110.53
1	C	122	ASN	CA-C-N	5.17	129.89	122.35
1	C	122	ASN	C-N-CA	5.17	129.89	122.35
1	B	187	VAL	CA-C-O	-5.15	116.42	121.67
1	D	77	ASP	N-CA-C	5.15	117.56	111.33
1	A	41	ALA	CA-C-N	5.14	128.82	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ALA	C-N-CA	5.14	128.82	120.60
1	B	18	ASP	CA-C-N	5.14	125.55	120.31
1	B	18	ASP	C-N-CA	5.14	125.55	120.31
1	A	75	LEU	N-CA-CB	5.14	119.14	110.77
1	A	142	LYS	CA-C-O	5.13	124.93	119.34
1	C	175	GLU	CA-CB-CG	5.12	124.35	114.10
1	D	78	GLY	N-CA-C	5.12	120.30	114.67
1	D	107	ASP	CA-C-N	5.12	127.09	120.44
1	D	107	ASP	C-N-CA	5.12	127.09	120.44
1	C	171	ASP	CB-CA-C	5.11	116.98	110.13
1	D	14	VAL	CA-C-N	5.10	130.35	123.11
1	D	14	VAL	C-N-CA	5.10	130.35	123.11
1	A	91	ASP	O-C-N	-5.10	117.51	123.27
1	B	89	MET	N-CA-C	5.09	117.69	109.40
1	A	153	SER	O-C-N	-5.07	116.10	122.24
1	A	166	ARG	CD-NE-CZ	5.07	131.50	124.40
1	D	149	ILE	CA-CB-CG2	5.07	119.12	110.50
1	A	18	ASP	CA-C-N	5.07	124.78	119.92
1	A	18	ASP	C-N-CA	5.07	124.78	119.92
1	B	18	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	190	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	18	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	35	PHE	O-C-N	-5.05	116.77	122.12
1	B	127	LYS	N-CA-C	5.05	116.86	111.36
1	B	124	VAL	O-C-N	-5.04	116.27	122.57
1	A	76	ARG	CA-C-N	5.04	127.53	120.28
1	A	76	ARG	C-N-CA	5.04	127.53	120.28
1	B	69	LEU	CA-C-N	5.04	127.86	120.71
1	B	69	LEU	C-N-CA	5.04	127.86	120.71
1	C	132	LYS	O-C-N	-5.04	117.00	122.84
1	A	89	MET	N-CA-C	5.02	117.76	109.72
1	B	110	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	133	ALA	O-C-N	-5.01	116.81	122.12
1	C	60	LYS	N-CA-C	5.01	116.56	108.34
1	B	171	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	134	LYS	CA-C-N	5.00	127.91	120.31
1	C	134	LYS	C-N-CA	5.00	127.91	120.31

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	TYR	Mainchain
1	A	27	VAL	Mainchain
1	A	41	ALA	Mainchain
1	A	54	THR	Mainchain
1	B	123	LYS	Mainchain
1	B	206	THR	Mainchain
1	B	27	VAL	Mainchain
1	B	54	THR	Mainchain
1	C	33	GLY	Mainchain
1	C	54	THR	Mainchain
1	D	190	ASP	Mainchain
1	D	54	THR	Mainchain
1	D	91	ASP	Mainchain

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	1612	0	1626	7	0
1	B	1635	0	1649	7	2
1	C	1628	0	1642	8	2
1	D	1628	0	1642	15	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	12	1	0
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	56	0	0	0	0
4	B	9	0	0	0	0
4	C	73	0	0	0	1
4	D	72	0	0	0	0
All	All	6829	0	6607	37	3

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 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ILE:HG22	1:D:136:ILE:O	1.82	0.78
1:D:134:LYS:H	1:D:134:LYS:HE2	1.49	0.78
1:D:138:PHE:O	1:D:138:PHE:HD1	1.71	0.73
1:B:158:GLU:HB3	1:B:179:MET:HE1	1.70	0.73
1:D:158:GLU:HB3	1:D:179:MET:HE1	1.77	0.67
1:C:158:GLU:HB3	1:C:179:MET:HE1	1.77	0.67
1:A:158:GLU:HB3	1:A:179:MET:HE1	1.79	0.64
1:D:127:LYS:O	1:D:128:ASP:HB2	1.98	0.63
1:D:138:PHE:O	1:D:138:PHE:CD1	2.53	0.61
1:A:140:ARG:O	1:A:140:ARG:HG3	2.00	0.60
1:D:136:ILE:O	1:D:136:ILE:CG2	2.48	0.60
1:C:134:LYS:HE3	1:C:134:LYS:H	1.67	0.59
1:A:142:LYS:O	1:A:143:ASN:HB3	2.08	0.53
1:C:101:VAL:HB	1:C:102:PRO:HD3	1.91	0.52
1:C:103:ASN:HB3	1:C:106:ARG:HH11	1.75	0.51
1:D:129:ARG:HH11	1:D:132:LYS:HA	1.76	0.50
1:A:40:VAL:O	1:A:41:ALA:C	2.53	0.50
1:B:118:VAL:HG11	1:B:160:PRO:HB3	1.95	0.48
1:D:132:LYS:HB3	1:D:134:LYS:HE3	1.96	0.47
1:B:143:ASN:HD22	1:B:143:ASN:HA	1.62	0.47
1:D:103:ASN:HB3	1:D:106:ARG:HH11	1.81	0.45
1:A:81:ILE:O	1:A:82:GLN:HB2	2.17	0.44
1:C:103:ASN:HB3	1:C:106:ARG:NH1	2.32	0.43
1:B:112:CYS:O	1:B:113:GLU:HB2	2.18	0.43
1:D:129:ARG:HD3	1:D:132:LYS:HA	2.01	0.43
1:D:72:PHE:HD2	1:D:106:ARG:HH12	1.67	0.42
1:D:118:VAL:HG23	1:D:164:LEU:HD21	2.01	0.42
1:C:159:LYS:HB2	1:C:160:PRO:HD3	2.01	0.42
1:A:59:ILE:HG21	1:A:169:ILE:HD11	2.02	0.42
1:A:123:LYS:HE2	3:A:704:GDP:N9	2.34	0.41
1:B:150:SER:HB3	1:B:155:TYR:HB3	2.03	0.41
1:B:159:LYS:HB2	1:B:160:PRO:HD3	2.02	0.41
1:C:134:LYS:H	1:C:134:LYS:CE	2.33	0.41
1:D:139:HIS:O	1:D:144:LEU:HD23	2.20	0.41
1:D:133:ALA:HB3	1:D:134:LYS:HE2	2.03	0.41
1:B:117:ILE:O	1:B:144:LEU:HA	2.21	0.40
1:C:6:GLU:HA	1:C:7:PRO:HD3	1.93	0.40

All (3) 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)
1:B:202:GLU:OE1	4:C:727:HOH:O[2_646]	1.51	0.69
1:C:28:LYS:NZ	1:D:113:GLU:OE1[2_656]	1.69	0.51
1:B:202:GLU:OE2	1:C:41:ALA:CB[2_646]	1.94	0.26

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	199/216 (92%)	183 (92%)	12 (6%)	4 (2%)	6	2
1	B	202/216 (94%)	191 (95%)	10 (5%)	1 (0%)	24	20
1	C	201/216 (93%)	198 (98%)	3 (2%)	0	100	100
1	D	201/216 (93%)	185 (92%)	13 (6%)	3 (2%)	8	4
All	All	803/864 (93%)	757 (94%)	38 (5%)	8 (1%)	12	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	B	137	VAL
1	D	128	ASP
1	D	138	PHE
1	A	140	ARG
1	D	114	ASN
1	A	139	HIS
1	A	41	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	173/185 (94%)	161 (93%)	12 (7%)	14	9
1	B	176/185 (95%)	163 (93%)	13 (7%)	13	8
1	C	175/185 (95%)	162 (93%)	13 (7%)	13	8
1	D	175/185 (95%)	162 (93%)	13 (7%)	13	8
All	All	699/740 (94%)	648 (93%)	51 (7%)	13	8

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	50	LEU
1	A	54	THR
1	A	56	ARG
1	A	76	ARG
1	A	109	VAL
1	A	132	LYS
1	A	134	LYS
1	A	138	PHE
1	A	144	LEU
1	A	159	LYS
1	A	193	LEU
1	B	15	LEU
1	B	42	THR
1	B	43	LEU
1	B	50	LEU
1	B	81	ILE
1	B	108	LEU
1	B	139	HIS
1	B	143	ASN
1	B	144	LEU
1	B	159	LYS
1	B	193	LEU
1	B	203	VAL
1	B	207	THR
1	C	15	LEU
1	C	42	THR
1	C	50	LEU
1	C	71	LYS
1	C	95	ARG
1	C	99	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	106	ARG
1	C	109	VAL
1	C	129	ARG
1	C	134	LYS
1	C	140	ARG
1	C	159	LYS
1	C	193	LEU
1	D	15	LEU
1	D	50	LEU
1	D	70	GLU
1	D	71	LYS
1	D	106	ARG
1	D	107	ASP
1	D	108	LEU
1	D	109	VAL
1	D	134	LYS
1	D	138	PHE
1	D	159	LYS
1	D	198	GLU
1	D	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	62	ASN
1	A	82	GLN
1	B	10	GLN
1	B	62	ASN
1	B	82	GLN
1	B	103	ASN
1	C	10	GLN
1	C	62	ASN
1	C	82	GLN
1	D	10	GLN
1	D	62	ASN
1	D	103	ASN

5.3.3 RNA ⓘ

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, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GDP	B	705	2	29,30,30	1.07	1 (3%)	45,47,47	0.94	3 (6%)
3	GDP	A	704	2	29,30,30	1.05	2 (6%)	45,47,47	1.21	6 (13%)
3	GDP	D	707	2	29,30,30	0.88	1 (3%)	45,47,47	1.13	3 (6%)
3	GDP	C	706	2	29,30,30	1.08	3 (10%)	45,47,47	1.04	4 (8%)

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	GDP	B	705	2	-	1/16/32/32	0/3/3/3
3	GDP	A	704	2	-	1/16/32/32	0/3/3/3
3	GDP	D	707	2	-	3/16/32/32	0/3/3/3
3	GDP	C	706	2	-	0/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	705	GDP	PA-O3A	-4.08	1.55	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	GDP	PA-O3A	-3.14	1.56	1.59
3	C	706	GDP	PA-O3A	-3.03	1.56	1.59
3	A	704	GDP	PB-O3B	-2.43	1.45	1.54
3	C	706	GDP	PB-O2B	-2.15	1.46	1.54
3	D	707	GDP	PB-O3B	-2.05	1.47	1.54
3	C	706	GDP	PA-O2A	-2.05	1.45	1.55

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	GDP	O4'-C1'-N9	3.50	116.29	108.36
3	C	706	GDP	O3B-PB-O3A	3.11	115.06	104.64
3	A	704	GDP	O3B-PB-O3A	2.80	114.03	104.64
3	D	707	GDP	O4'-C1'-N9	2.62	114.30	108.36
3	A	704	GDP	O2'-C2'-C1'	2.58	118.99	110.10
3	B	705	GDP	O4'-C1'-C2'	-2.50	101.26	106.62
3	A	704	GDP	O4'-C1'-C2'	-2.46	101.35	106.62
3	C	706	GDP	O2A-PA-O5'	2.36	118.28	107.57
3	C	706	GDP	O2B-PB-O3A	2.26	112.22	104.64
3	B	705	GDP	O2'-C2'-C1'	2.14	117.46	110.10
3	A	704	GDP	C2'-C1'-N9	-2.12	107.34	113.25
3	C	706	GDP	O4'-C1'-C2'	-2.11	102.11	106.62
3	A	704	GDP	O2B-PB-O3A	2.07	111.57	104.64
3	D	707	GDP	O2A-PA-O5'	2.06	116.90	107.57
3	D	707	GDP	O2B-PB-O3A	2.05	111.52	104.64
3	B	705	GDP	O2B-PB-O3A	2.04	111.48	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

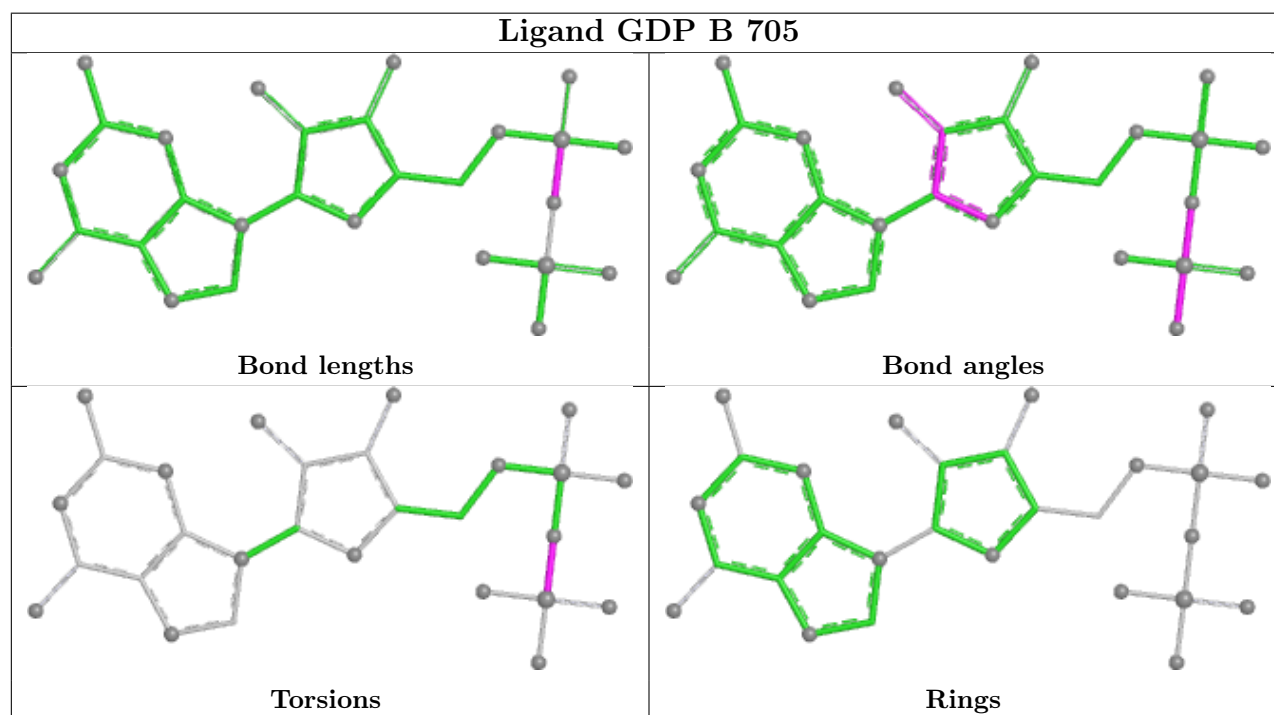
Mol	Chain	Res	Type	Atoms
3	D	707	GDP	O4'-C4'-C5'-O5'
3	D	707	GDP	C3'-C4'-C5'-O5'
3	A	704	GDP	PA-O3A-PB-O3B
3	B	705	GDP	PA-O3A-PB-O3B
3	D	707	GDP	PA-O3A-PB-O3B

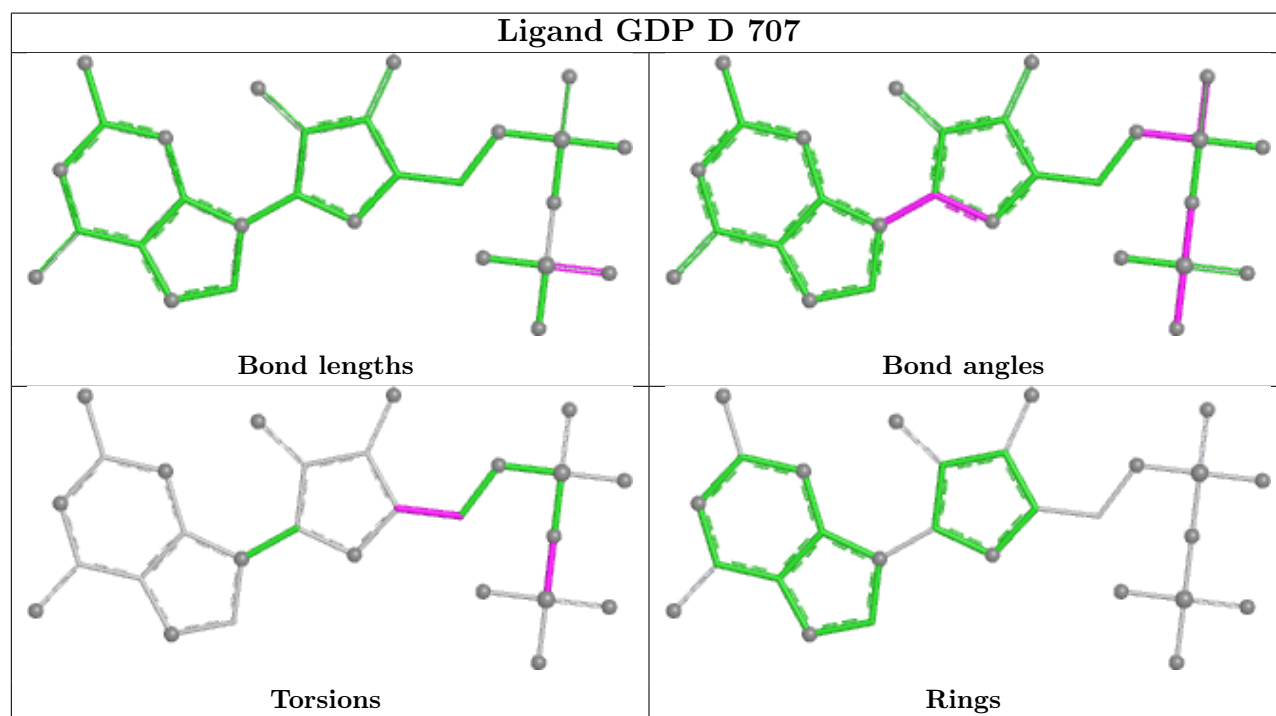
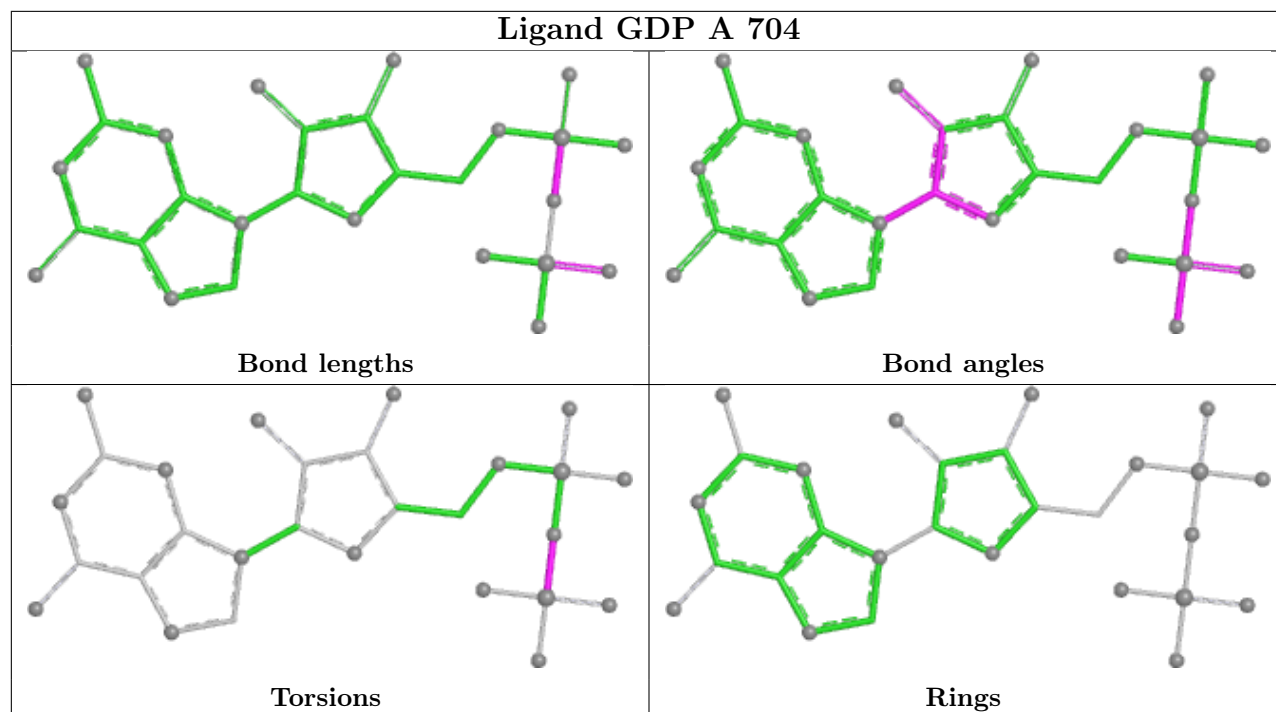
There are no ring outliers.

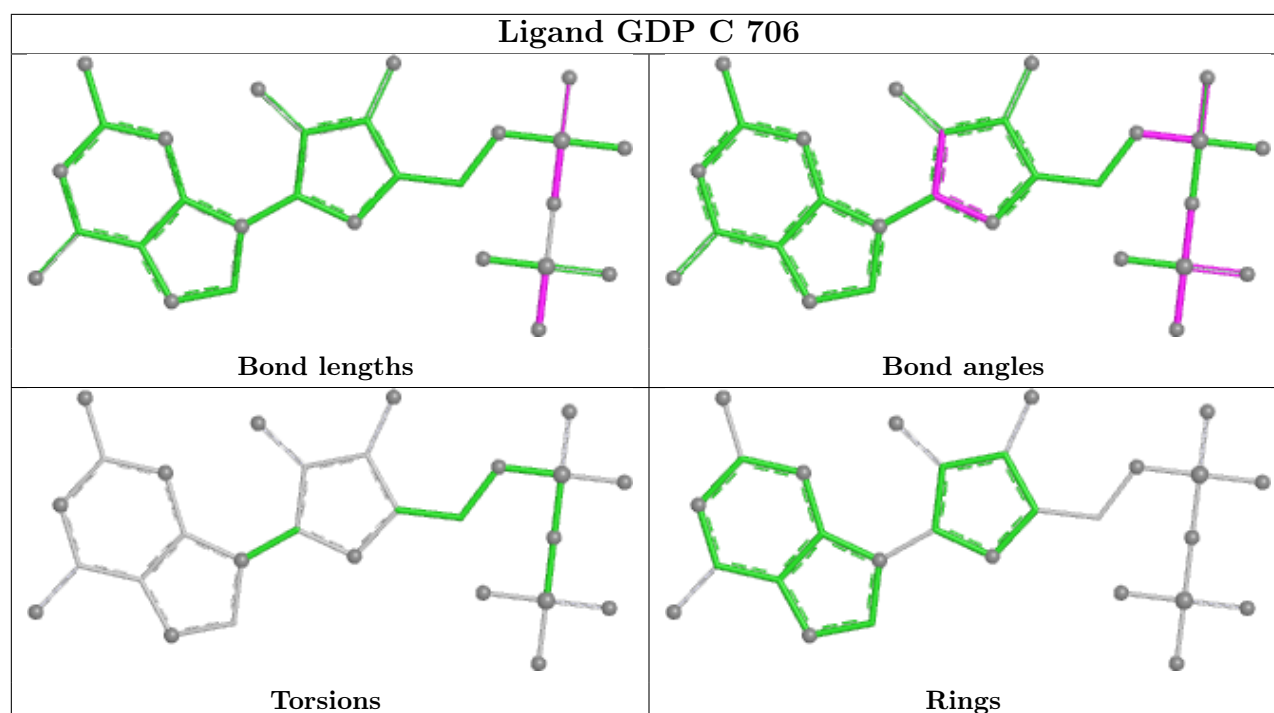
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	GDP	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.