



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 6S6D / pdb_00006s6d
Title : Crystal structure of RagA-Q66L-GTP/RagC-S75N-GDP GTPase heterodimer complex
Authors : Anandapadamanaban, M.; Masson, G.R.; Perisic, O.; Kaufman, J.; Williams, R.L.
Deposited on : 2019-07-02
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

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

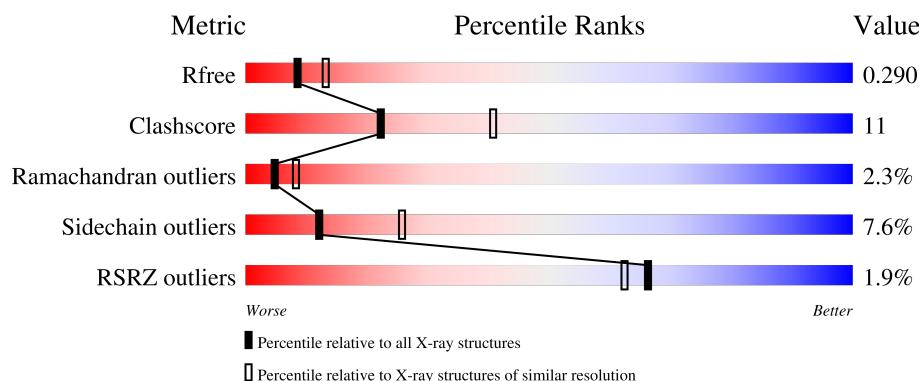
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	313	0% 73% 19% • •
1	B	313	0% 71% 20% • •
2	C	399	2% 54% 16% • 29%
2	D	399	2% 42% 21% 5% • 32%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9584 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 GTP-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2462	1564	429	452	17			
1	B	300	Total	C	N	O	S	0	1	0
			2461	1566	426	452	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	LEU	GLN	engineered mutation	UNP Q7L523
B	66	LEU	GLN	engineered mutation	UNP Q7L523

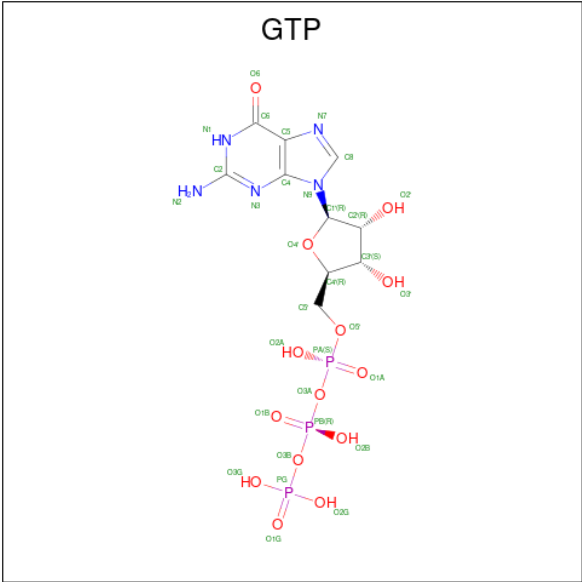
- Molecule 2 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	284	Total	C	N	O	S	0	1	0
			2288	1473	373	429	13			
2	D	272	Total	C	N	O	S	0	0	0
			2185	1403	359	411	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	75	ASN	SER	engineered mutation	UNP Q9HB90
D	75	ASN	SER	engineered mutation	UNP Q9HB90

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

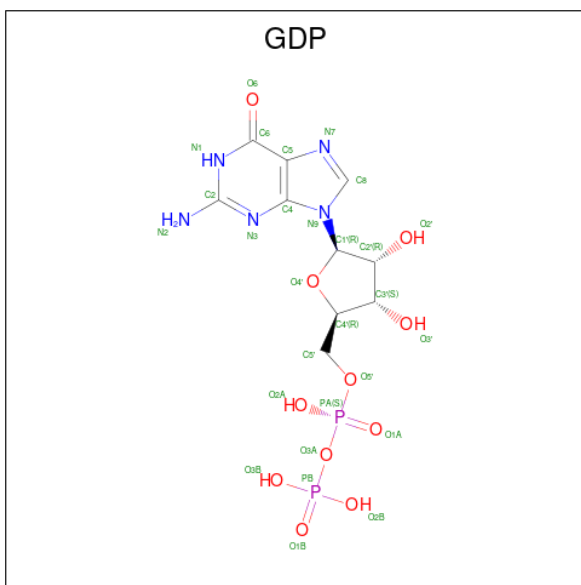


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

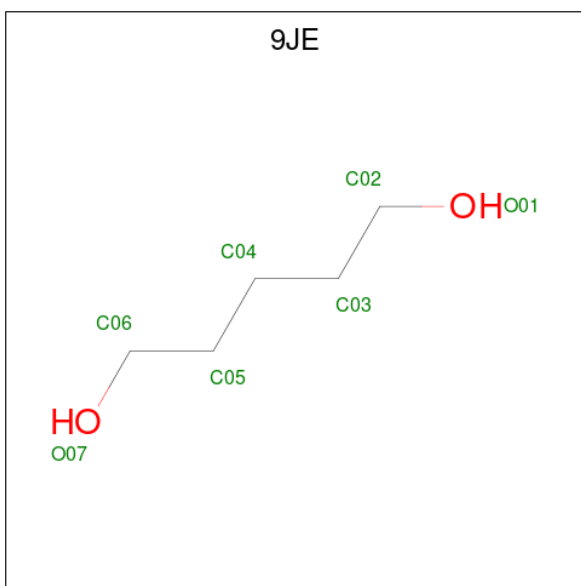
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is pentane-1,5-diol (CCD ID: 9JE) (formula: $\text{C}_5\text{H}_{12}\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 7 5 2	0	0
6	B	1	Total C O 7 5 2	0	0

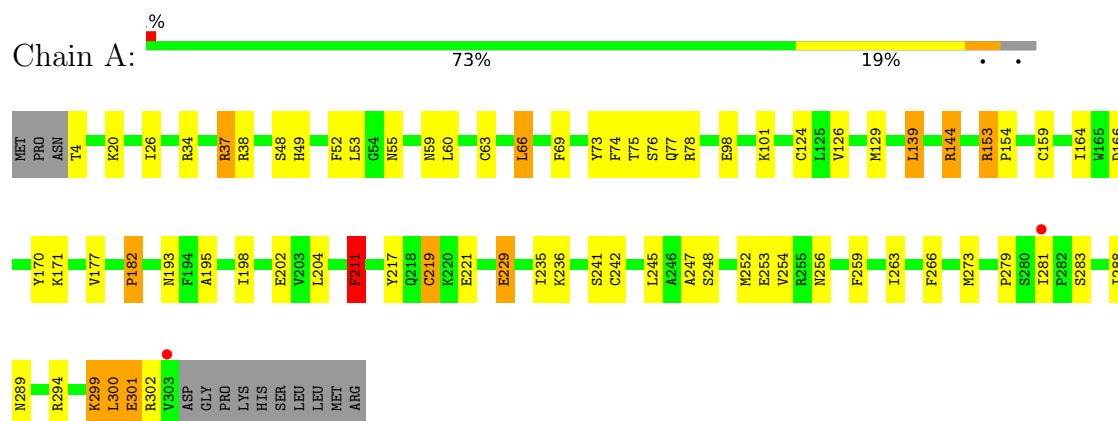
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total 14	O 14	0	0
7	C	15	Total 15	O 15	0	0
7	B	18	Total 18	O 18	0	0
7	D	5	Total 5	O 5	0	0

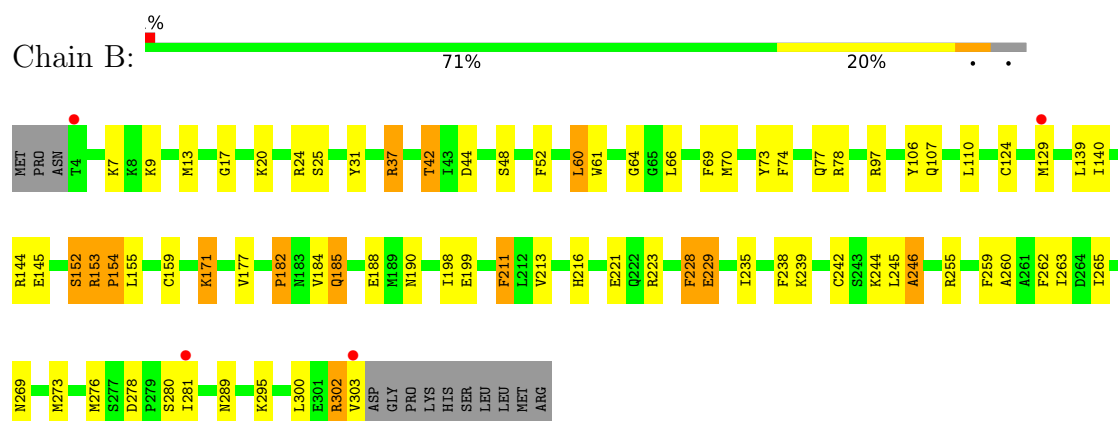
3 Residue-property plots

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 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.

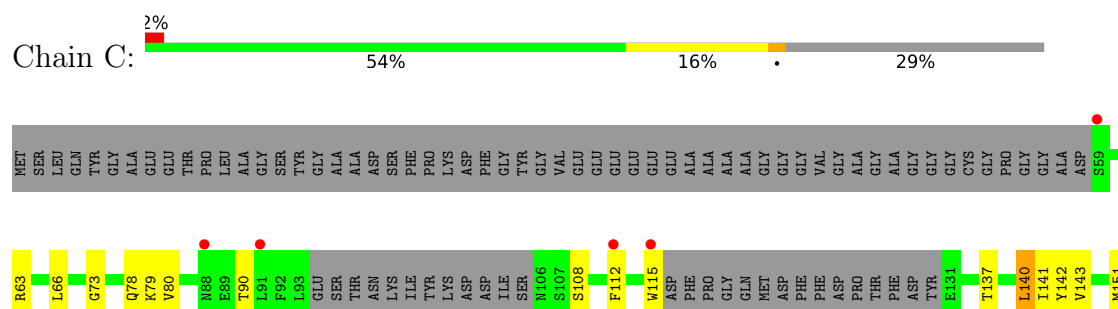
• Molecule 1: Ras-related GTP-binding protein A

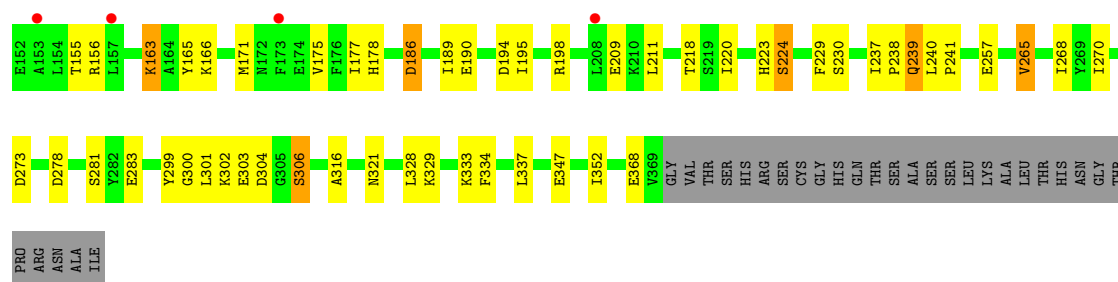


• Molecule 1: Ras-related GTP-binding protein A

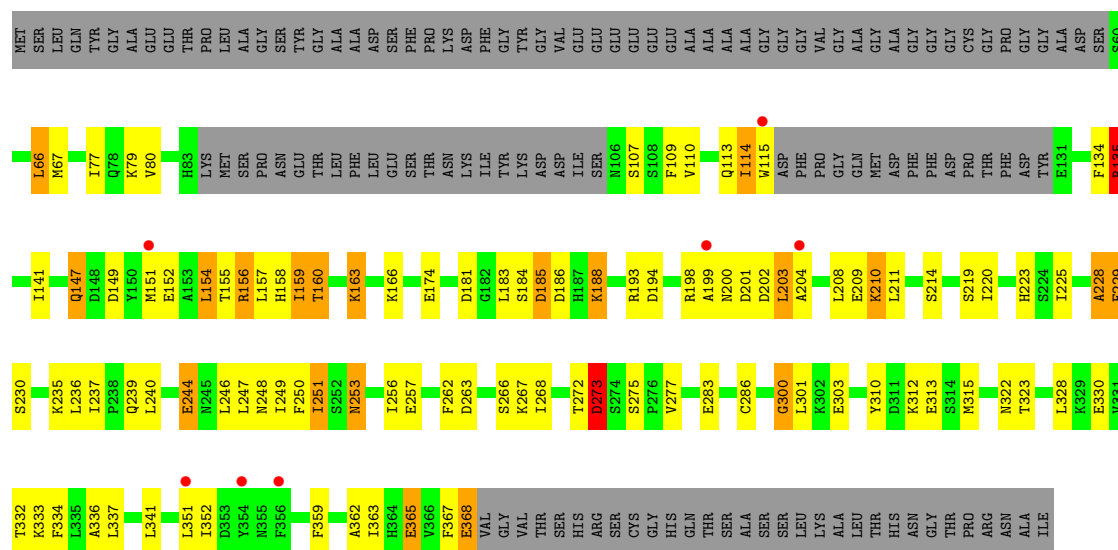
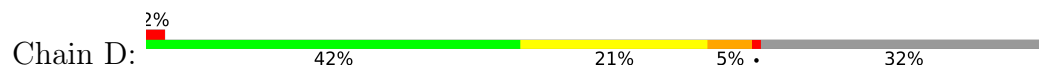


• Molecule 2: Ras-related GTP-binding protein C





• Molecule 2: Ras-related GTP-binding protein C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.50Å 81.44Å 246.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.50 49.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-2.50) 99.7 (49.29-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.287 0.214 , 0.290	Depositor DCC
R_{free} test set	2458 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9584	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 9JE, 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	1.08	0/2507	1.46	6/3376 (0.2%)
1	B	1.08	1/2509 (0.0%)	1.52	5/3380 (0.1%)
2	C	1.14	1/2335 (0.0%)	1.54	9/3149 (0.3%)
2	D	1.10	0/2224	1.53	5/2997 (0.2%)
All	All	1.10	2/9575 (0.0%)	1.51	25/12902 (0.2%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	229	PHE	C-O	5.84	1.30	1.24
1	B	153	ARG	N-CA	5.22	1.51	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	178	HIS	CB-CA-C	6.56	120.62	109.80
2	C	273	ASP	CA-CB-CG	-6.24	106.36	112.60
1	B	228	PHE	CA-C-N	5.74	127.97	120.28
1	B	228	PHE	C-N-CA	5.74	127.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	SER	CA-C-O	-5.56	113.06	119.56
1	A	229	GLU	CB-CA-C	-5.51	101.64	110.79
1	B	154	PRO	N-CA-C	-5.30	106.16	113.53
1	A	144	ARG	N-CA-C	-5.28	105.52	111.28
2	C	304	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	166	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	77	GLN	CA-C-N	5.20	127.50	120.38
1	A	77	GLN	C-N-CA	5.20	127.50	120.38
1	A	211	PHE	CA-CB-CG	-5.19	108.61	113.80
2	D	351	LEU	CA-C-N	5.19	127.57	120.46
2	D	351	LEU	C-N-CA	5.19	127.57	120.46
2	C	195	ILE	CA-C-N	5.13	127.42	120.44
2	C	195	ILE	C-N-CA	5.13	127.42	120.44
2	C	265	VAL	N-CA-C	-5.12	105.85	110.82
1	B	229	GLU	CB-CA-C	-5.09	102.34	110.79
2	C	73	GLY	CA-C-N	5.06	127.37	120.54
2	C	73	GLY	C-N-CA	5.06	127.37	120.54
2	D	186	ASP	CA-C-N	5.04	128.74	120.63
2	D	186	ASP	C-N-CA	5.04	128.74	120.63
2	C	352	ILE	N-CA-C	-5.02	105.09	110.36
2	D	273	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	152	SER	Peptide
1	B	255	ARG	Peptide
2	C	306	SER	Peptide
2	D	262	PHE	Peptide

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	2462	0	2462	49	0
1	B	2461	0	2463	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2288	0	2279	40	0
2	D	2185	0	2182	70	0
3	A	32	0	12	1	0
3	B	32	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	28	0	12	0	0
5	D	28	0	12	0	0
6	B	14	0	0	2	0
7	A	14	0	0	4	0
7	B	18	0	0	2	0
7	C	15	0	0	2	0
7	D	5	0	0	2	0
All	All	9584	0	9434	200	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 11.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASN:HD22	1:B:300:LEU:HD11	1.16	1.09
1:A:236:LYS:HE2	7:A:506:HOH:O	1.61	0.99
2:D:183:LEU:HB2	2:D:188:LYS:HE2	1.48	0.95
1:A:126:VAL:HG12	1:A:129:MET:HE1	1.49	0.95
1:A:252:MET:HE3	1:A:263:ILE:HD12	1.54	0.90
2:D:200:ASN:HA	2:D:203:LEU:HD21	1.53	0.89
1:A:217:TYR:HH	1:A:219:CYS:HG	1.11	0.84
2:C:186:ASP:O	2:C:190:GLU:HG3	1.86	0.75
2:D:183:LEU:CB	2:D:188:LYS:HE2	2.17	0.74
2:D:184:SER:C	2:D:188:LYS:HZ3	1.95	0.74
1:A:153:ARG:HB3	1:A:154:PRO:HD3	1.70	0.73
2:D:208:LEU:HA	2:D:210:LYS:HE3	1.71	0.73
1:A:153:ARG:CB	1:A:154:PRO:CD	2.67	0.72
1:B:185:GLN:H	1:B:185:GLN:CD	1.96	0.71
2:D:322:ASN:O	2:D:323:THR:OG1	2.08	0.71
1:A:37:ARG:NH1	3:A:401:GTP:O2'	2.25	0.69
2:D:199:ALA:O	2:D:203:LEU:CD2	2.43	0.67
1:B:190:ASN:ND2	1:B:300:LEU:HD11	2.00	0.66
1:A:248:SER:CB	2:C:321:ASN:HD22	2.08	0.66
1:B:24:ARG:HD3	1:B:60:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:ALA:O	2:D:203:LEU:HD21	1.95	0.65
1:A:171:LYS:HB2	1:A:229:GLU:HG2	1.79	0.65
1:A:248:SER:HB3	2:C:321:ASN:HD22	1.61	0.64
1:A:75:THR:OG1	1:A:76:SER:N	2.29	0.64
1:A:49:HIS:CE1	1:A:59:ASN:OD1	2.51	0.64
1:B:211:PHE:CZ	1:B:235:ILE:HG21	2.33	0.64
1:A:144:ARG:HD2	7:A:514:HOH:O	1.97	0.63
1:B:302:ARG:HH11	1:B:302:ARG:HG2	1.63	0.63
2:D:79:LYS:HB2	7:D:505:HOH:O	1.98	0.63
1:B:24:ARG:CD	1:B:60:LEU:HD13	2.30	0.60
1:A:153:ARG:HB3	1:A:154:PRO:CD	2.30	0.60
1:A:52:PHE:CZ	1:A:177:VAL:HG11	2.36	0.60
1:B:107:GLN:NE2	6:B:403:9JE:C06	2.65	0.60
2:D:200:ASN:CA	2:D:203:LEU:HD21	2.30	0.59
2:D:203:LEU:HD22	7:D:504:HOH:O	2.02	0.59
1:A:153:ARG:HB2	1:A:154:PRO:HD2	1.84	0.59
1:A:198:ILE:HG13	1:A:289:ASN:HD22	1.68	0.59
2:D:194:ASP:OD1	2:D:198:ARG:NE	2.31	0.59
1:B:42:THR:HB	3:B:401:GTP:O1G	2.02	0.59
2:C:218:THR:HA	2:C:224:SER:HB2	1.86	0.58
1:B:302:ARG:HG2	1:B:302:ARG:NH1	2.18	0.58
2:C:165:TYR:CD2	2:C:211:LEU:HD12	2.39	0.58
1:A:263:ILE:HG12	1:A:273:MET:HG3	1.86	0.58
1:A:281:ILE:HD12	1:A:281:ILE:O	2.04	0.57
2:D:183:LEU:HB2	2:D:188:LYS:CE	2.29	0.57
2:D:185:ASP:N	2:D:188:LYS:HZ3	2.01	0.57
1:B:66:LEU:HB2	1:B:69:PHE:CD2	2.40	0.57
2:D:109:PHE:O	2:D:109:PHE:CG	2.58	0.57
1:A:299:LYS:HG3	1:A:300:LEU:HD12	1.87	0.57
2:C:347:GLU:HB3	1:B:185:GLN:HG3	1.87	0.57
1:B:213:VAL:HG21	1:B:228:PHE:HB3	1.86	0.57
2:D:300:GLY:O	2:D:301:LEU:HD12	2.06	0.56
1:A:211:PHE:CE2	1:A:235:ILE:HG21	2.41	0.56
2:D:251:ILE:CD1	2:D:273:ASP:HB3	2.36	0.55
2:D:80:VAL:HG21	2:D:220:ILE:HB	1.88	0.55
2:C:299:TYR:O	2:C:300:GLY:C	2.47	0.55
2:D:159:ILE:C	2:D:163:LYS:HE3	2.32	0.55
2:C:239:GLN:H	2:C:239:GLN:HE21	1.55	0.55
2:D:246:LEU:HA	2:D:249:ILE:HD12	1.89	0.55
1:A:217:TYR:OH	1:A:219:CYS:SG	2.39	0.55
1:A:195:ALA:HB1	1:A:217:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:OE2	1:A:204:LEU:HD21	2.07	0.54
1:A:217:TYR:CD1	1:A:217:TYR:C	2.85	0.54
1:A:170:TYR:OH	1:A:236:LYS:HG2	2.09	0.53
2:D:203:LEU:HB2	2:D:208:LEU:O	2.08	0.53
2:D:184:SER:C	2:D:188:LYS:NZ	2.65	0.53
2:D:107:SER:HA	2:D:334:PHE:CE1	2.44	0.53
2:D:283:GLU:O	2:D:286:CYS:HB2	2.10	0.52
2:D:228:ALA:O	2:D:230:SER:N	2.43	0.52
2:C:79:LYS:CD	2:C:90:THR:HG22	2.40	0.52
2:D:367:PHE:O	2:D:368:GLU:C	2.53	0.52
2:D:249:ILE:O	2:D:253:ASN:HB2	2.09	0.52
1:A:144:ARG:CD	7:A:514:HOH:O	2.57	0.51
1:B:244:LYS:O	1:B:246:ALA:N	2.42	0.51
2:C:66:LEU:HD12	2:C:141:ILE:HB	1.91	0.51
1:B:302:ARG:NH1	1:B:302:ARG:O	2.37	0.51
2:C:163:LYS:O	2:C:166:LYS:HB3	2.11	0.51
1:A:153:ARG:HB2	1:A:154:PRO:CD	2.40	0.51
2:D:251:ILE:CD1	2:D:273:ASP:CB	2.89	0.51
1:A:124:CYS:O	1:A:159:CYS:HA	2.11	0.51
1:B:211:PHE:CE2	1:B:235:ILE:HG21	2.46	0.50
1:A:73:TYR:O	1:A:78:ARG:HA	2.11	0.50
2:D:310:TYR:OH	2:D:330:GLU:HA	2.12	0.50
1:A:248:SER:HB3	2:C:321:ASN:ND2	2.27	0.49
2:C:140:LEU:C	2:C:140:LEU:HD12	2.37	0.49
2:D:251:ILE:HG22	2:D:256:ILE:O	2.11	0.49
1:B:70:MET:HA	1:B:73:TYR:CD2	2.47	0.49
2:D:247:LEU:HD23	2:D:359:PHE:CE2	2.47	0.49
1:A:66:LEU:HB2	1:A:69:PHE:CD2	2.47	0.49
2:C:140:LEU:HD12	2:C:141:ILE:N	2.26	0.49
1:B:262:PHE:O	1:B:273:MET:HA	2.13	0.49
1:A:253:GLU:O	2:C:316:ALA:HA	2.13	0.49
2:C:79:LYS:HD3	2:C:90:THR:HG22	1.95	0.49
1:B:244:LYS:C	1:B:246:ALA:H	2.20	0.49
2:D:154:LEU:O	2:D:157:LEU:HB3	2.13	0.49
2:D:322:ASN:C	2:D:323:THR:HG1	2.18	0.49
2:C:223[A]:HIS:CD2	2:C:283:GLU:HG3	2.48	0.48
2:C:223[B]:HIS:CD2	2:C:283:GLU:HG3	2.48	0.48
2:C:328:LEU:HA	2:C:337:LEU:O	2.13	0.48
1:A:20:LYS:HE3	1:A:63:CYS:O	2.13	0.48
1:B:245:LEU:O	1:B:246:ALA:CB	2.62	0.48
1:B:44:ASP:OD1	1:B:77:GLN:NE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLU:HB3	1:A:101:LYS:HB3	1.96	0.47
2:C:211:LEU:HD23	2:C:211:LEU:C	2.38	0.47
2:D:193:ARG:O	2:D:194:ASP:C	2.56	0.47
1:B:185:GLN:CD	1:B:185:GLN:N	2.68	0.47
1:B:17:GLY:HA2	3:B:401:GTP:H5'	1.97	0.47
1:B:238:PHE:CE2	1:B:242:CYS:SG	3.08	0.47
2:D:263:ASP:HA	2:D:334:PHE:O	2.15	0.47
2:C:78:GLN:HE21	2:C:112:PHE:HE2	1.62	0.47
2:C:80:VAL:HG21	2:C:220:ILE:HB	1.96	0.47
2:C:137:THR:HG22	2:C:171:MET:HE2	1.95	0.47
1:B:66:LEU:HD12	1:B:69:PHE:HE2	1.80	0.47
2:C:211:LEU:HD23	2:C:211:LEU:O	2.16	0.46
2:D:113:GLN:O	2:D:114:ILE:HD12	2.16	0.46
2:D:203:LEU:O	2:D:208:LEU:N	2.49	0.46
2:D:201:ASP:O	2:D:204:ALA:N	2.48	0.46
2:C:238:PRO:HD2	2:C:239:GLN:NE2	2.31	0.46
2:D:152:GLU:O	2:D:156:ARG:HD3	2.15	0.46
1:B:74:PHE:O	1:B:78:ARG:HD2	2.16	0.45
1:B:110:LEU:HB3	1:B:155:LEU:CD1	2.47	0.45
2:D:141:ILE:HA	2:D:174:GLU:O	2.16	0.45
1:A:53:LEU:O	1:A:301:GLU:HB2	2.17	0.45
1:A:195:ALA:CB	1:A:217:TYR:CD1	2.98	0.45
1:B:13:MET:C	1:B:20:LYS:HD3	2.42	0.45
1:A:55:ASN:ND2	1:A:182:PRO:HD2	2.31	0.45
1:A:74:PHE:O	1:A:78:ARG:NH1	2.49	0.45
2:D:183:LEU:C	2:D:188:LYS:HE2	2.42	0.45
2:D:230:SER:HA	2:D:268:ILE:HG23	1.98	0.45
2:D:273:ASP:OD1	2:D:273:ASP:C	2.60	0.45
1:A:256:ASN:HB2	1:A:259:PHE:CD1	2.52	0.45
1:A:266:PHE:O	1:A:294:ARG:HD3	2.17	0.45
2:C:301:LEU:HD12	2:C:301:LEU:HA	1.82	0.45
1:A:171:LYS:CB	1:A:229:GLU:HG2	2.46	0.44
1:B:52:PHE:CZ	1:B:177:VAL:HG11	2.52	0.44
2:D:239:GLN:NE2	2:D:239:GLN:H	2.15	0.44
1:B:216:HIS:HD2	6:B:404:9JE:O07	2.01	0.44
2:D:66:LEU:HD12	2:D:141:ILE:HB	1.99	0.44
2:D:114:ILE:CG2	2:D:115:TRP:N	2.80	0.44
1:B:153:ARG:N	1:B:154:PRO:HD2	2.33	0.44
1:B:42:THR:HG22	1:B:64:GLY:CA	2.48	0.43
1:B:235:ILE:HD11	1:B:263:ILE:HD13	2.00	0.43
2:C:230:SER:HA	2:C:268:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:ILE:HA	2:D:341:LEU:HB3	2.01	0.43
2:D:359:PHE:O	2:D:362:ALA:HB3	2.19	0.43
1:A:248:SER:HB2	2:C:321:ASN:HD22	1.82	0.43
2:C:220:ILE:HA	7:C:504:HOH:O	2.19	0.43
2:C:303:GLU:OE2	2:C:303:GLU:HA	2.18	0.43
1:B:259:PHE:CD2	1:B:260:ALA:N	2.87	0.43
2:D:247:LEU:HD12	2:D:272:THR:C	2.43	0.43
1:B:221:GLU:OE2	1:B:221:GLU:HA	2.18	0.43
1:A:195:ALA:HB1	1:A:217:TYR:CE1	2.54	0.42
2:C:194:ASP:OD1	2:C:198:ARG:NE	2.43	0.42
1:B:171:LYS:HB2	1:B:229:GLU:HG2	2.01	0.42
1:B:185:GLN:H	1:B:185:GLN:NE2	2.17	0.42
2:C:240:LEU:HB3	2:C:241:PRO:HD3	2.01	0.42
2:C:278:ASP:O	2:C:281:SER:HB2	2.19	0.42
2:D:147:GLN:HE21	2:D:147:GLN:HB3	1.60	0.42
2:D:181:ASP:HB3	2:D:219:SER:OG	2.20	0.42
1:B:9:LYS:HE3	1:B:61:TRP:CE2	2.54	0.42
2:D:228:ALA:O	2:D:229:PHE:C	2.62	0.42
1:B:124:CYS:O	1:B:159:CYS:HA	2.20	0.42
1:B:188:GLU:HG3	7:B:509:HOH:O	2.19	0.42
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.88	0.42
2:C:151:MET:HE3	2:C:151:MET:HA	2.01	0.42
2:D:183:LEU:CB	2:D:188:LYS:CE	2.93	0.42
2:D:365:GLU:O	2:D:368:GLU:N	2.49	0.42
1:A:34:ARG:NH2	7:A:502:HOH:O	2.40	0.42
1:B:140:ILE:O	1:B:144:ARG:HG2	2.19	0.42
2:D:272:THR:HG21	2:D:277:VAL:HG21	2.02	0.42
1:A:241:SER:O	1:A:245:LEU:HG	2.19	0.42
2:D:77:ILE:HG23	2:D:225:ILE:HD11	2.00	0.42
1:A:26:ILE:CD1	1:A:164:ILE:HB	2.50	0.41
1:B:37:ARG:NE	7:B:505:HOH:O	2.53	0.41
1:B:198:ILE:HG13	1:B:289:ASN:HD22	1.85	0.41
2:D:158:HIS:C	2:D:160:THR:H	2.27	0.41
2:D:163:LYS:H	2:D:163:LYS:HE2	1.83	0.41
1:B:106:TYR:CZ	1:B:110:LEU:HD11	2.54	0.41
2:C:142:TYR:O	2:C:175:VAL:HA	2.19	0.41
2:C:333:LYS:HE3	2:C:334:PHE:CZ	2.55	0.41
2:D:149:ASP:O	2:D:151:MET:N	2.54	0.41
2:D:240:LEU:HG	2:D:244:GLU:OE2	2.21	0.41
2:D:266:SER:O	2:D:267:LYS:HB2	2.20	0.41
1:A:242:CYS:HB3	1:A:247:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:PHE:O	2:D:135:ARG:C	2.64	0.41
2:D:237:ILE:HG23	2:D:239:GLN:HE21	1.86	0.41
2:C:142:TYR:CE1	2:C:143:VAL:O	2.74	0.40
1:B:276:MET:HE2	1:B:281:ILE:HG12	2.03	0.40
2:D:247:LEU:O	2:D:251:ILE:HG13	2.21	0.40
2:D:310:TYR:OH	2:D:336:ALA:HB2	2.21	0.40
2:D:114:ILE:HG23	2:D:115:TRP:N	2.36	0.40
1:B:25:SER:HB2	1:B:31:TYR:CD1	2.57	0.40
2:D:214:SER:OG	2:D:235:LYS:NZ	2.55	0.40
2:D:244:GLU:O	2:D:248:ASN:ND2	2.54	0.40
2:C:220:ILE:CA	7:C:504:HOH:O	2.69	0.40
2:C:237:ILE:HD13	2:C:270:ILE:HB	2.03	0.40
2:C:301:LEU:O	2:C:302:LYS:HB2	2.21	0.40
1:B:199:GLU:O	1:B:276:MET:HE1	2.22	0.40
2:D:250:PHE:CE2	2:D:256:ILE:CD1	3.04	0.40
2:D:328:LEU:HA	2:D:337:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/313 (95%)	274 (92%)	17 (6%)	7 (2%)	5	8
1	B	299/313 (96%)	270 (90%)	24 (8%)	5 (2%)	7	13
2	C	279/399 (70%)	261 (94%)	15 (5%)	3 (1%)	11	22
2	D	266/399 (67%)	216 (81%)	39 (15%)	11 (4%)	2	3
All	All	1142/1424 (80%)	1021 (89%)	95 (8%)	26 (2%)	5	8

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	299	LYS
1	B	48	SER
1	B	246	ALA
1	B	280	SER
2	D	135	ARG
2	D	185	ASP
2	D	229	PHE
1	A	279	PRO
2	D	159	ILE
1	A	182	PRO
1	A	221	GLU
1	A	300	LEU
2	C	163	LYS
2	C	368	GLU
2	D	257	GLU
2	D	202	ASP
2	D	228	ALA
1	A	193	ASN
2	C	177	ILE
2	D	209	GLU
2	D	211	LEU
1	B	302	ARG
1	B	182	PRO
2	D	110	VAL
2	D	300	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	275/287 (96%)	261 (95%)	14 (5%)	21	43
1	B	275/287 (96%)	255 (93%)	20 (7%)	13	27
2	C	258/340 (76%)	243 (94%)	15 (6%)	18	38
2	D	246/340 (72%)	215 (87%)	31 (13%)	4	9
All	All	1054/1254 (84%)	974 (92%)	80 (8%)	12	26

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	37	ARG
1	A	38	ARG
1	A	48	SER
1	A	60	LEU
1	A	66	LEU
1	A	139	LEU
1	A	211	PHE
1	A	219	CYS
1	A	254	VAL
1	A	283	SER
1	A	288	ILE
1	A	301	GLU
1	A	302	ARG
2	C	63	ARG
2	C	108	SER
2	C	115	TRP
2	C	140	LEU
2	C	155	THR
2	C	156	ARG
2	C	186	ASP
2	C	189	ILE
2	C	209	GLU
2	C	224	SER
2	C	239	GLN
2	C	257	GLU
2	C	265	VAL
2	C	306	SER
2	C	329	LYS
1	B	7	LYS
1	B	37	ARG
1	B	42	THR
1	B	60	LEU
1	B	97	ARG
1	B	129	MET
1	B	139	LEU
1	B	145	GLU
1	B	171	LYS
1	B	182	PRO
1	B	184	VAL
1	B	185	GLN
1	B	211	PHE

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Mol	Chain	Res	Type
1	B	223	ARG
1	B	239	LYS
1	B	265	ILE
1	B	269	ASN
1	B	278	ASP
1	B	295	LYS
1	B	303	VAL
2	D	66	LEU
2	D	67	MET
2	D	114	ILE
2	D	135	ARG
2	D	147	GLN
2	D	154	LEU
2	D	155	THR
2	D	156	ARG
2	D	160	THR
2	D	163	LYS
2	D	166	LYS
2	D	188	LYS
2	D	203	LEU
2	D	210	LYS
2	D	223	HIS
2	D	236	LEU
2	D	244	GLU
2	D	251	ILE
2	D	253	ASN
2	D	273	ASP
2	D	275	SER
2	D	303	GLU
2	D	312	LYS
2	D	313	GLU
2	D	315	MET
2	D	332	THR
2	D	333	LYS
2	D	352	ILE
2	D	363	ILE
2	D	365	GLU
2	D	368	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	289	ASN
2	C	78	GLN
2	C	196	HIS
2	C	239	GLN
2	C	321	ASN
1	B	30	ASN
1	B	49	HIS
1	B	80	ASN
1	B	185	GLN
1	B	186	GLN
1	B	190	ASN
1	B	193	ASN
1	B	256	ASN
1	B	269	ASN
1	B	289	ASN
2	D	75	ASN
2	D	113	GLN
2	D	147	GLN
2	D	187	HIS
2	D	196	HIS
2	D	197	GLN
2	D	234	GLN
2	D	239	GLN
2	D	248	ASN
2	D	253	ASN
2	D	321	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	A	401	4	33,34,34	0.63	0	50,54,54	0.78	0
6	9JE	B	403	-	6,6,6	0.54	0	5,5,5	0.91	0
5	GDP	C	401	-	29,30,30	1.18	4 (13%)	45,47,47	1.82	13 (28%)
3	GTP	B	401	4	33,34,34	0.82	1 (3%)	50,54,54	0.67	1 (2%)
6	9JE	B	404	-	6,6,6	0.35	0	5,5,5	0.52	0
5	GDP	D	401	-	29,30,30	1.23	5 (17%)	45,47,47	1.70	7 (15%)

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	GTP	A	401	4	-	2/22/38/38	0/3/3/3
6	9JE	B	403	-	-	2/4/4/4	-
5	GDP	C	401	-	-	5/16/32/32	0/3/3/3
3	GTP	B	401	4	-	0/22/38/38	0/3/3/3
6	9JE	B	404	-	-	3/4/4/4	-
5	GDP	D	401	-	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	GDP	C4-N9	-2.80	1.30	1.38
5	D	401	GDP	C5-C4	2.78	1.46	1.38
5	C	401	GDP	C5-C4	2.72	1.46	1.38
3	B	401	GTP	PA-O3A	2.69	1.62	1.59
5	D	401	GDP	C5-N7	-2.49	1.34	1.39
5	D	401	GDP	PA-O3A	2.36	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	GDP	C6-N1	-2.29	1.34	1.38
5	C	401	GDP	C5-N7	-2.25	1.34	1.39
5	D	401	GDP	C4-N9	-2.21	1.32	1.38
5	C	401	GDP	C6-N1	-2.17	1.34	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	GDP	C5-C4-N3	-4.99	120.45	128.39
5	C	401	GDP	C2-N3-C4	4.29	119.70	112.30
5	C	401	GDP	C5-C4-N3	-4.13	121.81	128.39
5	D	401	GDP	C2-N3-C4	4.01	119.20	112.30
5	D	401	GDP	N9-C4-N3	3.73	133.41	125.95
5	C	401	GDP	C6-C5-N7	3.57	136.79	130.29
5	C	401	GDP	O3B-PB-O3A	3.25	115.55	104.64
5	D	401	GDP	C6-C5-N7	3.21	136.13	130.29
5	C	401	GDP	N9-C4-N3	3.04	132.04	125.95
5	C	401	GDP	O3'-C3'-C2'	-2.77	102.94	111.82
5	C	401	GDP	O3A-PA-O1A	-2.75	102.42	110.70
5	C	401	GDP	O4'-C4'-C5'	-2.74	100.57	109.33
3	B	401	GTP	O3G-PG-O3B	2.55	113.17	104.64
5	D	401	GDP	O6-C6-C5	-2.51	119.91	126.53
5	D	401	GDP	C4-C5-N7	-2.45	106.78	110.67
5	C	401	GDP	C1'-N9-C4	-2.17	120.07	126.49
5	C	401	GDP	O2A-PA-O3A	2.15	113.08	107.27
5	C	401	GDP	O6-C6-C5	-2.06	121.10	126.53
5	C	401	GDP	C4-C5-N7	-2.06	107.41	110.67
5	D	401	GDP	O2A-PA-O1A	2.05	121.99	112.44
5	C	401	GDP	C6-C5-C4	-2.01	115.80	118.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	GDP	C5'-O5'-PA-O3A
5	D	401	GDP	PA-O3A-PB-O3B
5	C	401	GDP	O4'-C4'-C5'-O5'
6	B	404	9JE	C03-C04-C05-C06
5	C	401	GDP	C3'-C4'-C5'-O5'
6	B	404	9JE	C02-C03-C04-C05
3	A	401	GTP	PA-O3A-PB-O1B
5	C	401	GDP	C5'-O5'-PA-O1A

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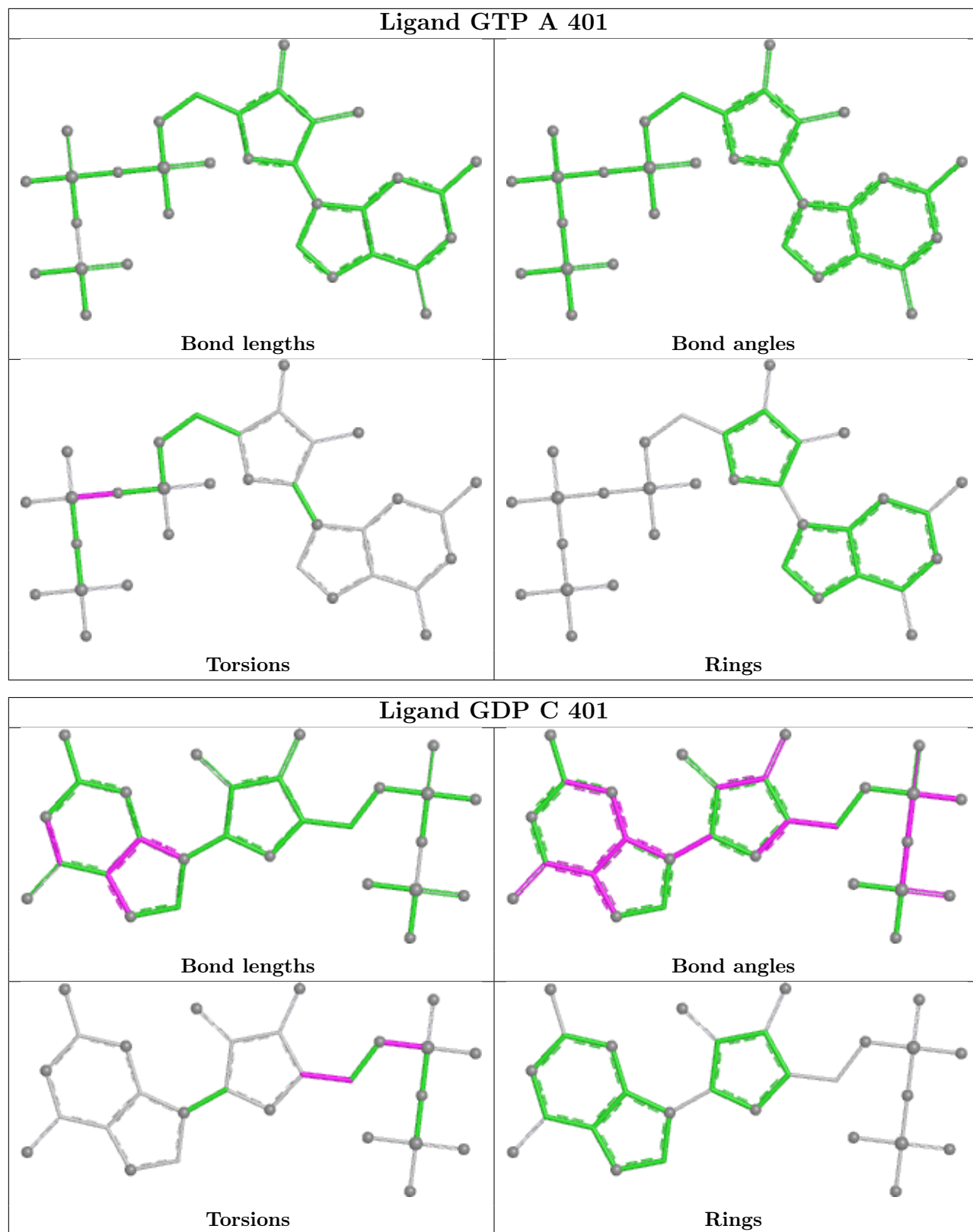
Mol	Chain	Res	Type	Atoms
5	C	401	GDP	C5'-O5'-PA-O2A
6	B	403	9JE	C03-C04-C05-C06
6	B	403	9JE	C02-C03-C04-C05
6	B	404	9JE	C04-C05-C06-O07
3	A	401	GTP	PA-O3A-PB-O2B
5	D	401	GDP	PA-O3A-PB-O1B

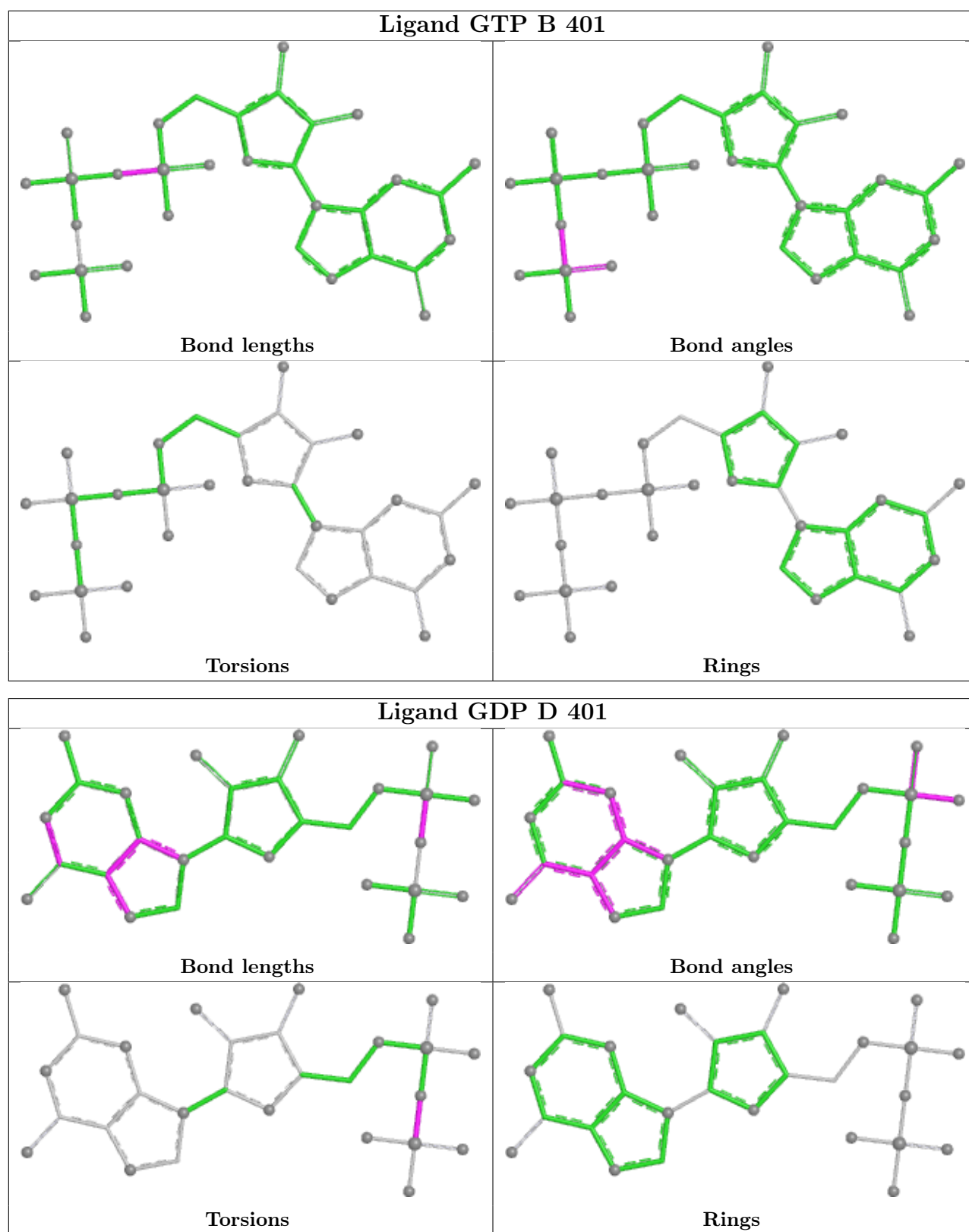
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GTP	1	0
6	B	403	9JE	1	0
3	B	401	GTP	2	0
6	B	404	9JE	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	300/313 (95%)	-0.01	2 (0%) 84 81	40, 61, 103, 154	0
1	B	300/313 (95%)	0.08	4 (1%) 75 71	38, 65, 106, 149	1 (0%)
2	C	284/399 (71%)	0.18	9 (3%) 50 46	38, 67, 114, 137	1 (0%)
2	D	272/399 (68%)	0.62	7 (2%) 57 52	59, 110, 150, 167	0
All	All	1156/1424 (81%)	0.21	22 (1%) 66 62	38, 72, 130, 167	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	5.6
1	A	281	ILE	3.9
1	B	281	ILE	3.8
2	D	115	TRP	3.3
2	D	204	ALA	3.1
1	B	4	THR	3.0
1	A	303	VAL	2.8
2	D	356	PHE	2.7
1	B	129	MET	2.7
2	C	59	SER	2.6
2	D	351	LEU	2.4
2	D	199	ALA	2.4
2	C	208	LEU	2.4
2	C	91	LEU	2.3
2	C	112	PHE	2.2
2	C	173	PHE	2.2
2	C	88	ASN	2.2
2	D	151	MET	2.1
2	C	153	ALA	2.1
2	D	354	TYR	2.1
2	C	157	LEU	2.0
2	C	115	TRP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

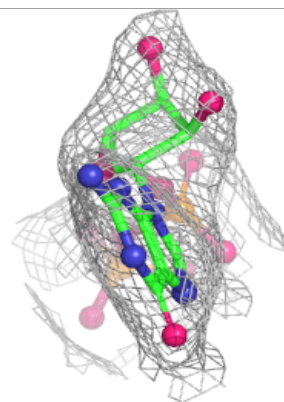
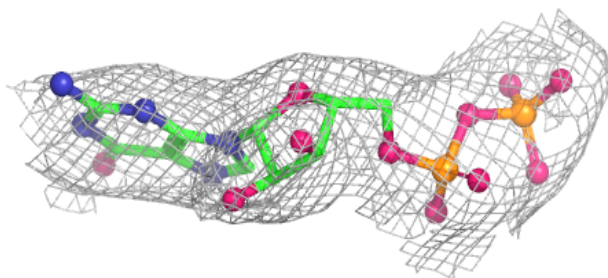
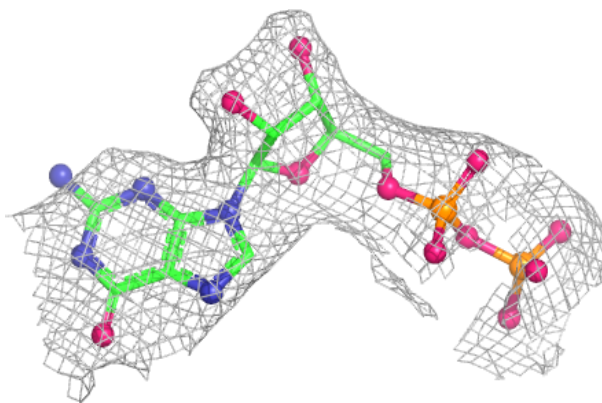
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	9JE	B	403	7/7	0.84	0.18	56,62,65,76	0
5	GDP	D	401	28/28	0.92	0.06	79,93,107,123	0
5	GDP	C	401	28/28	0.93	0.08	52,72,91,93	0
6	9JE	B	404	7/7	0.94	0.12	54,54,65,76	0
3	GTP	B	401	32/32	0.96	0.06	45,59,69,80	0
3	GTP	A	401	32/32	0.98	0.05	33,42,45,56	0
4	MG	B	402	1/1	0.98	0.09	58,58,58,58	0
4	MG	A	402	1/1	0.99	0.03	43,43,43,43	0

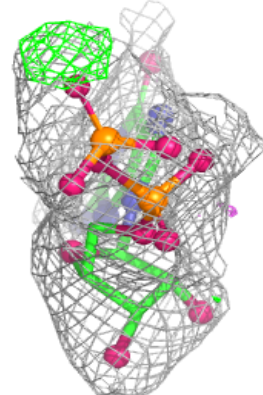
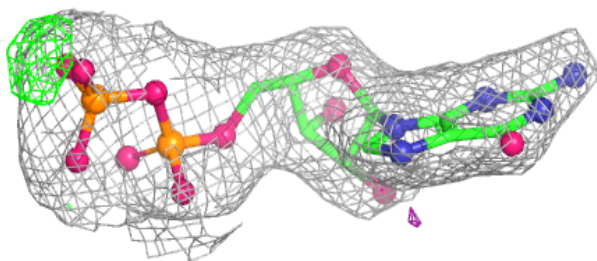
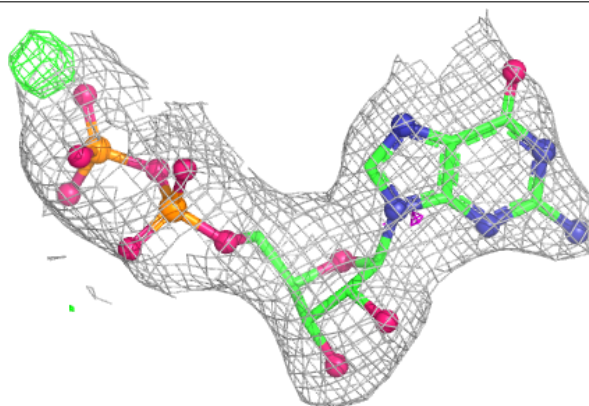
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP D 401:

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

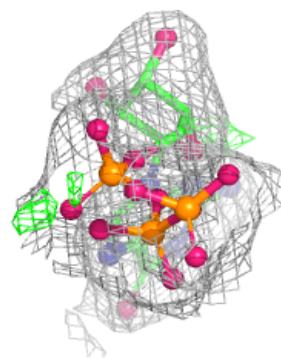
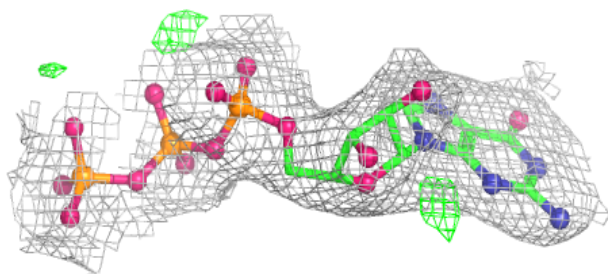
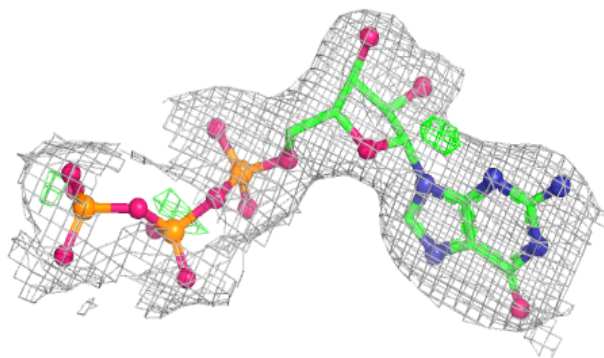
**Electron density around GDP C 401:**

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

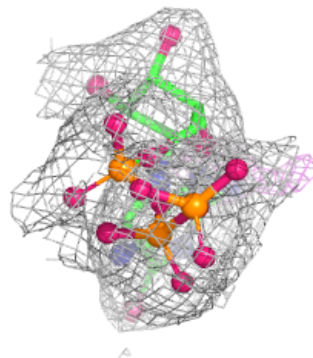
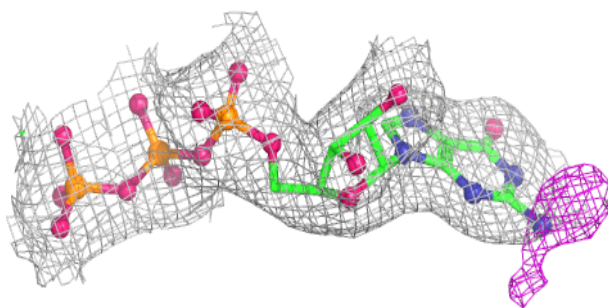
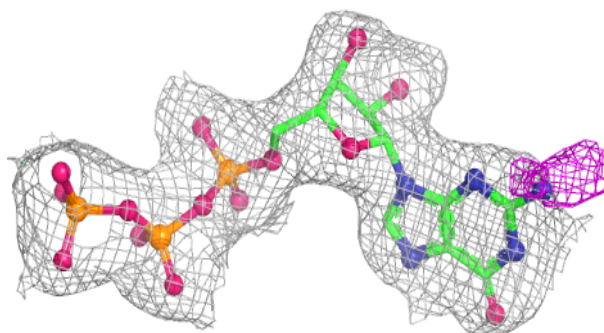


Electron density around GTP B 401:

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

**Electron density around GTP A 401:**

$2mF_o-DF_c$ (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.