



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:49 PM UTC

PDB ID : 5TDH / pdb_00005tdh
Title : The crystal structure of the dominant negative mutant G protein alpha(i)-1-beta-1-gamma-2 G203A/A326S
Authors : Liu, P.; Jia, M.-Z.; Zhou, X.E.; de Waal, P.W.; Dickson, B.M.; Liu, B.; Hou, L.; Yin, Y.-T.; Kang, Y.-Y.; Shi, Y.; Melcher, K.; Xu, H.E.; Jiang, Y.
Deposited on : 2016-09-19
Resolution : 3.00 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

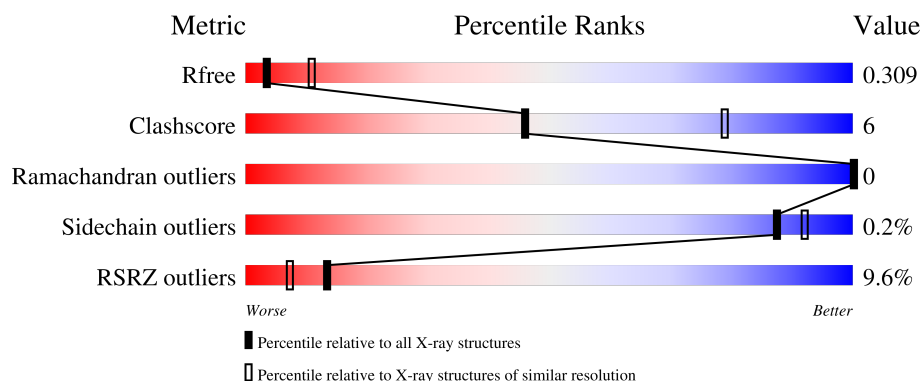
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	354	7% 85% 10% 5%
1	H	354	6% 82% 12% 5%
2	B	342	9% 80% 19% .
2	J	342	12% 82% 17% .

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Mol	Chain	Length	Quality of chain			
3	G	68	13%	72%	9%	19%
3	K	68	15%	65%	15%	19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11505 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2706	1713	464	514	15			
1	H	336	Total	C	N	O	S	0	0	0
			2697	1707	462	513	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ALA	SER	conflict	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096
H	98	ALA	SER	conflict	UNP P63096
H	203	ALA	GLY	engineered mutation	UNP P63096
H	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	0	0
			2599	1603	465	509	22			
2	J	339	Total	C	N	O	S	0	0	0
			2599	1603	465	509	22			

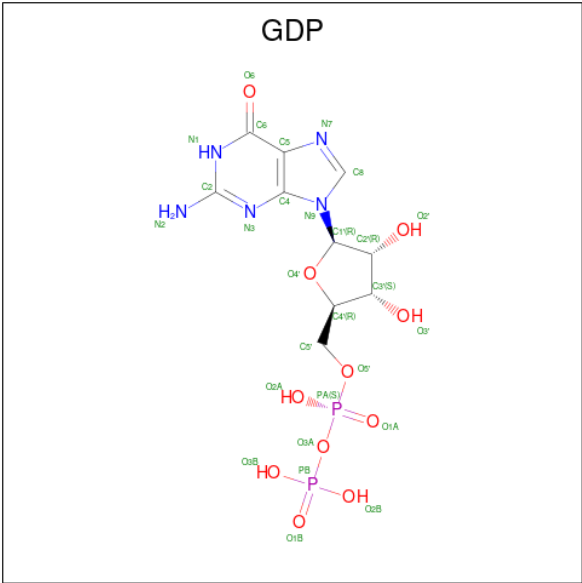
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP P54311
B	0	ALA	-	expression tag	UNP P54311
J	-1	SER	-	expression tag	UNP P54311
J	0	ALA	-	expression tag	UNP P54311

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	55	Total	C	N	O	S	0	0	0
			424	266	75	80	3			
3	K	55	Total	C	N	O	S	0	0	0
			424	266	75	80	3			

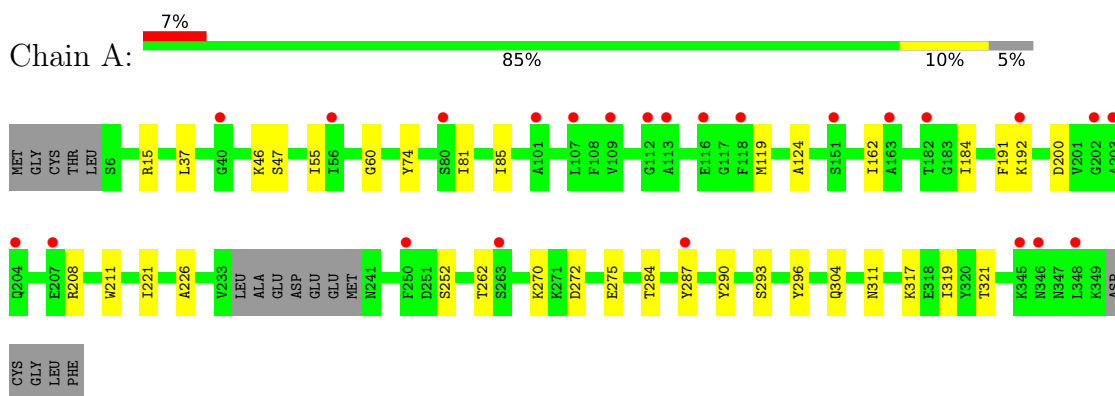
- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



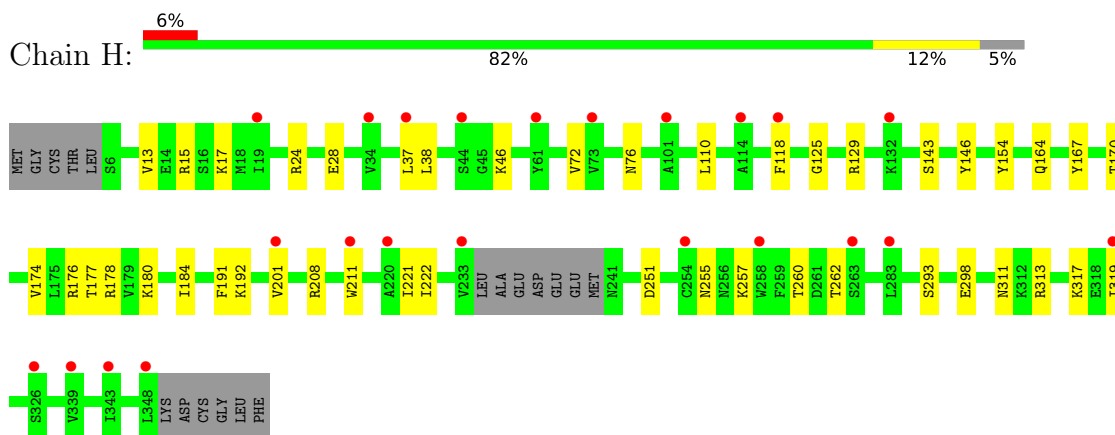
3 Residue-property plots

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.

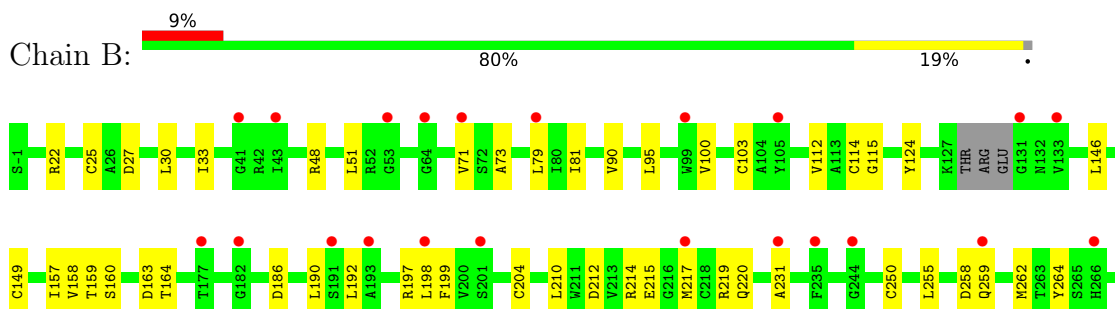
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

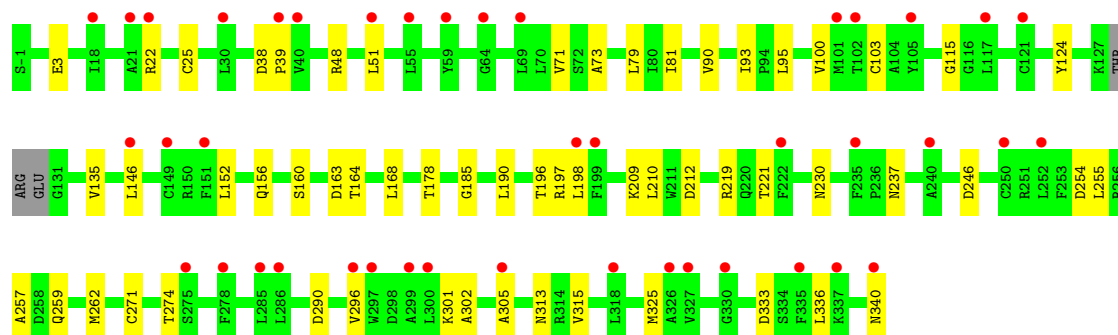
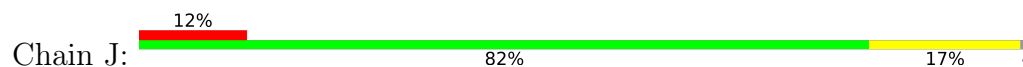


- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

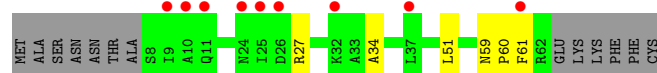
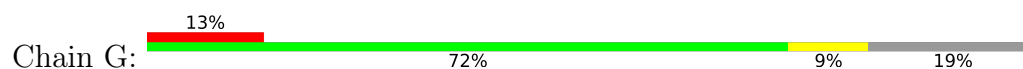




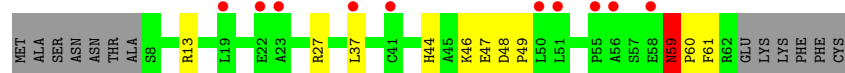
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.01Å 54.57Å 138.35Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	43.63 – 3.00 43.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.63-3.00) 98.3 (43.63-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.276 , 0.305 0.279 , 0.309	Depositor DCC
R_{free} test set	2556 reflections (7.24%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11505	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: 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	0.30	0/2751	0.74	0/3700
1	H	0.28	0/2742	0.71	0/3689
2	B	0.29	0/2645	0.74	0/3583
2	J	0.27	0/2645	0.72	0/3583
3	G	0.29	0/430	0.81	0/580
3	K	0.32	0/430	0.95	2/580 (0.3%)
All	All	0.29	0/11643	0.74	2/15715 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	59	ASN	CA-C-N	5.34	125.16	119.28
3	K	59	ASN	C-N-CA	5.34	125.16	119.28

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	2706	0	2695	20	0
1	H	2697	0	2682	29	0
2	B	2599	0	2505	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2599	0	2505	35	0
3	G	424	0	436	6	0
3	K	424	0	436	9	0
4	A	28	0	12	2	0
4	H	28	0	12	3	0
All	All	11505	0	11283	132	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 6.

All (132) 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:J:51:LEU:HB2	2:J:336:LEU:HB2	1.66	0.76
2:B:115:GLY:HA3	2:B:146:LEU:HD23	1.71	0.73
1:A:15:ARG:NH1	2:B:90:VAL:O	2.21	0.72
2:J:115:GLY:HA3	2:J:146:LEU:HD23	1.71	0.71
2:B:325:MET:O	2:B:340:ASN:ND2	2.24	0.70
1:A:304:GLN:HG3	1:A:321:THR:HG21	1.73	0.69
1:H:262:THR:O	1:H:317:LYS:NZ	2.23	0.69
3:K:59:ASN:ND2	3:K:61:PHE:O	2.22	0.69
2:B:71:VAL:HG12	2:B:81:ILE:HG12	1.74	0.68
2:J:71:VAL:HG12	2:J:81:ILE:HG12	1.77	0.67
2:J:325:MET:O	2:J:340:ASN:ND2	2.29	0.66
2:B:197:ARG:NH1	2:B:212:ASP:OD1	2.26	0.66
1:A:262:THR:O	1:A:317:LYS:NZ	2.28	0.65
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.78	0.64
2:B:212:ASP:OD2	2:B:219:ARG:NH2	2.31	0.64
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.80	0.62
1:H:184:ILE:HG12	1:H:201:VAL:HA	1.82	0.62
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.82	0.61
1:H:176:ARG:HA	4:H:401:GDP:O2'	2.00	0.61
1:A:208:ARG:HA	1:A:211:TRP:NE1	2.16	0.60
2:J:271:CYS:HB2	2:J:290:ASP:HB2	1.84	0.59
2:J:79:LEU:HG	2:J:95:LEU:HD21	1.85	0.59
2:B:146:LEU:HD11	2:B:159:THR:HB	1.84	0.58
2:J:237:ASN:HD21	3:K:37:LEU:HD23	1.68	0.58
2:B:214:ARG:HH12	3:K:46:LYS:HD3	1.69	0.58
1:H:46:LYS:NZ	4:H:401:GDP:O2B	2.36	0.57
2:J:22:ARG:HB3	2:J:259:GLN:NE2	2.20	0.57
2:J:212:ASP:OD2	2:J:219:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:168:LEU:HB3	2:J:178:THR:HB	1.86	0.56
2:B:25:CYS:SG	3:G:27:ARG:HB3	2.45	0.56
1:H:293:SER:OG	1:H:298:GLU:OE1	2.17	0.55
2:B:79:LEU:HG	2:B:95:LEU:HD21	1.89	0.55
2:B:262:MET:SD	2:B:302:ALA:HB2	2.46	0.55
2:J:274:THR:OG1	2:J:315:VAL:O	2.22	0.55
3:K:44:HIS:ND1	3:K:47:GLU:OE1	2.35	0.53
1:H:313:ARG:HD3	1:H:317:LYS:HG3	1.90	0.53
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.90	0.53
1:H:257:LYS:HA	1:H:313:ARG:HH22	1.72	0.53
1:H:260:THR:HA	1:H:313:ARG:HH12	1.73	0.53
2:B:48:ARG:HB3	3:G:61:PHE:HB3	1.91	0.53
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.91	0.53
1:H:260:THR:HA	1:H:313:ARG:NH1	2.24	0.53
1:A:47:SER:HB3	4:A:401:GDP:O1A	2.09	0.52
1:H:177:THR:O	4:H:401:GDP:O3'	2.27	0.52
1:H:164:GLN:HB2	1:H:167:TYR:HB2	1.91	0.52
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.92	0.52
2:J:230:ASN:ND2	2:J:246:ASP:OD1	2.42	0.52
2:J:152:LEU:HD22	2:J:196:THR:HB	1.92	0.52
1:H:110:LEU:O	1:H:118:PHE:HZ	1.93	0.51
1:A:290:TYR:OH	1:A:293:SER:O	2.22	0.51
2:J:22:ARG:HB3	2:J:259:GLN:HE21	1.74	0.51
2:J:197:ARG:NH1	2:J:212:ASP:OD1	2.33	0.51
1:H:208:ARG:HA	1:H:211:TRP:NE1	2.27	0.50
1:H:251:ASP:OD1	1:H:255:ASN:ND2	2.45	0.50
1:H:178:ARG:HH11	1:H:180:LYS:HE3	1.77	0.49
1:A:208:ARG:NH1	1:A:252:SER:OG	2.45	0.49
1:H:72:VAL:O	1:H:76:ASN:ND2	2.42	0.49
1:H:311:ASN:HB2	1:H:319:ILE:HD11	1.95	0.49
2:B:163:ASP:O	2:B:164:THR:OG1	2.28	0.48
2:B:313:ASN:HB3	2:B:332:TRP:HB2	1.95	0.48
2:B:215:GLU:HB3	2:B:217:MET:HE3	1.95	0.48
2:J:210:LEU:HD22	2:J:255:LEU:HD22	1.95	0.48
2:B:321:THR:OG1	2:B:323:ASP:OD1	2.26	0.48
1:H:13:VAL:HG12	1:H:17:LYS:HE2	1.94	0.48
2:B:264:TYR:OH	2:B:299:ALA:O	2.22	0.48
1:H:125:GLY:O	1:H:129:ARG:HG3	2.14	0.48
2:J:39:PRO:HG3	2:J:301:LYS:HE2	1.95	0.48
2:B:22:ARG:HB3	2:B:259:GLN:NE2	2.27	0.48
2:B:112:VAL:HG13	2:B:124:TYR:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:PHE:CE2	1:H:192:LYS:HE3	2.48	0.48
3:G:59:ASN:ND2	3:G:61:PHE:O	2.46	0.48
2:B:48:ARG:HG3	2:B:340:ASN:HB3	1.97	0.47
2:B:79:LEU:HD11	2:B:114:CYS:SG	2.54	0.47
2:B:192:LEU:HD23	2:B:199:PHE:HB3	1.97	0.47
2:B:274:THR:OG1	2:B:315:VAL:O	2.32	0.47
1:A:191:PHE:CZ	1:A:192:LYS:HE2	2.50	0.47
2:B:296:VAL:O	2:B:305:ALA:N	2.42	0.47
2:J:3:GLU:OE2	3:K:13:ARG:NH2	2.48	0.47
1:A:81:ILE:O	1:A:85:ILE:HG12	2.15	0.47
1:A:275:GLU:HG3	1:A:296:TYR:HB2	1.97	0.47
2:B:158:VAL:HG11	2:B:192:LEU:HD21	1.96	0.47
2:B:220:GLN:NE2	2:B:258:ASP:OD1	2.33	0.46
2:B:186:ASP:HB2	2:B:204:CYS:SG	2.56	0.46
1:H:143:SER:HA	1:H:146:TYR:CE2	2.51	0.46
2:J:209:LYS:NZ	2:J:221:THR:OG1	2.45	0.46
1:H:257:LYS:HA	1:H:313:ARG:NH2	2.31	0.46
2:B:22:ARG:HB3	2:B:259:GLN:HE21	1.80	0.46
2:B:149:CYS:HB2	2:B:157:ILE:HD11	1.98	0.46
2:B:198:LEU:HB3	2:B:210:LEU:HD11	1.98	0.46
2:J:160:SER:HB3	2:J:190:LEU:HD23	1.97	0.46
2:B:231:ALA:HB1	2:B:276:VAL:HG22	1.99	0.45
1:H:15:ARG:NH1	2:J:90:VAL:O	2.50	0.45
2:B:33:ILE:HG21	3:G:34:ALA:HB1	1.98	0.45
2:J:313:ASN:HB2	2:J:333:ASP:HB3	1.98	0.45
2:B:27:ASP:OD1	2:B:27:ASP:N	2.39	0.45
2:J:262:MET:SD	2:J:302:ALA:HB2	2.56	0.45
1:A:311:ASN:HB2	1:A:319:ILE:HD11	1.98	0.45
2:J:79:LEU:HB2	2:J:93:ILE:HB	1.99	0.45
2:B:214:ARG:NH1	3:K:46:LYS:HD3	2.31	0.44
2:B:73:ALA:HB2	2:B:103:CYS:HB3	2.00	0.44
2:B:283:ARG:HB3	3:G:51:LEU:HD11	1.98	0.44
1:A:46:LYS:NZ	4:A:401:GDP:O1B	2.46	0.44
1:H:170:THR:O	1:H:174:VAL:HG23	2.18	0.44
2:J:124:TYR:HA	2:J:135:VAL:HA	1.99	0.44
1:H:260:THR:OG1	1:H:313:ARG:NH2	2.51	0.43
1:A:74:TYR:HE1	1:A:162:ILE:HG22	1.83	0.43
1:A:119:MET:HE3	1:A:124:ALA:HB2	2.00	0.43
2:B:198:LEU:HD13	2:B:210:LEU:HD11	2.01	0.43
1:H:154:TYR:CE2	1:H:176:ARG:HG3	2.53	0.43
2:J:164:THR:HG22	2:J:185:GLY:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:254:ASP:HB3	2:J:257:ALA:HB3	2.00	0.42
2:J:25:CYS:SG	3:K:27:ARG:HB3	2.59	0.42
2:J:198:LEU:HB3	2:J:210:LEU:HD11	2.01	0.42
1:A:272:ASP:OD1	1:A:272:ASP:N	2.52	0.42
2:J:48:ARG:HG3	2:J:340:ASN:HB3	2.01	0.42
1:A:226:ALA:HB1	1:A:270:LYS:HD2	2.02	0.42
1:H:24:ARG:O	1:H:28:GLU:HG3	2.20	0.42
2:J:152:LEU:HB2	2:J:156:GLN:HB2	2.00	0.42
2:J:163:ASP:O	2:J:164:THR:OG1	2.30	0.41
3:K:48:ASP:HA	3:K:49:PRO:HD3	1.82	0.41
3:G:59:ASN:HA	3:G:60:PRO:HD3	1.86	0.41
1:H:38:LEU:HD23	1:H:222:ILE:HB	2.02	0.41
2:J:73:ALA:HB2	2:J:103:CYS:HB3	2.01	0.41
2:B:331:SER:OG	2:B:332:TRP:N	2.54	0.41
2:J:38:ASP:HA	2:J:39:PRO:HD3	1.92	0.41
1:A:184:ILE:HG13	1:A:200:ASP:O	2.20	0.41
1:H:37:LEU:HB3	1:H:221:ILE:HG12	2.02	0.41
1:A:37:LEU:HB3	1:A:221:ILE:HG12	2.03	0.40
2:B:30:LEU:HB3	2:B:262:MET:HE3	2.01	0.40
1:A:284:THR:HA	1:A:287:TYR:O	2.21	0.40
3:K:59:ASN:HA	3:K:60:PRO:HD3	1.76	0.40
2:J:296:VAL:O	2:J:305:ALA:N	2.53	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	333/354 (94%)	328 (98%)	5 (2%)	0	100	100
1	H	332/354 (94%)	327 (98%)	5 (2%)	0	100	100
2	B	335/342 (98%)	328 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	335/342 (98%)	328 (98%)	7 (2%)	0	100	100
3	G	53/68 (78%)	51 (96%)	2 (4%)	0	100	100
3	K	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
All	All	1441/1528 (94%)	1412 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/305 (95%)	291 (100%)	0	100	100
1	H	290/305 (95%)	290 (100%)	0	100	100
2	B	281/284 (99%)	280 (100%)	1 (0%)	84	90
2	J	281/284 (99%)	280 (100%)	1 (0%)	84	90
3	G	45/56 (80%)	45 (100%)	0	100	100
3	K	45/56 (80%)	44 (98%)	1 (2%)	45	74
All	All	1233/1290 (96%)	1230 (100%)	3 (0%)	87	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	100	VAL
2	J	100	VAL
3	K	59	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
1	A	322	HIS

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Mol	Chain	Res	Type
2	B	75	GLN
2	B	156	GLN
2	B	259	GLN
2	J	125	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
4	GDP	H	401	-	29,30,30	1.17	3 (10%)	45,47,47	1.84	9 (20%)
4	GDP	A	401	-	29,30,30	1.21	3 (10%)	45,47,47	1.78	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
4	GDP	H	401	-	-	3/16/32/32	0/3/3/3
4	GDP	A	401	-	-	2/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	401	GDP	C5-C4	3.15	1.47	1.38
4	A	401	GDP	C5-C4	3.13	1.47	1.38
4	H	401	GDP	C6-N1	-2.52	1.34	1.38
4	A	401	GDP	C6-N1	-2.43	1.34	1.38
4	A	401	GDP	PA-O3A	2.38	1.62	1.59
4	H	401	GDP	C5-N7	-2.00	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	401	GDP	C5-C4-N3	-6.14	118.62	128.39
4	A	401	GDP	C5-C4-N3	-5.90	118.99	128.39
4	H	401	GDP	C2-N3-C4	5.00	120.91	112.30
4	H	401	GDP	N9-C4-N3	4.83	135.61	125.95
4	A	401	GDP	C2-N3-C4	4.72	120.44	112.30
4	A	401	GDP	N9-C4-N3	4.36	134.67	125.95
4	A	401	GDP	C6-C5-N7	3.27	136.24	130.29
4	H	401	GDP	C2'-C1'-N9	-3.22	104.29	113.25
4	H	401	GDP	C6-C5-N7	3.03	135.81	130.29
4	A	401	GDP	O2A-PA-O3A	2.72	114.62	107.27
4	H	401	GDP	C3'-C2'-C1'	2.65	106.48	101.46
4	A	401	GDP	C4-C5-N7	-2.58	106.59	110.67
4	H	401	GDP	O6-C6-C5	-2.34	120.37	126.53
4	H	401	GDP	C5-C6-N1	2.15	118.73	113.25
4	H	401	GDP	C4-C5-N7	-2.13	107.30	110.67
4	A	401	GDP	O6-C6-C5	-2.07	121.07	126.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

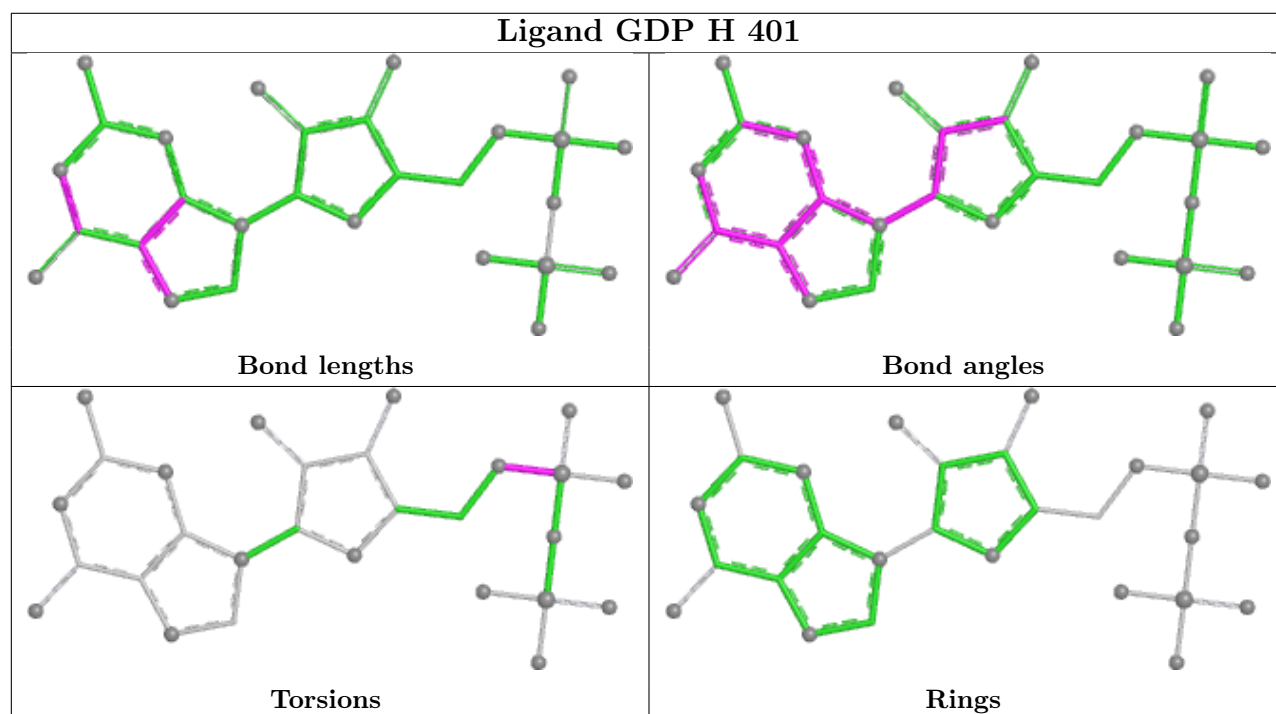
Mol	Chain	Res	Type	Atoms
4	H	401	GDP	C5'-O5'-PA-O3A
4	H	401	GDP	C5'-O5'-PA-O1A
4	H	401	GDP	C5'-O5'-PA-O2A
4	A	401	GDP	O4'-C4'-C5'-O5'
4	A	401	GDP	C3'-C4'-C5'-O5'

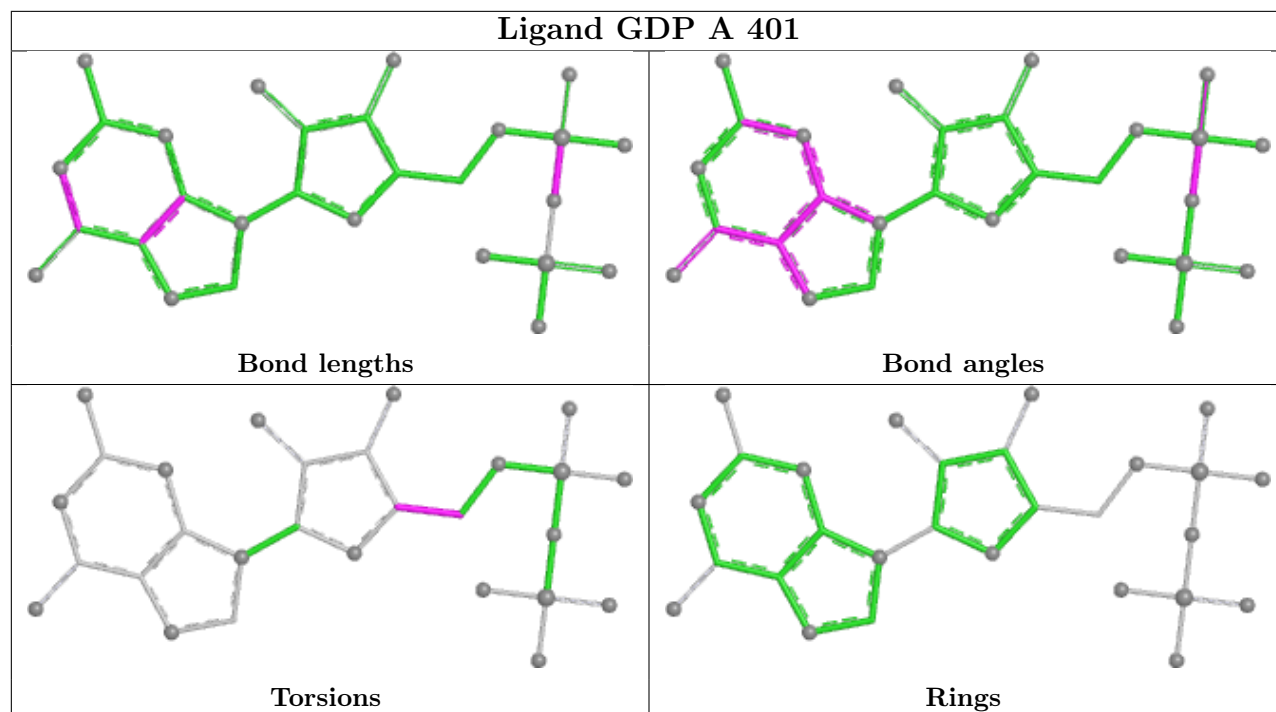
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	401	GDP	3	0
4	A	401	GDP	2	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	337/354 (95%)	0.91	24 (7%)	22 11	33, 62, 109, 150	0
1	H	336/354 (94%)	0.93	23 (6%)	23 12	46, 93, 159, 176	0
2	B	339/342 (99%)	1.02	32 (9%)	14 7	28, 61, 92, 134	0
2	J	339/342 (99%)	1.20	42 (12%)	8 5	90, 132, 169, 197	0
3	G	55/68 (80%)	1.27	9 (16%)	4 3	37, 84, 116, 122	0
3	K	55/68 (80%)	1.49	10 (18%)	3 2	96, 162, 181, 188	0
All	All	1461/1528 (95%)	1.04	140 (9%)	13 7	28, 85, 161, 197	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	SER	4.9
3	G	26	ASP	4.0
1	A	118	PHE	3.8
1	H	254	CYS	3.6
3	K	41	CYS	3.5
3	K	51	LEU	3.5
1	H	44	SER	3.4
2	J	285	LEU	3.3
2	B	133	VAL	3.3
2	B	231	ALA	3.3
1	A	109	VAL	3.3
2	J	299	ALA	3.3
2	J	326	ALA	3.2
1	H	101	ALA	3.2
2	B	41	GLY	3.1
1	A	348	LEU	3.0
3	G	9	ILE	3.0
2	J	330	GLY	3.0
2	J	199	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	116	GLU	2.9
1	H	339	VAL	2.9
2	J	55	LEU	2.9
3	G	11	GLN	2.9
2	J	327	VAL	2.8
2	B	43	ILE	2.8
2	B	198	LEU	2.8
1	H	326	SER	2.8
2	J	102	THR	2.8
2	J	149	CYS	2.8
1	H	348	LEU	2.8
2	J	146	LEU	2.8
2	B	244	GLY	2.8
2	B	71	VAL	2.8
2	J	278	PHE	2.7
2	B	295	ASN	2.7
3	G	24	ASN	2.7
3	K	23	ALA	2.7
3	K	55	PRO	2.7
3	K	37	LEU	2.7
2	B	317	CYS	2.7
3	G	61	PHE	2.7
1	H	233	VAL	2.7
3	K	50	LEU	2.7
2	J	22	ARG	2.6
2	B	276	VAL	2.6
1	A	112	GLY	2.6
3	K	56	ALA	2.6
2	J	121	CYS	2.6
2	B	53	GLY	2.6
2	B	131	GLY	2.6
1	A	113	ALA	2.6
1	A	56	ILE	2.6
2	B	319	GLY	2.6
2	J	340	ASN	2.6
1	A	101	ALA	2.6
2	J	335	PHE	2.5
1	A	287	TYR	2.5
2	J	117	LEU	2.5
1	A	182	THR	2.5
2	B	105	TYR	2.5
2	B	266	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	240	ALA	2.5
1	A	107	LEU	2.5
2	B	340	ASN	2.5
2	J	222	PHE	2.5
2	B	327	VAL	2.5
2	B	191	SER	2.4
1	H	211	TRP	2.4
1	H	37	LEU	2.4
3	G	25	ILE	2.4
2	B	201	SER	2.4
2	J	297	TRP	2.4
1	H	61	TYR	2.4
1	H	201	VAL	2.4
2	B	193	ALA	2.4
3	K	22	GLU	2.4
2	J	286	LEU	2.4
2	J	296	VAL	2.4
1	A	204	GLN	2.4
1	H	263	SER	2.4
1	A	40	GLY	2.4
1	A	202	GLY	2.4
2	J	337	LYS	2.4
1	A	203	ALA	2.3
2	J	21	ALA	2.3
2	J	40	VAL	2.3
1	A	263	SER	2.3
2	B	99	TRP	2.3
1	A	163	ALA	2.3
1	A	250	PHE	2.3
1	H	283	LEU	2.3
2	J	30	LEU	2.3
2	B	182	GLY	2.3
2	B	313	ASN	2.3
2	J	39	PRO	2.3
1	H	114	ALA	2.2
2	B	64	GLY	2.2
2	J	250	CYS	2.2
2	J	105	TYR	2.2
3	G	10	ALA	2.2
1	H	73	VAL	2.2
1	H	343	ILE	2.2
1	H	220	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	151	PHE	2.2
2	B	286	LEU	2.2
3	G	37	LEU	2.2
2	J	235	PHE	2.2
2	J	69	LEU	2.1
3	K	19	LEU	2.1
1	A	207	GLU	2.1
1	H	319	ILE	2.1
2	J	101	MET	2.1
2	J	305	ALA	2.1
1	H	118	PHE	2.1
1	A	192	LYS	2.1
2	B	79	LEU	2.1
2	J	51	LEU	2.1
2	J	300	LEU	2.1
3	G	32	LYS	2.1
2	B	235	PHE	2.1
1	H	19	ILE	2.1
2	J	198	LEU	2.1
1	A	151	SER	2.1
1	A	346	ASN	2.1
2	B	177	THR	2.1
3	K	58	GLU	2.1
2	B	308	LEU	2.0
2	J	252	LEU	2.0
1	H	258	TRP	2.0
2	B	217	MET	2.0
2	J	59	TYR	2.0
2	B	259	GLN	2.0
2	J	64	GLY	2.0
1	A	345	LYS	2.0
1	H	34	VAL	2.0
2	J	18	ILE	2.0
2	J	275	SER	2.0
1	H	132	LYS	2.0
2	B	318	LEU	2.0
2	J	318	LEU	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 [i](#)

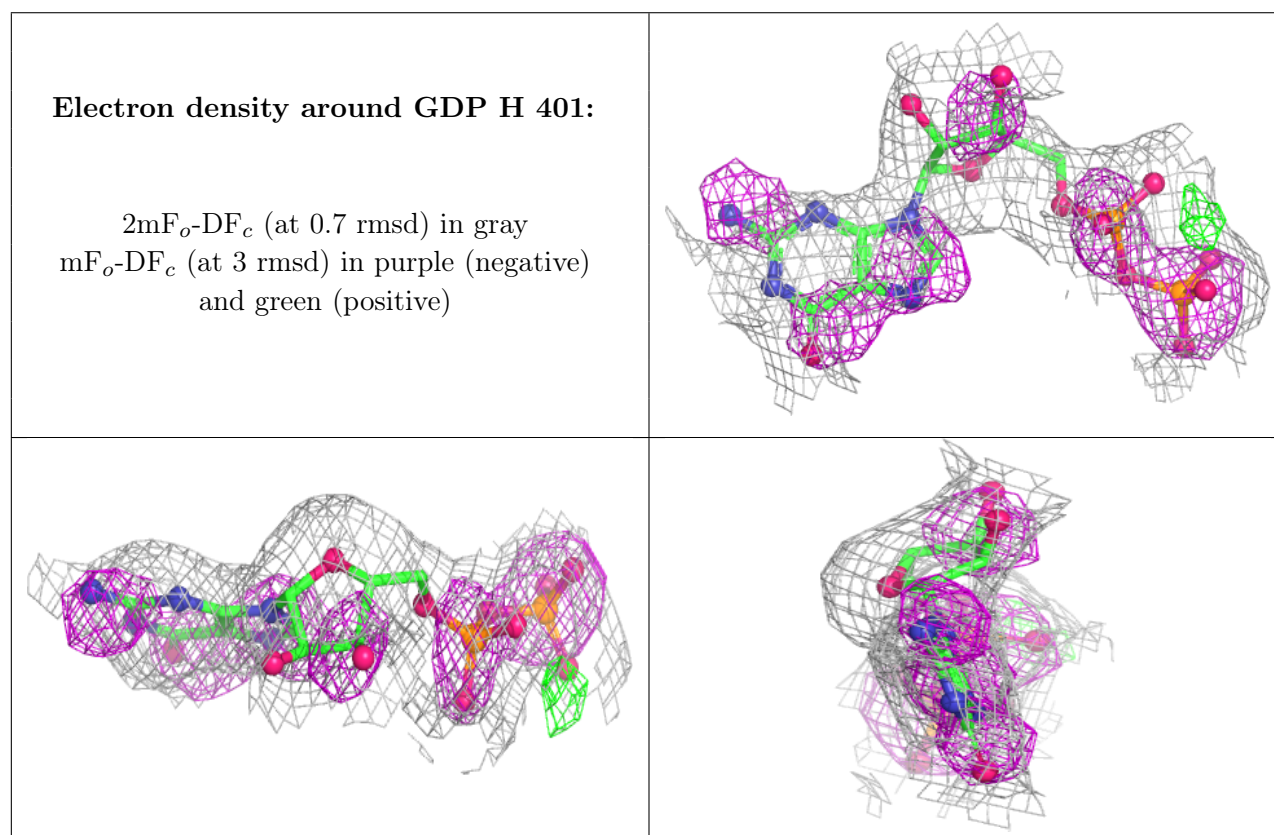
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

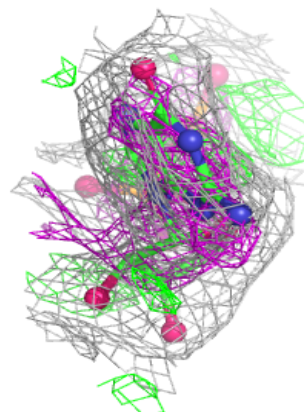
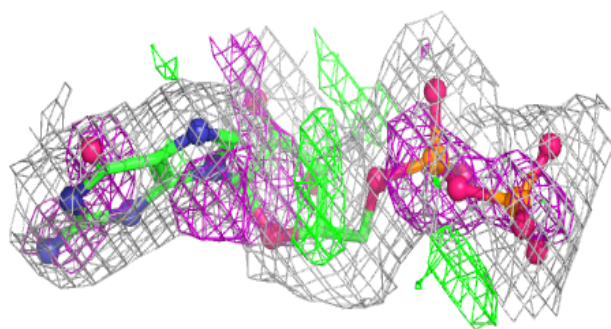
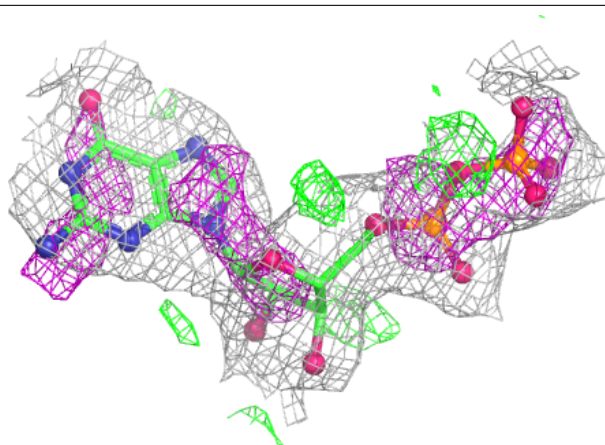
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GDP	H	401	28/28	0.73	0.14	30,38,43,44	0
4	GDP	A	401	28/28	0.85	0.13	20,26,29,29	0

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 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.