



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:19 AM EDT

PDB ID : 1TAD / pdb_00001tad
Title : GTPASE MECHANISM OF GPROTEINS FROM THE 1.7-ANGSTROM
CRYSTAL STRUCTURE OF TRANSDUCIN ALPHA-GDP-ALF4-
Authors : Sondek, J.; Lambright, D.G.; Noel, J.P.; Hamm, H.E.; Sigler, P.B.
Deposited on : 1995-01-05
Resolution : 1.70 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)	:	2.50

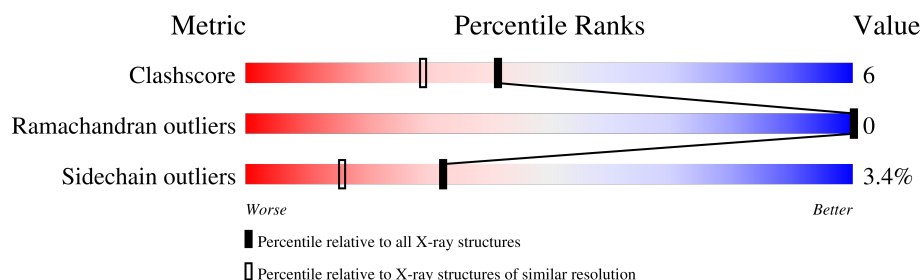
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	324	 83% 13% ..
1	B	324	 81% 16% ..
1	C	324	 81% 16% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8773 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.

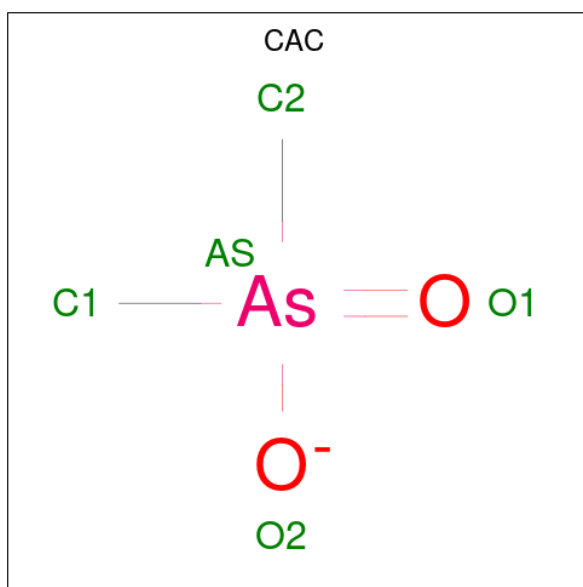
- Molecule 1 is a protein called TRANSDUCIN-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2539	1610	428	483	18			
1	B	316	Total	C	N	O	S	0	0	0
			2539	1610	428	483	18			
1	C	318	Total	C	N	O	S	0	0	0
			2555	1620	431	486	18			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

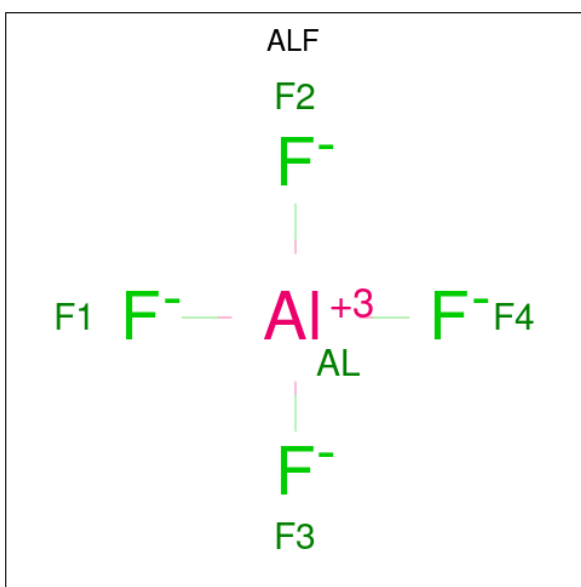
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



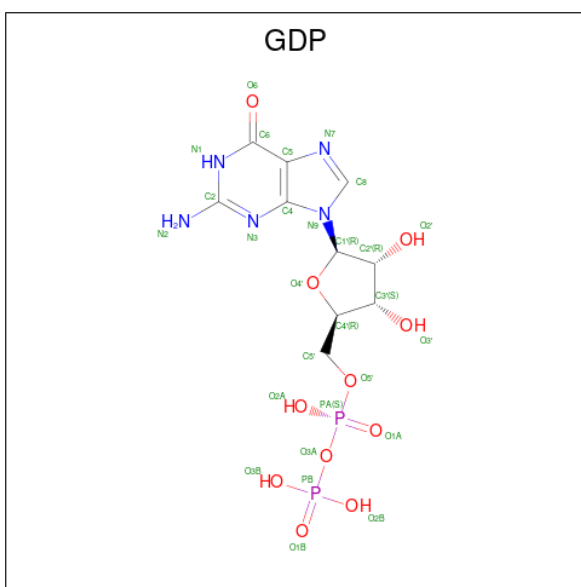
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			4	1	2	1		
3	A	1	Total	As	C	O	0	0
			4	1	2	1		
3	B	1	Total	As	C	O	0	0
			4	1	2	1		
3	B	1	Total	As	C	O	0	0
			4	1	2	1		
3	C	1	Total	As	C	O	0	0
			4	1	2	1		
3	C	1	Total	As	C	O	0	0
			4	1	2	1		

- Molecule 4 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	Al 1	F 4	0	0
4	B	1	Total 5	Al 1	F 4	0	0
4	C	1	Total 5	Al 1	F 4	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

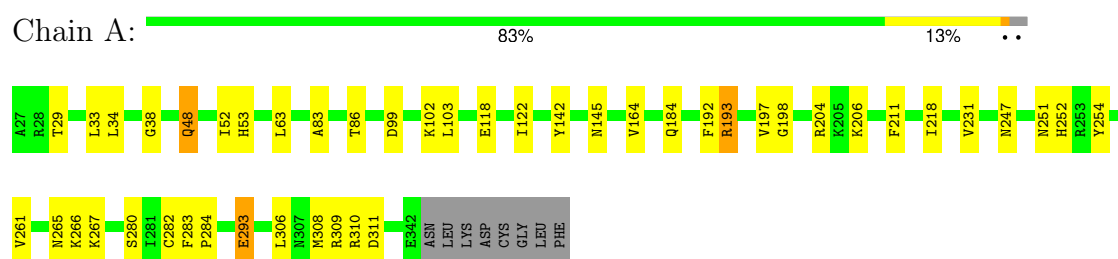
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	378	Total	O	0	0
			378	378		
6	B	316	Total	O	0	0
			316	316		
6	C	320	Total	O	0	0
			320	320		

3 Residue-property plots

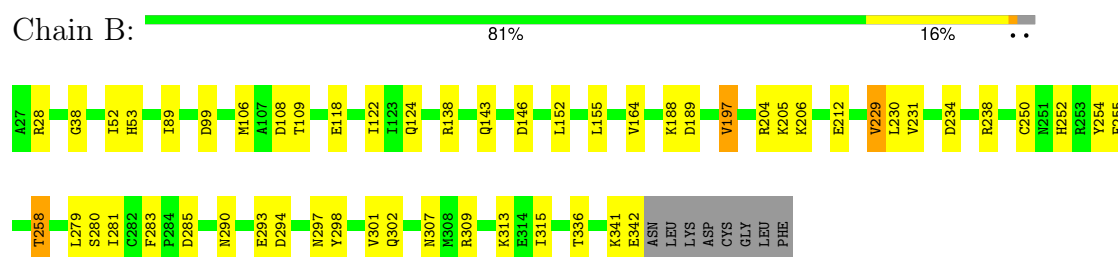
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

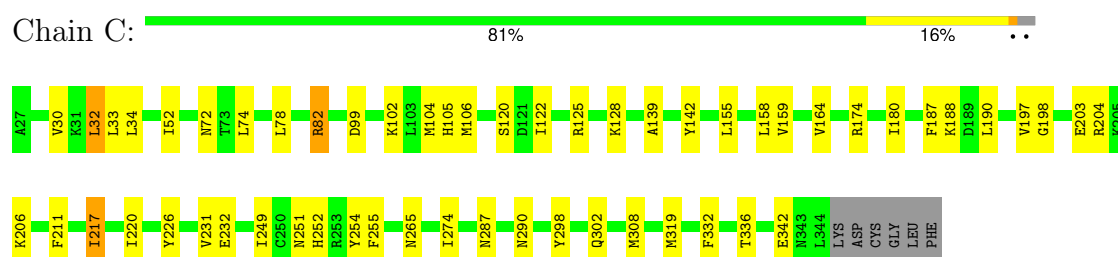
• Molecule 1: TRANSDUCIN-ALPHA



• Molecule 1: TRANSDUCIN-ALPHA



• Molecule 1: TRANSDUCIN-ALPHA



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	74.90Å 108.20Å 79.00Å 90.00° 111.70° 90.00°	Depositor
Resolution (Å)	8.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.209 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8773	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: CAC, GDP, CA, ALF

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	0.43	0/2584	0.85	4/3484 (0.1%)
1	B	0.42	0/2584	0.84	3/3484 (0.1%)
1	C	0.43	0/2600	0.87	8/3506 (0.2%)
All	All	0.43	0/7768	0.85	15/10474 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	ILE	N-CA-C	6.87	117.48	110.82
1	C	211	PHE	N-CA-C	6.03	120.50	113.20
1	C	249	ILE	N-CA-C	6.00	116.06	110.42
1	A	52	ILE	N-CA-C	5.83	116.47	110.82
1	A	204	ARG	N-CA-C	5.77	118.35	111.71
1	C	204	ARG	N-CA-C	5.67	118.40	111.82
1	A	211	PHE	N-CA-C	5.61	119.87	113.19
1	A	265	ASN	N-CA-C	5.50	117.62	110.53
1	B	52	ILE	N-CA-C	5.46	116.12	110.82
1	B	204	ARG	N-CA-C	5.44	118.13	111.82
1	C	319	MET	N-CA-C	-5.27	100.70	109.46
1	C	226	TYR	N-CA-C	5.27	117.77	111.71
1	C	217	ILE	CB-CA-C	-5.15	103.01	110.63
1	B	281	ILE	N-CA-C	-5.12	105.40	110.62
1	C	265	ASN	N-CA-C	5.08	117.08	110.53

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	2539	0	2517	31	0
1	B	2539	0	2517	31	0
1	C	2555	0	2534	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	2	0
3	C	8	0	0	4	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
5	A	28	0	12	1	0
5	B	28	0	12	0	0
5	C	28	0	12	0	0
6	A	378	0	0	7	0
6	B	316	0	0	5	0
6	C	320	0	0	5	0
All	All	8773	0	7604	98	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 (98) 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:A:266:LYS:HB2	6:A:759:HOH:O	1.77	0.83
1:B:197:VAL:HG11	3:B:354:CAC:C1	2.13	0.78
1:A:252:HIS:HD2	1:A:254:TYR:HB2	1.49	0.76
1:C:99:ASP:HA	1:C:102:LYS:HE2	1.65	0.76
1:C:251:ASN:HD21	1:C:308:MET:H	1.36	0.73
1:A:310:ARG:HG2	1:A:311:ASP:H	1.53	0.72
1:C:231:VAL:HG21	6:C:1390:HOH:O	1.93	0.68
1:B:188:LYS:HG3	1:B:336:THR:HG21	1.75	0.67
1:C:252:HIS:HD2	1:C:254:TYR:H	1.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASN:HD21	1:C:174:ARG:H	1.47	0.62
1:C:155:LEU:O	1:C:159:VAL:HG22	2.01	0.61
1:B:250:CYS:SG	1:B:315:ILE:HD11	2.41	0.60
1:B:231:VAL:HG12	6:B:786:HOH:O	2.01	0.59
1:A:197:VAL:HG22	1:A:198:GLY:N	2.17	0.58
1:A:99:ASP:HB3	1:A:122:ILE:HG23	1.84	0.58
1:A:251:ASN:HD21	1:A:308:MET:H	1.52	0.57
1:A:48:GLN:HE21	1:A:48:GLN:HA	1.68	0.57
1:C:197:VAL:HG22	1:C:198:GLY:N	2.19	0.57
1:A:310:ARG:HG2	1:A:311:ASP:N	2.19	0.57
1:C:232:GLU:HB2	6:C:1295:HOH:O	2.04	0.57
1:A:293:GLU:H	1:A:293:GLU:CD	2.13	0.57
1:A:34:LEU:HD23	1:A:218:ILE:HB	1.86	0.57
1:B:99:ASP:HB3	1:B:122:ILE:HG23	1.86	0.56
1:C:30:VAL:HG12	1:C:32:LEU:HD12	1.88	0.56
1:A:252:HIS:CD2	1:A:254:TYR:HB2	2.37	0.56
1:C:187:PHE:CD2	1:C:336:THR:HG21	2.40	0.56
1:C:82:ARG:HD3	1:C:104:MET:HE1	1.87	0.56
1:B:252:HIS:HB3	1:B:255:PHE:CD2	2.43	0.54
1:C:336:THR:HB	6:C:1285:HOH:O	2.08	0.53
1:B:188:LYS:O	1:B:189:ASP:HB3	2.09	0.53
1:A:266:LYS:HG2	5:A:351:GDP:C6	2.44	0.52
1:C:99:ASP:HB3	1:C:122:ILE:HG23	1.91	0.52
1:C:197:VAL:HB	3:C:354:CAC:C2	2.41	0.51
1:A:145:ASN:HB3	6:A:464:HOH:O	2.11	0.50
1:B:212:GLU:HB3	6:B:518:HOH:O	2.11	0.50
1:A:251:ASN:HB3	1:A:309:ARG:NH2	2.27	0.50
1:B:124:GLN:HG3	1:B:155:LEU:HD23	1.94	0.50
1:B:279:LEU:H	1:B:290:ASN:ND2	2.11	0.49
1:B:255:PHE:HA	1:B:258:THR:HG23	1.94	0.49
1:C:102:LYS:O	1:C:106:MET:HG3	2.12	0.49
1:B:297:ASN:O	1:B:301:VAL:HG23	2.13	0.49
1:C:125:ARG:HA	1:C:128:LYS:HZ2	1.78	0.48
1:B:164:VAL:HG12	3:B:353:CAC:C1	2.43	0.48
1:A:252:HIS:HD2	1:A:254:TYR:CB	2.22	0.48
1:A:267:LYS:HE2	6:A:1017:HOH:O	2.13	0.48
1:B:146:ASP:HB3	6:B:1260:HOH:O	2.13	0.48
1:B:280:SER:HA	1:B:283:PHE:O	2.14	0.48
1:B:252:HIS:HD2	1:B:254:TYR:H	1.60	0.48
1:B:89:ILE:HD11	1:B:138:ARG:HH11	1.79	0.47
1:B:307:ASN:ND2	1:B:313:LYS:O	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LYS:O	1:B:342:GLU:HB2	2.14	0.47
1:A:164:VAL:HG12	3:A:353:CAC:C2	2.44	0.47
1:A:247:ASN:HB2	1:A:306:LEU:HD13	1.97	0.47
1:C:105:HIS:HB2	6:C:668:HOH:O	2.14	0.47
1:C:188:LYS:HB2	6:C:1285:HOH:O	2.15	0.47
1:C:217:ILE:HD11	1:C:255:PHE:CD1	2.50	0.47
1:B:229:VAL:HG21	1:B:234:ASP:O	2.14	0.47
1:B:252:HIS:CD2	1:B:254:TYR:H	2.34	0.46
1:B:118:GLU:HB2	6:B:1372:HOH:O	2.15	0.46
1:B:106:MET:HE1	1:B:118:GLU:HG3	1.98	0.46
1:A:83:ALA:HA	1:A:86:THR:OG1	2.16	0.46
1:A:53:HIS:HD2	6:A:734:HOH:O	1.98	0.45
1:A:197:VAL:CG2	1:A:198:GLY:N	2.79	0.45
1:C:203:GLU:O	1:C:206:LYS:HG2	2.17	0.45
1:C:217:ILE:HD11	1:C:255:PHE:CG	2.51	0.45
1:C:139:ALA:HA	1:C:142:TYR:CE1	2.52	0.44
1:C:197:VAL:HG22	1:C:198:GLY:H	1.83	0.44
1:B:38:GLY:HA2	4:B:355:ALF:F1	2.08	0.44
1:B:229:VAL:HG13	1:B:234:ASP:HA	2.00	0.44
1:A:280:SER:HA	1:A:283:PHE:O	2.17	0.44
1:B:230:LEU:HD23	1:B:238:ARG:HG2	1.99	0.44
1:C:102:LYS:HG3	1:C:122:ILE:HD13	2.00	0.43
1:A:142:TYR:HB3	6:A:481:HOH:O	2.17	0.43
1:B:293:GLU:HG3	1:B:294:ASP:N	2.33	0.43
1:B:53:HIS:HD2	6:B:531:HOH:O	2.00	0.43
1:C:187:PHE:HD2	1:C:336:THR:HG21	1.80	0.43
1:C:180:ILE:HG23	3:C:354:CAC:C2	2.48	0.43
1:C:164:VAL:HG12	3:C:353:CAC:O1	2.19	0.43
1:B:106:MET:HA	1:B:109:THR:HB	2.01	0.42
1:C:72:ASN:ND2	1:C:174:ARG:H	2.14	0.42
1:C:34:LEU:HD22	1:C:220:ILE:HD11	2.01	0.42
1:A:192:PHE:C	1:A:193:ARG:HE	2.27	0.42
1:C:30:VAL:HG12	1:C:32:LEU:CD1	2.48	0.42
1:A:184:GLN:HE21	1:A:193:ARG:NH1	2.18	0.41
1:C:251:ASN:HD21	1:C:308:MET:N	2.11	0.41
1:C:274:ILE:O	1:C:290:ASN:ND2	2.48	0.41
1:A:218:ILE:HG12	1:A:261:VAL:CG2	2.50	0.41
1:B:279:LEU:H	1:B:290:ASN:HD21	1.67	0.41
1:A:197:VAL:HG23	6:A:447:HOH:O	2.20	0.41
1:B:298:TYR:O	1:B:302:GLN:HG2	2.21	0.41
1:C:30:VAL:HG21	1:C:190:LEU:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:PHE:O	1:C:336:THR:HG23	2.21	0.41
1:A:29:THR:HG23	1:A:193:ARG:HD2	2.03	0.41
1:C:197:VAL:HG21	3:C:354:CAC:C1	2.52	0.40
1:A:282:CYS:O	1:A:284:PRO:HD3	2.21	0.40
1:C:298:TYR:O	1:C:302:GLN:HG2	2.21	0.40
1:A:38:GLY:HA2	4:A:355:ALF:F3	2.12	0.40
1:A:231:VAL:HG21	6:A:1067:HOH:O	2.20	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	314/324 (97%)	306 (98%)	8 (2%)	0	100	100
1	B	314/324 (97%)	308 (98%)	6 (2%)	0	100	100
1	C	316/324 (98%)	313 (99%)	3 (1%)	0	100	100
All	All	944/972 (97%)	927 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	281/288 (98%)	272 (97%)	9 (3%)	34	17
1	B	281/288 (98%)	270 (96%)	11 (4%)	28	12
1	C	283/288 (98%)	274 (97%)	9 (3%)	34	17
All	All	845/864 (98%)	816 (97%)	29 (3%)	32	16

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	48	GLN
1	A	63	LEU
1	A	102	LYS
1	A	103	LEU
1	A	118	GLU
1	A	193	ARG
1	A	206	LYS
1	A	293	GLU
1	B	28	ARG
1	B	108	ASP
1	B	143	GLN
1	B	152	LEU
1	B	197	VAL
1	B	205	LYS
1	B	206	LYS
1	B	229	VAL
1	B	258	THR
1	B	285	ASP
1	B	309	ARG
1	C	32	LEU
1	C	33	LEU
1	C	74	LEU
1	C	78	LEU
1	C	82	ARG
1	C	120	SER
1	C	158	LEU
1	C	287	ASN
1	C	342	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	48	GLN
1	A	53	HIS
1	A	88	ASN
1	A	97	GLN
1	A	184	GLN
1	A	191	ASN
1	A	200	GLN
1	A	240	HIS
1	A	247	ASN
1	A	251	ASN
1	A	252	HIS
1	A	318	HIS
1	B	53	HIS
1	B	97	GLN
1	B	105	HIS
1	B	252	HIS
1	B	290	ASN
1	B	302	GLN
1	B	326	GLN
1	C	53	HIS
1	C	72	ASN
1	C	124	GLN
1	C	200	GLN
1	C	247	ASN
1	C	251	ASN
1	C	252	HIS
1	C	343	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 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	CAC	A	353	1	0,3,4	-	-	0,3,6	-	-
5	GDP	A	351	4,2	29,30,30	0.86	1 (3%)	45,47,47	0.72	1 (2%)
3	CAC	C	354	1	0,3,4	-	-	0,3,6	-	-
4	ALF	A	355	6,5	4,4,4	1.44	0	-	-	-
5	GDP	C	351	4,2	29,30,30	0.85	2 (6%)	45,47,47	0.78	1 (2%)
3	CAC	C	353	1	0,3,4	-	-	0,3,6	-	-
3	CAC	A	354	1	0,3,4	-	-	0,3,6	-	-
5	GDP	B	351	4,2	29,30,30	0.72	1 (3%)	45,47,47	0.79	1 (2%)
4	ALF	B	355	6,5	4,4,4	1.44	0	-	-	-
4	ALF	C	355	6,5	4,4,4	1.44	0	-	-	-
3	CAC	B	353	1	0,3,4	-	-	0,3,6	-	-
3	CAC	B	354	1	0,3,4	-	-	0,3,6	-	-

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
5	GDP	B	351	4,2	-	3/16/32/32	0/3/3/3
5	GDP	C	351	4,2	-	2/16/32/32	0/3/3/3
5	GDP	A	351	4,2	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	351	GDP	PA-O3A	2.61	1.62	1.59
5	C	351	GDP	PB-O2B	-2.33	1.46	1.54
5	A	351	GDP	PB-O2B	-2.05	1.47	1.54
5	B	351	GDP	PB-O2B	-2.02	1.47	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	351	GDP	O2B-PB-O1B	2.36	120.02	110.83
5	C	351	GDP	O2B-PB-O1B	2.20	119.40	110.83
5	A	351	GDP	O2B-PB-O1B	2.19	119.36	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	351	GDP	PA-O3A-PB-O2B
5	B	351	GDP	PA-O3A-PB-O2B
5	C	351	GDP	PA-O3A-PB-O2B
5	C	351	GDP	PA-O3A-PB-O1B
5	A	351	GDP	PA-O3A-PB-O1B
5	B	351	GDP	PA-O3A-PB-O1B
5	A	351	GDP	PA-O3A-PB-O3B
5	B	351	GDP	PA-O3A-PB-O3B

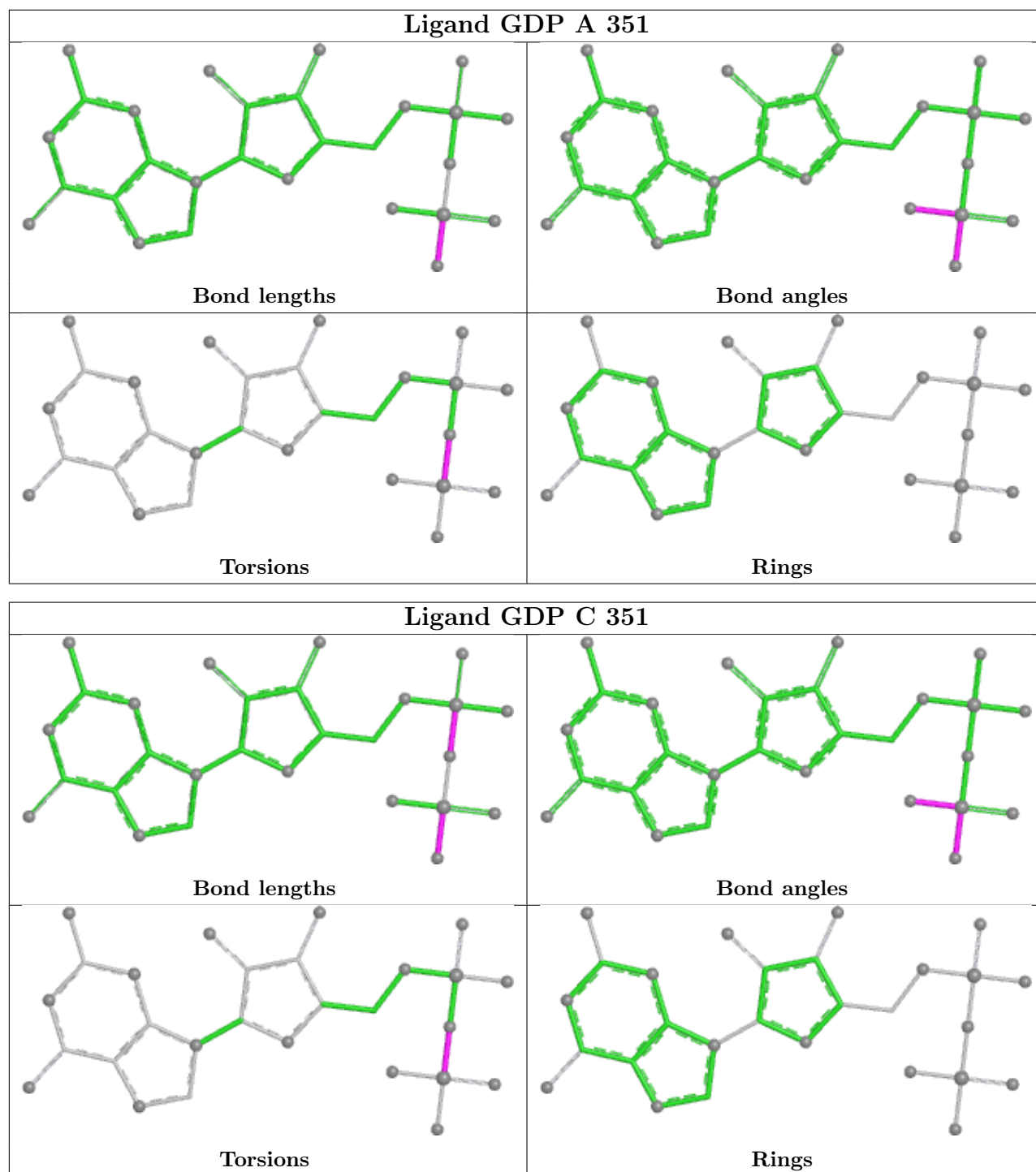
There are no ring outliers.

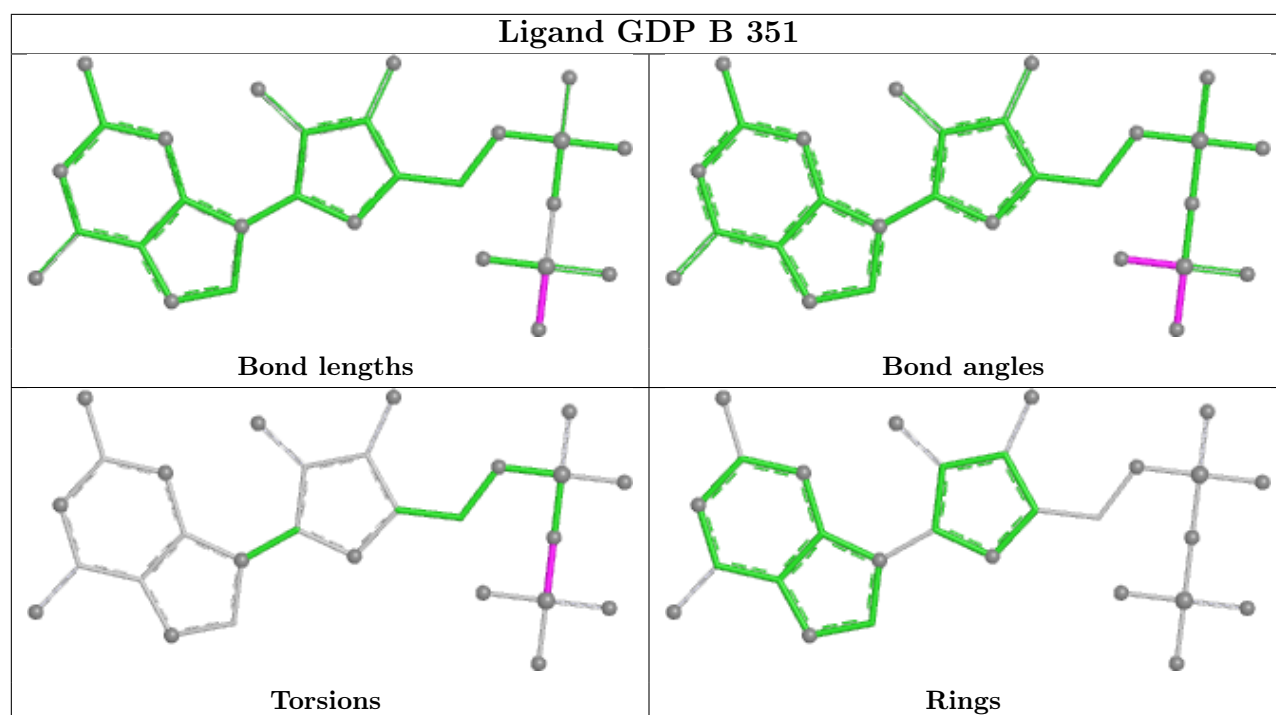
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	353	CAC	1	0
5	A	351	GDP	1	0
3	C	354	CAC	3	0
4	A	355	ALF	1	0
3	C	353	CAC	1	0
4	B	355	ALF	1	0
3	B	353	CAC	1	0
3	B	354	CAC	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.