



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:57 AM UTC

PDB ID : 1GP2 / pdb_00001gp2
Title : G PROTEIN HETEROTRIMER GI_ALPHA_1 BETA_1 GAMMA_2
WITH GDP BOUND
Authors : Wall, M.A.; Sprang, S.R.
Deposited on : 1996-11-13
Resolution : 2.30 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

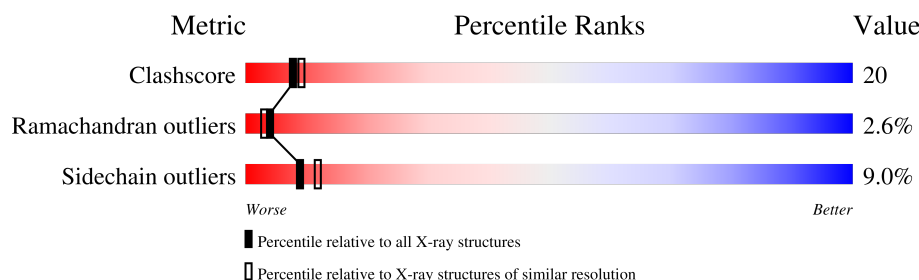
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	353	 60% 34% • •
2	B	340	 53% 40% 7%
3	G	71	 38% 27% 8% • 24%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6197 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 G PROTEIN GI ALPHA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	60	0	0
			2759	1745	470	528	16			

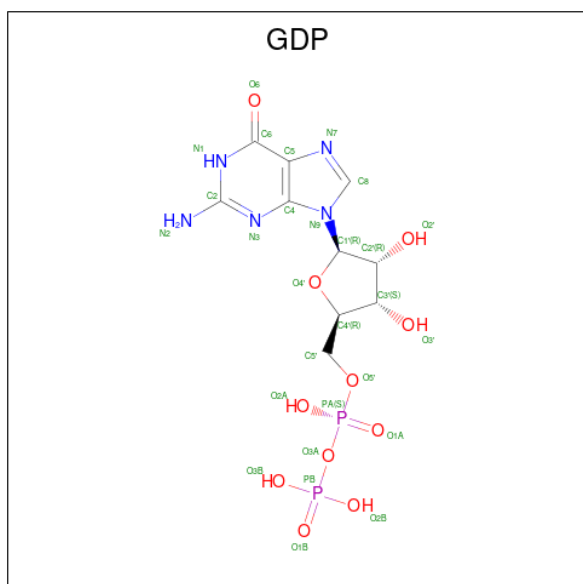
- Molecule 2 is a protein called G PROTEIN GI BETA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	27	0	0
			2607	1607	468	511	21			

- Molecule 3 is a protein called G PROTEIN GI GAMMA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	54	Total	C	N	O	S	0	0	0
			413	260	71	79	3			

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 5 is water.

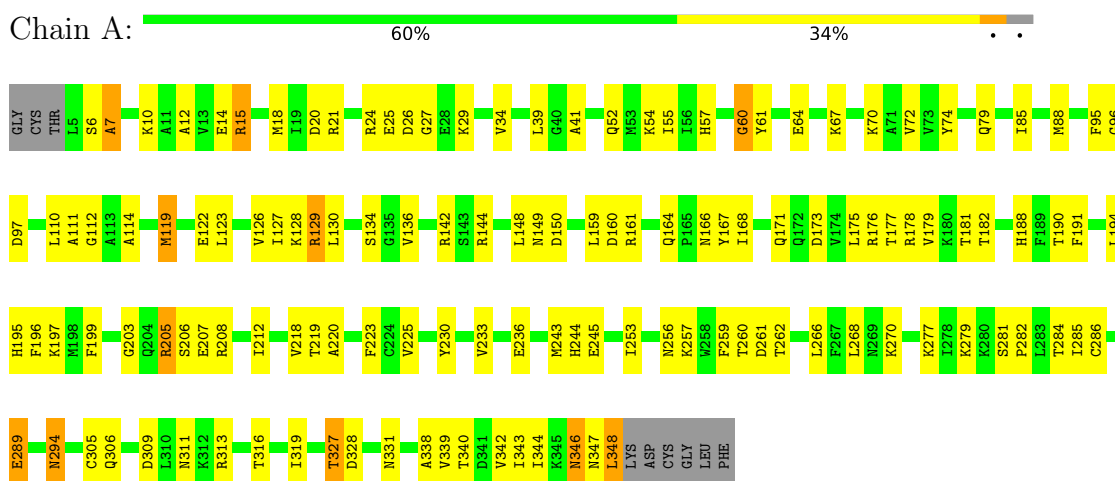
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	225	Total 225	O 225	0	0
5	B	142	Total 142	O 142	0	0
5	G	23	Total 23	O 23	0	0

3 Residue-property plots

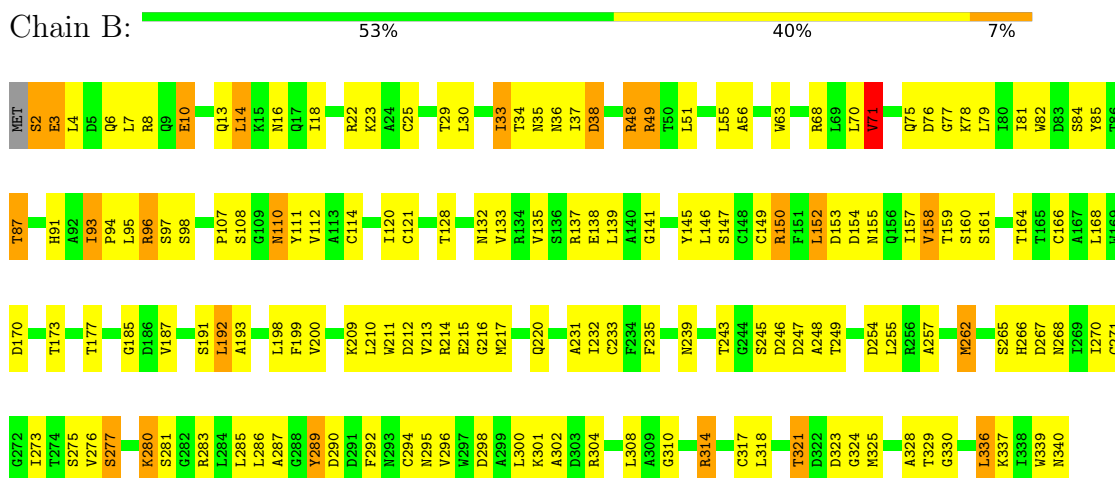
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: G PROTEIN GI ALPHA 1



• Molecule 2: G PROTEIN GI BETA 1



• Molecule 3: G PROTEIN GI GAMMA 2



MET	ALA	SER	ASN	ASN	THR	ALA	S8	R13	E17	Q18	M21	E22	A23	N24	I25	D26	R27	I28	K29	D36	L37	M38	A39	Y40	C41	A45	K46	E47	D48	L51	T52	P53	V54	P55	A56	N59	P60	F61	ARG	GLU	LYS	LYS	PHE	SER	ALA	ILE	LEU
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	84.29Å 84.29Å 132.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	89.8 (15.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.226 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6197	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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: 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	0.62	0/2805	1.01	7/3775 (0.2%)
2	B	0.58	0/2654	1.05	12/3597 (0.3%)
3	G	0.58	0/419	1.19	5/566 (0.9%)
All	All	0.60	0/5878	1.04	24/7938 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	VAL	N-CA-C	8.85	121.89	108.71
2	B	152	LEU	N-CA-C	-7.78	101.64	112.45
1	A	57	HIS	N-CA-C	7.32	122.23	113.16
3	G	54	VAL	CA-C-N	6.55	128.02	119.84
3	G	54	VAL	C-N-CA	6.55	128.02	119.84
2	B	314	ARG	N-CA-C	6.25	118.36	110.24
3	G	51	LEU	N-CA-C	-6.13	104.78	112.93
3	G	48	ASP	CA-C-N	6.02	125.70	119.56
3	G	48	ASP	C-N-CA	6.02	125.70	119.56
2	B	161	SER	N-CA-C	5.78	117.97	109.24
2	B	289	TYR	N-CA-C	5.75	119.06	110.14
1	A	164	GLN	CA-C-N	5.64	126.89	119.84
1	A	164	GLN	C-N-CA	5.64	126.89	119.84
2	B	93	ILE	CA-C-N	5.60	126.84	119.84
2	B	93	ILE	C-N-CA	5.60	126.84	119.84
2	B	235	PHE	N-CA-C	-5.52	101.39	109.50
2	B	71	VAL	CB-CA-C	-5.46	103.74	111.38
2	B	38	ASP	N-CA-C	-5.38	102.87	109.65
2	B	262	MET	N-CA-C	5.33	117.17	109.07
1	A	279	LYS	CA-C-N	5.30	127.84	120.63
1	A	279	LYS	C-N-CA	5.30	127.84	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	SER	N-CA-C	5.25	117.17	109.24
1	A	15	ARG	N-CA-C	-5.12	105.39	111.69
1	A	60	GLY	N-CA-C	-5.04	102.64	112.02

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	2759	0	2739	87	0
2	B	2607	0	2510	130	0
3	G	413	0	423	21	0
4	A	28	0	12	1	0
5	A	225	0	0	10	0
5	B	142	0	0	5	0
5	G	23	0	0	2	0
All	All	6197	0	5684	225	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 20.

All (225) 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:128:LYS:HG3	1:A:159:LEU:HD23	1.38	1.06
1:A:181:THR:O	1:A:203:GLY:HA3	1.70	0.90
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.59	0.82
1:A:149:ASN:OD1	1:A:178:ARG:HD3	1.80	0.81
1:A:311:ASN:HB2	1:A:319:ILE:HD11	1.62	0.81
2:B:48:ARG:HD3	2:B:340:ASN:HB2	1.65	0.79
1:A:112:GLY:HA2	5:A:405:HOH:O	1.84	0.77
1:A:282:PRO:HA	1:A:294:ASN:HD21	1.49	0.76
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.67	0.75
1:A:129:ARG:HH11	1:A:129:ARG:HG2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LEU:HG	2:B:95:LEU:HD21	1.68	0.73
2:B:289:TYR:CE1	2:B:295:ASN:HB2	2.24	0.73
2:B:198:LEU:HA	2:B:213:VAL:HG23	1.71	0.72
2:B:51:LEU:HD23	2:B:87:THR:HG22	1.70	0.72
2:B:48:ARG:HG2	3:G:61:PHE:HB3	1.73	0.71
1:A:7:ALA:HB3	5:A:359:HOH:O	1.91	0.70
1:A:230:TYR:O	1:A:286:CYS:HB2	1.91	0.70
1:A:282:PRO:HA	1:A:294:ASN:ND2	2.07	0.70
2:B:262:MET:SD	2:B:302:ALA:HB2	2.32	0.70
2:B:121:CYS:HB3	2:B:139:LEU:HB2	1.75	0.69
2:B:79:LEU:HD11	2:B:114:CYS:SG	2.32	0.68
2:B:212:ASP:HB3	2:B:215:GLU:HB2	1.75	0.67
2:B:6:GLN:O	2:B:10:GLU:HB2	1.94	0.67
1:A:52:GLN:NE2	1:A:175:LEU:HD21	2.10	0.67
1:A:88:MET:HE1	1:A:95:PHE:CE1	2.29	0.67
2:B:96:ARG:HD3	2:B:96:ARG:H	1.61	0.66
2:B:48:ARG:HD3	2:B:340:ASN:CB	2.27	0.64
3:G:54:VAL:HG13	3:G:55:PRO:HD2	1.78	0.64
2:B:286:LEU:HD22	2:B:296:VAL:HG22	1.80	0.64
2:B:8:ARG:HG3	2:B:8:ARG:HH11	1.63	0.63
2:B:286:LEU:CD2	2:B:296:VAL:HG13	2.28	0.63
2:B:152:LEU:HD23	2:B:192:LEU:HD21	1.80	0.63
1:A:342:VAL:O	1:A:346:ASN:HB2	1.98	0.63
2:B:239:ASN:HA	2:B:255:LEU:HD12	1.80	0.62
2:B:166:CYS:SG	2:B:187:VAL:HG11	2.41	0.61
2:B:249:THR:HG22	2:B:265:SER:HB3	1.82	0.61
2:B:71:VAL:HG13	2:B:81:ILE:HG12	1.83	0.60
1:A:188:HIS:CD2	1:A:197:LYS:HG2	2.37	0.60
3:G:22:GLU:HB2	5:G:78:HOH:O	2.01	0.60
2:B:51:LEU:HD13	2:B:82:TRP:CG	2.37	0.59
1:A:266:LEU:HD21	1:A:268:LEU:HD21	1.84	0.59
1:A:61:TYR:HB2	1:A:171:GLN:HG2	1.85	0.59
2:B:340:ASN:HD22	3:G:61:PHE:HB2	1.68	0.58
1:A:188:HIS:HD2	1:A:197:LYS:HG2	1.68	0.58
3:G:52:THR:O	3:G:54:VAL:N	2.37	0.58
2:B:71:VAL:HG11	2:B:112:VAL:HG21	1.86	0.58
2:B:150:ARG:C	2:B:157:ILE:HG13	2.29	0.57
1:A:70:LYS:HE3	1:A:167:TYR:HD2	1.70	0.57
2:B:29:THR:O	2:B:33:ILE:HG23	2.05	0.57
2:B:96:ARG:HH21	2:B:97:SER:CB	2.18	0.56
1:A:67:LYS:HE2	5:A:388:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:HE2	5:A:476:HOH:O	2.04	0.56
3:G:36:ASP:O	3:G:39:ALA:HB3	2.05	0.56
2:B:200:VAL:HA	2:B:209:LYS:O	2.05	0.56
2:B:283:ARG:HB3	3:G:51:LEU:HD11	1.86	0.56
1:A:39:LEU:HD13	1:A:253:ILE:HG12	1.87	0.55
2:B:77:GLY:C	2:B:78:LYS:HD2	2.31	0.55
3:G:51:LEU:O	3:G:53:PRO:HD3	2.06	0.55
2:B:37:ILE:HG22	2:B:38:ASP:N	2.22	0.55
2:B:271:CYS:CB	2:B:290:ASP:HB2	2.36	0.54
2:B:147:SER:OG	2:B:187:VAL:O	2.24	0.54
2:B:168:LEU:O	2:B:177:THR:N	2.40	0.54
1:A:18:MET:HA	1:A:21:ARG:NH1	2.22	0.54
2:B:75:GLN:HG2	2:B:98:SER:O	2.07	0.54
2:B:275:SER:HB3	5:B:395:HOH:O	2.07	0.54
1:A:12:ALA:O	1:A:15:ARG:HG2	2.07	0.53
1:A:72:VAL:HG11	1:A:179:VAL:HG12	1.91	0.53
2:B:51:LEU:HB3	2:B:82:TRP:CE3	2.43	0.53
1:A:338:ALA:O	1:A:342:VAL:HG23	2.09	0.53
2:B:271:CYS:SG	2:B:290:ASP:HB2	2.49	0.53
2:B:233:CYS:HB2	2:B:276:VAL:HG23	1.91	0.53
2:B:37:ILE:HG12	3:G:38:MET:HE3	1.91	0.53
2:B:209:LYS:HD2	2:B:211:TRP:CZ2	2.44	0.53
2:B:270:ILE:O	2:B:270:ILE:HG22	2.09	0.53
1:A:256:ASN:HB3	1:A:259:PHE:HD2	1.74	0.53
1:A:313:ARG:HB3	1:A:316:THR:HB	1.91	0.53
1:A:230:TYR:HB3	1:A:243:MET:HE3	1.90	0.53
2:B:3:GLU:HA	2:B:6:GLN:OE1	2.09	0.53
2:B:246:ASP:C	2:B:248:ALA:H	2.18	0.52
1:A:168:ILE:O	1:A:168:ILE:HG13	2.09	0.52
1:A:328:ASP:HB3	1:A:331:ASN:HB3	1.92	0.52
2:B:14:LEU:O	2:B:18:ILE:HG13	2.08	0.52
1:A:67:LYS:HE3	1:A:168:ILE:HG22	1.91	0.52
1:A:305:CYS:O	1:A:309:ASP:HB2	2.09	0.52
2:B:271:CYS:HB2	2:B:290:ASP:CB	2.39	0.52
1:A:344:ILE:HG23	1:A:348:LEU:HD12	1.91	0.52
2:B:153:ASP:O	2:B:155:ASN:N	2.43	0.52
2:B:108:SER:OG	2:B:110:ASN:HB2	2.10	0.52
2:B:191:SER:O	2:B:199:PHE:HB2	2.10	0.52
2:B:49:ARG:HD2	2:B:84:SER:O	2.09	0.52
2:B:49:ARG:HG2	2:B:87:THR:HG23	1.91	0.52
2:B:51:LEU:HB3	2:B:82:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:MET:HG2	1:A:286:CYS:SG	2.50	0.51
1:A:244:HIS:HE1	1:A:286:CYS:O	1.92	0.51
2:B:110:ASN:HB3	2:B:111:TYR:CD1	2.46	0.51
2:B:18:ILE:HG12	3:G:23:ALA:HA	1.93	0.51
2:B:7:LEU:HD22	3:G:13:ARG:HG2	1.93	0.50
2:B:48:ARG:HG2	3:G:61:PHE:CB	2.39	0.50
1:A:256:ASN:HB3	1:A:259:PHE:CD2	2.46	0.50
1:A:306:GLN:NE2	1:A:306:GLN:HA	2.26	0.50
2:B:51:LEU:CD2	2:B:87:THR:HG22	2.40	0.50
2:B:34:THR:O	2:B:36:ASN:N	2.45	0.50
2:B:267:ASP:O	2:B:268:ASN:HB2	2.11	0.50
2:B:96:ARG:HH21	2:B:97:SER:HB3	1.76	0.49
1:A:129:ARG:HG2	1:A:129:ARG:NH1	2.24	0.49
1:A:85:ILE:HD13	1:A:88:MET:HE2	1.94	0.49
2:B:13:GLN:HA	2:B:16:ASN:HD22	1.77	0.49
2:B:317:CYS:SG	2:B:330:GLY:HA3	2.53	0.49
1:A:128:LYS:HG3	1:A:159:LEU:CD2	2.27	0.49
2:B:120:ILE:HG21	2:B:138:GLU:HB3	1.95	0.49
2:B:318:LEU:HD23	2:B:329:THR:HG22	1.94	0.49
2:B:281:SER:HB3	3:G:48:ASP:HB2	1.94	0.48
1:A:188:HIS:HB3	1:A:195:HIS:CE1	2.47	0.48
2:B:308:LEU:HB3	2:B:339:TRP:CZ3	2.48	0.48
3:G:46:LYS:O	3:G:46:LYS:HD3	2.14	0.48
2:B:152:LEU:CD2	2:B:192:LEU:HD21	2.44	0.48
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.95	0.48
3:G:17:GLU:HG3	5:G:89:HOH:O	2.13	0.48
2:B:266:HIS:CD2	2:B:304:ARG:HH11	2.32	0.48
2:B:149:CYS:HA	2:B:158:VAL:O	2.14	0.48
2:B:63:TRP:CZ3	2:B:70:LEU:HD23	2.49	0.48
1:A:166:ASN:HB2	5:A:441:HOH:O	2.13	0.47
1:A:130:LEU:O	1:A:136:VAL:HG21	2.13	0.47
2:B:68:ARG:NH1	2:B:85:TYR:HD2	2.11	0.47
3:G:46:LYS:HD3	3:G:46:LYS:C	2.39	0.47
2:B:275:SER:O	2:B:287:ALA:HA	2.14	0.47
1:A:61:TYR:H	1:A:171:GLN:NE2	2.12	0.47
1:A:122:GLU:O	1:A:126:VAL:HG23	2.14	0.47
1:A:270:LYS:HG2	4:A:355:GDP:C6	2.49	0.47
1:A:289:GLU:CD	1:A:289:GLU:H	2.23	0.47
1:A:52:GLN:OE1	1:A:52:GLN:HA	2.14	0.47
1:A:52:GLN:HE22	1:A:175:LEU:HD21	1.75	0.47
1:A:179:VAL:HG22	5:A:532:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HB	1:A:196:PHE:CD2	2.50	0.46
2:B:107:PRO:HD2	5:B:397:HOH:O	2.14	0.46
1:A:27:GLY:HA2	2:B:55:LEU:HD11	1.96	0.46
1:A:191:PHE:CE2	1:A:340:THR:HG21	2.50	0.46
2:B:191:SER:HB2	2:B:232:ILE:HG23	1.98	0.46
3:G:18:GLN:O	3:G:21:MET:HB2	2.15	0.46
1:A:55:ILE:HA	1:A:60:GLY:CA	2.39	0.46
2:B:79:LEU:HB2	2:B:93:ILE:HB	1.98	0.46
2:B:292:PHE:HA	2:B:314:ARG:HA	1.98	0.46
2:B:298:ASP:CG	2:B:301:LYS:HB2	2.41	0.46
1:A:20:ASP:O	1:A:24:ARG:HG3	2.16	0.45
2:B:96:ARG:H	2:B:96:ARG:CD	2.22	0.45
2:B:289:TYR:HE1	2:B:295:ASN:HB2	1.79	0.45
2:B:193:ALA:HB2	2:B:198:LEU:HD12	1.97	0.45
1:A:127:ILE:HB	1:A:159:LEU:HD21	1.98	0.45
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.81	0.45
2:B:280:LYS:HB2	2:B:324:GLY:HA3	1.99	0.45
2:B:159:THR:O	2:B:166:CYS:HA	2.15	0.45
1:A:203:GLY:O	1:A:205:ARG:N	2.48	0.45
1:A:282:PRO:HB2	1:A:284:THR:HG22	1.99	0.44
2:B:30:LEU:HD23	2:B:262:MET:HB2	1.99	0.44
2:B:96:ARG:HD3	2:B:96:ARG:N	2.30	0.44
2:B:254:ASP:HB3	2:B:257:ALA:HB3	1.99	0.44
1:A:34:VAL:HG13	1:A:219:THR:HG21	2.00	0.44
1:A:85:ILE:HA	1:A:88:MET:HE2	1.99	0.44
2:B:56:ALA:H	2:B:76:ASP:HB3	1.81	0.44
1:A:110:LEU:O	1:A:112:GLY:N	2.50	0.44
1:A:181:THR:HG23	5:A:447:HOH:O	2.17	0.44
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.98	0.44
1:A:74:TYR:CE1	1:A:119:MET:HG2	2.52	0.44
1:A:54:LYS:HE3	1:A:60:GLY:O	2.18	0.44
1:A:266:LEU:CD2	1:A:268:LEU:HD21	2.47	0.44
1:A:281:SER:OG	1:A:285:ILE:HD12	2.18	0.44
2:B:81:ILE:HB	2:B:91:HIS:HB2	2.00	0.44
2:B:232:ILE:HG13	2:B:243:THR:HG22	1.99	0.44
1:A:206:SER:HB3	2:B:145:TYR:HE1	1.83	0.43
2:B:137:ARG:HG2	2:B:137:ARG:HH11	1.83	0.43
2:B:337:LYS:HB2	2:B:339:TRP:HE1	1.83	0.43
2:B:160:SER:HB2	2:B:187:VAL:HG12	2.00	0.43
2:B:239:ASN:ND2	5:B:472:HOH:O	2.51	0.43
1:A:260:THR:HG22	1:A:261:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:THR:O	2:B:37:ILE:HG13	2.17	0.43
2:B:276:VAL:HA	2:B:286:LEU:O	2.17	0.43
2:B:292:PHE:N	2:B:292:PHE:CD1	2.87	0.43
1:A:212:ILE:HD12	1:A:212:ILE:HA	1.84	0.43
1:A:188:HIS:HB3	1:A:195:HIS:HE1	1.84	0.43
2:B:193:ALA:CB	2:B:198:LEU:HD12	2.48	0.43
2:B:277:SER:O	2:B:285:LEU:HD12	2.17	0.43
1:A:161:ARG:HD2	5:A:439:HOH:O	2.18	0.43
2:B:164:THR:HG22	2:B:185:GLY:C	2.44	0.43
2:B:146:LEU:HD11	2:B:159:THR:HB	1.99	0.43
2:B:96:ARG:HH21	2:B:97:SER:HB2	1.83	0.43
2:B:340:ASN:ND2	3:G:61:PHE:HB2	2.33	0.43
1:A:225:VAL:HB	1:A:268:LEU:HD23	2.00	0.43
5:A:465:HOH:O	2:B:55:LEU:HD13	2.18	0.43
2:B:210:LEU:HB3	2:B:220:GLN:H	1.83	0.43
2:B:318:LEU:CD2	2:B:329:THR:HG22	2.49	0.43
1:A:95:PHE:HB3	1:A:97:ASP:O	2.19	0.42
2:B:25:CYS:HB3	3:G:29:LYS:HA	1.99	0.42
1:A:39:LEU:HD13	1:A:253:ILE:CG1	2.49	0.42
2:B:93:ILE:HA	2:B:94:PRO:HD3	1.81	0.42
1:A:123:LEU:O	1:A:127:ILE:HG13	2.17	0.42
1:A:220:ALA:HA	1:A:262:THR:HG23	2.01	0.42
1:A:179:VAL:HA	5:A:515:HOH:O	2.19	0.42
2:B:18:ILE:O	2:B:22:ARG:HG3	2.19	0.42
2:B:328:ALA:HA	2:B:337:LYS:O	2.19	0.42
2:B:150:ARG:O	2:B:157:ILE:HG13	2.20	0.42
2:B:301:LYS:O	2:B:302:ALA:HB3	2.20	0.42
2:B:8:ARG:HG3	2:B:8:ARG:NH1	2.32	0.42
2:B:231:ALA:HB2	2:B:275:SER:HA	2.02	0.42
1:A:176:ARG:HD3	1:A:327:THR:HG21	2.01	0.41
1:A:340:THR:O	1:A:343:ILE:HB	2.19	0.41
2:B:68:ARG:HG3	2:B:85:TYR:CD2	2.55	0.41
1:A:25:GLU:O	1:A:29:LYS:HG3	2.21	0.41
2:B:339:TRP:N	2:B:339:TRP:CD1	2.88	0.41
2:B:2:SER:O	2:B:4:LEU:N	2.53	0.41
1:A:148:LEU:HD12	1:A:148:LEU:HA	1.89	0.41
2:B:192:LEU:HD12	2:B:192:LEU:HA	1.80	0.41
1:A:142:ARG:C	1:A:144:ARG:H	2.28	0.41
2:B:212:ASP:O	2:B:216:GLY:N	2.45	0.41
1:A:223:PHE:CD1	1:A:223:PHE:C	2.99	0.41
2:B:192:LEU:HD23	5:B:360:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:ARG:NH2	5:B:480:HOH:O	2.54	0.41
2:B:170:ASP:CG	2:B:173:THR:HG22	2.45	0.40
2:B:96:ARG:HE	2:B:97:SER:HB3	1.86	0.40
2:B:300:LEU:HD21	3:G:41:CYS:SG	2.61	0.40
2:B:321:THR:HB	2:B:323:ASP:OD1	2.21	0.40
1:A:96:GLY:HA3	1:A:134:SER:OG	2.21	0.40
3:G:59:ASN:O	3:G:61:PHE:N	2.55	0.40
1:A:173:ASP:O	1:A:177:THR:HG23	2.22	0.40
2:B:77:GLY:O	2:B:78:LYS:HD2	2.21	0.40
2:B:273:ILE:HG13	2:B:289:TYR:CE2	2.57	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	342/353 (97%)	314 (92%)	21 (6%)	7 (2%)	6	5
2	B	337/340 (99%)	307 (91%)	23 (7%)	7 (2%)	5	4
3	G	52/71 (73%)	39 (75%)	8 (15%)	5 (10%)	0	0
All	All	731/764 (96%)	660 (90%)	52 (7%)	19 (3%)	4	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	ASN
3	G	55	PRO
3	G	60	PRO
1	A	7	ALA
1	A	114	ALA
1	A	236	GLU
2	B	3	GLU

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Mol	Chain	Res	Type
2	B	128	THR
2	B	154	ASP
3	G	45	ALA
3	G	56	ALA
1	A	41	ALA
1	A	119	MET
1	A	6	SER
2	B	247	ASP
1	A	111	ALA
2	B	310	GLY
3	G	53	PRO
2	B	141	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	296/303 (98%)	271 (92%)	25 (8%)	10	14
2	B	282/283 (100%)	260 (92%)	22 (8%)	11	16
3	G	44/58 (76%)	35 (80%)	9 (20%)	1	1
All	All	622/644 (97%)	566 (91%)	56 (9%)	9	12

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	14	GLU
1	A	26	ASP
1	A	64	GLU
1	A	79	GLN
1	A	129	ARG
1	A	150	ASP
1	A	160	ASP
1	A	182	THR
1	A	190	THR

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	199	PHE
1	A	205	ARG
1	A	207	GLU
1	A	218	VAL
1	A	233	VAL
1	A	245	GLU
1	A	257	LYS
1	A	289	GLU
1	A	294	ASN
1	A	327	THR
1	A	339	VAL
1	A	346	ASN
1	A	347	ASN
1	A	348	LEU
2	B	2	SER
2	B	10	GLU
2	B	14	LEU
2	B	23	LYS
2	B	33	ILE
2	B	48	ARG
2	B	49	ARG
2	B	71	VAL
2	B	87	THR
2	B	96	ARG
2	B	110	ASN
2	B	132	ASN
2	B	135	VAL
2	B	150	ARG
2	B	158	VAL
2	B	192	LEU
2	B	217	MET
2	B	277	SER
2	B	280	LYS
2	B	321	THR
2	B	325	MET
2	B	336	LEU
3	G	8	SER
3	G	25	ILE
3	G	26	ASP
3	G	27	ARG
3	G	36	ASP

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Mol	Chain	Res	Type
3	G	54	VAL
3	G	55	PRO
3	G	59	ASN
3	G	60	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	188	HIS
1	A	195	HIS
1	A	306	GLN
1	A	346	ASN
2	B	16	ASN
2	B	110	ASN
2	B	132	ASN
2	B	175	GLN
2	B	176	GLN
2	B	266	HIS
2	B	340	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](#)

1 ligand is 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	A	355	-	29,30,30	1.54	6 (20%)	45,47,47	1.73	9 (20%)

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	A	355	-	-	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	A	355	GDP	O4'-C1'	4.50	1.52	1.42
4	A	355	GDP	PA-O3A	3.10	1.62	1.59
4	A	355	GDP	C6-N1	2.34	1.43	1.38
4	A	355	GDP	C1'-N9	2.23	1.53	1.47
4	A	355	GDP	C4-N3	2.09	1.39	1.34
4	A	355	GDP	PB-O3B	-2.04	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	355	GDP	O4'-C1'-N9	6.97	124.15	108.36
4	A	355	GDP	O3A-PB-O1B	-3.13	94.58	111.04
4	A	355	GDP	O3'-C3'-C4'	-2.55	103.76	111.08
4	A	355	GDP	O2'-C2'-C3'	2.32	119.26	111.82
4	A	355	GDP	O2B-PB-O1B	2.29	119.77	110.83
4	A	355	GDP	C2'-C1'-N9	-2.11	107.36	113.25
4	A	355	GDP	O4'-C4'-C5'	2.11	116.09	109.33
4	A	355	GDP	N9-C8-N7	2.07	117.24	113.40
4	A	355	GDP	C5'-C4'-C3'	-2.02	107.93	115.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

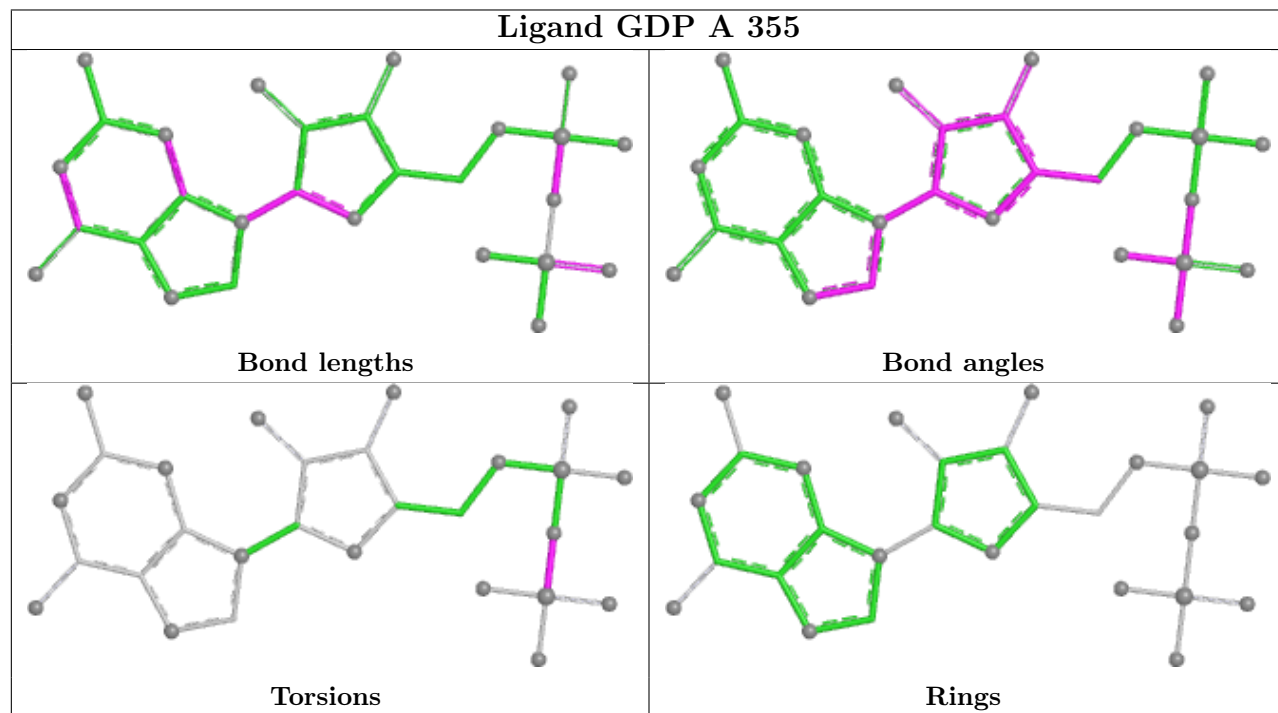
Mol	Chain	Res	Type	Atoms
4	A	355	GDP	PA-O3A-PB-O2B
4	A	355	GDP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	355	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 ⓘ

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

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.