



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:07 PM UTC

PDB ID : 1GLB / pdb_00001glb
Title : STRUCTURE OF THE REGULATORY COMPLEX OF ESCHERICHIA COLI IIIGLC WITH GLYCEROL KINASE
Authors : Hurley, J.H.; Worthylake, D.; Faber, H.R.; Meadow, N.D.; Roseman, S.; Pettigrew, D.W.; Remington, S.J.
Deposited on : 1992-10-28
Resolution : 2.60 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

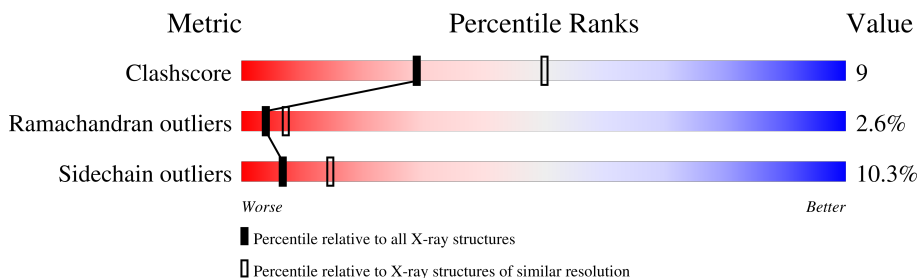
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	F	168	 65% 26% 6% •
2	G	501	 63% 29% 5% ••

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5018 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.

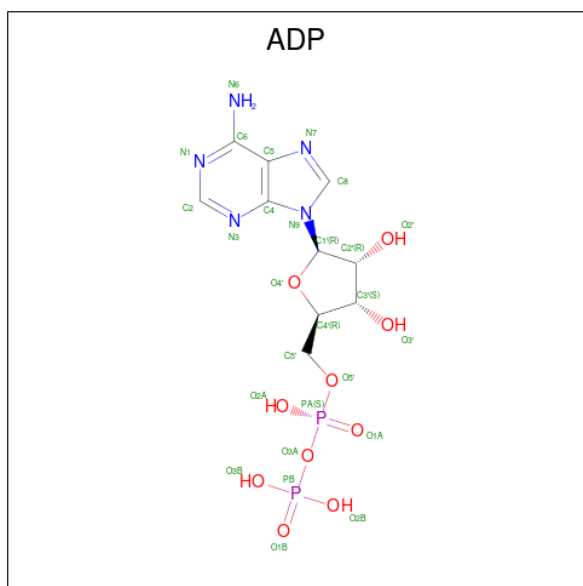
- Molecule 1 is a protein called GLUCOSE-SPECIFIC PROTEIN IIIGlc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	162	Total	C	N	O	S	0	0	1
			1202	769	191	240	2			

- Molecule 2 is a protein called GLYCEROL KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	490	Total	C	N	O	S	0	0	1
			3783	2387	655	722	19			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



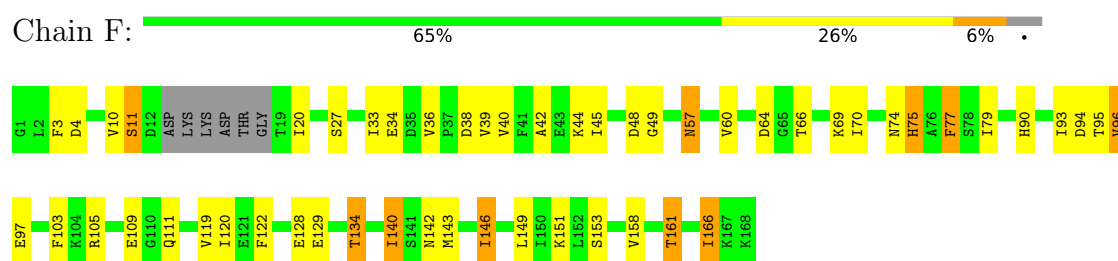
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots [i](#)

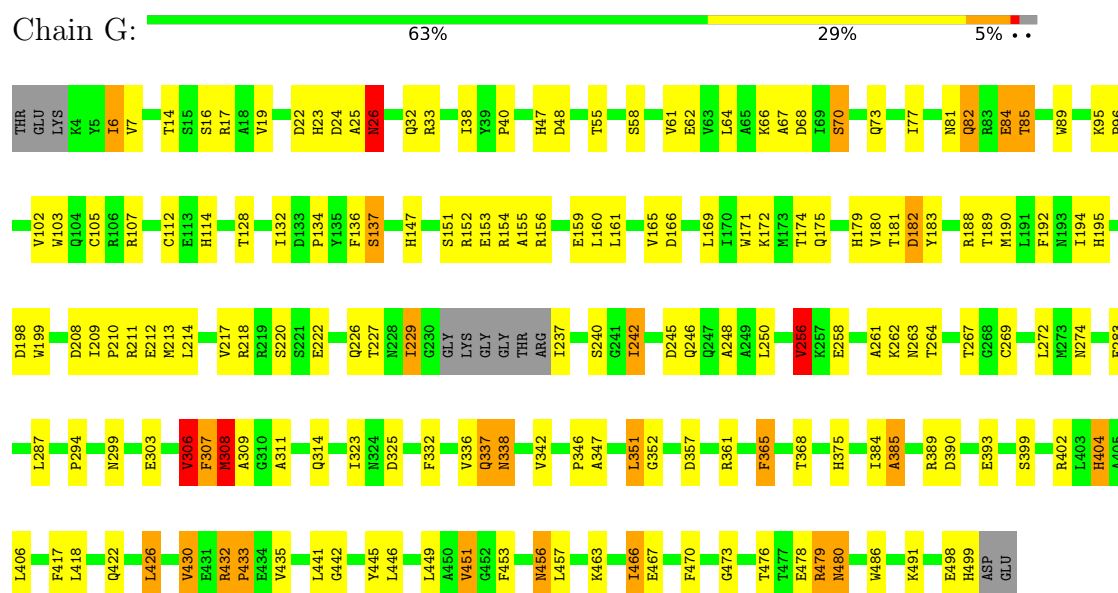
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: GLYCEROL KINASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.70Å 124.90Å 134.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.205 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: ADP, GOL

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	F	0.94	3/1217 (0.2%)	1.80	30/1647 (1.8%)
2	G	1.00	17/3861 (0.4%)	1.83	83/5251 (1.6%)
All	All	0.99	20/5078 (0.4%)	1.82	113/6898 (1.6%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	11	SER	C-N	-7.25	1.23	1.33
2	G	375	HIS	CD2-NE2	-7.20	1.29	1.37
2	G	147	HIS	CD2-NE2	-6.71	1.30	1.37
2	G	229	ILE	C-N	-6.54	1.24	1.33
1	F	75	HIS	CD2-NE2	-6.53	1.30	1.37
2	G	306	VAL	CA-CB	6.51	1.62	1.54
2	G	47	HIS	CD2-NE2	-6.48	1.30	1.37
2	G	114	HIS	CD2-NE2	-6.32	1.30	1.37
2	G	85	THR	CA-CB	6.29	1.62	1.53
2	G	195	HIS	CD2-NE2	-6.26	1.30	1.37
1	F	90	HIS	CD2-NE2	-6.18	1.31	1.37
2	G	23	HIS	CD2-NE2	-6.10	1.31	1.37
2	G	404	HIS	CD2-NE2	-6.00	1.31	1.37
2	G	179	HIS	CD2-NE2	-5.85	1.31	1.37
2	G	499	HIS	CD2-NE2	-5.80	1.31	1.37
2	G	430	VAL	CA-CB	5.72	1.61	1.54
2	G	19	VAL	CA-CB	5.42	1.62	1.54
2	G	194	ILE	CA-CB	5.36	1.61	1.54
2	G	375	HIS	CG-ND1	-5.08	1.32	1.38
2	G	195	HIS	CG-ND1	-5.00	1.32	1.38

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	336	VAL	N-CA-C	10.72	121.03	111.81
2	G	147	HIS	CA-CB-CG	-10.24	103.56	113.80
2	G	457	LEU	N-CA-C	10.23	125.64	112.34
1	F	111	GLN	N-CA-C	9.81	124.25	109.25
2	G	245	ASP	CA-CB-CG	9.66	122.27	112.60
1	F	60	VAL	N-CA-CB	-9.28	100.63	112.60
1	F	57	ASN	N-CA-C	9.15	130.30	110.80
1	F	10	VAL	N-CA-C	9.14	120.97	108.17
1	F	146	ILE	N-CA-C	8.91	121.46	108.53
2	G	137	SER	N-CA-C	8.58	121.71	111.33
2	G	256	VAL	N-CA-CB	-8.53	101.27	112.36
1	F	70	ILE	N-CA-C	-8.36	96.40	108.36
2	G	323	ILE	N-CA-C	7.93	125.84	109.34
2	G	180	VAL	N-CA-C	7.91	120.16	108.45
1	F	142	ASN	CA-CB-CG	7.59	120.19	112.60
2	G	308	MET	N-CA-CB	-7.50	99.75	111.23
2	G	308	MET	N-CA-C	7.46	120.79	108.49
2	G	263	ASN	OD1-CG-ND2	-7.20	115.40	122.60
2	G	68	ASP	CA-CB-CG	7.13	119.73	112.60
2	G	22	ASP	CA-CB-CG	6.98	119.58	112.60
2	G	432	ARG	CA-C-N	6.94	126.93	119.78
2	G	432	ARG	C-N-CA	6.94	126.93	119.78
2	G	451	VAL	N-CA-CB	-6.91	99.83	111.23
1	F	140	ILE	N-CA-C	-6.83	98.02	107.99
1	F	44	LYS	N-CA-C	6.81	120.89	111.90
2	G	325	ASP	CA-CB-CG	6.75	119.35	112.60
2	G	307	PHE	N-CA-C	6.67	120.67	112.54
2	G	136	PHE	O-C-N	6.57	130.39	122.96
2	G	385	ALA	N-CA-C	6.54	118.49	111.36
2	G	161	LEU	N-CA-C	6.53	119.34	109.23
2	G	303	GLU	N-CA-C	6.46	119.13	108.99
1	F	109	GLU	N-CA-C	6.38	119.05	111.33
2	G	165	VAL	N-CA-C	6.37	119.01	111.05
2	G	404	HIS	CA-CB-CG	-6.26	107.54	113.80
1	F	64	ASP	CA-CB-CG	6.18	118.78	112.60
1	F	3	PHE	N-CA-C	6.16	120.83	112.88
2	G	240	SER	N-CA-C	6.14	121.70	113.72
2	G	314	GLN	CG-CD-NE2	6.11	125.57	116.40
2	G	242	ILE	CB-CA-C	-6.07	99.97	110.65
1	F	57	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	F	10	VAL	N-CA-CB	-6.01	103.08	111.25
2	G	256	VAL	CB-CA-C	5.97	117.50	110.93
2	G	73	GLN	N-CA-C	-5.93	104.19	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	134	THR	CA-CB-OG1	-5.91	100.74	109.60
2	G	491	LYS	CA-CB-CG	5.91	125.92	114.10
2	G	417	PHE	CA-C-O	-5.91	114.80	121.00
2	G	456	ASN	N-CA-C	5.85	123.26	110.80
2	G	147	HIS	CB-CG-CD2	-5.84	123.60	131.20
2	G	47	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	F	4	ASP	N-CA-C	5.77	118.51	111.82
1	F	77	PHE	CA-CB-CG	5.73	119.53	113.80
2	G	390	ASP	CA-CB-CG	5.71	118.31	112.60
2	G	198	ASP	CA-CB-CG	5.70	118.30	112.60
1	F	103	PHE	CA-CB-CG	-5.69	108.11	113.80
1	F	75	HIS	CB-CG-CD2	-5.69	123.81	131.20
2	G	182	ASP	CA-CB-CG	5.65	118.25	112.60
2	G	26	ASN	CA-CB-CG	5.64	118.24	112.60
1	F	122	PHE	CA-CB-CG	5.63	119.43	113.80
2	G	338	ASN	CB-CG-ND2	5.63	124.84	116.40
1	F	161	THR	CA-C-N	5.58	125.49	119.85
1	F	161	THR	C-N-CA	5.58	125.49	119.85
2	G	220	SER	N-CA-C	5.58	119.35	112.54
2	G	151	SER	N-CA-C	5.56	118.06	111.33
2	G	314	GLN	OE1-CD-NE2	-5.56	117.04	122.60
2	G	453	PHE	CA-CB-CG	5.55	119.35	113.80
2	G	14	THR	CA-CB-OG1	-5.49	101.36	109.60
2	G	179	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	F	90	HIS	CB-CG-CD2	-5.45	124.11	131.20
1	F	134	THR	CA-CB-CG2	5.42	119.72	110.50
2	G	183	TYR	N-CA-C	5.42	117.26	111.36
2	G	169	LEU	N-CA-C	5.40	117.17	111.28
2	G	70	SER	N-CA-C	5.40	117.17	108.32
2	G	337	GLN	N-CA-CB	5.39	119.61	110.49
2	G	357	ASP	CA-C-N	5.39	124.90	119.19
2	G	357	ASP	C-N-CA	5.39	124.90	119.19
2	G	48	ASP	CA-C-N	5.37	125.44	119.32
2	G	48	ASP	C-N-CA	5.37	125.44	119.32
2	G	82	GLN	OE1-CD-NE2	-5.37	117.23	122.60
2	G	84	GLU	N-CA-C	5.37	122.23	110.80
2	G	85	THR	CA-C-N	5.36	129.17	121.50
2	G	85	THR	C-N-CA	5.36	129.17	121.50
2	G	82	GLN	CG-CD-NE2	5.33	124.40	116.40
2	G	103	TRP	CG-CD2-CE3	5.33	139.23	133.90
2	G	309	ALA	CA-C-O	-5.31	116.31	119.55
2	G	258	GLU	N-CA-C	5.30	118.12	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	180	VAL	N-CA-CB	-5.28	102.79	111.45
2	G	445	TYR	CB-CA-C	-5.28	102.03	110.79
1	F	109	GLU	O-C-N	-5.27	116.54	122.12
2	G	384	ILE	CA-C-N	5.26	127.77	120.29
2	G	384	ILE	C-N-CA	5.26	127.77	120.29
2	G	337	GLN	CB-CA-C	-5.25	99.97	110.42
2	G	23	HIS	CA-CB-CG	-5.24	108.56	113.80
2	G	466	ILE	N-CA-CB	-5.22	102.62	111.23
2	G	365	PHE	CA-CB-CG	5.22	119.02	113.80
1	F	38	ASP	O-C-N	5.17	129.46	122.59
2	G	199	TRP	CE2-CD2-CG	-5.16	101.01	107.20
2	G	67	ALA	N-CA-C	-5.16	98.88	107.80
2	G	181	THR	N-CA-CB	5.15	119.55	111.20
1	F	129	GLU	CA-CB-CG	5.15	124.40	114.10
2	G	209	ILE	N-CA-C	-5.13	101.99	108.05
2	G	332	PHE	CA-CB-CG	-5.12	108.68	113.80
2	G	261	ALA	N-CA-C	5.11	116.84	109.07
1	F	39	VAL	N-CA-C	5.09	118.19	111.17
2	G	89	TRP	CG-CD2-CE3	5.08	138.98	133.90
2	G	486	TRP	CG-CD2-CE3	5.07	138.97	133.90
2	G	134	PRO	CA-C-N	5.06	127.37	120.54
2	G	134	PRO	C-N-CA	5.06	127.37	120.54
2	G	357	ASP	CA-CB-CG	5.05	117.65	112.60
1	F	57	ASN	O-C-N	-5.04	115.88	122.59
2	G	433	PRO	N-CA-C	5.04	119.22	111.21
2	G	17	ARG	CA-CB-CG	5.02	124.14	114.10
1	F	153	SER	N-CA-C	5.02	115.67	108.74
2	G	466	ILE	CB-CA-C	5.01	119.51	111.29

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	F	1202	0	1217	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3783	0	3637	65	0
3	G	27	0	12	0	0
4	G	6	0	8	0	0
All	All	5018	0	4874	86	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 9.

All (86) 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:F:20:ILE:HD12	1:F:166:ILE:HD11	1.59	0.82
2:G:33:ARG:HG3	2:G:55:THR:HG22	1.72	0.71
1:F:48:ASP:HB3	1:F:143:MET:HE2	1.73	0.71
1:F:40:VAL:HA	1:F:45:ILE:HD12	1.74	0.70
1:F:143:MET:SD	1:F:146:ILE:HD11	2.33	0.68
2:G:137:SER:HB2	2:G:189:THR:HA	1.79	0.64
2:G:26:ASN:HD22	2:G:26:ASN:H	1.43	0.64
2:G:7:VAL:HB	2:G:77:ILE:HD13	1.80	0.63
2:G:256:VAL:HG13	2:G:294:PRO:HG3	1.82	0.62
2:G:476:THR:O	2:G:479:ARG:HB2	2.00	0.61
2:G:307:PHE:H	2:G:308:MET:HE2	1.64	0.61
2:G:85:THR:HB	2:G:102:VAL:HA	1.81	0.61
2:G:269:CYS:HB2	2:G:306:VAL:HG22	1.81	0.61
2:G:274:ASN:HD21	2:G:299:ASN:HD22	1.49	0.60
2:G:227:THR:HG22	2:G:237:ILE:HA	1.83	0.60
1:F:74:ASN:HD21	1:F:105:ARG:HD2	1.68	0.59
1:F:75:HIS:HD2	1:F:95:THR:HB	1.66	0.58
1:F:74:ASN:ND2	1:F:105:ARG:HD2	2.18	0.58
2:G:58:SER:O	2:G:62:GLU:HB2	2.04	0.57
2:G:248:ALA:O	2:G:442:GLY:HA3	2.05	0.56
2:G:81:ASN:ND2	2:G:166:ASP:HB3	2.22	0.55
2:G:267:THR:HG23	2:G:311:ALA:HB2	1.87	0.55
2:G:38:ILE:HG22	2:G:40:PRO:HD3	1.88	0.55
2:G:62:GLU:O	2:G:66:LYS:HB2	2.07	0.55
2:G:192:PHE:HE1	2:G:217:VAL:HG11	1.72	0.54
2:G:154:ARG:HG2	2:G:159:GLU:HB2	1.90	0.53
2:G:430:VAL:HB	2:G:470:PHE:HB2	1.89	0.53
1:F:34:GLU:HA	1:F:42:ALA:HA	1.90	0.53
2:G:174:THR:HG22	2:G:226:GLN:O	2.08	0.53
2:G:105:CYS:SG	2:G:107:ARG:HB3	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ASP:O	1:F:97:GLU:HG2	2.08	0.52
2:G:105:CYS:SG	2:G:107:ARG:NH1	2.82	0.52
2:G:128:THR:HG21	2:G:190:MET:HA	1.90	0.52
2:G:422:GLN:NE2	2:G:426:LEU:HD13	2.25	0.52
1:F:69:LYS:O	1:F:77:PHE:HA	2.09	0.52
1:F:74:ASN:ND2	1:F:105:ARG:HB2	2.25	0.51
1:F:75:HIS:CD2	1:F:95:THR:HB	2.43	0.51
2:G:64:LEU:HD22	2:G:70:SER:HA	1.93	0.51
2:G:156:ARG:HA	2:G:212:GLU:OE1	2.11	0.50
1:F:74:ASN:HD21	1:F:105:ARG:HH11	1.59	0.50
2:G:182:ASP:HB3	2:G:242:ILE:HB	1.94	0.49
2:G:128:THR:HG23	2:G:192:PHE:O	2.12	0.49
2:G:189:THR:O	2:G:190:MET:HB3	2.13	0.49
2:G:211:ARG:HG3	2:G:214:LEU:HD12	1.95	0.48
2:G:435:VAL:HG11	2:G:441:LEU:HD11	1.96	0.47
2:G:422:GLN:O	2:G:426:LEU:HB2	2.13	0.47
1:F:96:VAL:HG21	2:G:478:GLU:HG2	1.96	0.47
2:G:171:TRP:CE3	2:G:172:LYS:HE2	2.50	0.47
2:G:246:GLN:HB3	2:G:272:LEU:HD11	1.96	0.47
2:G:153:GLU:HA	2:G:156:ARG:HH11	1.79	0.46
2:G:171:TRP:HE3	2:G:172:LYS:HE2	1.81	0.46
1:F:20:ILE:HB	1:F:166:ILE:HG13	1.98	0.45
1:F:77:PHE:CZ	1:F:119:VAL:HG21	2.52	0.45
2:G:155:ALA:CB	2:G:210:PRO:HG3	2.47	0.45
2:G:435:VAL:HG11	2:G:441:LEU:CD1	2.46	0.45
2:G:385:ALA:HA	2:G:422:GLN:OE1	2.17	0.45
2:G:389:ARG:HH12	2:G:479:ARG:HG2	1.82	0.45
2:G:347:ALA:HB2	2:G:351:LEU:HD13	1.99	0.44
2:G:308:MET:HB2	2:G:346:PRO:HB2	1.98	0.44
1:F:140:ILE:HD12	1:F:149:LEU:HD11	1.99	0.44
1:F:143:MET:HE1	1:F:149:LEU:HD13	1.99	0.44
2:G:82:GLN:OE1	2:G:85:THR:HG21	2.17	0.44
2:G:188:ARG:HH22	2:G:287:LEU:HD13	1.83	0.44
2:G:210:PRO:HG2	2:G:213:MET:HG3	2.00	0.44
2:G:347:ALA:O	2:G:361:ARG:HA	2.18	0.44
2:G:152:ARG:HD3	2:G:208:ASP:OD2	2.18	0.43
2:G:264:THR:O	2:G:269:CYS:HA	2.19	0.43
2:G:152:ARG:HG2	2:G:156:ARG:NH1	2.33	0.43
2:G:308:MET:H	2:G:308:MET:HG2	1.64	0.43
2:G:16:SER:O	2:G:32:GLN:HA	2.19	0.43
2:G:26:ASN:H	2:G:26:ASN:ND2	2.15	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:402:ARG:HE	2:G:404:HIS:HE1	1.67	0.42
2:G:480:ASN:HD22	2:G:480:ASN:N	2.17	0.42
1:F:49:GLY:O	1:F:151:LYS:HE3	2.20	0.42
2:G:112:CYS:HB3	2:G:132:ILE:HG22	2.00	0.42
2:G:155:ALA:HB2	2:G:160:LEU:HD11	2.02	0.42
2:G:342:VAL:HA	2:G:365:PHE:O	2.20	0.42
2:G:432:ARG:HA	2:G:433:PRO:HD2	1.87	0.41
2:G:473:GLY:O	2:G:476:THR:HG22	2.20	0.41
2:G:250:LEU:HD22	2:G:272:LEU:HD22	2.02	0.41
1:F:66:THR:O	1:F:79:ILE:HG13	2.21	0.41
2:G:6:ILE:HD12	2:G:6:ILE:N	2.35	0.41
1:F:27:SER:OG	1:F:158:VAL:HG12	2.20	0.40
2:G:389:ARG:NH1	2:G:479:ARG:HG2	2.36	0.40
2:G:95:LYS:HA	2:G:96:PRO:HD3	1.91	0.40
1:F:33:ILE:O	1:F:36:VAL:HG23	2.22	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	F	158/168 (94%)	141 (89%)	15 (10%)	2 (1%)	9	21
2	G	486/501 (97%)	438 (90%)	33 (7%)	15 (3%)	3	5
All	All	644/669 (96%)	579 (90%)	48 (8%)	17 (3%)	4	7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	57	ASN
2	G	84	GLU
2	G	175	GLN

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Mol	Chain	Res	Type
2	G	229	ILE
2	G	479	ARG
2	G	25	ALA
2	G	222	GLU
2	G	337	GLN
1	F	11	SER
2	G	24	ASP
2	G	463	LYS
2	G	467	GLU
2	G	26	ASN
2	G	218	ARG
2	G	399	SER
2	G	61	VAL
2	G	352	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	F	73/145 (50%)	66 (90%)	7 (10%)	8	17
2	G	190/412 (46%)	170 (90%)	20 (10%)	6	14
All	All	263/557 (47%)	236 (90%)	27 (10%)	7	15

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	93	ILE
1	F	96	VAL
1	F	120	ILE
1	F	128	GLU
1	F	134	THR
1	F	161	THR
1	F	166	ILE
2	G	6	ILE
2	G	256	VAL

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Mol	Chain	Res	Type
2	G	262	LYS
2	G	283	GLU
2	G	306	VAL
2	G	308	MET
2	G	338	ASN
2	G	351	LEU
2	G	368	THR
2	G	393	GLU
2	G	406	LEU
2	G	418	LEU
2	G	426	LEU
2	G	446	LEU
2	G	449	LEU
2	G	451	VAL
2	G	456	ASN
2	G	466	ILE
2	G	480	ASN
2	G	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	253	GLN
2	G	263	ASN
2	G	284	ASN
2	G	299	ASN
2	G	324	ASN
2	G	404	HIS
2	G	480	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 [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	GOL	G	503	-	5,5,5	0.44	0	5,5,5	0.36	0
3	ADP	G	502	-	28,29,29	0.90	1 (3%)	43,45,45	0.92	2 (4%)

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	GOL	G	503	-	-	0/4/4/4	-
3	ADP	G	502	-	-	0/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	502	ADP	PB-O2B	-2.04	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	502	ADP	O3'-C3'-C4'	-2.55	103.75	111.08
3	G	502	ADP	O3B-PB-O3A	-2.04	97.79	104.64

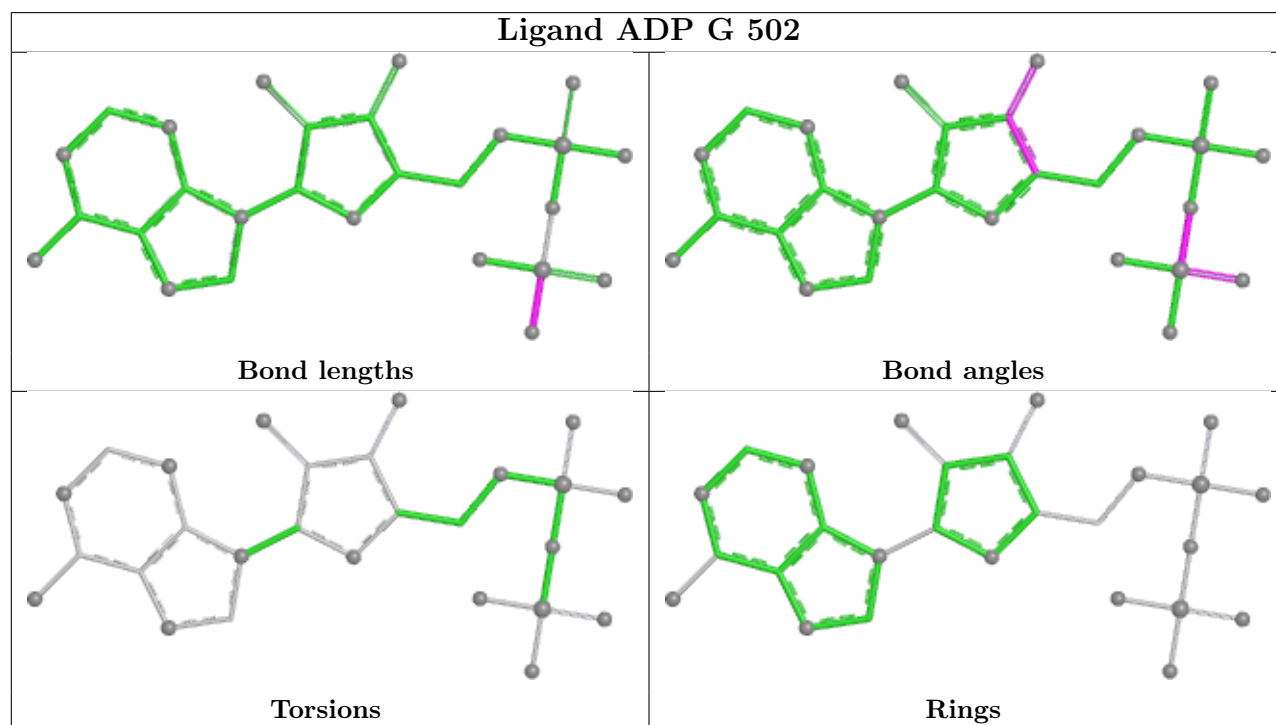
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.