



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:28 AM UTC

PDB ID : 1DAR / pdb_00001dar
Title : ELONGATION FACTOR G IN COMPLEX WITH GDP
Authors : Al-Karadaghi, S.; Aevansson, A.; Garber, M.; Zheltonosova, J.; Liljas, A.
Deposited on : 1996-02-15
Resolution : 2.40 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

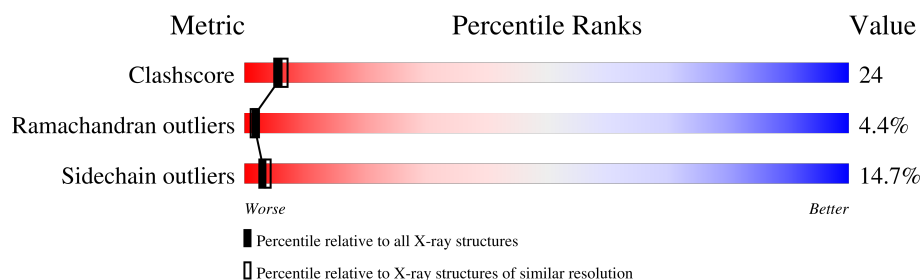
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	691	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4893 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 ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	619	4732	3005	817	892	18	277	0	4

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 3 is water.

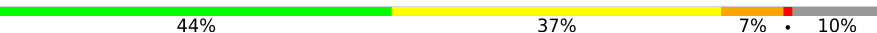
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	133	Total 133 O 133	0	0

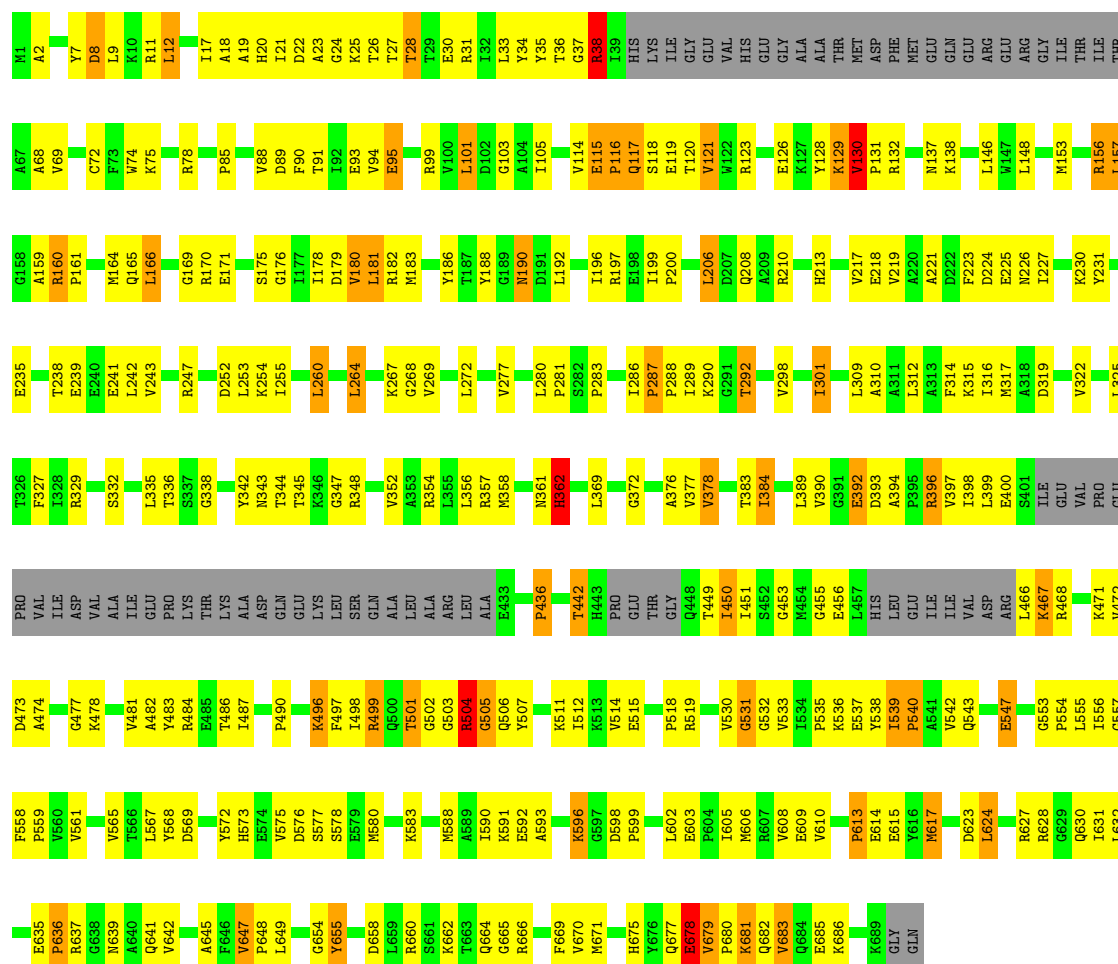
3 Residue-property plots

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: ELONGATION FACTOR G

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.30Å 106.40Å 115.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4893	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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	0.85	5/4817 (0.1%)	1.20	34/6524 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	VAL	CA-CB	6.11	1.60	1.53
1	A	38	ARG	C-N	-5.32	1.25	1.33
1	A	400	GLU	C-N	-5.24	1.26	1.33
1	A	442	THR	C-N	-5.18	1.26	1.33
1	A	456	GLU	C-N	-5.06	1.26	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	GLY	N-CA-C	-7.67	103.52	112.73
1	A	394	ALA	N-CA-C	-7.37	100.14	110.31
1	A	115	GLU	CA-C-N	7.28	128.94	119.84
1	A	115	GLU	C-N-CA	7.28	128.94	119.84
1	A	169	GLY	N-CA-C	-7.16	102.21	112.81
1	A	436	PRO	N-CA-CB	6.99	110.59	103.25
1	A	208	GLN	N-CA-C	-6.91	103.74	111.28
1	A	471	LYS	N-CA-C	6.66	119.78	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	LYS	N-CA-C	-6.38	104.25	111.14
1	A	310	ALA	N-CA-C	-6.05	98.39	108.32
1	A	613	PRO	N-CA-C	-5.92	101.21	110.50
1	A	670	VAL	N-CA-C	-5.79	100.70	108.35
1	A	269	VAL	N-CA-C	5.78	115.97	110.42
1	A	301	ILE	N-CA-C	5.69	115.76	106.72
1	A	268	GLY	N-CA-C	5.68	122.30	114.92
1	A	264	LEU	N-CA-C	5.66	119.70	112.34
1	A	467	LYS	N-CA-C	5.59	122.72	110.80
1	A	598	ASP	CA-C-N	5.59	125.54	119.78
1	A	598	ASP	C-N-CA	5.59	125.54	119.78
1	A	660	ARG	N-CA-C	-5.45	104.37	111.02
1	A	505	GLY	N-CA-C	-5.43	100.31	113.18
1	A	105	ILE	CB-CA-C	-5.41	104.78	111.32
1	A	78	ARG	N-CA-C	-5.35	100.59	109.46
1	A	451	ILE	N-CA-C	5.34	111.92	106.21
1	A	130	VAL	N-CA-C	5.33	112.82	107.55
1	A	287	PRO	N-CA-C	5.30	117.16	110.70
1	A	678	GLU	N-CA-C	5.27	117.86	109.96
1	A	362	HIS	N-CA-C	5.22	121.91	110.80
1	A	219	VAL	CB-CA-C	-5.21	105.19	112.02
1	A	301	ILE	N-CA-CB	-5.15	105.92	112.15
1	A	539	ILE	CB-CA-C	-5.14	108.81	113.70
1	A	148	LEU	N-CA-C	-5.04	105.79	111.28
1	A	287	PRO	CA-C-N	5.02	126.11	119.84
1	A	287	PRO	C-N-CA	5.02	126.11	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	568	TYR	Sidechain

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	4732	0	4702	212	0
2	A	28	0	12	3	0
3	A	133	0	0	4	0
All	All	4893	0	4714	212	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 24.

All (212) 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:18:ALA:HB1	1:A:121:VAL:HG11	1.34	1.08
1:A:159:ALA:O	1:A:161:PRO:HD3	1.71	0.90
1:A:129:LYS:HG2	1:A:253:LEU:HD11	1.56	0.87
1:A:24:GLY:O	1:A:28:THR:HG23	1.74	0.85
1:A:511:LYS:HD3	1:A:569:ASP:HB3	1.60	0.82
1:A:95:GLU:HG2	1:A:128:TYR:OH	1.78	0.82
1:A:486:THR:HG22	1:A:487:ILE:H	1.44	0.82
1:A:680:PRO:HD2	1:A:683:VAL:HG21	1.62	0.81
1:A:319:ASP:HB2	1:A:325:LEU:HD12	1.65	0.79
1:A:117:GLN:O	1:A:121:VAL:HG23	1.83	0.78
1:A:627:ARG:HH11	1:A:627:ARG:HG2	1.47	0.78
1:A:18:ALA:CB	1:A:121:VAL:HG11	2.12	0.78
1:A:496:LYS:O	1:A:588:MET:HE1	1.84	0.78
1:A:679:VAL:HG13	1:A:683:VAL:HB	1.68	0.74
1:A:396:ARG:H	1:A:396:ARG:HD2	1.54	0.73
1:A:317:MET:HG3	1:A:327:PHE:HE2	1.56	0.71
1:A:239:GLU:O	1:A:243:VAL:HG23	1.91	0.70
1:A:392:GLU:HG3	1:A:393:ASP:H	1.57	0.70
1:A:119:GLU:OE2	1:A:666:ARG:HD2	1.93	0.69
1:A:345:THR:HG21	3:A:801:HOH:O	1.93	0.69
1:A:658:ASP:O	1:A:662:LYS:HD3	1.93	0.69
1:A:556:ILE:HG13	1:A:558:PHE:HD1	1.59	0.68
1:A:317:MET:HG3	1:A:327:PHE:CE2	2.28	0.68
1:A:165:GLN:NE2	1:A:260:LEU:H	1.92	0.68
1:A:88:VAL:HG11	1:A:121:VAL:HG22	1.76	0.67
1:A:539:ILE:HB	1:A:540:PRO:HD3	1.77	0.67
1:A:396:ARG:HD2	1:A:396:ARG:N	2.10	0.67
1:A:486:THR:HG22	1:A:487:ILE:N	2.10	0.66
1:A:34:TYR:HD2	1:A:35:TYR:CD1	2.13	0.66
1:A:636:PRO:HG3	1:A:641:GLN:HE22	1.61	0.66
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:N	1:A:398:ILE:HD12	2.11	0.65
1:A:535:PRO:HB2	1:A:538:TYR:CD2	2.31	0.65
1:A:170:ARG:HD3	1:A:171:GLU:HG3	1.79	0.65
1:A:627:ARG:HG2	1:A:627:ARG:NH1	2.09	0.65
1:A:20:HIS:HD2	1:A:117:GLN:H	1.43	0.65
1:A:190:ASN:HD22	1:A:192:LEU:H	1.42	0.65
1:A:606:MET:HE2	1:A:649:LEU:HD13	1.78	0.64
1:A:573:HIS:ND1	1:A:576:ASP:HB2	2.12	0.64
1:A:680:PRO:HD2	1:A:683:VAL:CG2	2.28	0.64
1:A:609:GLU:O	1:A:669:PHE:HA	1.97	0.64
1:A:17:ILE:O	1:A:25:LYS:HE2	1.97	0.64
1:A:132:ARG:HG2	1:A:132:ARG:HH11	1.63	0.64
1:A:91:THR:O	1:A:95:GLU:HB2	1.96	0.64
1:A:20:HIS:CD2	1:A:117:GLN:HB2	2.34	0.63
1:A:27:THR:O	1:A:31:ARG:HG2	2.00	0.62
1:A:530:VAL:O	1:A:533:VAL:HG23	1.99	0.62
1:A:486:THR:HG21	3:A:817:HOH:O	1.99	0.62
1:A:345:THR:HG22	1:A:398:ILE:HG23	1.82	0.61
1:A:31:ARG:O	1:A:35:TYR:HD1	1.83	0.60
1:A:114:VAL:HG21	1:A:157:LEU:HD22	1.83	0.60
1:A:617:MET:O	1:A:617:MET:HG2	2.01	0.60
1:A:165:GLN:HA	1:A:178:ILE:O	2.02	0.59
1:A:69:VAL:CG2	1:A:314:PHE:HZ	2.14	0.59
1:A:506:GLN:HE22	1:A:578:SER:CB	2.15	0.58
1:A:309:LEU:HA	1:A:332:SER:O	2.03	0.58
1:A:68:ALA:HB2	1:A:315:LYS:HG2	1.87	0.57
1:A:453:GLY:O	1:A:468:ARG:HA	2.05	0.57
1:A:344:THR:HG23	1:A:390:VAL:HG22	1.86	0.56
1:A:289:ILE:HG23	1:A:301:ILE:HB	1.87	0.56
1:A:132:ARG:HG2	1:A:132:ARG:NH1	2.21	0.56
1:A:514:VAL:HG21	1:A:593:ALA:HB1	1.87	0.56
1:A:466:LEU:O	1:A:468:ARG:N	2.39	0.55
1:A:12:LEU:HD13	1:A:372:GLY:O	2.06	0.55
1:A:338:GLY:HA2	1:A:352:VAL:O	2.06	0.55
1:A:450:ILE:HA	1:A:473:ASP:HA	1.87	0.55
1:A:218:GLU:HG3	1:A:231:TYR:CE2	2.42	0.55
1:A:316:ILE:CD1	1:A:384:ILE:HA	2.37	0.55
1:A:21:ILE:O	1:A:22:ASP:HB2	2.06	0.55
1:A:605:ILE:HG21	1:A:675:HIS:CE1	2.42	0.54
1:A:555:LEU:HD11	1:A:599:PRO:HB2	1.90	0.54
1:A:179:ASP:OD2	1:A:182:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLY:O	1:A:38:ARG:HB3	2.07	0.53
1:A:483:TYR:O	1:A:484:ARG:HD3	2.09	0.53
1:A:316:ILE:HD11	1:A:384:ILE:HA	1.90	0.53
1:A:514:VAL:HG21	1:A:593:ALA:CB	2.39	0.53
1:A:319:ASP:HB2	1:A:325:LEU:CD1	2.35	0.53
1:A:101:LEU:C	1:A:101:LEU:HD23	2.33	0.52
1:A:156:ARG:O	1:A:639:ASN:ND2	2.42	0.52
1:A:238:THR:OG1	1:A:241:GLU:HB2	2.09	0.52
1:A:635:GLU:HB3	1:A:642:VAL:CG2	2.39	0.52
1:A:36:THR:HG21	1:A:72:CYS:SG	2.49	0.52
1:A:153:MET:HA	1:A:157:LEU:HD22	1.91	0.52
1:A:213:HIS:O	1:A:217:VAL:HG23	2.08	0.52
1:A:596:LYS:NZ	1:A:596:LYS:HB3	2.25	0.52
1:A:160:ARG:HG2	1:A:255:ILE:HG22	1.90	0.52
1:A:206:LEU:O	1:A:210:ARG:HD2	2.10	0.52
1:A:490:PRO:HB3	1:A:515:GLU:HB2	1.92	0.52
1:A:361:ASN:O	1:A:362:HIS:ND1	2.43	0.51
1:A:115:GLU:O	1:A:118:SER:HB2	2.11	0.51
1:A:88:VAL:HB	1:A:117:GLN:HG2	1.92	0.51
1:A:190:ASN:ND2	1:A:192:LEU:H	2.07	0.51
1:A:199:ILE:HB	1:A:200:PRO:HD2	1.93	0.51
1:A:342:TYR:HE1	1:A:347:GLY:O	1.94	0.51
1:A:218:GLU:O	1:A:221:ALA:HB3	2.12	0.50
1:A:292:THR:HA	1:A:298:VAL:HA	1.92	0.50
1:A:498:ILE:HD11	1:A:507:TYR:CD2	2.45	0.50
1:A:519:ARG:NH1	1:A:602:LEU:HD11	2.26	0.50
1:A:119:GLU:CD	1:A:666:ARG:HH11	2.20	0.50
1:A:623:ASP:HB3	3:A:737:HOH:O	2.11	0.50
1:A:264:LEU:O	1:A:264:LEU:HG	2.11	0.49
1:A:632:LEU:HG	1:A:645:ALA:HA	1.95	0.49
1:A:609:GLU:HB3	3:A:806:HOH:O	2.12	0.49
1:A:624:LEU:HD23	1:A:631:ILE:CD1	2.43	0.49
1:A:179:ASP:O	1:A:183:MET:N	2.46	0.49
1:A:497:PHE:O	1:A:498:ILE:HD13	2.12	0.49
1:A:129:LYS:CG	1:A:253:LEU:HD11	2.37	0.49
1:A:613:PRO:O	1:A:615:GLU:N	2.46	0.49
1:A:119:GLU:OE1	1:A:666:ARG:NH1	2.46	0.48
1:A:392:GLU:CG	1:A:393:ASP:H	2.19	0.48
1:A:126:GLU:OE1	1:A:132:ARG:NH2	2.46	0.48
1:A:165:GLN:HE22	1:A:260:LEU:H	1.61	0.48
1:A:252:ASP:O	1:A:253:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLN:NE2	1:A:578:SER:OG	2.46	0.48
1:A:19:ALA:HB1	1:A:23:ALA:HB3	1.95	0.48
1:A:503:GLY:C	1:A:504:ARG:HD3	2.39	0.48
1:A:138:LYS:HE2	2:A:692:GDP:C4	2.49	0.47
1:A:238:THR:O	1:A:241:GLU:HB2	2.14	0.47
1:A:498:ILE:CD1	1:A:507:TYR:CD2	2.97	0.47
1:A:342:TYR:CD1	1:A:348:ARG:O	2.68	0.47
1:A:19:ALA:HB3	1:A:25:LYS:HB2	1.96	0.47
1:A:254:LYS:HA	1:A:254:LYS:HE2	1.97	0.47
1:A:496:LYS:H	1:A:588:MET:CE	2.28	0.47
1:A:7:TYR:CG	1:A:8:ASP:N	2.82	0.47
1:A:506:GLN:HE22	1:A:578:SER:HB3	1.81	0.47
1:A:123:ARG:HD2	1:A:637:ARG:HG2	1.97	0.46
1:A:397:VAL:C	1:A:398:ILE:HD12	2.39	0.46
1:A:636:PRO:CG	1:A:641:GLN:HE22	2.28	0.46
1:A:357:ARG:HH11	1:A:357:ARG:CG	2.27	0.46
1:A:608:VAL:HG22	1:A:671:MET:HB3	1.96	0.46
1:A:319:ASP:HB3	1:A:322:VAL:H	1.81	0.46
1:A:603:GLU:HB3	1:A:679:VAL:HG23	1.96	0.46
1:A:392:GLU:HG3	1:A:393:ASP:N	2.26	0.46
1:A:69:VAL:HG23	1:A:314:PHE:HZ	1.80	0.46
1:A:504:ARG:HB2	1:A:505:GLY:H	1.41	0.46
1:A:129:LYS:HD3	1:A:129:LYS:O	2.16	0.46
1:A:342:TYR:HD1	1:A:348:ARG:O	1.99	0.45
1:A:344:THR:CG2	1:A:390:VAL:HG22	2.46	0.45
1:A:486:THR:CG2	1:A:487:ILE:H	2.23	0.45
1:A:512:ILE:HG22	1:A:567:LEU:HA	1.99	0.45
1:A:247:ARG:NH2	1:A:280:LEU:O	2.50	0.45
1:A:34:TYR:CD2	1:A:35:TYR:CD1	2.99	0.45
1:A:9:LEU:HD22	1:A:283:PRO:HB2	1.99	0.45
1:A:21:ILE:HG22	1:A:22:ASP:OD1	2.17	0.44
1:A:126:GLU:CD	1:A:132:ARG:HH22	2.25	0.44
1:A:190:ASN:HD22	1:A:190:ASN:C	2.25	0.44
1:A:327:PHE:CZ	1:A:358:MET:HE3	2.52	0.44
1:A:610:VAL:HG22	1:A:669:PHE:HB3	1.99	0.44
1:A:85:PRO:HG3	1:A:93:GLU:HB3	1.98	0.44
1:A:680:PRO:O	1:A:681:LYS:C	2.61	0.44
1:A:342:TYR:HE1	1:A:347:GLY:C	2.25	0.44
1:A:680:PRO:O	1:A:683:VAL:N	2.51	0.44
1:A:680:PRO:HB2	1:A:683:VAL:HG23	1.99	0.44
1:A:654:GLY:O	1:A:655:TYR:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:GLN:C	1:A:666:ARG:H	2.25	0.44
1:A:103:GLY:HA2	1:A:130:VAL:HG23	2.00	0.43
1:A:247:ARG:NH2	1:A:281:PRO:HA	2.33	0.43
1:A:126:GLU:OE2	1:A:253:LEU:HD22	2.18	0.43
1:A:287:PRO:HA	1:A:288:PRO:HD3	1.93	0.43
1:A:506:GLN:HE21	1:A:506:GLN:HA	1.82	0.43
1:A:553:GLY:O	1:A:557:GLY:HA2	2.17	0.43
1:A:606:MET:CG	1:A:649:LEU:HB2	2.49	0.43
1:A:649:LEU:O	1:A:649:LEU:HG	2.18	0.43
1:A:95:GLU:HG2	1:A:128:TYR:CZ	2.54	0.43
1:A:450:ILE:HA	1:A:472:VAL:O	2.18	0.43
1:A:226:ASN:O	1:A:230:LYS:HG3	2.19	0.43
1:A:506:GLN:NE2	1:A:506:GLN:HA	2.34	0.42
1:A:129:LYS:O	1:A:129:LYS:CD	2.67	0.42
1:A:230:LYS:HB3	1:A:235:GLU:HB3	2.00	0.42
1:A:361:ASN:O	1:A:362:HIS:CB	2.66	0.42
1:A:223:PHE:CE1	1:A:254:LYS:HG3	2.54	0.42
1:A:354:ARG:HB2	1:A:378:VAL:HG23	2.01	0.42
1:A:25:LYS:N	2:A:692:GDP:O2B	2.52	0.42
1:A:322:VAL:O	1:A:322:VAL:HG12	2.19	0.42
1:A:531:GLY:O	1:A:532:GLY:C	2.63	0.42
1:A:223:PHE:HE1	1:A:254:LYS:HG3	1.84	0.42
1:A:627:ARG:O	1:A:647:VAL:HG23	2.19	0.42
1:A:138:LYS:HE2	2:A:692:GDP:N9	2.35	0.42
1:A:176:GLY:HA2	1:A:186:TYR:O	2.20	0.42
1:A:224:ASP:HB3	1:A:227:ILE:HG13	2.02	0.42
1:A:343:ASN:OD1	1:A:343:ASN:C	2.62	0.42
1:A:572:TYR:HB2	1:A:577:SER:OG	2.20	0.42
1:A:166:LEU:HD22	1:A:180:VAL:CG1	2.50	0.41
1:A:507:TYR:CD1	1:A:507:TYR:C	2.97	0.41
1:A:669:PHE:CD1	1:A:669:PHE:N	2.84	0.41
1:A:677:GLN:HG2	1:A:678:GLU:N	2.34	0.41
1:A:137:ASN:O	1:A:138:LYS:HB2	2.21	0.41
1:A:358:MET:HE1	1:A:376:ALA:HB3	2.03	0.41
1:A:325:LEU:HD21	1:A:356:LEU:HD12	2.01	0.41
1:A:499:ARG:HG2	1:A:501:THR:HG22	2.01	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.67	0.41
1:A:543:GLN:O	1:A:547:GLU:HB2	2.20	0.41
1:A:554:PRO:HG3	1:A:591:LYS:HD2	2.01	0.41
1:A:114:VAL:HG11	1:A:157:LEU:HD13	2.03	0.41
1:A:357:ARG:CG	1:A:357:ARG:NH1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ILE:HG13	1:A:558:PHE:CD1	2.47	0.41
1:A:682:GLN:O	1:A:683:VAL:C	2.62	0.41
1:A:123:ARG:HH12	1:A:639:ASN:HD21	1.67	0.41
1:A:312:LEU:HD23	1:A:399:LEU:HB2	2.03	0.41
1:A:314:PHE:CD1	1:A:315:LYS:HB2	2.56	0.41
1:A:74:TRP:O	1:A:75:LYS:C	2.64	0.41
1:A:114:VAL:HG11	1:A:157:LEU:CD1	2.51	0.41
1:A:188:TYR:CD2	1:A:267:LYS:HG2	2.56	0.41
1:A:573:HIS:HB3	1:A:576:ASP:HB2	2.03	0.40
1:A:486:THR:HG23	1:A:561:VAL:O	2.21	0.40
1:A:218:GLU:HG3	1:A:231:TYR:CZ	2.56	0.40
1:A:289:ILE:HG13	1:A:290:LYS:N	2.36	0.40
1:A:181:LEU:HD12	1:A:181:LEU:C	2.46	0.40
1:A:354:ARG:HB2	1:A:378:VAL:CG2	2.51	0.40
1:A:20:HIS:HD2	1:A:117:GLN:HB2	1.85	0.40
1:A:90:PHE:O	1:A:94:VAL:HG23	2.22	0.40
1:A:553:GLY:HA2	1:A:554:PRO:HD3	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	609/691 (88%)	540 (89%)	42 (7%)	27 (4%)	2 1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	89	ASP
1	A	362	HIS
1	A	392	GLU

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Mol	Chain	Res	Type
1	A	436	PRO
1	A	467	LYS
1	A	617	MET
1	A	8	ASP
1	A	442	THR
1	A	450	ILE
1	A	482	ALA
1	A	614	GLU
1	A	2	ALA
1	A	175	SER
1	A	449	THR
1	A	536	LYS
1	A	628	ARG
1	A	474	ALA
1	A	504	ARG
1	A	477	GLY
1	A	531	GLY
1	A	655	TYR
1	A	681	LYS
1	A	116	PRO
1	A	636	PRO
1	A	665	GLY
1	A	455	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	491/582 (84%)	419 (85%)	72 (15%)	3 4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	12	LEU
1	A	26	THR

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Mol	Chain	Res	Type
1	A	28	THR
1	A	30	GLU
1	A	33	LEU
1	A	95	GLU
1	A	99	ARG
1	A	101	LEU
1	A	116	PRO
1	A	117	GLN
1	A	120	THR
1	A	121	VAL
1	A	129	LYS
1	A	130	VAL
1	A	131	PRO
1	A	146	LEU
1	A	156	ARG
1	A	157	LEU
1	A	160	ARG
1	A	164	MET
1	A	166	LEU
1	A	180	VAL
1	A	181	LEU
1	A	190	ASN
1	A	196	ILE
1	A	197	ARG
1	A	206	LEU
1	A	225	GLU
1	A	242	LEU
1	A	260	LEU
1	A	272	LEU
1	A	277	VAL
1	A	286	ILE
1	A	292	THR
1	A	329	ARG
1	A	335	LEU
1	A	336	THR
1	A	369	LEU
1	A	377	VAL
1	A	378	VAL
1	A	383	THR
1	A	384	ILE
1	A	389	LEU
1	A	396	ARG

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Mol	Chain	Res	Type
1	A	478	LYS
1	A	481	VAL
1	A	496	LYS
1	A	499	ARG
1	A	501	THR
1	A	504	ARG
1	A	518	PRO
1	A	537	GLU
1	A	540	PRO
1	A	542	VAL
1	A	547	GLU
1	A	559	PRO
1	A	565	VAL
1	A	575	VAL
1	A	580	MET
1	A	590	ILE
1	A	592	GLU
1	A	596	LYS
1	A	624	LEU
1	A	630	GLN
1	A	647	VAL
1	A	648	PRO
1	A	678	GLU
1	A	679	VAL
1	A	683	VAL
1	A	685	GLU
1	A	686	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	112	GLN
1	A	117	GLN
1	A	165	GLN
1	A	190	ASN
1	A	506	GLN
1	A	509	HIS
1	A	595	GLN
1	A	639	ASN
1	A	641	GLN

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 ⓘ

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	$\# Z > 2$
2	GDP	A	692	-	29,30,30	1.70	6 (20%)	45,47,47	2.18	12 (26%)

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
2	GDP	A	692	-	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	692	GDP	PA-O3A	-4.44	1.54	1.59
2	A	692	GDP	PB-O3B	2.97	1.65	1.54
2	A	692	GDP	C4-N9	-2.84	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	692	GDP	O4'-C1'	2.71	1.48	1.42
2	A	692	GDP	PB-O1B	-2.53	1.42	1.50
2	A	692	GDP	C6-N1	-2.47	1.34	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	692	GDP	O2B-PB-O3A	9.97	138.06	104.64
2	A	692	GDP	O2B-PB-O1B	-3.40	97.59	110.83
2	A	692	GDP	C2'-C3'-C4'	3.22	108.83	102.61
2	A	692	GDP	O4'-C1'-C2'	-3.13	99.91	106.62
2	A	692	GDP	O2'-C2'-C3'	-2.98	102.27	111.82
2	A	692	GDP	O2'-C2'-C1'	2.72	119.48	110.10
2	A	692	GDP	O3A-PB-O1B	-2.60	97.38	111.04
2	A	692	GDP	C8-N7-C5	-2.42	99.95	104.26
2	A	692	GDP	O3B-PB-O2B	-2.41	98.78	107.80
2	A	692	GDP	O3B-PB-O3A	2.29	112.32	104.64
2	A	692	GDP	O3'-C3'-C2'	-2.15	104.92	111.82
2	A	692	GDP	O2A-PA-O5'	2.00	116.65	107.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	692	GDP	PB-O3A-PA-O5'
2	A	692	GDP	O4'-C4'-C5'-O5'
2	A	692	GDP	PA-O3A-PB-O3B

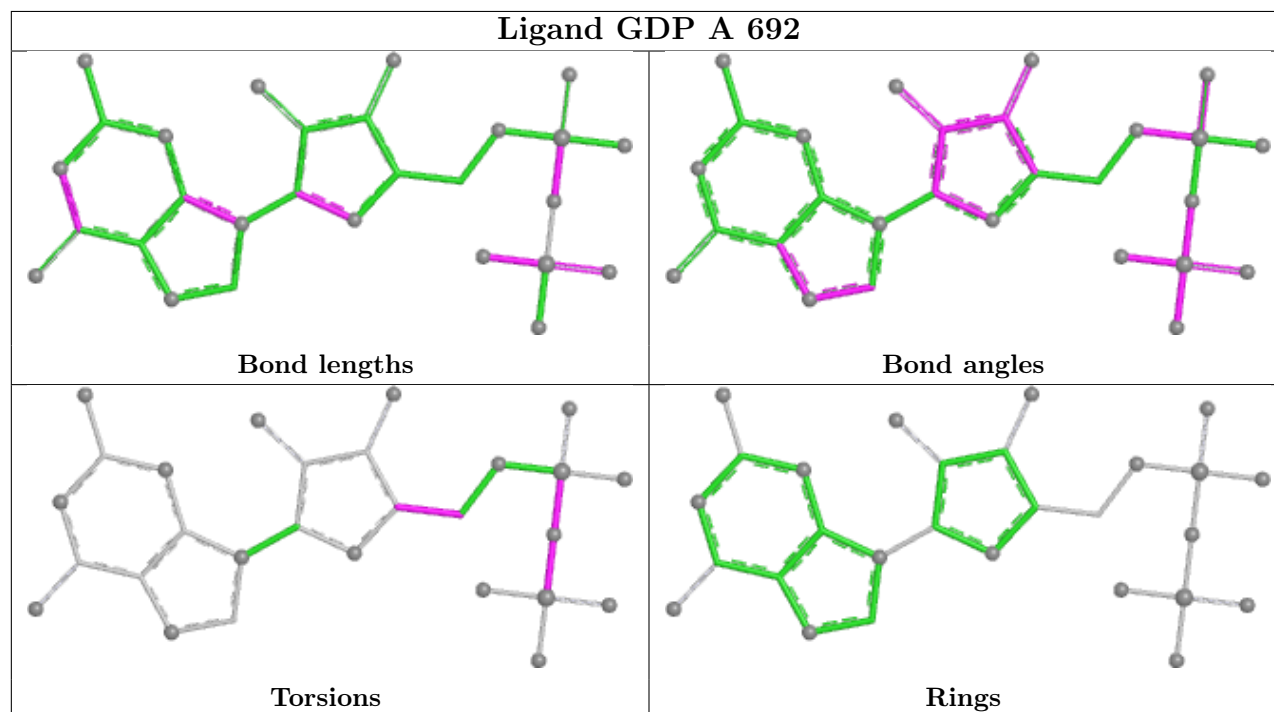
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	692	GDP	3	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.