



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:56 PM GMT

PDB ID : 1DAR
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

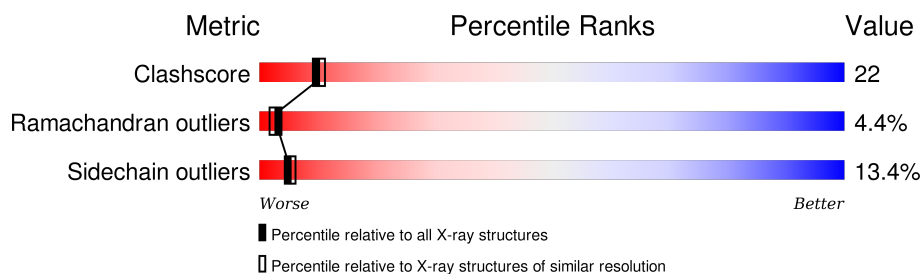
1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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
1	A	619	Total	C	N	O	S	277	0	4
			4732	3005	817	892	18			

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

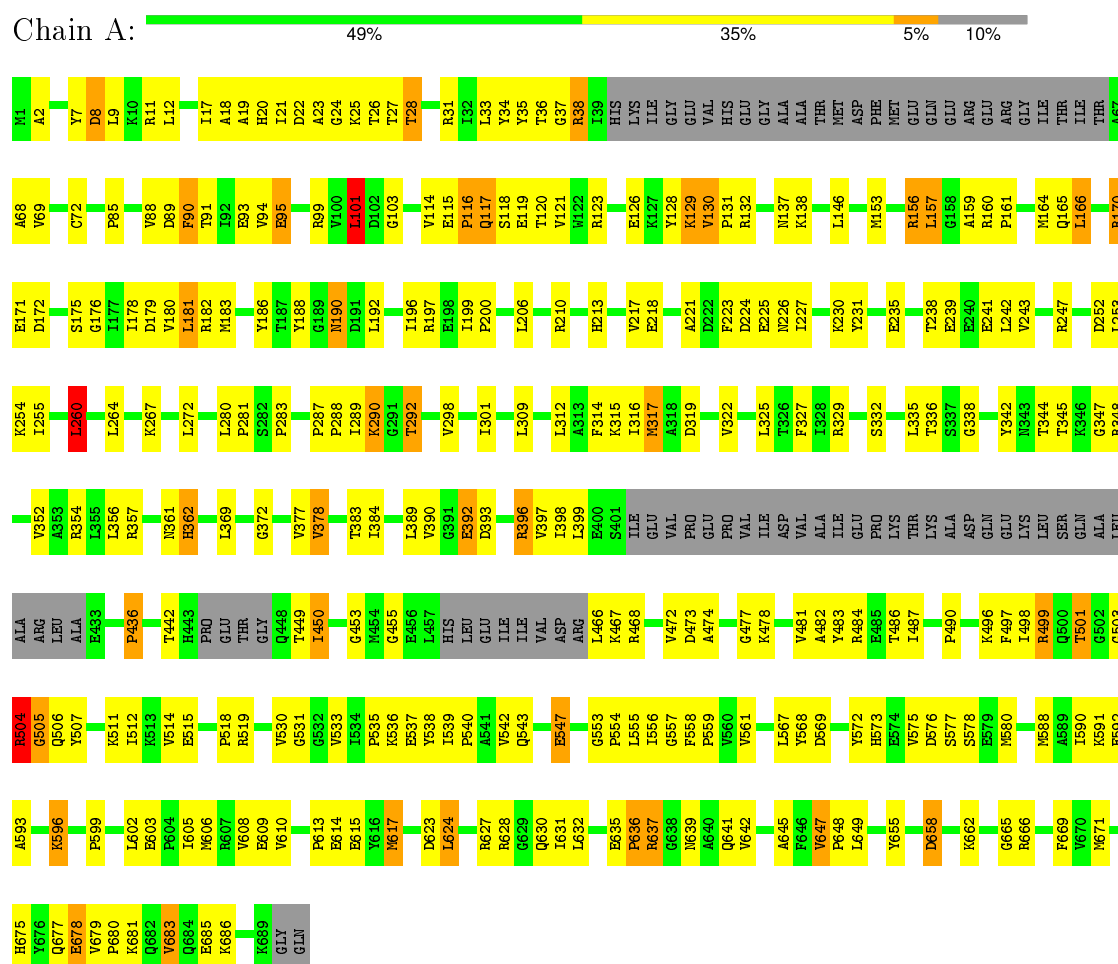


3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ELONGATION FACTOR G



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.30 Å 106.40 Å 115.60 Å 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	0.63	0/4817	0.86	5/6524 (0.1%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	436	PRO	N-CA-CB	6.08	110.59	103.30
1	A	260	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	181	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	101	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	505	GLY	N-CA-C	-5.12	100.31	113.10

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	199	0
2	A	28	0	12	3	0
3	A	133	0	0	4	0
All	All	4893	0	4714	199	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 22.

All (199) 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:679:VAL:HG13	1:A:683:VAL:HB	1.68	0.74
1:A:396:ARG:HD2	1:A:396:ARG:H	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:496:LYS:O	1:A:588:MET:HE1	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:396:ARG:HD2	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
1:A:398:ILE:HD12	1:A:398:ILE:N	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:NH1	1:A:627:ARG:HG2	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: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:132:ARG:HH11	1:A:132:ARG:HG2	1.63	0.64
1:A:17:ILE:O	1:A:25:LYS:HE2	1.97	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:NH1	1:A:132:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:GLY:O	1:A:38:ARG:HB3	2.07	0.54
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
1:A:483:TYR:O	1:A:484:ARG:HD3	2.09	0.53
1:A:514:VAL:HG21	1:A:593:ALA:CB	2.39	0.53
1:A:316:ILE:HD11	1:A:384:ILE:HA	1.90	0.53
1:A:319:ASP:HB2	1:A:325:LEU:CD1	2.35	0.53
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:156:ARG:O	1:A:639:ASN:ND2	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:252:ASP:O	1:A:253:LEU:HB2	2.14	0.48
1:A:165:GLN:HE22	1:A:260:LEU:H	1.61	0.48
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:101:LEU:C	1:A:101:LEU:HD23	2.33	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:496:LYS:H	1:A:588:MET:CE	2.28	0.47
1:A:254:LYS:HA	1:A:254:LYS:HE2	1.97	0.47
1:A:506:GLN:HE22	1:A:578:SER:HB3	1.81	0.47
1:A:7:TYR:CG	1:A:8:ASP:N	2.82	0.47
1:A:636:PRO:CG	1:A:641:GLN:HE22	2.28	0.46
1:A:123:ARG:HD2	1:A:637:ARG:HG2	1.97	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:603:GLU:HB3	1:A:679:VAL:HG23	1.96	0.46
1:A:319:ASP:HB3	1:A:322:VAL:H	1.81	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:O	1:A:129:LYS:HD3	2.16	0.46
1:A:119:GLU:CD	1:A:666:ARG:HH11	2.20	0.45
1:A:342:TYR:HD1	1:A:348:ARG:O	1.99	0.45
1:A:486:THR:CG2	1:A:487:ILE:H	2.23	0.45
1:A:344:THR:CG2	1:A:390:VAL:HG22	2.46	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: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:HB2	1:A:683:VAL:HG23	1.99	0.44
1:A:680:PRO:O	1:A:683:VAL:N	2.51	0.44
1:A:247:ARG:NH2	1:A:281:PRO:HA	2.33	0.43
1:A:103:GLY:HA2	1:A:130:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:OE2	1:A:253:LEU:HD22	2.18	0.43
1:A:503:GLY:C	1:A:504:ARG:HD3	2.39	0.43
1:A:287:PRO:HA	1:A:288:PRO:HD3	1.93	0.43
1:A:506:GLN:HA	1:A:506:GLN:HE21	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:HG	1:A:649:LEU:O	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:HA	1:A:506:GLN:NE2	2.34	0.42
1:A:129:LYS:O	1:A:129:LYS:CD	2.67	0.42
1:A:361:ASN:O	1:A:362:HIS:CB	2.66	0.42
1:A:230:LYS:HB3	1:A:235:GLU:HB3	2.00	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:322:VAL:HG12	1:A:322:VAL:O	2.19	0.42
1:A:25:LYS:N	2:A:692:GDP:O2B	2.52	0.42
1:A:627:ARG:O	1:A:647:VAL:HG23	2.19	0.42
1:A:223:PHE:HE1	1:A:254:LYS:HG3	1.84	0.42
1:A:397:VAL:C	1:A:398:ILE:HD12	2.39	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:572:TYR:HB2	1:A:577:SER:OG	2.20	0.42
1:A:224:ASP:HB3	1:A:227:ILE:HG13	2.02	0.42
1:A:669:PHE:N	1:A:669:PHE:CD1	2.84	0.41
1:A:166:LEU:HD22	1:A:180:VAL:CG1	2.50	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:596:LYS:HZ3	1:A:596:LYS:HB3	1.83	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:554:PRO:HG3	1:A:591:LYS:HD2	2.01	0.41
1:A:543:GLN:O	1:A:547:GLU:HB2	2.20	0.41
1:A:556:ILE:HG13	1:A:558:PHE:CD1	2.47	0.41
1:A:357:ARG:NH1	1:A:357:ARG:CG	2.84	0.41
1:A:114:VAL:HG11	1:A:157:LEU:HD13	2.03	0.41
1:A:314:PHE:CD1	1:A:315:LYS:HB2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:289:ILE:HG13	1:A:290:LYS:N	2.36	0.40
1:A:218:GLU:HG3	1:A:231:TYR:CZ	2.56	0.40
1:A:606:MET:HE2	1:A:649:LEU:HD13	2.04	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:553:GLY:HA2	1:A:554:PRO:HD3	1.81	0.40
1:A:90:PHE:O	1:A:94: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	A	609/691 (88%)	540 (89%)	42 (7%)	27 (4%)	3 2

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
1	A	436	PRO
1	A	467	LYS
1	A	617	MET
1	A	8	ASP
1	A	442	THR
1	A	450	ILE

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Mol	Chain	Res	Type
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%)	425 (87%)	66 (13%)	5 6

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	26	THR
1	A	28	THR
1	A	33	LEU
1	A	90	PHE
1	A	95	GLU
1	A	99	ARG
1	A	101	LEU
1	A	116	PRO

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Mol	Chain	Res	Type
1	A	117	GLN
1	A	120	THR
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	164	MET
1	A	166	LEU
1	A	170	ARG
1	A	172	ASP
1	A	181	LEU
1	A	190	ASN
1	A	196	ILE
1	A	197	ARG
1	A	225	GLU
1	A	242	LEU
1	A	260	LEU
1	A	272	LEU
1	A	290	LYS
1	A	292	THR
1	A	317	MET
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	389	LEU
1	A	396	ARG
1	A	478	LYS
1	A	481	VAL
1	A	499	ARG
1	A	501	THR
1	A	504	ARG
1	A	518	PRO
1	A	537	GLU
1	A	542	VAL
1	A	547	GLU
1	A	559	PRO

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Mol	Chain	Res	Type
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	637	ARG
1	A	647	VAL
1	A	648	PRO
1	A	658	ASP
1	A	678	GLU
1	A	683	VAL
1	A	685	GLU
1	A	686	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	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 carbohydrates 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	-	23,30,30	1.91	6 (26%)	30,47,47	3.30	13 (43%)

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	-	-	0/12/32/32	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	C4-N3	-2.87	1.31	1.35
2	A	692	GDP	PB-O1B	-2.61	1.42	1.51
2	A	692	GDP	C8-N7	-2.59	1.29	1.34
2	A	692	GDP	C5-C4	-2.27	1.35	1.40
2	A	692	GDP	PB-O3B	3.09	1.65	1.54
2	A	692	GDP	O4'-C1'	5.58	1.48	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	692	GDP	C5-C6-N1	-9.52	110.57	123.59
2	A	692	GDP	O2B-PB-O1B	-4.04	97.59	110.58
2	A	692	GDP	O2'-C2'-C3'	-2.94	102.27	111.83
2	A	692	GDP	PA-O3A-PB	-2.83	123.19	132.67
2	A	692	GDP	C1'-N9-C4	-2.30	123.47	126.94
2	A	692	GDP	O3B-PB-O2B	-2.26	98.78	107.38
2	A	692	GDP	O3'-C3'-C2'	-2.12	104.92	111.83
2	A	692	GDP	C4-C5-N7	3.00	112.24	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	692	GDP	C2'-C3'-C4'	3.02	108.83	102.61
2	A	692	GDP	C4'-O4'-C1'	3.23	113.27	109.72
2	A	692	GDP	O3A-PA-O5'	5.16	116.63	102.94
2	A	692	GDP	O2B-PB-O3A	7.27	138.06	105.09
2	A	692	GDP	C6-N1-C2	7.36	126.15	115.94

There are no chirality outliers.

There are no torsion outliers.

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.