Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:34 PM GMT

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PDB ID	:	4M1K
Title	:	Crystal structure of elongation factor G (EFG)
Authors	:	Liu, G.; Dong, J.; Gong, W.; Qin, Y.
Deposited on	:	2013-08-02
Resolution	:	2.95 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
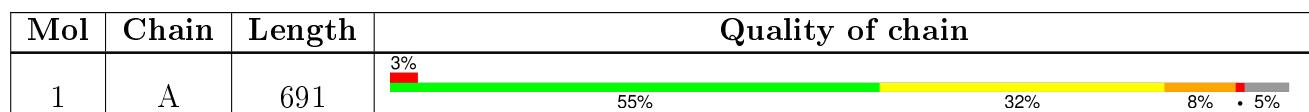
The reported resolution of this entry is 2.95 Å.

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	Percentile Ranks	Value
Rfree		0.290
Clashscore		19
Ramachandran outliers		2.8%
Sidechain outliers		15.7%
RSRZ outliers		2.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	691	3% ▮ 55% / 32% / 8% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5133 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	656	5104	3245	872	969	18	0	0	0
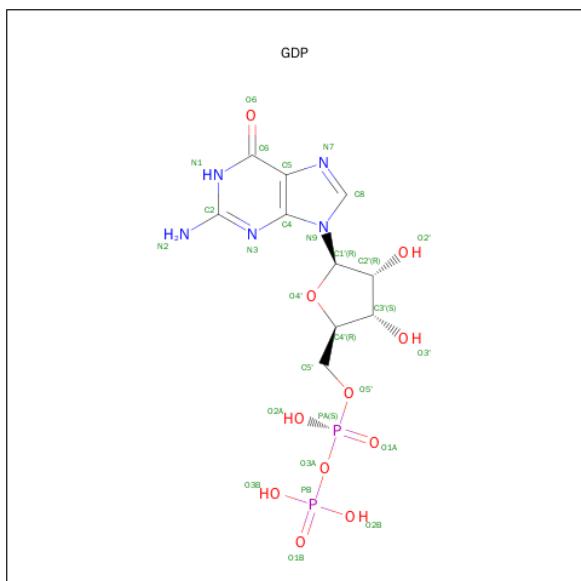
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	LEU	GLN	ENGINEERED MUTATION	UNP P13551

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
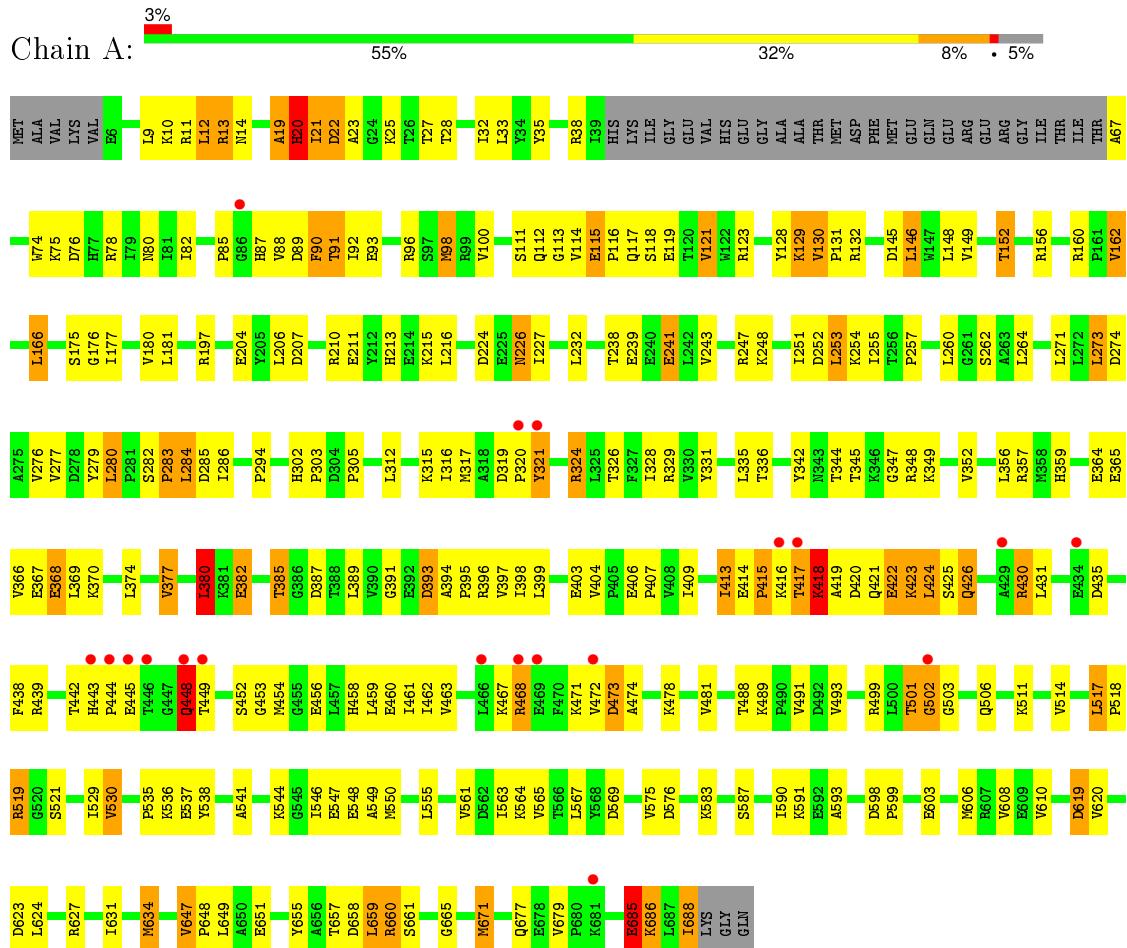
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	28	10	5	11	2	0	0

3 Residue-property plots (i)

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.

- Molecule 1: Elongation factor G

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.99Å 86.77Å 123.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.99 – 2.95 37.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.99-2.95) 99.7 (37.99-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.194 , 0.292 0.192 , 0.290	Depositor DCC
R_{free} test set	899 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 17641 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5133	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: GDP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.43	0/5199	0.62	0/7047

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ALA	Peptide

5.2 Too-close contacts (i)

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	5104	0	5151	195	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	12	3	0
All	All	5133	0	5163	195	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 19.

All (195) 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:544:LYS:HD3	1:A:583:LYS:HD2	1.33	1.03
1:A:19:ALA:HB3	1:A:25:LYS:HB2	1.43	0.99
1:A:114:VAL:HG13	1:A:152:THR:HB	1.54	0.89
1:A:20:HIS:ND1	1:A:117:GLN:HG2	1.96	0.80
1:A:413:ILE:HD11	1:A:449:THR:HB	1.66	0.77
1:A:419:ALA:O	1:A:422:GLU:HB2	1.85	0.77
1:A:467:LYS:HG2	1:A:472:VAL:O	1.86	0.76
1:A:442:THR:O	1:A:444:PRO:HD3	1.88	0.73
1:A:226:ASN:OD1	1:A:226:ASN:N	2.19	0.73
1:A:414:GLU:O	1:A:474:ALA:HB1	1.88	0.72
1:A:502:GLY:N	1:A:503:GLY:HA2	2.06	0.70
1:A:348:ARG:CZ	1:A:382:GLU:HB2	2.23	0.68
1:A:321:TYR:HD2	1:A:321:TYR:H	1.42	0.68
1:A:316:ILE:HG12	1:A:385:THR:HG22	1.76	0.68
1:A:660:ARG:HG2	1:A:665:GLY:HA2	1.78	0.66
1:A:377:VAL:HG22	1:A:380:LEU:HD22	1.77	0.65
1:A:21:ILE:HG23	1:A:22:ASP:HB2	1.79	0.65
1:A:535:PRO:HG2	1:A:538:TYR:HD2	1.62	0.65
1:A:114:VAL:HG13	1:A:152:THR:CB	2.27	0.64
1:A:443:HIS:CE1	1:A:445:GLU:HB2	2.32	0.64
1:A:502:GLY:H	1:A:503:GLY:CA	2.12	0.63
1:A:113:GLY:HA2	1:A:149:VAL:HG22	1.81	0.63
1:A:413:ILE:CD1	1:A:449:THR:HB	2.29	0.62
1:A:417:THR:O	1:A:419:ALA:N	2.34	0.61
1:A:541:ALA:O	1:A:583:LYS:HA	2.01	0.61
1:A:92:ILE:HG23	1:A:93:GLU:H	1.64	0.61
1:A:13:ARG:HD2	1:A:277:VAL:HA	1.83	0.60
1:A:28:THR:O	1:A:32:ILE:HG13	2.01	0.60
1:A:10:LYS:O	1:A:13:ARG:NH2	2.34	0.60
1:A:417:THR:C	1:A:419:ALA:H	2.04	0.60
1:A:92:ILE:HG23	1:A:93:GLU:N	2.17	0.59
1:A:619:ASP:OD2	1:A:619:ASP:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ARG:CZ	1:A:660:ARG:HB3	2.31	0.59
1:A:359:HIS:CE1	1:A:364:GLU:OE2	2.55	0.59
1:A:549:ALA:HB3	1:A:590:ILE:HG21	1.83	0.59
1:A:22:ASP:H	3:A:702:GDP:PB	2.25	0.59
1:A:549:ALA:HB1	1:A:591:LYS:HE3	1.84	0.59
1:A:271:LEU:O	1:A:274:ASP:HB2	2.03	0.58
1:A:359:HIS:HE1	1:A:364:GLU:OE2	1.87	0.57
1:A:206:LEU:O	1:A:210:ARG:HG3	2.02	0.57
1:A:11:ARG:HD2	1:A:76:ASP:O	2.04	0.57
1:A:20:HIS:HB3	1:A:23:ALA:HB2	1.87	0.56
1:A:575:VAL:HG13	1:A:576:ASP:OD2	2.07	0.55
1:A:394:ALA:HB1	1:A:395:PRO:HD2	1.89	0.55
1:A:377:VAL:CG2	1:A:380:LEU:HD22	2.37	0.54
1:A:514:VAL:HG13	1:A:565:VAL:HG22	1.89	0.54
1:A:502:GLY:N	1:A:503:GLY:CA	2.69	0.54
1:A:74:TRP:CE2	1:A:273:LEU:HB3	2.42	0.54
1:A:502:GLY:H	1:A:503:GLY:HA2	1.70	0.54
1:A:180:VAL:O	1:A:213:HIS:ND1	2.30	0.54
1:A:511:LYS:HD2	1:A:569:ASP:HB3	1.90	0.53
1:A:608:VAL:HG22	1:A:671:MET:HG2	1.90	0.53
1:A:417:THR:C	1:A:419:ALA:N	2.61	0.53
1:A:416:LYS:HG2	1:A:473:ASP:O	2.09	0.53
1:A:608:VAL:HG22	1:A:671:MET:CG	2.38	0.53
1:A:608:VAL:HG21	1:A:647:VAL:HG13	1.90	0.53
1:A:166:LEU:HD22	1:A:180:VAL:CG1	2.38	0.52
1:A:610:VAL:HG13	1:A:659:LEU:HD11	1.91	0.52
1:A:114:VAL:CG1	1:A:152:THR:HB	2.35	0.52
1:A:546:ILE:HG23	1:A:590:ILE:HG12	1.90	0.52
1:A:238:THR:OG1	1:A:241:GLU:HB2	2.09	0.52
1:A:13:ARG:NH1	1:A:277:VAL:O	2.42	0.51
1:A:587:SER:O	1:A:591:LYS:HG3	2.10	0.51
1:A:251:ILE:HD13	1:A:285:ASP:HB3	1.92	0.51
1:A:90:PHE:CD1	1:A:90:PHE:N	2.78	0.51
1:A:549:ALA:HB3	1:A:590:ILE:CG2	2.41	0.51
1:A:324:ARG:HG3	1:A:324:ARG:HH11	1.75	0.51
1:A:176:GLY:C	1:A:177:ILE:HG13	2.31	0.51
1:A:264:LEU:HB2	3:A:702:GDP:C5	2.46	0.50
1:A:458:HIS:O	1:A:462:ILE:HG13	2.11	0.50
1:A:423:LYS:HA	1:A:426:GLN:HE21	1.77	0.50
1:A:493:VAL:HG21	1:A:593:ALA:HB2	1.93	0.50
1:A:294:PRO:HG3	1:A:396:ARG:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:O	1:A:152:THR:OG1	2.29	0.50
1:A:98:MET:HG3	1:A:130:VAL:HG11	1.94	0.50
1:A:544:LYS:HD3	1:A:583:LYS:CD	2.24	0.49
1:A:162:VAL:HG13	1:A:257:PRO:HA	1.94	0.49
1:A:603:GLU:HG2	1:A:679:VAL:HG12	1.94	0.49
1:A:424:LEU:HB2	1:A:472:VAL:HG11	1.94	0.49
1:A:439:ARG:HB2	1:A:452:SER:HB2	1.94	0.49
1:A:9:LEU:HD22	1:A:283:PRO:HB2	1.94	0.49
1:A:359:HIS:CE1	1:A:364:GLU:HB3	2.48	0.49
1:A:359:HIS:HE1	1:A:364:GLU:HB3	1.78	0.49
1:A:499:ARG:HB2	1:A:506:GLN:HB2	1.95	0.48
1:A:634:MET:H	1:A:634:MET:CE	2.26	0.48
1:A:416:LYS:HE2	1:A:416:LYS:HA	1.94	0.48
1:A:415:PRO:CB	1:A:421:GLN:HB2	2.43	0.48
1:A:489:LYS:HE3	1:A:598:ASP:CG	2.33	0.48
1:A:391:GLY:O	1:A:393:ASP:N	2.41	0.48
1:A:418:LYS:N	1:A:418:LYS:HD2	2.28	0.48
1:A:211:GLU:O	1:A:215:LYS:HG3	2.12	0.48
1:A:544:LYS:O	1:A:548:GLU:HG3	2.14	0.47
1:A:397:VAL:HG12	1:A:398:ILE:N	2.29	0.47
1:A:160:ARG:HG2	1:A:255:ILE:HG22	1.96	0.47
1:A:319:ASP:CG	1:A:320:PRO:HD2	2.34	0.47
1:A:20:HIS:ND1	1:A:21:ILE:O	2.48	0.47
1:A:324:ARG:NH1	1:A:324:ARG:HG3	2.30	0.47
1:A:9:LEU:HB3	1:A:284:LEU:HD22	1.96	0.47
1:A:627:ARG:HB3	1:A:651:GLU:HB3	1.96	0.47
1:A:21:ILE:CG2	1:A:22:ASP:HB2	2.43	0.47
1:A:409:ILE:CD1	1:A:649:LEU:HD21	2.45	0.47
1:A:448:GLN:HG3	1:A:448:GLN:H	1.59	0.46
1:A:67:ALA:HA	1:A:317:MET:HE1	1.96	0.46
1:A:321:TYR:N	1:A:321:TYR:CD2	2.80	0.46
1:A:608:VAL:HG21	1:A:647:VAL:CG1	2.46	0.46
1:A:224:ASP:HB3	1:A:227:ILE:HD12	1.96	0.46
1:A:357:ARG:HG3	1:A:366:VAL:HG11	1.98	0.46
1:A:119:GLU:O	1:A:123:ARG:HG2	2.15	0.46
1:A:85:PRO:HB3	1:A:90:PHE:CD2	2.51	0.46
1:A:453:GLY:N	1:A:459:LEU:HD21	2.31	0.46
1:A:627:ARG:NH2	1:A:658:ASP:OD1	2.45	0.46
1:A:342:TYR:HD1	1:A:349:LYS:HD3	1.80	0.46
1:A:344:THR:HG22	1:A:396:ARG:HG3	1.97	0.46
1:A:407:PRO:HA	1:A:453:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PRO:HB3	1:A:370:LYS:HD3	1.98	0.46
1:A:87:HIS:HB3	1:A:90:PHE:CZ	2.51	0.45
1:A:685:GLU:HG2	1:A:685:GLU:O	2.15	0.45
1:A:423:LYS:NZ	1:A:471:LYS:O	2.45	0.45
1:A:598:ASP:N	1:A:599:PRO:CD	2.78	0.45
1:A:12:LEU:HD11	1:A:78:ARG:HD2	1.99	0.45
1:A:145:ASP:HB3	1:A:148:LEU:HB3	1.98	0.45
1:A:166:LEU:HD22	1:A:180:VAL:HG11	1.98	0.45
1:A:129:LYS:O	1:A:131:PRO:HD3	2.16	0.45
1:A:90:PHE:O	1:A:92:ILE:N	2.49	0.45
1:A:685:GLU:O	1:A:686:LYS:HB2	2.16	0.45
1:A:146:LEU:HD22	1:A:146:LEU:O	2.16	0.45
1:A:115:GLU:H	1:A:118:SER:HB2	1.81	0.45
1:A:356:LEU:HD23	1:A:365:GLU:HA	1.99	0.44
1:A:239:GLU:O	1:A:243:VAL:HG23	2.16	0.44
1:A:426:GLN:O	1:A:430:ARG:NH1	2.51	0.44
1:A:74:TRP:NE1	1:A:273:LEU:HB3	2.31	0.44
1:A:606:MET:HG3	1:A:671:MET:SD	2.57	0.44
1:A:116:PRO:HB3	1:A:665:GLY:HA3	2.00	0.44
1:A:254:LYS:HD3	1:A:254:LYS:HA	1.67	0.44
1:A:544:LYS:NZ	1:A:583:LYS:HE3	2.33	0.44
1:A:89:ASP:C	1:A:91:THR:H	2.21	0.44
1:A:252:ASP:O	1:A:253:LEU:HB2	2.17	0.44
1:A:461:ILE:HG13	1:A:462:ILE:N	2.33	0.44
1:A:620:VAL:O	1:A:624:LEU:HG	2.17	0.44
1:A:561:VAL:O	1:A:563:ILE:HG23	2.18	0.43
1:A:329:ARG:HG2	1:A:331:TYR:CZ	2.53	0.43
1:A:409:ILE:HD11	1:A:649:LEU:HD21	2.00	0.43
1:A:544:LYS:HE2	1:A:548:GLU:OE2	2.19	0.43
1:A:335:LEU:O	1:A:368:GLU:HA	2.19	0.43
1:A:328:ILE:HD13	1:A:377:VAL:HG12	2.00	0.43
1:A:74:TRP:HD1	1:A:277:VAL:HG11	1.84	0.43
1:A:453:GLY:H	1:A:459:LEU:HD21	1.84	0.43
1:A:243:VAL:HG13	1:A:279:TYR:CE1	2.53	0.43
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.85	0.43
1:A:631:ILE:N	1:A:631:ILE:HD12	2.34	0.43
1:A:395:PRO:HB2	1:A:397:VAL:HG23	2.00	0.43
1:A:98:MET:HG2	1:A:128:TYR:CD2	2.53	0.43
1:A:302:HIS:HA	1:A:303:PRO:HD3	1.57	0.42
1:A:659:LEU:HD23	1:A:659:LEU:HA	1.86	0.42
1:A:20:HIS:CE1	1:A:21:ILE:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG22	1:A:156:ARG:HD3	2.01	0.42
1:A:88:VAL:HG11	1:A:121:VAL:HG12	2.01	0.42
1:A:247:ARG:NH2	1:A:285:ASP:OD2	2.46	0.42
1:A:413:ILE:HG13	1:A:449:THR:O	2.19	0.42
1:A:647:VAL:HA	1:A:648:PRO:HD3	1.92	0.42
1:A:529:ILE:HG12	1:A:567:LEU:HG	2.01	0.42
1:A:655:TYR:CE2	1:A:659:LEU:HG	2.54	0.42
1:A:456:GLU:O	1:A:460:GLU:HG3	2.20	0.42
1:A:422:GLU:O	1:A:426:GLN:NE2	2.53	0.41
1:A:14:ASN:OD1	1:A:80:ASN:HB2	2.19	0.41
1:A:276:VAL:O	1:A:280:LEU:HB2	2.20	0.41
1:A:575:VAL:HG13	1:A:576:ASP:N	2.35	0.41
1:A:329:ARG:HA	1:A:374:LEU:HG	2.02	0.41
1:A:82:ILE:HG12	1:A:100:VAL:HG12	2.00	0.41
1:A:549:ALA:CB	1:A:591:LYS:HE3	2.51	0.41
1:A:75:LYS:HE3	1:A:274:ASP:OD1	2.20	0.41
1:A:623:ASP:O	1:A:627:ARG:HG3	2.20	0.41
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.90	0.41
1:A:345:THR:HB	1:A:387:ASP:OD1	2.20	0.41
1:A:493:VAL:HG11	1:A:593:ALA:HA	2.03	0.41
1:A:367:GLU:O	1:A:368:GLU:HB2	2.20	0.41
1:A:286:ILE:HG13	1:A:286:ILE:O	2.20	0.41
1:A:435:ASP:HB3	1:A:438:PHE:CE1	2.56	0.41
1:A:535:PRO:HG2	1:A:538:TYR:CD2	2.49	0.41
1:A:92:ILE:CG2	1:A:93:GLU:N	2.84	0.41
1:A:394:ALA:HB1	1:A:395:PRO:CD	2.50	0.41
1:A:518:PRO:HG2	1:A:521:SER:OG	2.20	0.41
1:A:547:GLU:HA	1:A:550:MET:HE2	2.01	0.41
1:A:488:THR:OG1	1:A:598:ASP:O	2.31	0.41
1:A:20:HIS:ND1	1:A:21:ILE:N	2.68	0.41
1:A:421:GLN:NE2	1:A:421:GLN:O	2.54	0.41
1:A:216:LEU:HD23	1:A:216:LEU:C	2.41	0.41
1:A:517:LEU:HD13	1:A:564:LYS:HB2	2.03	0.41
1:A:519:ARG:HD3	1:A:519:ARG:HA	1.38	0.41
1:A:13:ARG:HH21	1:A:282:SER:HB3	1.85	0.41
1:A:22:ASP:N	3:A:702:GDP:O2B	2.54	0.40
1:A:426:GLN:HB2	1:A:426:GLN:HE21	1.62	0.40
1:A:555:LEU:O	1:A:688:ILE:HG23	2.21	0.40
1:A:443:HIS:HE1	1:A:445:GLU:HB2	1.84	0.40
1:A:35:TYR:HD2	1:A:38:ARG:NH2	2.18	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	652/691 (94%)	584 (90%)	50 (8%)	18 (3%)	6	28

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	91	THR
1	A	418	LYS
1	A	501	THR
1	A	530	VAL
1	A	347	GLY
1	A	368	GLU
1	A	415	PRO
1	A	448	GLN
1	A	502	GLY
1	A	685	GLU
1	A	686	LYS
1	A	241	GLU
1	A	380	LEU
1	A	468	ARG
1	A	90	PHE
1	A	283	PRO
1	A	403	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	547/582 (94%)	461 (84%)	86 (16%)	3	13

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	ARG
1	A	20	HIS
1	A	21	ILE
1	A	22	ASP
1	A	27	THR
1	A	33	LEU
1	A	96	ARG
1	A	98	MET
1	A	111	SER
1	A	112	GLN
1	A	115	GLU
1	A	121	VAL
1	A	129	LYS
1	A	130	VAL
1	A	132	ARG
1	A	146	LEU
1	A	152	THR
1	A	162	VAL
1	A	166	LEU
1	A	175	SER
1	A	181	LEU
1	A	197	ARG
1	A	204	GLU
1	A	207	ASP
1	A	226	ASN
1	A	232	LEU
1	A	248	LYS
1	A	253	LEU
1	A	260	LEU
1	A	262	SER
1	A	273	LEU
1	A	280	LEU
1	A	284	LEU
1	A	312	LEU
1	A	315	LYS
1	A	321	TYR
1	A	324	ARG

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Mol	Chain	Res	Type
1	A	326	THR
1	A	336	THR
1	A	352	VAL
1	A	369	LEU
1	A	377	VAL
1	A	380	LEU
1	A	382	GLU
1	A	385	THR
1	A	389	LEU
1	A	393	ASP
1	A	399	LEU
1	A	404	VAL
1	A	406	GLU
1	A	413	ILE
1	A	417	THR
1	A	418	LYS
1	A	420	ASP
1	A	422	GLU
1	A	423	LYS
1	A	424	LEU
1	A	425	SER
1	A	426	GLN
1	A	430	ARG
1	A	448	GLN
1	A	454	MET
1	A	463	VAL
1	A	468	ARG
1	A	473	ASP
1	A	478	LYS
1	A	481	VAL
1	A	491	VAL
1	A	501	THR
1	A	517	LEU
1	A	519	ARG
1	A	530	VAL
1	A	536	LYS
1	A	537	GLU
1	A	619	ASP
1	A	634	MET
1	A	647	VAL
1	A	657	THR
1	A	659	LEU

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Mol	Chain	Res	Type
1	A	660	ARG
1	A	661	SER
1	A	671	MET
1	A	677	GLN
1	A	685	GLU
1	A	688	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	426	GLN
1	A	443	HIS

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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
3	GDP	A	702	2	23,30,30	1.34	3 (13%)	30,47,47	1.94	8 (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
3	GDP	A	702	2	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GDP	O4'-C1'	2.19	1.44	1.41
3	A	702	GDP	C5-C4	3.46	1.48	1.40
3	A	702	GDP	C6-C5	3.93	1.49	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	GDP	C5-C6-N1	-4.29	117.73	123.59
3	A	702	GDP	C6-C5-C4	-3.46	116.76	120.90
3	A	702	GDP	N3-C2-N1	-3.42	122.24	127.44
3	A	702	GDP	PA-O3A-PB	-2.56	124.08	132.67
3	A	702	GDP	C4-C5-N7	-2.53	107.15	109.48
3	A	702	GDP	C2'-C1'-N9	-2.06	111.14	114.29
3	A	702	GDP	O4'-C1'-N9	3.07	114.52	108.10
3	A	702	GDP	C6-N1-C2	5.20	123.15	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
3	A	702	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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	656/691 (94%)	-0.21	19 (2%) 55	35	21, 46, 109, 171	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	THR	5.4
1	A	502	GLY	4.1
1	A	469	GLU	4.0
1	A	429	ALA	4.0
1	A	417	THR	3.8
1	A	448	GLN	3.5
1	A	444	PRO	3.2
1	A	434	GLU	3.1
1	A	468	ARG	3.0
1	A	86	GLY	2.8
1	A	445	GLU	2.6
1	A	321	TYR	2.5
1	A	449	THR	2.4
1	A	416	LYS	2.4
1	A	681	LYS	2.4
1	A	472	VAL	2.3
1	A	443	HIS	2.3
1	A	466	LEU	2.2
1	A	320	PRO	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GDP	A	702	28/28	0.93	0.17	0.74	68,84,101,128	0
2	MG	A	701	1/1	0.86	0.11	-	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.