Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BM0
Title	:	RIBOSOMAL ELONGATION FACTOR G (EF-G) FUSIDIC ACID RESISTANT MUTANT T84A
Authors	:	Hansson, S.; Singh, R.; Gudkov, A.T.; Liljas, A.; Logan, D.T.
Deposited on	:	2005-03-09
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:

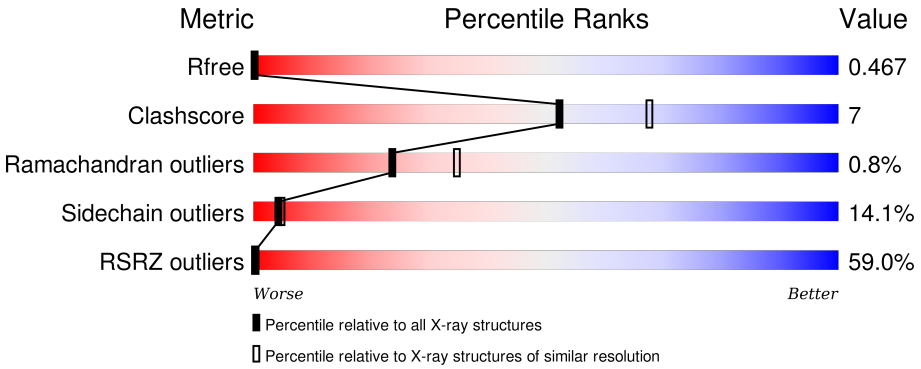
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 <=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	57% 71% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5363 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.

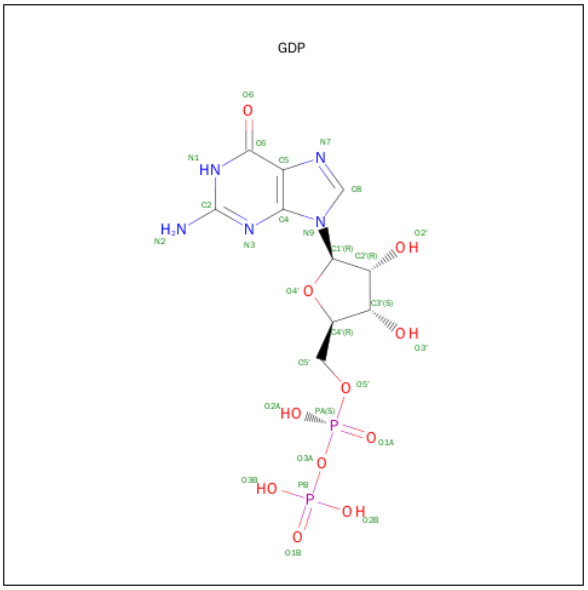
- Molecule 1 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5190	3299	889	984	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	GLY	CONFLICT	UNP P13551
A	84	ALA	THR	ENGINEERED MUTATION	UNP P13551

- Molecule 2 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		
2	A	1	28	10	5	11	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

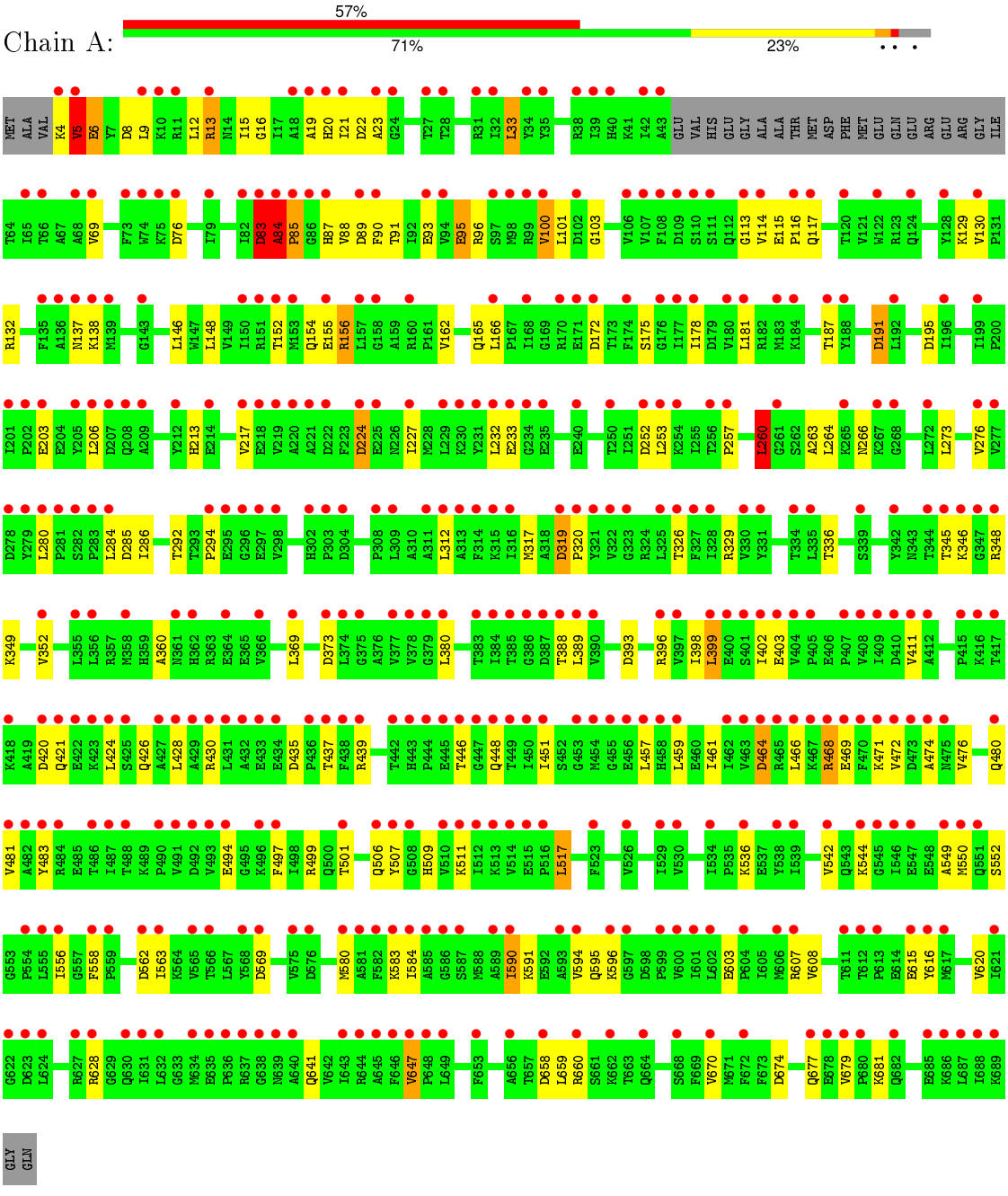
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	144	Total O 144 144	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.20Å 88.50Å 116.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 14.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.40) 81.6 (14.75-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.210 , 0.274 0.460 , 0.467	Depositor DCC
R_{free} test set	1192 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.5	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 23328 reflections	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	5363	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.58	1/5288 (0.0%)	0.85	24/7165 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	PRO	C-N	16.82	1.63	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	ALA	O-C-N	11.16	142.31	121.10
1	A	84	ALA	C-N-CD	8.91	147.11	128.40
1	A	191	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	13	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	83	ASP	C-N-CA	6.58	138.16	121.70
1	A	84	ALA	CA-C-N	-6.49	98.93	117.10
1	A	658	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	195	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	285	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	224	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	435	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	569	ASP	CB-CG-OD2	5.86	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	420	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	319	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	172	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	252	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	674	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	393	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	8	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	84	ALA	C-N-CA	-5.31	99.69	122.00
1	A	76	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	13	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	464	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	260	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	ASP	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	5190	0	5229	70	0
2	A	28	0	12	1	0
3	A	1	0	0	0	0
4	A	144	0	0	4	0
All	All	5363	0	5241	70	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 7.

All (70) 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:137:ASN:ND2	1:A:137:ASN:O	1.92	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ASP:OD1	4:A:2122:HOH:O	1.85	0.93
1:A:84:ALA:N	1:A:85:PRO:CD	2.32	0.92
1:A:84:ALA:N	1:A:85:PRO:HD2	1.91	0.84
1:A:148:LEU:O	1:A:152:THR:HG22	1.81	0.81
1:A:137:ASN:CG	1:A:137:ASN:O	2.22	0.76
1:A:398:ILE:HG21	1:A:402:ILE:HD11	1.74	0.68
1:A:428:LEU:HD21	1:A:451:ILE:HD11	1.81	0.61
1:A:616:TYR:O	1:A:620:VAL:HG23	2.01	0.61
1:A:497:PHE:CD1	1:A:584:ILE:HG21	2.36	0.60
1:A:137:ASN:HD21	1:A:263:ALA:H	1.49	0.60
1:A:4:LYS:O	1:A:5:VAL:HG23	2.01	0.59
1:A:83:ASP:CG	1:A:84:ALA:N	2.56	0.59
1:A:641:GLN:NE2	4:A:2135:HOH:O	2.38	0.57
1:A:608:VAL:HG21	1:A:647:VAL:HG13	1.87	0.55
1:A:137:ASN:ND2	1:A:263:ALA:H	2.05	0.54
1:A:13:ARG:HG2	1:A:276:VAL:HG12	1.90	0.53
1:A:83:ASP:OD2	1:A:85:PRO:HD2	2.08	0.53
1:A:87:HIS:CE1	1:A:461:ILE:HG21	2.45	0.52
1:A:138:LYS:HG2	2:A:1690:GDP:C6	2.45	0.52
1:A:87:HIS:HB3	1:A:88:VAL:O	2.09	0.52
1:A:203:GLU:HA	4:A:2050:HOH:O	2.10	0.51
1:A:88:VAL:O	1:A:89:ASP:HB2	2.12	0.50
1:A:424:LEU:HD12	1:A:472:VAL:HG11	1.93	0.49
1:A:91:THR:HG21	1:A:670:VAL:HG12	1.94	0.49
1:A:517:LEU:HD22	1:A:563:ILE:C	2.32	0.49
1:A:165:GLN:NE2	1:A:260:LEU:H	2.11	0.49
1:A:556:ILE:HD12	1:A:558:PHE:CD2	2.48	0.49
1:A:474:ALA:O	1:A:476:VAL:HG23	2.12	0.49
1:A:583:LYS:HD2	4:A:2120:HOH:O	2.13	0.49
1:A:591:LYS:O	1:A:595:GLN:HG3	2.13	0.48
1:A:87:HIS:HB3	1:A:88:VAL:HB	1.95	0.48
1:A:88:VAL:HG12	1:A:88:VAL:O	2.13	0.48
1:A:224:ASP:HB3	1:A:227:ILE:HD12	1.96	0.48
1:A:590:ILE:O	1:A:594:VAL:HG23	2.14	0.47
1:A:608:VAL:HG21	1:A:647:VAL:CG1	2.44	0.47
1:A:213:HIS:O	1:A:217:VAL:HG23	2.15	0.47
1:A:19:ALA:HB1	1:A:23:ALA:HB3	1.96	0.46
1:A:165:GLN:HA	1:A:178:ILE:O	2.15	0.46
1:A:116:PRO:HA	1:A:156:ARG:HH22	1.80	0.46
1:A:91:THR:CG2	1:A:670:VAL:HG12	2.47	0.45
1:A:162:VAL:HG13	1:A:257:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HB3	1:A:88:VAL:C	2.37	0.45
1:A:481:VAL:HG22	1:A:483:TYR:CE2	2.52	0.45
1:A:294:PRO:HD3	1:A:396:ARG:O	2.18	0.44
1:A:603:GLU:HG2	1:A:679:VAL:HG12	1.99	0.44
1:A:165:GLN:HE22	1:A:260:LEU:H	1.64	0.44
1:A:20:HIS:NE2	1:A:117:GLN:HB2	2.33	0.43
1:A:424:LEU:CD1	1:A:472:VAL:HG11	2.47	0.43
1:A:550:MET:SD	1:A:563:ILE:HD11	2.58	0.43
1:A:494:GLU:HG2	1:A:511:LYS:HG2	2.00	0.43
1:A:100:VAL:O	1:A:329:ARG:NH1	2.52	0.43
1:A:388:THR:HG23	1:A:399:LEU:HD22	2.00	0.43
1:A:16:GLY:HA3	1:A:101:LEU:HD22	2.00	0.42
1:A:13:ARG:HG2	1:A:276:VAL:CG1	2.49	0.42
1:A:191:ASP:O	1:A:266:ASN:ND2	2.44	0.42
1:A:114:VAL:O	1:A:115:GLU:HG2	2.19	0.42
1:A:494:GLU:OE1	1:A:509:HIS:NE2	2.53	0.42
1:A:286:ILE:HG13	1:A:286:ILE:H	1.74	0.42
1:A:411:VAL:HG23	1:A:459:LEU:HD23	2.01	0.42
1:A:507:TYR:CD1	1:A:507:TYR:C	2.93	0.42
1:A:345:THR:HG23	1:A:402:ILE:HD12	2.00	0.42
1:A:33:LEU:HG	1:A:360:ALA:HB2	2.01	0.42
1:A:464:ASP:O	1:A:468:ARG:HB2	2.19	0.42
1:A:95:GLU:HG3	1:A:96:ARG:N	2.32	0.41
1:A:549:ALA:HB1	1:A:591:LYS:HD3	2.02	0.41
1:A:87:HIS:HB3	1:A:88:VAL:CB	2.51	0.41
1:A:15:ILE:HA	1:A:103:GLY:O	2.20	0.41
1:A:87:HIS:HB3	1:A:88:VAL:CA	2.51	0.41
1:A:319:ASP:HA	1:A:320:PRO:HD3	1.93	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	662/691 (96%)	627 (95%)	30 (4%)	5 (1%)	24 35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	5	VAL
1	A	6	GLU
1	A	113	GLY
1	A	380	LEU

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	555/581 (96%)	477 (86%)	78 (14%)	4 5

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	GLU
1	A	9	LEU
1	A	12	LEU
1	A	21	ILE
1	A	22	ASP
1	A	33	LEU
1	A	69	VAL
1	A	90	PHE
1	A	93	GLU
1	A	95	GLU
1	A	100	VAL
1	A	129	LYS
1	A	130	VAL
1	A	132	ARG
1	A	146	LEU

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Mol	Chain	Res	Type
1	A	154	GLN
1	A	155	GLU
1	A	156	ARG
1	A	166	LEU
1	A	175	SER
1	A	181	LEU
1	A	187	THR
1	A	206	LEU
1	A	232	LEU
1	A	233	GLU
1	A	253	LEU
1	A	260	LEU
1	A	264	LEU
1	A	273	LEU
1	A	280	LEU
1	A	284	LEU
1	A	292	THR
1	A	312	LEU
1	A	317	MET
1	A	326	THR
1	A	336	THR
1	A	346	LYS
1	A	348	ARG
1	A	349	LYS
1	A	352	VAL
1	A	369	LEU
1	A	373	ASP
1	A	389	LEU
1	A	399	LEU
1	A	403	GLU
1	A	421	GLN
1	A	426	GLN
1	A	430	ARG
1	A	437	THR
1	A	439	ARG
1	A	446	THR
1	A	448	GLN
1	A	457	LEU
1	A	466	LEU
1	A	468	ARG
1	A	469	GLU
1	A	471	LYS

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	499	ARG
1	A	501	THR
1	A	506	GLN
1	A	517	LEU
1	A	536	LYS
1	A	542	VAL
1	A	544	LYS
1	A	552	SER
1	A	580	MET
1	A	590	ILE
1	A	596	LYS
1	A	607	ARG
1	A	615	GLU
1	A	628	ARG
1	A	647	VAL
1	A	659	LEU
1	A	660	ARG
1	A	677	GLN
1	A	681	LYS

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

Mol	Chain	Res	Type
1	A	40	HIS
1	A	117	GLN
1	A	137	ASN
1	A	165	GLN
1	A	208	GLN
1	A	226	ASN
1	A	270	GLN
1	A	421	GLN
1	A	506	GLN
1	A	543	GLN
1	A	641	GLN
1	A	684	GLN

5.3.3 RNA

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	$\#\|Z\| > 2$
2	GDP	A	1690	3	23,30,30	1.14	2 (8%)	30,47,47	2.11	9 (30%)

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	1690	3	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1690	GDP	C2-N1	2.84	1.40	1.35
2	A	1690	GDP	C6-N1	3.89	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1690	GDP	N3-C2-N1	-4.98	119.86	127.44
2	A	1690	GDP	C1'-N9-C4	-3.88	121.09	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1690	GDP	C5-C6-N1	-3.77	118.44	123.59
2	A	1690	GDP	PA-O3A-PB	-3.73	120.17	132.67
2	A	1690	GDP	C2'-C1'-N9	-2.57	110.37	114.29
2	A	1690	GDP	O4'-C4'-C3'	2.14	109.46	105.15
2	A	1690	GDP	O4'-C1'-N9	2.62	113.57	108.10
2	A	1690	GDP	N2-C2-N1	3.23	122.55	117.20
2	A	1690	GDP	C6-N1-C2	3.61	120.95	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1690	GDP	1	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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(Å^2)	Q<0.9
1	A	666/691 (96%)	2.49	393 (59%)	0	0	17, 28, 58, 72	0

All (393) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	GLN	11.8
1	A	86	GLY	9.2
1	A	471	LYS	9.2
1	A	472	VAL	8.3
1	A	429	ALA	7.8
1	A	470	PHE	7.5
1	A	114	VAL	7.5
1	A	420	ASP	7.4
1	A	143	GLY	7.0
1	A	424	LEU	6.7
1	A	5	VAL	6.6
1	A	439	ARG	6.5
1	A	444	PRO	6.4
1	A	418	LYS	6.4
1	A	530	VAL	6.2
1	A	448	GLN	6.0
1	A	90	PHE	5.9
1	A	646	PHE	5.9
1	A	235	GLU	5.8
1	A	445	GLU	5.6
1	A	110	SER	5.6
1	A	42	ILE	5.6
1	A	66	THR	5.5
1	A	43	ALA	5.4
1	A	84	ALA	5.4
1	A	401	SER	5.3
1	A	171	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	582	PHE	5.3
1	A	613	PRO	5.3
1	A	467	LYS	5.3
1	A	334	THR	5.2
1	A	589	ALA	5.2
1	A	662	LYS	5.2
1	A	158	GLY	5.2
1	A	558	PHE	5.2
1	A	436	PRO	5.1
1	A	229	LEU	5.0
1	A	326	THR	5.0
1	A	526	VAL	5.0
1	A	481	VAL	5.0
1	A	686	LYS	5.0
1	A	24	GLY	4.9
1	A	417	THR	4.9
1	A	408	VAL	4.8
1	A	586	GLY	4.8
1	A	584	ILE	4.8
1	A	458	HIS	4.7
1	A	457	LEU	4.7
1	A	199	ILE	4.7
1	A	99	ARG	4.7
1	A	534	ILE	4.7
1	A	464	ASP	4.7
1	A	281	PRO	4.6
1	A	501	THR	4.6
1	A	581	ALA	4.6
1	A	416	LYS	4.6
1	A	450	ILE	4.6
1	A	356	LEU	4.6
1	A	389	LEU	4.6
1	A	428	LEU	4.5
1	A	510	VAL	4.5
1	A	284	LEU	4.5
1	A	11	ARG	4.5
1	A	214	GLU	4.5
1	A	361	ASN	4.5
1	A	634	MET	4.4
1	A	404	VAL	4.4
1	A	590	ILE	4.4
1	A	325	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	40	HIS	4.3
1	A	19	ALA	4.3
1	A	482	ALA	4.3
1	A	449	THR	4.2
1	A	486	THR	4.2
1	A	434	GLU	4.2
1	A	437	THR	4.2
1	A	491	VAL	4.2
1	A	396	ARG	4.1
1	A	644	ARG	4.1
1	A	575	VAL	4.1
1	A	538	TYR	4.1
1	A	628	ARG	4.1
1	A	82	ILE	4.1
1	A	490	PRO	4.0
1	A	555	LEU	4.0
1	A	645	ALA	4.0
1	A	201	ILE	4.0
1	A	616	TYR	4.0
1	A	400	GLU	3.9
1	A	639	ASN	3.9
1	A	664	GLN	3.9
1	A	562	ASP	3.9
1	A	206	LEU	3.9
1	A	432	ALA	3.9
1	A	155	GLU	3.9
1	A	468	ARG	3.9
1	A	649	LEU	3.9
1	A	97	SER	3.9
1	A	455	GLY	3.9
1	A	585	ALA	3.8
1	A	279	TYR	3.8
1	A	180	VAL	3.8
1	A	369	LEU	3.8
1	A	668	SER	3.8
1	A	425	SER	3.8
1	A	352	VAL	3.8
1	A	653	PHE	3.8
1	A	150	ILE	3.8
1	A	276	VAL	3.7
1	A	466	LEU	3.7
1	A	492	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	453	GLY	3.7
1	A	122	TRP	3.7
1	A	265	LYS	3.7
1	A	69	VAL	3.7
1	A	546	ILE	3.7
1	A	205	TYR	3.7
1	A	411	VAL	3.6
1	A	76	ASP	3.6
1	A	497	PHE	3.6
1	A	514	VAL	3.6
1	A	277	VAL	3.6
1	A	469	GLU	3.6
1	A	670	VAL	3.5
1	A	513	LYS	3.5
1	A	459	LEU	3.5
1	A	624	LEU	3.5
1	A	74	TRP	3.5
1	A	314	PHE	3.5
1	A	366	VAL	3.5
1	A	536	LYS	3.5
1	A	475	ASN	3.5
1	A	280	LEU	3.5
1	A	230	LYS	3.5
1	A	320	PRO	3.4
1	A	13	ARG	3.4
1	A	335	LEU	3.4
1	A	506	GLN	3.4
1	A	116	PRO	3.4
1	A	319	ASP	3.4
1	A	21	ILE	3.4
1	A	547	GLU	3.4
1	A	222	ASP	3.4
1	A	594	VAL	3.4
1	A	473	ASP	3.4
1	A	682	GLN	3.4
1	A	184	LYS	3.4
1	A	596	LYS	3.4
1	A	181	LEU	3.4
1	A	124	GLN	3.4
1	A	308	PRO	3.4
1	A	302	HIS	3.4
1	A	647	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	415	PRO	3.3
1	A	79	ILE	3.3
1	A	507	TYR	3.3
1	A	298	VAL	3.3
1	A	397	VAL	3.3
1	A	422	GLU	3.3
1	A	631	ILE	3.2
1	A	113	GLY	3.2
1	A	423	LYS	3.2
1	A	296	GLY	3.2
1	A	168	ILE	3.2
1	A	677	GLN	3.2
1	A	688	ILE	3.2
1	A	23	ALA	3.2
1	A	207	ASP	3.2
1	A	32	ILE	3.2
1	A	640	ALA	3.2
1	A	327	PHE	3.1
1	A	172	ASP	3.1
1	A	380	LEU	3.1
1	A	433	GLU	3.1
1	A	39	ILE	3.1
1	A	342	TYR	3.1
1	A	523	PHE	3.1
1	A	630	GLN	3.1
1	A	383	THR	3.1
1	A	430	ARG	3.1
1	A	9	LEU	3.1
1	A	157	LEU	3.1
1	A	295	GLU	3.1
1	A	117	GLN	3.1
1	A	321	TYR	3.0
1	A	187	THR	3.0
1	A	637	ARG	3.0
1	A	28	THR	3.0
1	A	94	VAL	3.0
1	A	232	LEU	3.0
1	A	480	GLN	3.0
1	A	328	ILE	3.0
1	A	384	ILE	3.0
1	A	89	ASP	3.0
1	A	465	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	331	TYR	3.0
1	A	487	ILE	3.0
1	A	549	ALA	3.0
1	A	108	PHE	3.0
1	A	267	LYS	2.9
1	A	496	LYS	2.9
1	A	689	LYS	2.9
1	A	107	VAL	2.9
1	A	160	ARG	2.9
1	A	438	PHE	2.9
1	A	672	PHE	2.9
1	A	34	TYR	2.9
1	A	451	ILE	2.9
1	A	390	VAL	2.9
1	A	128	TYR	2.9
1	A	462	ILE	2.9
1	A	358	MET	2.9
1	A	120	THR	2.9
1	A	660	ARG	2.9
1	A	379	GLY	2.9
1	A	508	GLY	2.9
1	A	272	LEU	2.9
1	A	83	ASP	2.9
1	A	539	ILE	2.9
1	A	212	TYR	2.9
1	A	409	ILE	2.9
1	A	106	VAL	2.8
1	A	166	LEU	2.8
1	A	152	THR	2.8
1	A	209	ALA	2.8
1	A	638	GLY	2.8
1	A	621	ILE	2.8
1	A	565	VAL	2.8
1	A	202	PRO	2.8
1	A	31	ARG	2.8
1	A	484	ARG	2.8
1	A	617	MET	2.8
1	A	176	GLY	2.8
1	A	234	GLY	2.8
1	A	345	THR	2.8
1	A	542	VAL	2.8
1	A	225	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	427	ALA	2.8
1	A	587	SER	2.8
1	A	612	THR	2.7
1	A	111	SER	2.7
1	A	362	HIS	2.7
1	A	446	THR	2.7
1	A	224	ASP	2.7
1	A	512	ILE	2.7
1	A	139	MET	2.7
1	A	18	ALA	2.7
1	A	178	ILE	2.7
1	A	252	ASP	2.7
1	A	303	PRO	2.7
1	A	648	PRO	2.7
1	A	27	THR	2.7
1	A	85	PRO	2.7
1	A	257	PRO	2.7
1	A	511	LYS	2.7
1	A	373	ASP	2.6
1	A	348	ARG	2.6
1	A	355	LEU	2.6
1	A	550	MET	2.6
1	A	35	TYR	2.6
1	A	188	TYR	2.6
1	A	515	GLU	2.6
1	A	593	ALA	2.6
1	A	10	LYS	2.6
1	A	607	ARG	2.6
1	A	102	ASP	2.6
1	A	304	ASP	2.6
1	A	322	VAL	2.6
1	A	377	VAL	2.6
1	A	192	LEU	2.6
1	A	73	PHE	2.6
1	A	268	GLY	2.6
1	A	407	PRO	2.6
1	A	559	PRO	2.6
1	A	545	GLY	2.5
1	A	231	TYR	2.5
1	A	283	PRO	2.5
1	A	563	ILE	2.5
1	A	635	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	339	SER	2.5
1	A	516	PRO	2.5
1	A	680	PRO	2.5
1	A	87	HIS	2.5
1	A	233	GLU	2.5
1	A	454	MET	2.5
1	A	602	LEU	2.5
1	A	632	LEU	2.5
1	A	250	THR	2.5
1	A	316	ILE	2.5
1	A	261	GLY	2.5
1	A	403	GLU	2.5
1	A	636	PRO	2.5
1	A	597	GLY	2.5
1	A	601	ILE	2.4
1	A	221	ALA	2.4
1	A	474	ALA	2.4
1	A	410	ASP	2.4
1	A	456	GLU	2.4
1	A	678	GLU	2.4
1	A	611	THR	2.4
1	A	604	PRO	2.4
1	A	323	GLY	2.4
1	A	431	LEU	2.4
1	A	138	LYS	2.4
1	A	580	MET	2.4
1	A	218	GLU	2.4
1	A	253	LEU	2.4
1	A	399	LEU	2.4
1	A	600	VAL	2.4
1	A	4	LYS	2.4
1	A	170	ARG	2.4
1	A	623	ASP	2.4
1	A	196	ILE	2.4
1	A	402	ILE	2.4
1	A	151	ARG	2.4
1	A	658	ASP	2.3
1	A	100	VAL	2.3
1	A	488	THR	2.3
1	A	606	MET	2.3
1	A	685	GLU	2.3
1	A	687	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	493	VAL	2.3
1	A	20	HIS	2.3
1	A	576	ASP	2.3
1	A	374	LEU	2.3
1	A	208	GLN	2.3
1	A	347	GLY	2.3
1	A	109	ASP	2.3
1	A	98	MET	2.3
1	A	529	ILE	2.3
1	A	551	GLN	2.3
1	A	312	LEU	2.3
1	A	388	THR	2.3
1	A	447	GLY	2.3
1	A	183	MET	2.2
1	A	386	GLY	2.2
1	A	568	TYR	2.2
1	A	311	ALA	2.2
1	A	643	ILE	2.2
1	A	278	ASP	2.2
1	A	297	GLU	2.2
1	A	599	PRO	2.2
1	A	387	ASP	2.2
1	A	256	THR	2.2
1	A	330	VAL	2.2
1	A	622	GLY	2.2
1	A	385	THR	2.2
1	A	566	THR	2.2
1	A	93	GLU	2.2
1	A	38	ARG	2.2
1	A	254	LYS	2.2
1	A	294	PRO	2.2
1	A	627	ARG	2.2
1	A	483	TYR	2.2
1	A	544	LYS	2.2
1	A	220	ALA	2.1
1	A	135	PHE	2.1
1	A	442	THR	2.1
1	A	130	VAL	2.1
1	A	75	LYS	2.1
1	A	569	ASP	2.1
1	A	240	GLU	2.1
1	A	364	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	346	LYS	2.1
1	A	344	THR	2.1
1	A	656	ALA	2.1
1	A	615	GLU	2.1
1	A	405	PRO	2.1
1	A	282	SER	2.1
1	A	65	ILE	2.1
1	A	136	ALA	2.1
1	A	313	ALA	2.1
1	A	412	ALA	2.1
1	A	217	VAL	2.1
1	A	463	VAL	2.1
1	A	556	ILE	2.1
1	A	68	ALA	2.0
1	A	153	MET	2.0
1	A	219	VAL	2.0
1	A	177	ILE	2.0
1	A	443	HIS	2.0
1	A	583	LYS	2.0
1	A	174	PHE	2.0
1	A	309	LEU	2.0
1	A	554	PRO	2.0
1	A	137	ASN	2.0
1	A	315	LYS	2.0
1	A	378	VAL	2.0
1	A	375	GLY	2.0
1	A	203	GLU	2.0
1	A	679	VAL	2.0
1	A	227	ILE	2.0
1	A	494	GLU	2.0

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

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, 95^{th} 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
2	GDP	A	1690	28/28	0.76	0.29	-0.27	58,62,65,66	0
3	MG	A	1691	1/1	0.68	0.31	-	75,75,75,75	0

6.5 Other polymers

There are no such residues in this entry.