Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:18 PM GMT

PDB ID	:	1A4R
Title	:	G12V MUTANT OF HUMAN PLACENTAL CDC42 GTPASE IN THE GDP FORM
Authors	:	Rudolph, M.G.; Vetter, I.R.; Wittinghofer, A.
Deposited on	:	1998-02-02
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

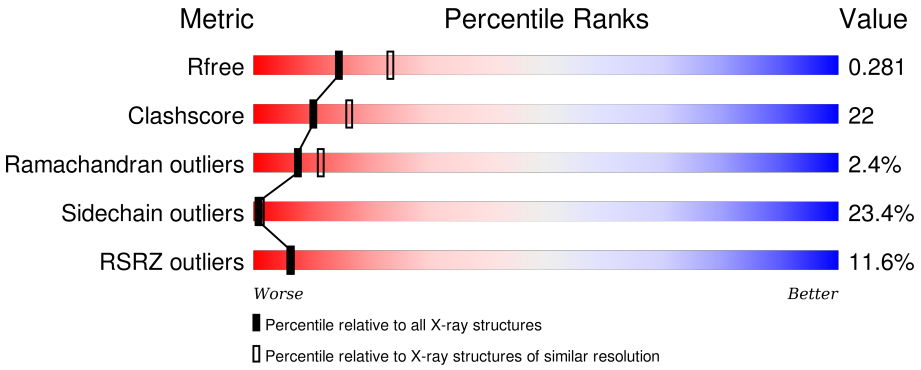
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	191	5% 50% 42% 7% •
1	B	191	18% 41% 46% 12% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3087 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 G25K GTP-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1488	957	241	282	8			
1	B	190	Total	C	N	O	S	0	0	0
			1488	957	241	282	8			

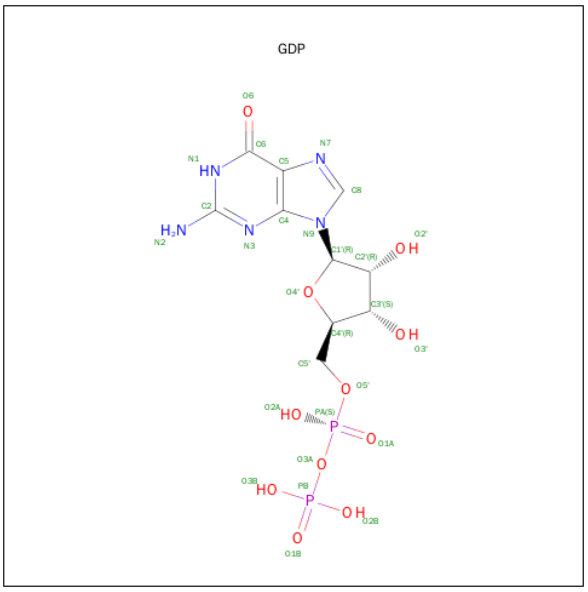
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	VAL	GLY	ENGINEERED	UNP P60953
B	212	VAL	GLY	ENGINEERED	UNP P60953

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

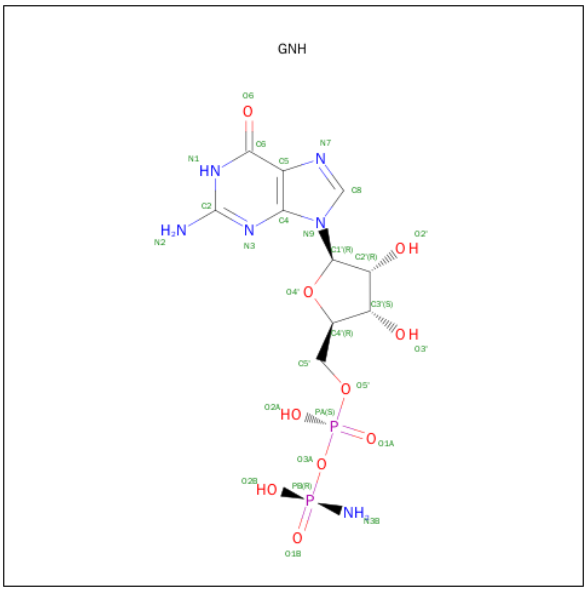
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- 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
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is AMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNH) (formula: $C_{10}H_{16}N_6O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			28	10	6	10	2		

- Molecule 5 is water.

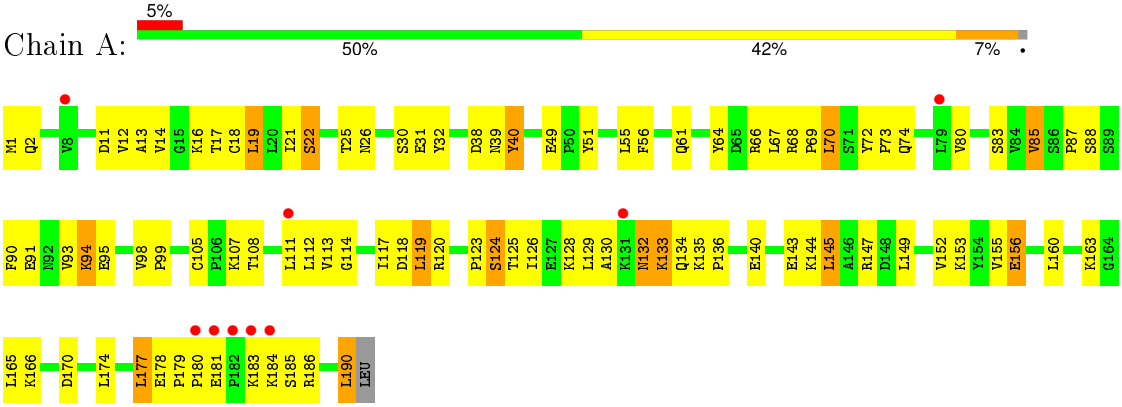
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	6	Total O 6 6	0	0

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.

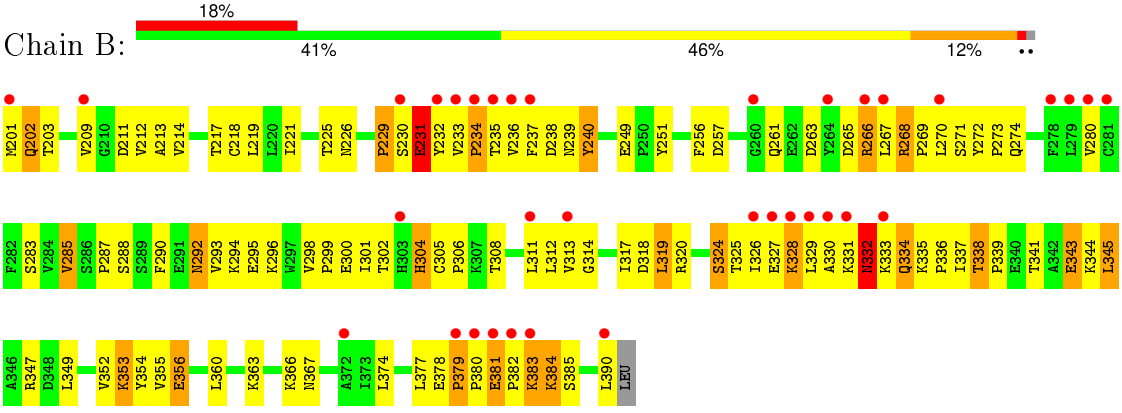
- Molecule 1: G25K GTP-BINDING PROTEIN

Chain A:



- Molecule 1: G25K GTP-BINDING PROTEIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.65Å 98.65Å 104.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (30.00-2.50) 96.0 (29.88-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.228 , 0.280 0.228 , 0.281	Depositor DCC
R_{free} test set	1738 reflections (9.87%)	DCC
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 18210 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3087	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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, GNH, 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	0.38	0/1521	0.63	0/2070
1	B	0.37	0/1521	0.60	0/2070
All	All	0.38	0/3042	0.62	0/4140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1488	0	1518	52	1
1	B	1488	0	1515	81	0
2	A	1	0	0	0	0
3	A	28	0	12	0	0
4	B	28	0	14	3	0
5	A	48	0	0	1	0
5	B	6	0	0	0	0
All	All	3087	0	3059	132	1

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 (132) 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:B:221:ILE:HG21	1:B:229:PRO:HG3	1.50	0.91
1:B:213:ALA:H	4:B:400:GNH:HN32	1.18	0.89
1:B:298:VAL:HG21	1:B:349:LEU:HD13	1.53	0.88
1:B:293:VAL:O	1:B:298:VAL:HG23	1.87	0.74
1:A:190:LEU:N	1:A:190:LEU:HD23	2.02	0.74
1:A:190:LEU:H	1:A:190:LEU:HD23	1.53	0.73
1:A:117:ILE:HG21	1:A:156:GLU:HB2	1.71	0.71
1:B:317:ILE:HG21	1:B:356:GLU:HB2	1.74	0.70
1:A:120:ARG:O	1:A:126:ILE:HD11	1.90	0.70
1:A:132:ASN:O	1:A:133:LYS:HG2	1.90	0.70
1:A:135:LYS:HG2	1:A:136:PRO:HD2	1.73	0.69
1:B:268:ARG:HB3	1:B:269:PRO:HD3	1.74	0.69
1:B:273:PRO:O	1:B:274:GLN:HB2	1.92	0.69
1:B:325:THR:HA	1:B:328:LYS:HE3	1.75	0.68
1:B:221:ILE:CG2	1:B:229:PRO:HG3	2.23	0.68
1:B:381:GLU:O	1:B:383:LYS:N	2.28	0.66
1:A:17:THR:HG22	1:A:21:ILE:HD12	1.78	0.66
1:A:124:SER:O	1:A:128:LYS:HG3	1.96	0.66
1:B:304:HIS:H	1:B:304:HIS:HD1	1.45	0.65
1:B:298:VAL:HG21	1:B:349:LEU:CD1	2.26	0.65
1:B:238:ASP:CG	1:B:239:ASN:H	2.01	0.64
1:B:267:LEU:H	1:B:267:LEU:HD12	1.65	0.62
1:B:240:TYR:N	1:B:240:TYR:CD1	2.68	0.62
1:B:326:ILE:HA	1:B:329:LEU:HB2	1.81	0.61
1:A:73:PRO:O	1:A:74:GLN:HB2	1.99	0.61
1:B:320:ARG:HH22	1:B:356:GLU:CD	2.04	0.61
1:B:305:CYS:HB3	1:B:308:THR:OG1	2.01	0.61
1:B:332:ASN:O	1:B:334:GLN:HG2	2.02	0.59
1:A:87:PRO:HG2	1:A:134:GLN:HG2	1.84	0.59
1:A:68:ARG:HB3	1:A:69:PRO:HD3	1.84	0.59
1:A:120:ARG:HH22	1:A:156:GLU:CD	2.06	0.59
1:A:40:TYR:N	1:A:40:TYR:CD1	2.70	0.59
1:B:267:LEU:N	1:B:267:LEU:HD12	2.18	0.59
1:A:111:LEU:HD12	1:A:152:VAL:HB	1.85	0.58
1:A:61:GLN:HB2	1:A:64:TYR:CE1	2.39	0.58
1:B:311:LEU:HD12	1:B:352:VAL:HB	1.86	0.58
1:A:94:LYS:HG3	1:A:95:GLU:N	2.18	0.58
1:A:18:CYS:O	1:A:22:SER:HB2	2.04	0.57
1:B:229:PRO:O	1:B:233:VAL:HG22	2.04	0.57
1:A:2:GLN:HG2	1:A:51:TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:GLU:HB3	1:B:379:PRO:CD	2.35	0.56
1:B:325:THR:O	1:B:329:LEU:HD23	2.05	0.56
1:B:274:GLN:NE2	1:B:274:GLN:HA	2.21	0.55
1:B:325:THR:HA	1:B:328:LYS:CE	2.36	0.55
1:B:213:ALA:N	4:B:400:GNH:HN32	1.96	0.55
1:B:339:PRO:O	1:B:343:GLU:N	2.34	0.55
1:A:11:ASP:O	1:A:14:VAL:HG13	2.06	0.54
1:B:313:VAL:HA	1:B:355:VAL:O	2.07	0.54
1:B:345:LEU:CD2	1:B:349:LEU:HG	2.38	0.53
1:B:209:VAL:HG21	1:B:301:ILE:HD11	1.91	0.53
1:A:145:LEU:CD2	1:A:149:LEU:HG	2.39	0.53
1:B:202:GLN:NE2	1:B:203:THR:H	2.07	0.53
1:B:266:ARG:HB3	1:B:267:LEU:HD12	1.89	0.53
1:A:61:GLN:HB2	1:A:64:TYR:CD1	2.45	0.52
1:B:345:LEU:HD22	1:B:349:LEU:HG	1.92	0.52
1:B:287:PRO:HG2	1:B:334:GLN:NE2	2.24	0.52
1:A:118:ASP:OD2	1:A:119:LEU:HD13	2.10	0.52
1:B:298:VAL:HB	1:B:299:PRO:HD3	1.92	0.51
1:A:16:LYS:HA	1:A:19:LEU:HD23	1.92	0.51
1:B:324:SER:O	1:B:328:LYS:HE3	2.11	0.51
1:A:120:ARG:NH2	1:A:156:GLU:OE2	2.43	0.51
1:B:320:ARG:NH2	1:B:356:GLU:OE2	2.44	0.50
1:B:330:ALA:C	1:B:332:ASN:H	2.14	0.50
1:B:283:SER:OG	1:B:285:VAL:HG23	2.12	0.50
1:B:304:HIS:O	1:B:306:PRO:HD3	2.12	0.50
1:B:296:LYS:O	1:B:299:PRO:HD2	2.12	0.50
1:A:67:LEU:O	1:A:70:LEU:HB2	2.12	0.49
1:A:132:ASN:C	1:A:133:LYS:HG2	2.32	0.49
1:A:12:VAL:O	1:A:13:ALA:HB3	2.12	0.49
1:A:113:VAL:HA	1:A:155:VAL:O	2.12	0.49
1:A:80:VAL:HG11	1:A:93:VAL:HG13	1.95	0.49
1:B:212:VAL:O	1:B:213:ALA:HB3	2.13	0.48
1:B:296:LYS:C	1:B:299:PRO:HD2	2.33	0.48
1:B:318:ASP:OD2	1:B:319:LEU:HD13	2.13	0.48
1:A:72:TYR:N	1:A:73:PRO:CD	2.76	0.48
1:B:272:TYR:N	1:B:272:TYR:CD1	2.81	0.48
1:A:132:ASN:ND2	1:A:133:LYS:HE3	2.29	0.47
1:B:294:LYS:HG3	1:B:295:GLU:N	2.27	0.47
1:B:211:ASP:O	1:B:214:VAL:HG13	2.14	0.47
1:A:140:GLU:CD	1:A:140:GLU:H	2.17	0.47
1:B:339:PRO:O	1:B:343:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:HA	1:A:55:LEU:O	2.15	0.47
1:B:217:THR:HG22	1:B:221:ILE:HD12	1.96	0.47
1:B:378:GLU:HB3	1:B:379:PRO:HD2	1.96	0.47
1:A:170:ASP:OD2	1:B:367:ASN:ND2	2.48	0.47
1:A:105:CYS:HB3	1:A:108:THR:OG1	2.15	0.47
1:A:98:VAL:N	1:A:99:PRO:CD	2.78	0.47
1:B:300:GLU:O	1:B:304:HIS:ND1	2.45	0.46
1:B:292:ASN:ND2	1:B:296:LYS:HB3	2.30	0.46
1:B:317:ILE:HD11	1:B:363:LYS:HD3	1.96	0.46
1:B:237:PHE:HB2	1:B:257:ASP:HB3	1.98	0.46
1:A:22:SER:HB3	1:A:165:LEU:HD21	1.98	0.46
1:B:295:GLU:O	1:B:299:PRO:HG2	2.15	0.46
1:A:83:SER:OG	1:A:85:VAL:HG23	2.16	0.46
1:A:90:PHE:CE1	1:A:145:LEU:HD12	2.52	0.45
1:A:117:ILE:HD11	1:A:163:LYS:HD3	1.97	0.45
1:A:73:PRO:HB3	1:A:190:LEU:CD2	2.47	0.45
1:B:317:ILE:CG2	1:B:356:GLU:HB2	2.42	0.45
1:A:145:LEU:HD22	1:A:149:LEU:HG	1.98	0.45
1:B:202:GLN:HB3	1:B:251:TYR:CD2	2.52	0.45
1:B:314:GLY:O	1:B:356:GLU:HA	2.15	0.45
1:B:353:LYS:HG3	1:B:354:TYR:N	2.32	0.44
1:B:256:PHE:N	1:B:256:PHE:CD1	2.86	0.44
1:A:25:THR:O	1:A:26:ASN:HB2	2.16	0.44
1:A:73:PRO:HB3	1:A:190:LEU:HD22	1.99	0.43
1:A:114:GLY:O	1:A:156:GLU:HA	2.18	0.43
1:B:338:THR:HG23	1:B:341:THR:OG1	2.18	0.43
1:B:234:PRO:C	1:B:236:VAL:H	2.20	0.43
1:B:335:LYS:HB3	1:B:336:PRO:HD2	1.99	0.43
1:A:186:ARG:NH1	5:A:1047:HOH:O	2.52	0.43
1:B:298:VAL:N	1:B:299:PRO:CD	2.82	0.42
1:A:130:ALA:HA	1:A:134:GLN:O	2.19	0.42
1:A:178:GLU:HB3	1:A:179:PRO:HD2	2.01	0.42
1:B:280:VAL:HG22	1:B:301:ILE:CD1	2.50	0.42
1:B:380:PRO:O	1:B:381:GLU:C	2.57	0.42
1:B:325:THR:HA	1:B:328:LYS:NZ	2.35	0.42
1:B:384:LYS:HZ2	1:B:384:LYS:HB2	1.85	0.42
1:A:56:PHE:N	1:A:56:PHE:CD1	2.88	0.41
1:B:292:ASN:O	1:B:292:ASN:ND2	2.31	0.41
1:B:274:GLN:NE2	1:B:274:GLN:CA	2.84	0.41
1:B:225:THR:O	1:B:226:ASN:HB2	2.20	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD12	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PRO:HB2	1:B:233:VAL:HG22	2.01	0.41
1:A:107:LYS:O	1:A:186:ARG:HG2	2.19	0.41
1:B:218:CYS:SG	4:B:400:GNH:H2'	2.60	0.41
1:B:381:GLU:OE1	1:B:384:LYS:HE3	2.20	0.41
1:B:332:ASN:HB3	1:B:334:GLN:HG2	2.02	0.41
1:B:231:GLU:HB2	1:B:232:TYR:H	1.61	0.41
1:B:298:VAL:O	1:B:302:THR:HG23	2.22	0.40
1:B:290:PHE:CD2	1:B:337:ILE:HD12	2.56	0.40
1:B:328:LYS:HG3	1:B:328:LYS:H	1.61	0.40
1:A:61:GLN:HB2	1:A:64:TYR:HE1	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:OH	1:A:64:TYR:OH[7_555]	1.81	0.39

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	188/191 (98%)	171 (91%)	15 (8%)	2 (1%)	17 31
1	B	188/191 (98%)	159 (85%)	22 (12%)	7 (4%)	4 5
All	All	376/382 (98%)	330 (88%)	37 (10%)	9 (2%)	7 11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	ASN
1	B	382	PRO
1	A	180	PRO

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Mol	Chain	Res	Type
1	B	231	GLU
1	A	123	PRO
1	B	234	PRO
1	B	268	ARG
1	B	379	PRO
1	B	229	PRO

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	171/172 (99%)	134 (78%)	37 (22%)	1 2
1	B	171/172 (99%)	128 (75%)	43 (25%)	1 1
All	All	342/344 (99%)	262 (77%)	80 (23%)	1 1

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	LEU
1	A	22	SER
1	A	30	SER
1	A	31	GLU
1	A	32	TYR
1	A	38	ASP
1	A	40	TYR
1	A	49	GLU
1	A	66	ARG
1	A	70	LEU
1	A	85	VAL
1	A	88	SER
1	A	91	GLU
1	A	94	LYS
1	A	112	LEU
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	124	SER
1	A	125	THR
1	A	129	LEU
1	A	132	ASN
1	A	133	LYS
1	A	143	GLU
1	A	144	LYS
1	A	145	LEU
1	A	147	ARG
1	A	153	LYS
1	A	156	GLU
1	A	160	LEU
1	A	166	LYS
1	A	174	LEU
1	A	177	LEU
1	A	181	GLU
1	A	183	LYS
1	A	184	LYS
1	A	185	SER
1	A	190	LEU
1	B	201	MET
1	B	202	GLN
1	B	219	LEU
1	B	230	SER
1	B	231	GLU
1	B	235	THR
1	B	240	TYR
1	B	249	GLU
1	B	261	GLN
1	B	263	ASP
1	B	265	ASP
1	B	266	ARG
1	B	270	LEU
1	B	271	SER
1	B	285	VAL
1	B	288	SER
1	B	292	ASN
1	B	304	HIS
1	B	312	LEU
1	B	319	LEU
1	B	324	SER
1	B	327	GLU

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Mol	Chain	Res	Type
1	B	328	LYS
1	B	331	LYS
1	B	332	ASN
1	B	333	LYS
1	B	334	GLN
1	B	338	THR
1	B	343	GLU
1	B	344	LYS
1	B	345	LEU
1	B	347	ARG
1	B	353	LYS
1	B	356	GLU
1	B	360	LEU
1	B	366	LYS
1	B	374	LEU
1	B	377	LEU
1	B	381	GLU
1	B	383	LYS
1	B	384	LYS
1	B	385	SER
1	B	390	LEU

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

Mol	Chain	Res	Type
1	A	74	GLN
1	A	134	GLN
1	A	162	GLN
1	B	202	GLN
1	B	274	GLN
1	B	334	GLN
1	B	367	ASN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	200	2	23,30,30	2.21	5 (21%)	30,47,47	2.23	7 (23%)
4	GNH	B	400	-	23,30,30	2.81	7 (30%)	27,47,47	2.41	8 (29%)

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	200	2	-	0/12/32/32	0/3/3/3
4	GNH	B	400	-	-	0/9/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	GNH	PB-O2B	-2.60	1.49	1.56
3	A	200	GDP	C6-C5	2.95	1.47	1.41
3	A	200	GDP	O4'-C1'	3.29	1.45	1.41
3	A	200	GDP	C2-N1	3.44	1.41	1.35
4	B	400	GNH	O4'-C1'	3.62	1.45	1.41
4	B	400	GNH	C6-C5	3.85	1.49	1.41
4	B	400	GNH	C2-N1	4.58	1.43	1.35
4	B	400	GNH	PB-O1B	4.75	1.51	1.46
3	A	200	GDP	C4-N3	5.56	1.44	1.35
3	A	200	GDP	C6-N1	5.76	1.43	1.33
4	B	400	GNH	C6-N1	6.48	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	GNH	C4-N3	7.02	1.46	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	200	GDP	C5-C6-N1	-7.02	113.99	123.59
4	B	400	GNH	C5-C6-N1	-6.82	114.26	123.59
4	B	400	GNH	N3-C2-N1	-3.70	121.81	127.44
3	A	200	GDP	N3-C2-N1	-3.49	122.12	127.44
3	A	200	GDP	O3A-PA-O5'	-3.22	94.39	102.94
4	B	400	GNH	O3A-PA-O5'	-2.85	95.37	102.94
4	B	400	GNH	O4'-C1'-N9	-2.78	102.28	108.10
3	A	200	GDP	C6-C5-C4	-2.41	118.02	120.90
4	B	400	GNH	C6-C5-C4	-2.25	118.20	120.90
3	A	200	GDP	C2'-C1'-N9	2.05	117.42	114.29
4	B	400	GNH	C2'-C1'-N9	2.61	118.28	114.29
3	A	200	GDP	O2B-PB-O1B	2.71	119.29	110.58
4	B	400	GNH	C4'-O4'-C1'	2.96	112.97	109.72
3	A	200	GDP	C6-N1-C2	6.43	124.86	115.94
4	B	400	GNH	C6-N1-C2	6.57	125.05	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
4	B	400	GNH	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

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	190/191 (99%)	0.24	9 (4%) 35 40	26, 43, 84, 100	0
1	B	190/191 (99%)	0.98	35 (18%) 2 2	35, 63, 99, 100	0
All	All	380/382 (99%)	0.61	44 (11%) 6 6	26, 52, 98, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	VAL	7.3
1	B	382	PRO	7.0
1	B	237	PHE	6.0
1	B	236	VAL	5.7
1	B	234	PRO	5.6
1	B	230	SER	4.9
1	B	235	THR	4.7
1	A	180	PRO	4.6
1	B	232	TYR	4.2
1	B	264	TYR	4.1
1	A	184	LYS	4.1
1	B	279	LEU	4.0
1	B	330	ALA	4.0
1	B	333	LYS	3.8
1	A	181	GLU	3.7
1	B	280	VAL	3.5
1	B	281	CYS	3.4
1	B	267	LEU	3.4
1	B	326	ILE	3.2
1	B	313	VAL	3.2
1	A	182	PRO	3.2
1	B	201	MET	3.1
1	B	266	ARG	2.8
1	B	209	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	183	LYS	2.6
1	B	311	LEU	2.6
1	B	390	LEU	2.6
1	B	328	LYS	2.6
1	B	303	HIS	2.6
1	B	260	GLY	2.6
1	A	111	LEU	2.5
1	B	270	LEU	2.5
1	B	327	GLU	2.4
1	B	331	LYS	2.4
1	A	79	LEU	2.3
1	B	329	LEU	2.3
1	B	380	PRO	2.3
1	A	131	LYS	2.2
1	B	278	PHE	2.2
1	B	381	GLU	2.1
1	A	8	VAL	2.1
1	B	379	PRO	2.1
1	B	372	ALA	2.1
1	B	383	LYS	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, 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
4	GNH	B	400	28/28	0.91	0.13	-0.63	28,64,79,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GDP	A	200	28/28	0.98	0.12	-0.67	23,34,41,46	0
2	MG	A	199	1/1	0.93	0.11	-	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.