



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 04:52 PM EDT

PDB ID : 1VG0
Title : The crystal structures of the REP-1 protein in complex with monoprenylated Rab7 protein
Authors : Rak, A.; Pylypenko, O.; Niculae, A.; Pyatkov, K.; Goody, R.S.; Alexandrov, K.
Deposited on : 2004-04-22
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

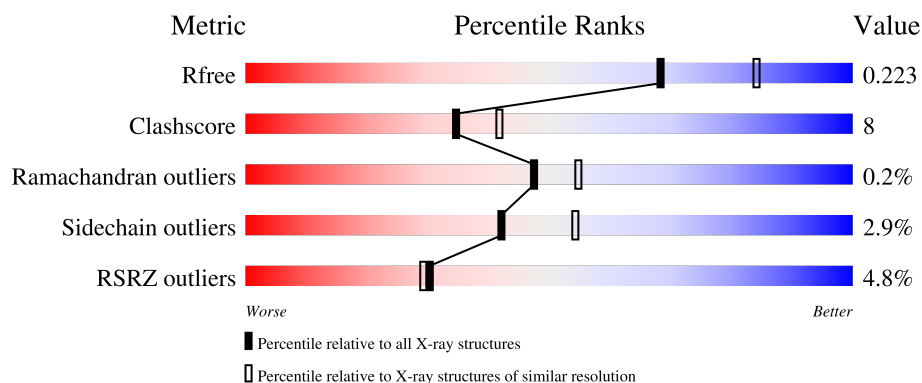
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	650	<div> <div>4%</div> <div>62%</div> <div>12%</div> <div>26%</div> </div>
2	B	207	<div> <div>4%</div> <div>67%</div> <div>20%</div> <div>12%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5773 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 Rab proteins geranylgeranyltransferase component A 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3819	2422	643	724	30			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	LYS	GLN	engineered mutation	UNP P37727
A	462	ARG	LYS	engineered mutation	UNP P37727
A	473	THR	ALA	engineered mutation	UNP P37727
A	483	ALA	GLY	engineered mutation	UNP P37727

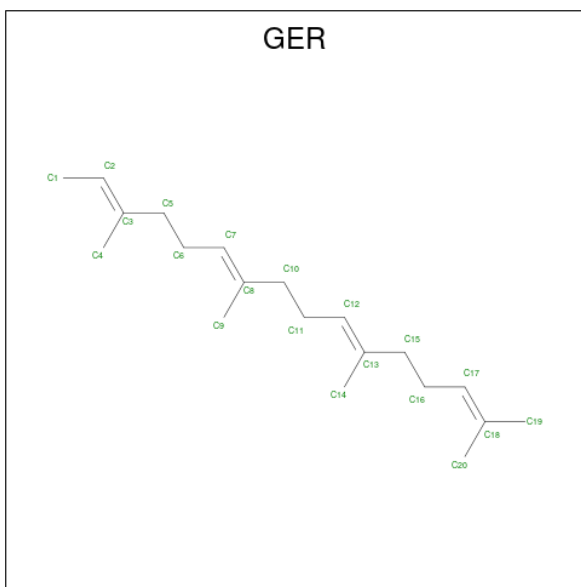
- Molecule 2 is a protein called Ras-related protein Rab-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1453	928	243	276	6			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is GERAN-8-YL GERAN (three-letter code: GER) (formula: C₂₀H₃₄).

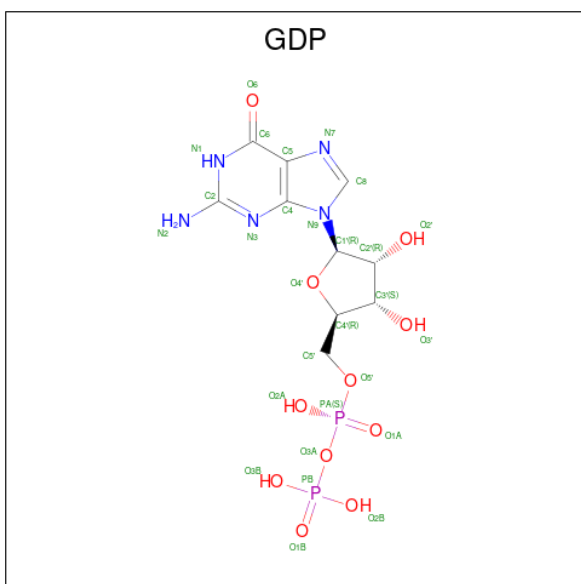


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 20 20	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

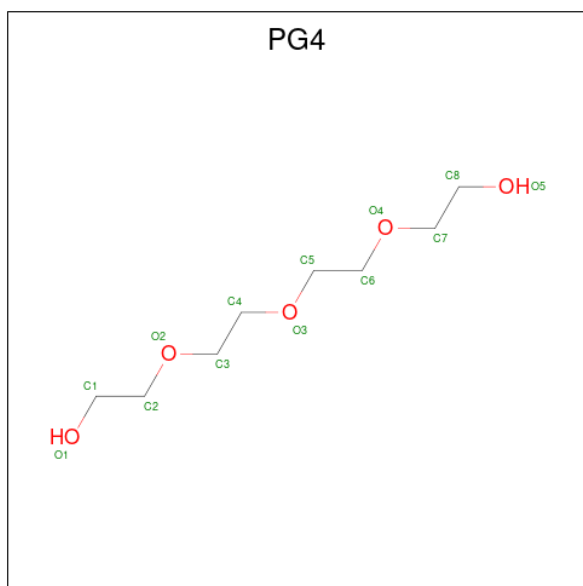
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		

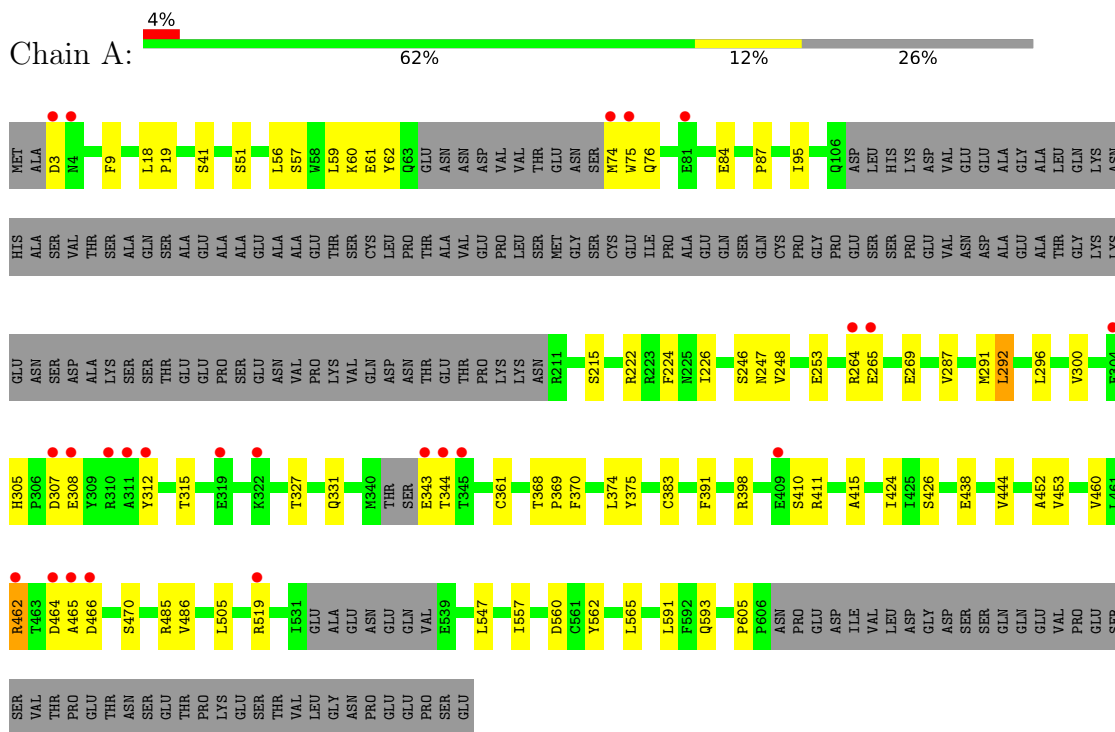
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	347	Total	O	0	0
			347	347		
8	B	91	Total	O	0	0
			91	91		

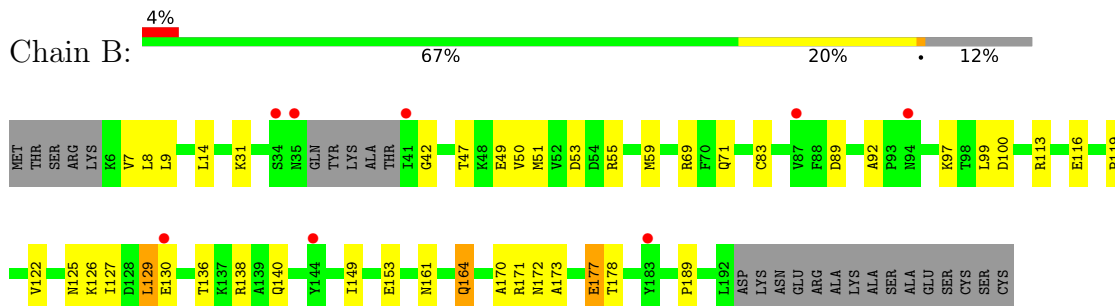
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Rab proteins geranylgeranyltransferase component A 1



- Molecule 2: Ras-related protein Rab-7



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.30Å 105.30Å 132.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.20 19.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (18.00-2.20) 97.6 (19.79-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.188 , 0.233 0.180 , 0.223	Depositor DCC
R_{free} test set	2266 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5773	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 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GER, CL, MG, PG4, 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	0.56	0/3894	0.72	0/5265
2	B	0.52	0/1481	0.66	0/2006
All	All	0.55	0/5375	0.70	0/7271

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	3819	0	3760	53	0
2	B	1453	0	1428	37	0
3	A	1	0	0	0	0
4	A	20	0	34	1	0
5	B	1	0	0	0	0
6	B	28	0	12	1	0
7	B	13	0	18	1	0
8	A	347	0	0	6	0
8	B	91	0	0	1	0
All	All	5773	0	5252	88	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 8.

All (88) 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)
2:B:161:ASN:HA	2:B:164:GLN:CG	2.11	0.81
1:A:462:ARG:NE	1:A:462:ARG:H	1.79	0.81
1:A:438:GLU:HG2	8:A:3277:HOH:O	1.82	0.79
1:A:287:VAL:O	1:A:291:MET:HG3	1.84	0.77
2:B:161:ASN:HA	2:B:164:GLN:HG2	1.67	0.77
1:A:560:ASP:HB2	8:A:3313:HOH:O	1.88	0.73
2:B:113:ARG:HH11	2:B:113:ARG:HG3	1.55	0.71
1:A:3:ASP:HB3	2:B:69:ARG:HE	1.53	0.71
1:A:74:MET:HG2	1:A:76:GLN:H	1.64	0.64
1:A:462:ARG:H	1:A:462:ARG:CD	2.09	0.63
1:A:57:SER:HA	1:A:60:LYS:HE2	1.80	0.62
1:A:519:ARG:HB2	8:A:3181:HOH:O	1.99	0.62
1:A:253:GLU:OE1	2:B:189:PRO:HG2	2.01	0.59
1:A:410:SER:O	1:A:411:ARG:HB2	2.03	0.59
2:B:59:MET:HE1	2:B:170:ALA:HA	1.84	0.59
1:A:361:CYS:HB2	1:A:369:PRO:HB3	1.85	0.58
1:A:415:ALA:HB1	1:A:424:ILE:O	2.04	0.58
1:A:485:ARG:HG3	8:A:3207:HOH:O	2.03	0.58
2:B:50:VAL:HG12	2:B:51:MET:N	2.19	0.57
2:B:89:ASP:HB3	2:B:92:ALA:HB3	1.86	0.57
2:B:122:VAL:HG23	2:B:149:ILE:HG21	1.87	0.55
2:B:161:ASN:CA	2:B:164:GLN:HG2	2.35	0.55
1:A:264:ARG:O	1:A:265:GLU:HB2	2.08	0.54
2:B:161:ASN:HA	2:B:164:GLN:HG3	1.86	0.54
2:B:71:GLN:HB3	7:B:5502:PG4:H62	1.90	0.54
1:A:56:LEU:HA	1:A:59:LEU:HD12	1.89	0.53
2:B:7:VAL:HG21	2:B:55:ARG:NH2	2.23	0.53
1:A:246:SER:O	1:A:247:ASN:HB2	2.08	0.53
1:A:51:SER:HA	1:A:224:PHE:O	2.09	0.52
1:A:486:VAL:HG22	1:A:505:LEU:HG	1.90	0.52
1:A:264:ARG:HB2	1:A:269:GLU:OE2	2.10	0.52
2:B:161:ASN:C	2:B:164:GLN:HG2	2.29	0.52
1:A:444:VAL:HG13	1:A:557:ILE:HD13	1.93	0.51
1:A:84:GLU:CD	1:A:411:ARG:HH12	2.14	0.51
1:A:9:PHE:O	1:A:426:SER:HA	2.11	0.51
2:B:126:LYS:HG2	6:B:1557:GDP:C6	2.46	0.51
2:B:126:LYS:HB3	2:B:129:LEU:HD22	1.92	0.51
1:A:368:THR:HB	1:A:369:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ASN:O	2:B:126:LYS:HB2	2.11	0.51
1:A:292:LEU:HD22	1:A:296:LEU:CD1	2.41	0.50
1:A:444:VAL:CG1	1:A:557:ILE:HD13	2.42	0.50
1:A:369:PRO:HG2	1:A:370:PHE:CE1	2.47	0.50
2:B:113:ARG:HG3	2:B:113:ARG:NH1	2.25	0.49
1:A:312:TYR:O	1:A:315:THR:HG22	2.13	0.49
1:A:462:ARG:CD	1:A:462:ARG:N	2.75	0.49
2:B:136:THR:O	2:B:140:GLN:HG3	2.12	0.48
2:B:59:MET:CE	2:B:170:ALA:HA	2.44	0.48
1:A:312:TYR:HB3	1:A:315:THR:CG2	2.43	0.47
1:A:61:GLU:OE2	1:A:61:GLU:N	2.45	0.47
2:B:97:LYS:HE2	2:B:138:ARG:NH2	2.29	0.47
1:A:75:TRP:HA	8:A:3239:HOH:O	2.15	0.47
2:B:97:LYS:NZ	2:B:138:ARG:HH21	2.13	0.47
2:B:127:ILE:HG21	2:B:153:GLU:HB3	1.98	0.46
1:A:374:LEU:O	1:A:375:TYR:HB2	2.15	0.46
2:B:8:LEU:HD23	2:B:8:LEU:C	2.36	0.46
1:A:3:ASP:CB	2:B:69:ARG:HE	2.23	0.45
1:A:292:LEU:HD22	1:A:296:LEU:HD11	1.96	0.45
1:A:305:HIS:HB3	1:A:308:GLU:HB2	1.98	0.45
1:A:343:GLU:OE2	1:A:344:THR:HG23	2.17	0.45
1:A:391:PHE:HZ	1:A:605:PRO:HB3	1.82	0.45
2:B:53:ASP:OD2	2:B:171:ARG:NH1	2.50	0.45
1:A:61:GLU:HG2	8:A:3034:HOH:O	2.17	0.44
4:A:952:GER:H92	4:A:952:GER:H41	1.99	0.44
2:B:177:GLU:HG3	2:B:178:THR:N	2.33	0.44
2:B:8:LEU:HD23	2:B:9:LEU:N	2.32	0.44
2:B:100:ASP:HB2	8:B:5525:HOH:O	2.17	0.44
2:B:9:LEU:CD2	2:B:177:GLU:HG2	2.48	0.44
1:A:18:LEU:HB3	1:A:19:PRO:HD3	2.00	0.43
1:A:410:SER:O	1:A:411:ARG:CB	2.66	0.43
2:B:119:PRO:HB3	2:B:172:ASN:HB3	2.01	0.42
1:A:296:LEU:O	1:A:300:VAL:HG23	2.19	0.42
2:B:50:VAL:CG1	2:B:51:MET:N	2.82	0.42
2:B:83:CYS:HB2	2:B:173:ALA:HB2	2.02	0.42
1:A:248:VAL:CG1	1:A:383:CYS:HB3	2.50	0.42
1:A:62:TYR:CD2	1:A:95:ILE:HB	2.55	0.42
1:A:327:THR:O	1:A:331:GLN:HG3	2.20	0.42
1:A:41:SER:HA	1:A:398:ARG:HG3	2.01	0.42
2:B:89:ASP:OD2	2:B:126:LYS:HD2	2.20	0.42
1:A:222:ARG:HD3	1:A:222:ARG:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:TYR:HB2	1:A:565:LEU:HD22	2.03	0.41
2:B:113:ARG:NH1	2:B:113:ARG:CG	2.83	0.41
1:A:452:ALA:HA	1:A:547:LEU:O	2.20	0.41
2:B:47:THR:HA	2:B:59:MET:O	2.19	0.41
1:A:464:ASP:CG	1:A:465:ALA:H	2.24	0.41
1:A:75:TRP:CH2	1:A:87:PRO:HG3	2.56	0.40
1:A:460:VAL:O	1:A:462:ARG:NH2	2.54	0.40
1:A:226:ILE:CG2	1:A:453:VAL:HG11	2.51	0.40
2:B:89:ASP:CG	2:B:126:LYS:HD2	2.41	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	471/650 (72%)	457 (97%)	14 (3%)	0	100	100
2	B	178/207 (86%)	170 (96%)	7 (4%)	1 (1%)	25	26
All	All	649/857 (76%)	627 (97%)	21 (3%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	42	GLY

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	429/581 (74%)	421 (98%)	8 (2%)	57	71
2	B	158/181 (87%)	149 (94%)	9 (6%)	20	24
All	All	587/762 (77%)	570 (97%)	17 (3%)	42	54

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	SER
1	A	292	LEU
1	A	307	ASP
1	A	462	ARG
1	A	466	ASP
1	A	470	SER
1	A	591	LEU
1	A	593	GLN
2	B	14	LEU
2	B	31	LYS
2	B	49	GLU
2	B	99	LEU
2	B	116	GLU
2	B	129	LEU
2	B	130	GLU
2	B	164	GLN
2	B	177	GLU

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

Mol	Chain	Res	Type
1	A	270	GLN
1	A	336	HIS
1	A	402	GLN
2	B	26	ASN
2	B	35	ASN
2	B	164	GLN
2	B	172	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
6	GDP	B	1557	5	24,30,30	1.64	3 (12%)	31,47,47	2.47	12 (38%)
7	PG4	B	5502	-	12,12,12	0.48	0	11,11,11	0.31	0
4	GER	A	952	-	19,19,19	1.87	8 (42%)	22,22,22	2.99	11 (50%)

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
6	GDP	B	1557	5	-	1/12/32/32	0/3/3/3
7	PG4	B	5502	-	-	5/10/10/10	-
4	GER	A	952	-	-	5/20/20/20	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1557	GDP	C6-N1	5.39	1.42	1.33
4	A	952	GER	C7-C8	2.88	1.39	1.33
4	A	952	GER	C12-C13	2.82	1.39	1.33
4	A	952	GER	C5-C3	2.73	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	952	GER	C17-C18	2.54	1.39	1.32
6	B	1557	GDP	C2'-C1'	-2.33	1.50	1.53
6	B	1557	GDP	C6-C5	2.13	1.45	1.41
4	A	952	GER	C10-C8	2.11	1.55	1.51
4	A	952	GER	C20-C18	2.10	1.56	1.50
4	A	952	GER	C9-C8	2.07	1.56	1.50
4	A	952	GER	C15-C13	2.01	1.55	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1557	GDP	C5-C6-N1	-7.55	113.10	123.43
4	A	952	GER	C9-C8-C10	6.67	126.49	115.27
6	B	1557	GDP	C6-N1-C2	5.91	125.32	115.93
4	A	952	GER	C20-C18-C19	5.85	127.52	114.60
4	A	952	GER	C6-C5-C3	4.32	127.17	112.98
4	A	952	GER	C4-C3-C5	4.00	122.00	115.27
6	B	1557	GDP	C6-C5-C4	-3.88	117.10	120.80
4	A	952	GER	C16-C15-C13	3.72	125.22	112.98
6	B	1557	GDP	C1'-N9-C4	-3.64	120.25	126.64
4	A	952	GER	C11-C10-C8	3.46	124.37	112.98
4	A	952	GER	C20-C18-C17	-3.41	112.80	122.65
4	A	952	GER	C10-C8-C7	-3.39	114.25	121.12
6	B	1557	GDP	N3-C2-N1	-3.23	122.91	127.22
6	B	1557	GDP	C2-N3-C4	-3.14	111.77	115.36
4	A	952	GER	C14-C13-C15	3.12	120.53	115.27
4	A	952	GER	C10-C11-C12	-2.93	102.25	111.88
4	A	952	GER	C4-C3-C2	-2.49	118.87	123.81
6	B	1557	GDP	O4'-C4'-C5'	2.30	116.93	109.37
6	B	1557	GDP	PA-O3A-PB	-2.19	125.30	132.83
6	B	1557	GDP	O3B-PB-O2B	-2.11	99.59	107.64
6	B	1557	GDP	N2-C2-N3	2.10	121.21	117.79
6	B	1557	GDP	O2A-PA-O5'	2.05	117.29	107.75
6	B	1557	GDP	O3'-C3'-C4'	-2.05	105.13	111.05

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	952	GER	C12-C13-C15-C16
4	A	952	GER	C14-C13-C15-C16
4	A	952	GER	C4-C3-C5-C6

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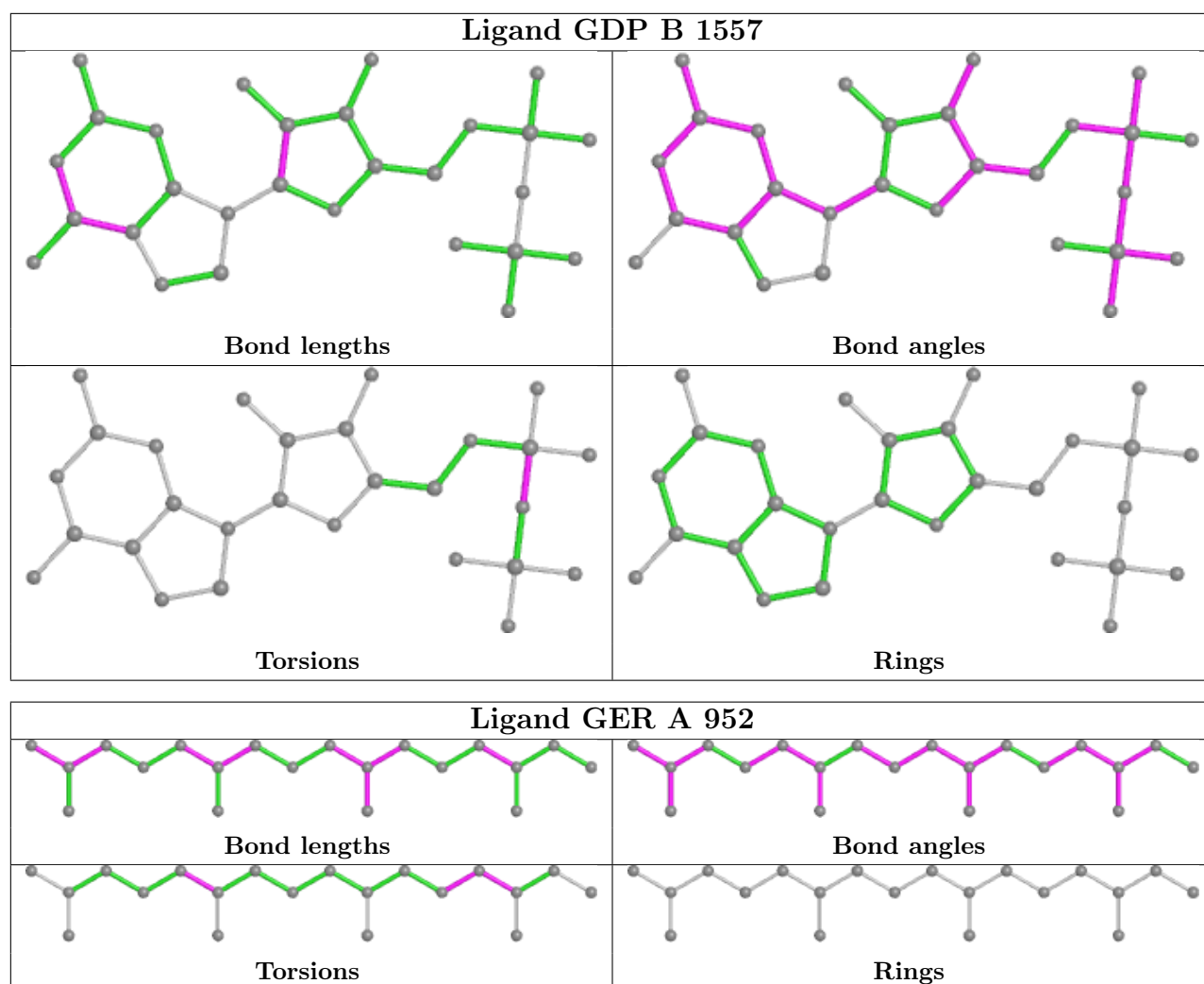
Mol	Chain	Res	Type	Atoms
4	A	952	GER	C2-C3-C5-C6
7	B	5502	PG4	O1-C1-C2-O2
7	B	5502	PG4	O2-C3-C4-O3
4	A	952	GER	C3-C5-C6-C7
7	B	5502	PG4	C6-C5-O3-C4
6	B	1557	GDP	PB-O3A-PA-O2A
7	B	5502	PG4	C5-C6-O4-C7
7	B	5502	PG4	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1557	GDP	1	0
7	B	5502	PG4	1	0
4	A	952	GER	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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(Å ²)	Q<0.9
1	A	481/650 (74%)	-0.32	24 (4%) 28 27	15, 26, 53, 65	0
2	B	182/207 (87%)	-0.08	8 (4%) 34 32	17, 36, 51, 61	0
All	All	663/857 (77%)	-0.26	32 (4%) 30 29	15, 29, 53, 65	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	ARG	4.9
2	B	35	ASN	4.7
1	A	465	ALA	4.4
1	A	344	THR	4.3
1	A	311	ALA	3.9
1	A	343	GLU	3.8
1	A	464	ASP	3.8
2	B	183	TYR	3.6
2	B	34	SER	3.6
1	A	310	ARG	3.4
1	A	3	ASP	3.3
1	A	265	GLU	3.3
1	A	74	MET	3.3
1	A	81	GLU	3.0
1	A	307	ASP	2.8
1	A	462	ARG	2.8
2	B	144	TYR	2.7
2	B	130	GLU	2.7
2	B	41	ILE	2.6
1	A	312	TYR	2.4
1	A	75	TRP	2.3
1	A	4	ASN	2.3
2	B	94	ASN	2.2
1	A	322	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	466	ASP	2.2
1	A	345	THR	2.1
1	A	308	GLU	2.1
1	A	519	ARG	2.1
2	B	87	VAL	2.1
1	A	319	GLU	2.1
1	A	409	GLU	2.1
1	A	304	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 monosaccharides in this entry.

6.4 Ligands [i](#)

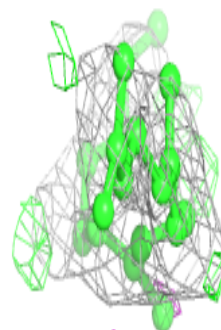
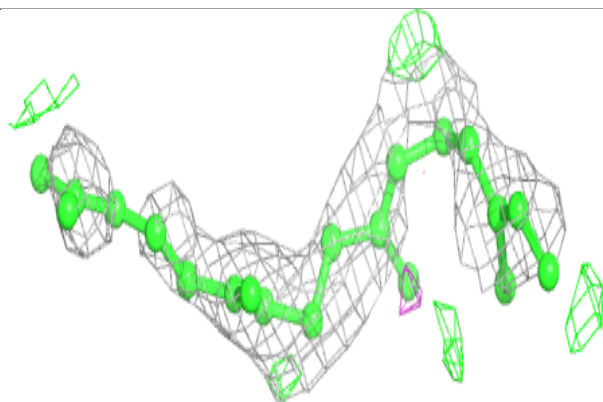
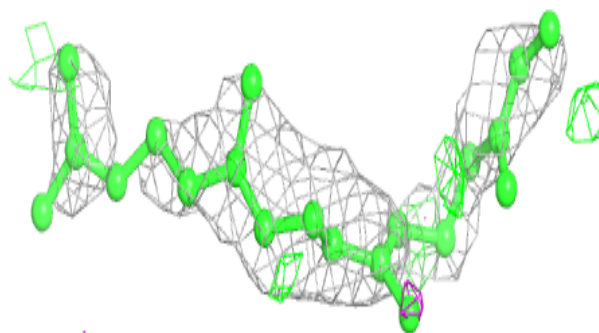
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GER	A	952	20/20	0.62	0.33	58,66,69,73	0
7	PG4	B	5502	13/13	0.90	0.14	42,49,52,55	0
5	MG	B	3000	1/1	0.95	0.06	27,27,27,27	0
6	GDP	B	1557	28/28	0.97	0.10	27,35,45,48	0
3	CL	A	3001	1/1	1.00	0.12	20,20,20,20	0

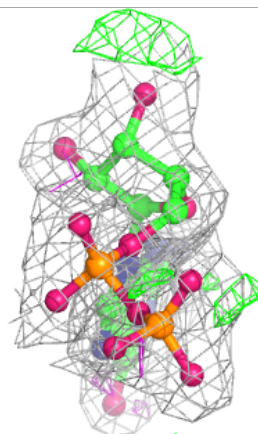
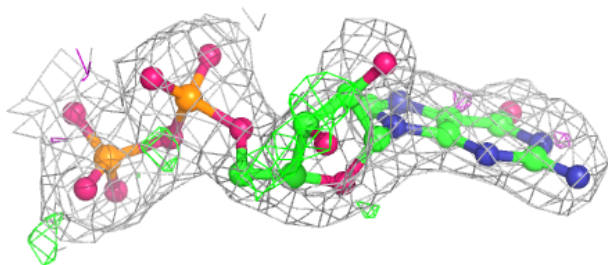
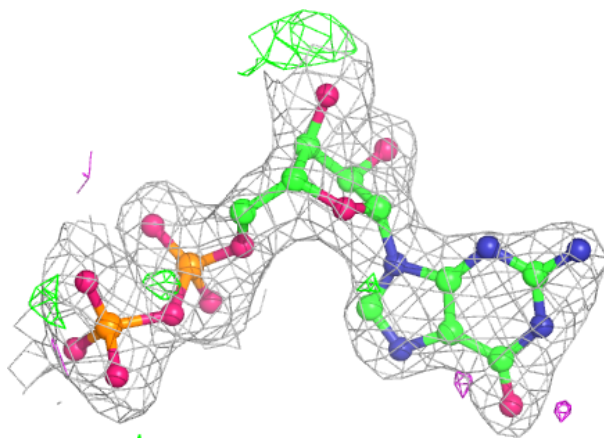
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GER A 952:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP B 1557:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.