



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:05 AM UTC

PDB ID : 2GVJ / pdb_00002gvj
Title : Crystal Structure of Human NMPRTase in complex with FK866
Authors : Khan, J.A.; Tao, X.; Tong, L.
Deposited on : 2006-05-02
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

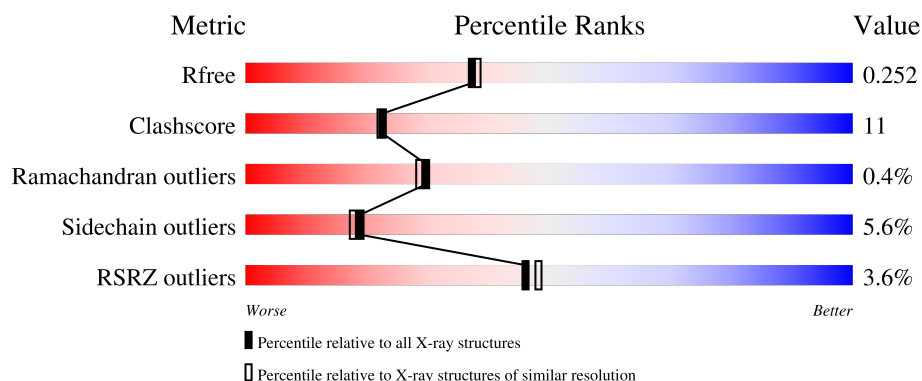
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	491	
1	B	491	

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	24	3	2		
2	B	1	Total	C	N	O	0	0
			29	24	3	2		

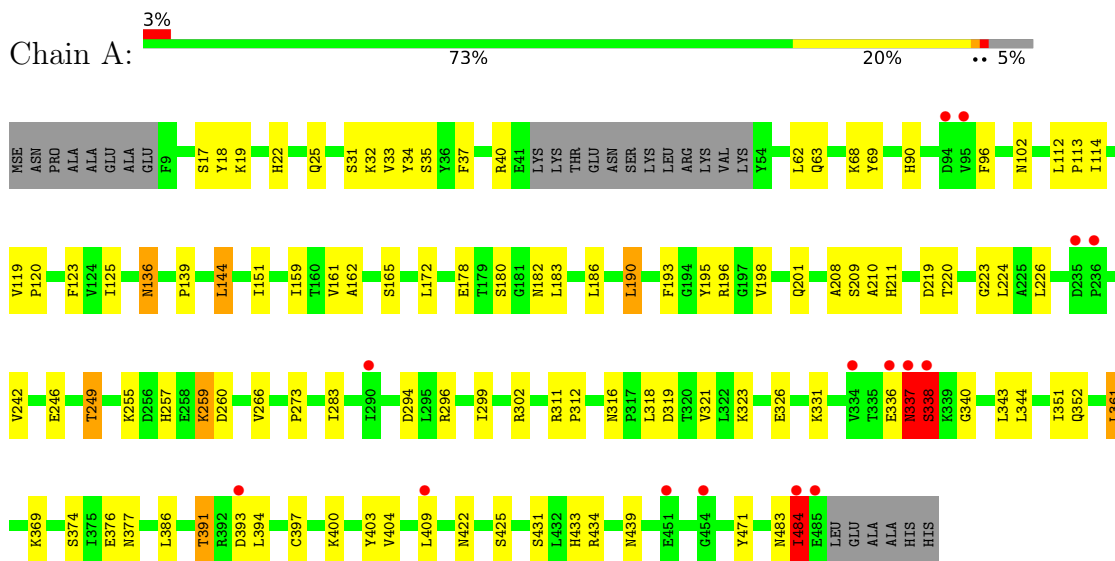
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	388	Total	O	0	0
			388	388		
3	B	387	Total	O	0	0
			387	387		

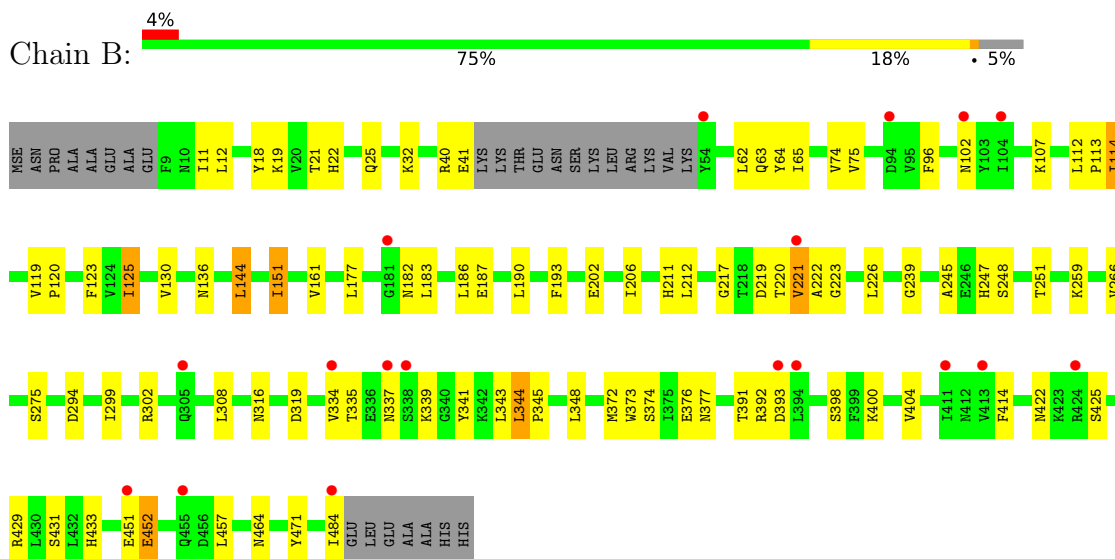
3 Residue-property plots

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: Nicotinamide phosphoribosyltransferase



- Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.78Å 105.90Å 83.43Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	82.76 – 2.10 82.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.76-2.10) 92.5 (82.76-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.247 , 0.298 0.247 , 0.252	Depositor DCC
R_{free} test set	4615 reflections (7.64%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8264	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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: DGB

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	0/3806	0.92	1/5155 (0.0%)
1	B	0.60	1/3797 (0.0%)	0.93	2/5143 (0.0%)
All	All	0.59	1/7603 (0.0%)	0.92	3/10298 (0.0%)

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	B	372	MSE	SE-CE	-5.40	1.79	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SER	N-CA-C	-8.74	101.98	114.12
1	B	182	ASN	N-CA-C	5.52	115.84	108.23
1	B	222	ALA	N-CA-C	-5.21	107.94	114.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	ASN	Peptide

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	3720	0	3692	87	0
1	B	3711	0	3686	75	0
2	A	29	0	31	1	0
2	B	29	0	31	2	0
3	A	388	0	0	26	0
3	B	387	0	0	20	0
All	All	8264	0	7440	157	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 11.

All (157) 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:114:ILE:HD13	1:B:144:LEU:HD13	1.40	1.04
1:A:283:ILE:HG12	3:A:1358:HOH:O	1.57	1.03
1:A:119:VAL:HG21	1:A:125:ILE:HD11	1.42	0.99
1:B:40:ARG:HD3	1:B:422:ASN:O	1.67	0.93
1:A:338:SER:HB3	3:A:1182:HOH:O	1.70	0.90
1:A:165:SER:HA	3:A:1359:HOH:O	1.71	0.89
1:A:249:THR:HG21	1:B:25:GLN:OE1	1.73	0.88
1:B:344:LEU:H	1:B:377:ASN:HD21	1.22	0.85
1:A:223:GLY:HA2	3:A:813:HOH:O	1.79	0.83
1:A:343:LEU:HD13	1:A:376:GLU:HG3	1.59	0.82
1:B:32:LYS:HD3	3:B:844:HOH:O	1.81	0.81
1:B:343:LEU:HD13	1:B:376:GLU:HG3	1.64	0.79
1:A:344:LEU:H	1:A:377:ASN:HD21	1.28	0.79
1:B:316:ASN:HD22	1:B:319:ASP:H	1.33	0.77
1:A:336:GLU:HG2	1:A:337:ASN:CB	2.15	0.77
1:B:64:TYR:CE2	1:B:206:ILE:HD11	2.19	0.77
1:B:221:VAL:C	3:B:1298:HOH:O	2.28	0.76
1:B:343:LEU:CD1	1:B:376:GLU:HG3	2.15	0.76
1:A:63:GLN:HE22	1:A:471:TYR:H	1.33	0.75
1:A:209:SER:HB3	3:A:813:HOH:O	1.89	0.72
1:A:40:ARG:HD3	1:A:422:ASN:O	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:815:HOH:O	1:B:251:THR:HG21	1.89	0.72
1:A:196:ARG:HG2	3:A:1301:HOH:O	1.90	0.71
1:A:312:PRO:HB3	3:A:1358:HOH:O	1.90	0.71
1:A:226:LEU:HB3	3:A:813:HOH:O	1.90	0.71
1:A:220:THR:HG22	3:A:708:HOH:O	1.89	0.70
1:A:374:SER:OG	1:A:376:GLU:HG2	1.91	0.70
1:B:130:VAL:HG22	3:B:1332:HOH:O	1.91	0.70
1:A:25:GLN:HE22	1:B:245:ALA:HA	1.57	0.70
1:A:17:SER:OG	1:A:90:HIS:HE1	1.75	0.70
1:B:211:HIS:HA	3:B:1304:HOH:O	1.92	0.69
1:A:336:GLU:HG2	1:A:337:ASN:N	2.06	0.69
1:A:259:LYS:HB2	1:A:259:LYS:NZ	2.08	0.68
1:B:63:GLN:HE22	1:B:471:TYR:H	1.40	0.67
1:A:40:ARG:CD	1:A:422:ASN:O	2.43	0.67
1:B:400:LYS:HD2	1:B:425:SER:HB3	1.77	0.67
1:A:338:SER:HB2	3:A:1005:HOH:O	1.94	0.66
1:B:344:LEU:H	1:B:377:ASN:ND2	1.92	0.66
1:B:348:LEU:HB3	3:B:1343:HOH:O	1.96	0.66
1:A:136:ASN:HD22	1:A:136:ASN:H	1.44	0.65
1:B:64:TYR:CZ	1:B:206:ILE:HD11	2.31	0.65
1:B:161:VAL:HG12	3:B:1304:HOH:O	1.97	0.65
1:A:302:ARG:NH1	3:A:1448:HOH:O	2.17	0.64
1:A:316:ASN:HD22	1:A:319:ASP:H	1.45	0.64
1:A:400:LYS:HD2	1:A:425:SER:HB3	1.79	0.63
1:A:259:LYS:HB2	1:A:259:LYS:HZ2	1.62	0.62
1:A:195:TYR:OH	1:A:201:GLN:NE2	2.31	0.62
1:B:193:PHE:CZ	2:B:501:DGB:HAD1	2.34	0.62
1:B:220:THR:HG22	3:B:769:HOH:O	1.98	0.62
1:A:249:THR:HG23	1:B:25:GLN:HB3	1.83	0.61
1:A:337:ASN:HA	1:A:340:GLY:H	1.66	0.61
1:A:296:ARG:NH1	1:A:331:LYS:O	2.34	0.61
1:B:348:LEU:CB	3:B:1343:HOH:O	2.49	0.60
1:A:336:GLU:HG2	1:A:337:ASN:HB2	1.83	0.60
1:A:338:SER:CB	3:A:1005:HOH:O	2.49	0.60
1:A:35:SER:HB3	3:A:1324:HOH:O	2.02	0.59
1:B:206:ILE:HD13	1:B:226:LEU:HD11	1.86	0.58
1:B:113:PRO:HA	1:B:464:ASN:HD22	1.69	0.58
1:B:398:SER:HA	3:B:1322:HOH:O	2.03	0.58
1:B:221:VAL:HG12	1:B:221:VAL:O	2.03	0.58
3:A:611:HOH:O	1:B:391:THR:HG23	2.05	0.57
1:A:161:VAL:HG12	3:A:722:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HB	1:A:302:ARG:HH21	1.69	0.55
1:B:64:TYR:CE2	1:B:206:ILE:CD1	2.88	0.55
1:A:32:LYS:HA	1:A:136:ASN:HD21	1.71	0.55
1:A:178:GLU:HG3	3:A:888:HOH:O	2.05	0.55
1:A:182:ASN:ND2	3:A:952:HOH:O	2.40	0.54
1:A:400:LYS:HD2	1:A:425:SER:CB	2.37	0.54
1:A:34:TYR:HB3	1:A:403:TYR:HB3	1.90	0.54
1:A:343:LEU:CD1	1:A:376:GLU:HG3	2.33	0.53
1:B:248:SER:HA	1:B:251:THR:HG22	1.89	0.53
1:B:343:LEU:HD13	1:B:376:GLU:CG	2.36	0.53
1:A:336:GLU:CG	1:A:337:ASN:N	2.72	0.53
1:A:19:LYS:HA	1:A:22:HIS:CD2	2.44	0.53
1:B:433:HIS:HA	1:B:457:LEU:HD13	1.90	0.53
1:A:321:VAL:HG23	1:A:352:GLN:HE21	1.74	0.52
1:B:247:HIS:O	1:B:251:THR:HG22	2.09	0.52
1:A:193:PHE:CZ	2:A:502:DGB:HAD1	2.45	0.52
1:A:190:LEU:CD1	3:A:1359:HOH:O	2.57	0.52
1:A:255:LYS:HG2	3:A:1314:HOH:O	2.09	0.51
1:A:483:ASN:O	1:A:484:ILE:C	2.53	0.51
1:B:21:THR:HA	3:B:1341:HOH:O	2.11	0.51
1:B:337:ASN:HB3	1:B:339:LYS:H	1.76	0.51
1:B:373:TRP:NE1	3:B:1311:HOH:O	2.44	0.51
1:B:316:ASN:ND2	1:B:319:ASP:H	2.06	0.50
1:A:32:LYS:O	1:A:404:VAL:HG23	2.12	0.50
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.46	0.50
1:A:33:VAL:H	1:A:136:ASN:HD21	1.59	0.50
1:A:299:ILE:HA	1:A:302:ARG:HD2	1.94	0.50
1:B:374:SER:OG	1:B:376:GLU:HG2	2.12	0.49
1:A:172:LEU:HD21	1:A:361:LEU:HD21	1.94	0.49
1:B:40:ARG:O	1:B:41:GLU:HB3	2.13	0.49
1:A:344:LEU:H	1:A:377:ASN:ND2	2.04	0.49
1:B:12:LEU:HD23	1:B:96:PHE:HZ	1.76	0.49
1:A:33:VAL:H	1:A:136:ASN:ND2	2.11	0.48
1:B:275:SER:CB	2:B:501:DGB:HAP1	2.43	0.48
1:A:136:ASN:H	1:A:136:ASN:ND2	2.10	0.48
1:A:17:SER:OG	1:A:90:HIS:CE1	2.62	0.48
1:A:63:GLN:HE22	1:A:471:TYR:N	2.06	0.48
1:A:159:ILE:HD11	3:A:773:HOH:O	2.14	0.48
1:A:316:ASN:HB3	1:A:319:ASP:HB2	1.96	0.48
1:A:90:HIS:HD2	1:B:239:GLY:O	1.97	0.48
1:B:120:PRO:O	1:B:123:PHE:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:HB	1:B:302:ARG:HH21	1.79	0.48
1:B:40:ARG:CD	1:B:422:ASN:O	2.50	0.47
1:A:40:ARG:HD2	1:A:422:ASN:O	2.14	0.47
1:B:414:PHE:CB	3:B:1317:HOH:O	2.62	0.47
1:B:113:PRO:HD2	1:B:144:LEU:CD1	2.45	0.47
1:B:259:LYS:HD2	1:B:294:ASP:HB3	1.96	0.47
1:A:391:THR:CG2	1:A:393:ASP:H	2.28	0.46
1:B:74:VAL:HG23	1:B:75:VAL:HG23	1.97	0.46
1:B:391:THR:HG22	1:B:392:ARG:N	2.29	0.46
1:A:210:ALA:C	3:A:722:HOH:O	2.58	0.45
1:A:162:ALA:HA	3:A:722:HOH:O	2.16	0.45
1:B:119:VAL:HG22	1:B:120:PRO:HD2	1.98	0.45
1:A:431:SER:OG	1:A:433:HIS:HE1	2.00	0.45
1:B:187:GLU:HG2	3:B:933:HOH:O	2.17	0.45
1:B:223:GLY:N	3:B:769:HOH:O	2.50	0.45
1:A:259:LYS:HZ1	1:A:294:ASP:HB3	1.80	0.44
1:A:211:HIS:HA	3:A:722:HOH:O	2.17	0.44
1:B:119:VAL:HG21	1:B:125:ILE:HD11	1.99	0.44
1:B:202:GLU:O	1:B:206:ILE:HG12	2.18	0.44
1:B:113:PRO:HD2	1:B:144:LEU:HD12	2.00	0.43
1:A:178:GLU:OE1	1:A:369:LYS:HE3	2.18	0.43
1:B:429:ARG:NH1	3:B:786:HOH:O	2.51	0.43
1:A:311:ARG:HG3	1:A:351:ILE:HG23	2.00	0.43
1:B:114:ILE:HD12	1:B:136:ASN:HA	2.01	0.43
1:B:345:PRO:HG2	3:B:1343:HOH:O	2.19	0.43
1:A:63:GLN:NE2	1:A:471:TYR:H	2.09	0.42
1:A:336:GLU:HG2	1:A:337:ASN:CA	2.49	0.42
1:A:112:LEU:HA	1:A:113:PRO:HD3	1.86	0.42
1:B:211:HIS:CA	3:B:1304:HOH:O	2.60	0.42
1:A:323:LYS:HA	1:A:326:GLU:HG2	2.01	0.42
1:A:31:SER:O	1:A:139:PRO:HA	2.20	0.42
1:A:208:ALA:HB3	3:A:708:HOH:O	2.19	0.42
1:A:242:VAL:HG11	1:A:273:PRO:HB2	2.01	0.41
1:A:37:PHE:CZ	1:A:397:CYS:HB3	2.55	0.41
1:B:431:SER:OG	1:B:433:HIS:CE1	2.73	0.41
1:B:65:ILE:HG23	1:B:151:ILE:HD13	2.02	0.41
1:A:120:PRO:HB2	1:A:123:PHE:CD1	2.56	0.41
1:A:484:ILE:H	1:A:484:ILE:HG13	1.57	0.41
1:B:299:ILE:CD1	1:B:308:LEU:HD22	2.51	0.41
1:A:400:LYS:CD	1:A:425:SER:HB3	2.48	0.41
1:B:65:ILE:HG23	1:B:151:ILE:CD1	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLU:OE2	1:B:19:LYS:NZ	2.35	0.41
1:B:337:ASN:HB2	1:B:341:TYR:H	1.86	0.41
1:A:114:ILE:HG12	1:A:144:LEU:HD13	2.03	0.41
1:B:112:LEU:HA	1:B:113:PRO:HD3	1.87	0.41
1:B:266:VAL:O	1:B:302:ARG:NH2	2.55	0.40
1:B:452:GLU:HB2	3:B:1204:HOH:O	2.21	0.40
1:B:484:ILE:H	1:B:484:ILE:HD12	1.86	0.40
1:B:217:GLY:HA3	3:B:631:HOH:O	2.22	0.40
1:B:392:ARG:NH1	3:B:803:HOH:O	2.42	0.40
1:A:68:LYS:HD3	1:A:69:TYR:CZ	2.56	0.40
1:A:257:HIS:HD2	1:A:260:ASP:OD2	2.04	0.40
1:B:316:ASN:HB3	1:B:319:ASP:HB2	2.03	0.40
1:A:439:ASN:HB3	3:A:1450:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/491 (94%)	440 (95%)	18 (4%)	3 (1%)	18	15
1	B	460/491 (94%)	443 (96%)	16 (4%)	1 (0%)	43	44
All	All	921/982 (94%)	883 (96%)	34 (4%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	ILE
1	A	96	PHE
1	A	337	ASN
1	B	221	VAL

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	409/427 (96%)	385 (94%)	24 (6%)	18	16
1	B	408/427 (96%)	386 (95%)	22 (5%)	20	18
All	All	817/854 (96%)	771 (94%)	46 (6%)	19	18

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	62	LEU
1	A	102	ASN
1	A	136	ASN
1	A	144	LEU
1	A	151	ILE
1	A	180	SER
1	A	183	LEU
1	A	186	LEU
1	A	190	LEU
1	A	198	VAL
1	A	219	ASP
1	A	224	LEU
1	A	249	THR
1	A	259	LYS
1	A	318	LEU
1	A	338	SER
1	A	361	LEU
1	A	386	LEU
1	A	391	THR
1	A	394	LEU
1	A	409	LEU
1	A	434	ARG
1	A	484	ILE
1	B	11	ILE
1	B	18	TYR
1	B	62	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	102	ASN
1	B	107	LYS
1	B	114	ILE
1	B	125	ILE
1	B	144	LEU
1	B	151	ILE
1	B	177	LEU
1	B	183	LEU
1	B	186	LEU
1	B	190	LEU
1	B	212	LEU
1	B	219	ASP
1	B	334	VAL
1	B	335	THR
1	B	344	LEU
1	B	393	ASP
1	B	404	VAL
1	B	451	GLU
1	B	452	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	25	GLN
1	A	63	GLN
1	A	90	HIS
1	A	92	GLN
1	A	97	ASN
1	A	102	ASN
1	A	129	ASN
1	A	136	ASN
1	A	201	GLN
1	A	257	HIS
1	A	264	HIS
1	A	268	GLN
1	A	316	ASN
1	A	337	ASN
1	A	352	GLN
1	A	377	ASN
1	A	433	HIS
1	A	464	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	479	ASN
1	A	481	GLN
1	A	483	ASN
1	B	22	HIS
1	B	63	GLN
1	B	90	HIS
1	B	97	ASN
1	B	102	ASN
1	B	129	ASN
1	B	146	ASN
1	B	257	HIS
1	B	264	HIS
1	B	268	GLN
1	B	316	ASN
1	B	337	ASN
1	B	370	GLN
1	B	377	ASN
1	B	433	HIS
1	B	464	ASN
1	B	479	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DGB	B	501	-	31,31,31	1.22	1 (3%)	39,39,39	1.38	3 (7%)
2	DGB	A	502	-	31,31,31	1.21	1 (3%)	39,39,39	1.23	5 (12%)

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	DGB	B	501	-	-	1/21/31/31	0/3/3/3
2	DGB	A	502	-	-	0/21/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	DGB	CAC-CAX	-6.34	1.34	1.48
2	B	501	DGB	CAC-CAX	-6.19	1.35	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	DGB	CAP-NAW-CAX	5.51	130.41	122.46
2	B	501	DGB	CAN-CAP-NAW	-3.39	102.68	112.20
2	A	502	DGB	CAN-CAP-NAW	-3.22	103.17	112.20
2	A	502	DGB	CAP-NAW-CAX	3.18	127.04	122.46
2	A	502	DGB	CAZ-CAD-CAC	-2.97	120.42	126.92
2	A	502	DGB	CAR-CAT-NBC	-2.22	106.31	110.66
2	B	501	DGB	CAI-NAV-CAM	2.11	120.56	116.85
2	A	502	DGB	CAI-NAV-CAM	2.04	120.43	116.85

There are no chirality outliers.

All (1) torsion outliers are listed below:

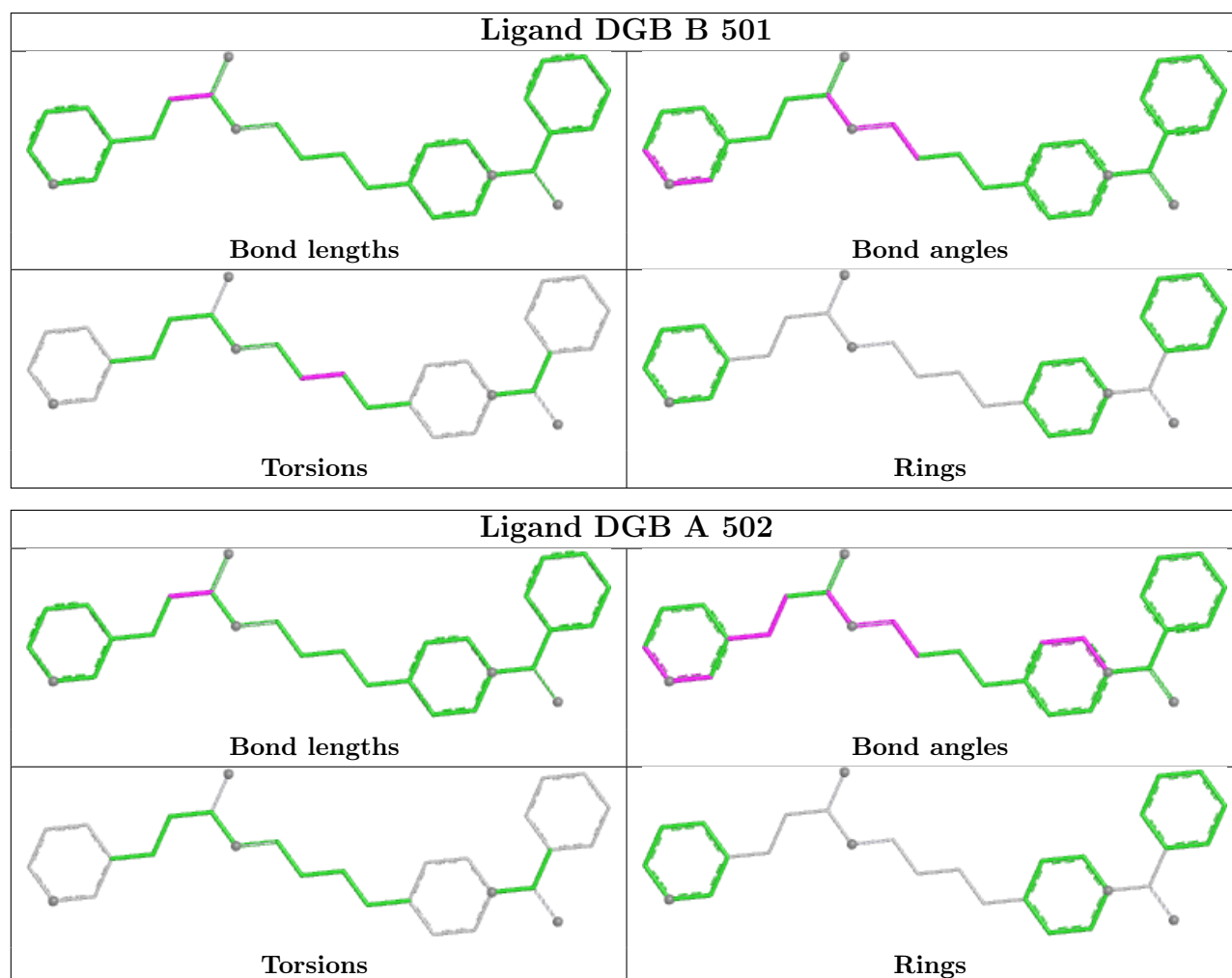
Mol	Chain	Res	Type	Atoms
2	B	501	DGB	CAP-CAN-CAO-CAQ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	DGB	2	0
2	A	502	DGB	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	463/491 (94%)	0.67	15 (3%) 50 53	4, 13, 21, 34	0
1	B	462/491 (94%)	0.57	18 (3%) 43 45	5, 13, 21, 31	0
All	All	925/982 (94%)	0.62	33 (3%) 46 48	4, 13, 21, 34	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	ASN	5.7
1	A	95	VAL	5.0
1	A	338	SER	3.9
1	B	484	ILE	3.8
1	A	484	ILE	3.7
1	B	221	VAL	3.4
1	B	451	GLU	3.4
1	A	451	GLU	3.3
1	A	94	ASP	3.2
1	B	455	GLN	3.1
1	B	411	ILE	3.1
1	B	338	SER	3.0
1	B	181	GLY	2.9
1	B	413	VAL	2.8
1	A	454	GLY	2.8
1	B	337	ASN	2.7
1	B	94	ASP	2.6
1	B	334	VAL	2.5
1	A	235	ASP	2.5
1	B	305	GLN	2.4
1	A	236	PRO	2.4
1	A	393	ASP	2.4
1	A	290	ILE	2.4
1	B	102	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	393	ASP	2.3
1	A	334	VAL	2.2
1	A	409	LEU	2.2
1	A	485	GLU	2.1
1	B	394	LEU	2.1
1	A	336	GLU	2.1
1	B	104	ILE	2.0
1	B	424	ARG	2.0
1	B	54	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

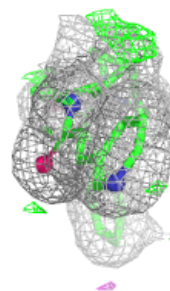
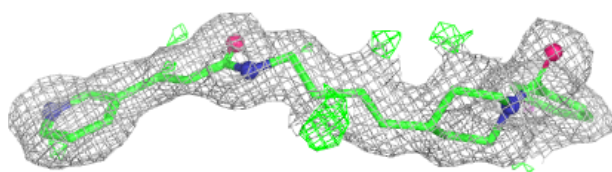
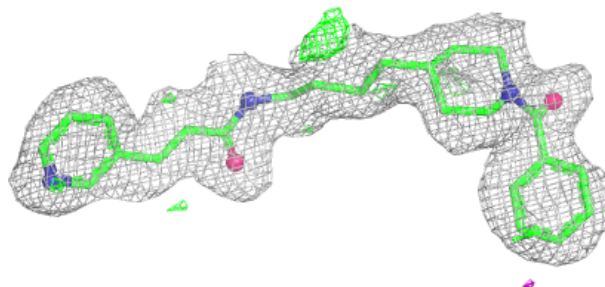
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DGB	A	502	29/29	0.87	0.11	11,12,13,14	0
2	DGB	B	501	29/29	0.89	0.09	11,12,14,14	0

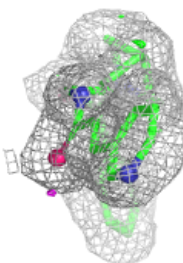
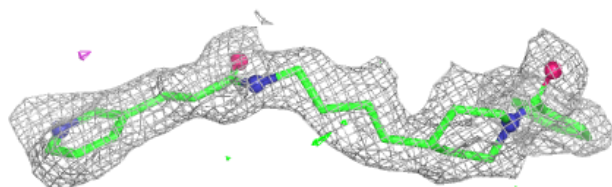
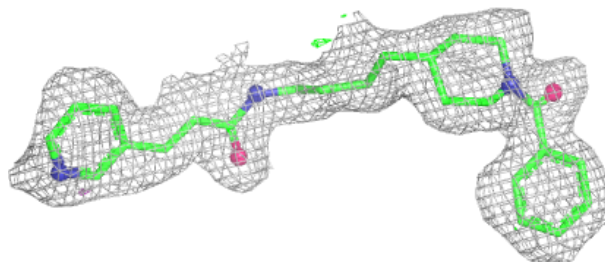
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGB A 502:

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

**Electron density around DGB B 501:**

$2mF_o-DF_c$ (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.