



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 AM UTC

PDB ID : 3B8X / pdb_00003b8x
Title : Crystal structure of GDP-4-keto-6-deoxymannose-3-dehydratase (ColD)
H188N mutant with bound GDP-perosamine
Authors : Cook, P.D.; Holden, H.M.
Deposited on : 2007-11-02
Resolution : 1.70 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

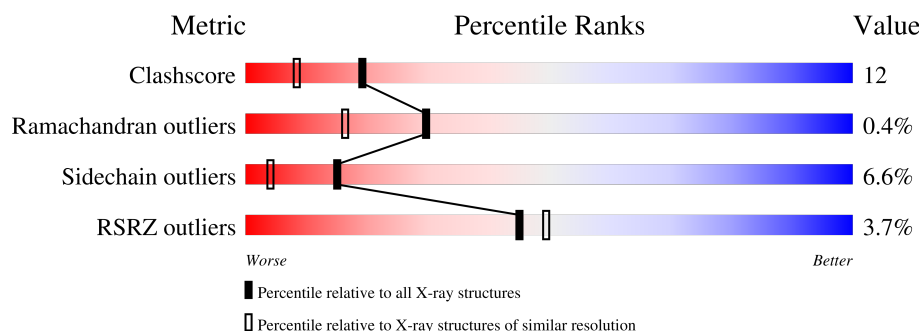
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	390	5% 75% 19% 5% .
1	B	390	3% 71% 23% 5% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7020 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 Pyridoxamine 5-phosphate-dependent dehydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	4	0
			3105	1993	506	591	15			
1	B	388	Total	C	N	O	S	0	4	0
			3124	2006	508	594	16			

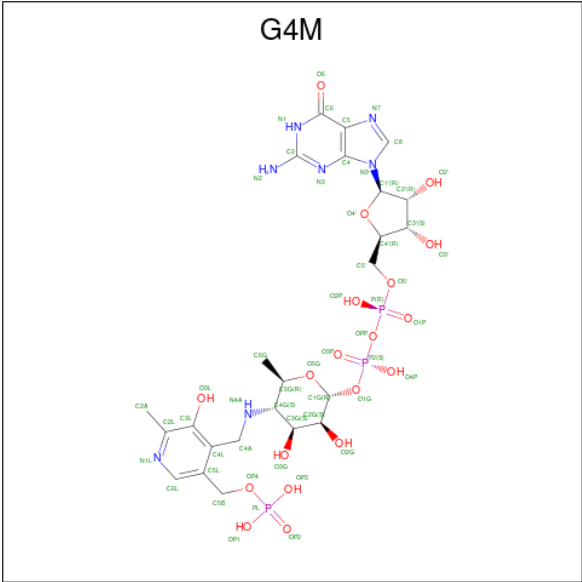
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9F118
A	0	HIS	-	expression tag	UNP Q9F118
A	188	ASN	HIS	engineered mutation	UNP Q9F118
B	-1	GLY	-	expression tag	UNP Q9F118
B	0	HIS	-	expression tag	UNP Q9F118
B	188	ASN	HIS	engineered mutation	UNP Q9F118

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

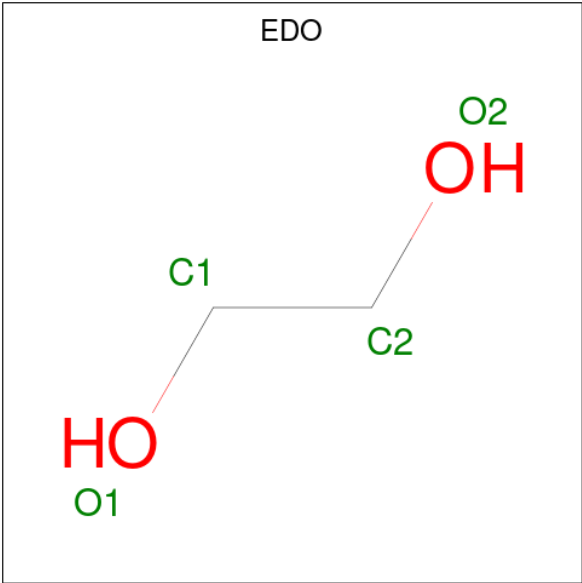
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Na	0	0
			4	4		
2	B	4	Total	Na	0	0
			4	4		

- Molecule 3 is [(2R,3S,4R,5R)-5-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)-3,4-dihydroxy tetrahydrofuran-2-yl]methyl (2R,3S,4S,5S,6R)-3,4-dihydroxy-5-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl)amino]-6-methyltetrahydro-2H-pyran-2-yl dihydrogen diphosphate (CCD ID: G4M) (formula: C₂₄H₃₆N₇O₁₉P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	24	7	19	3		
3	B	1	Total	C	N	O	P	0	0
			53	24	7	19	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

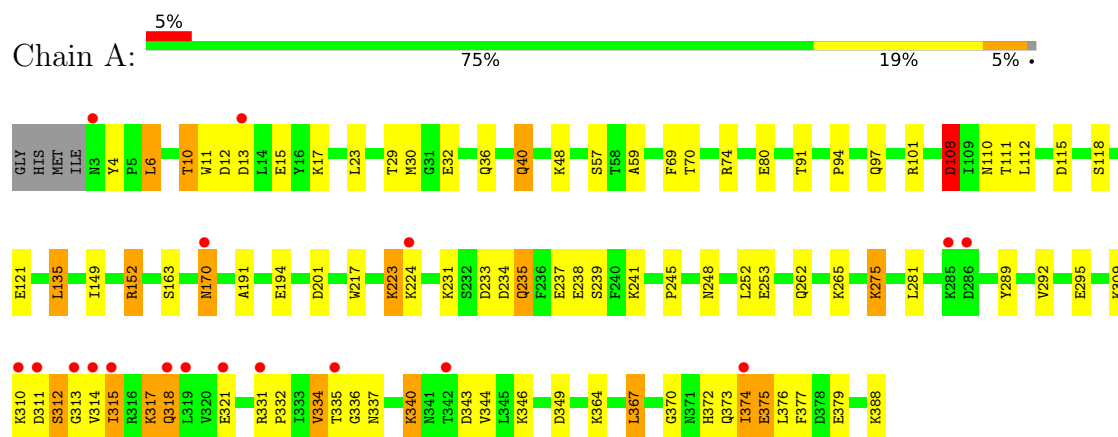
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	330	Total	O	0	0
			330	330		
5	B	335	Total	O	0	0
			335	335		

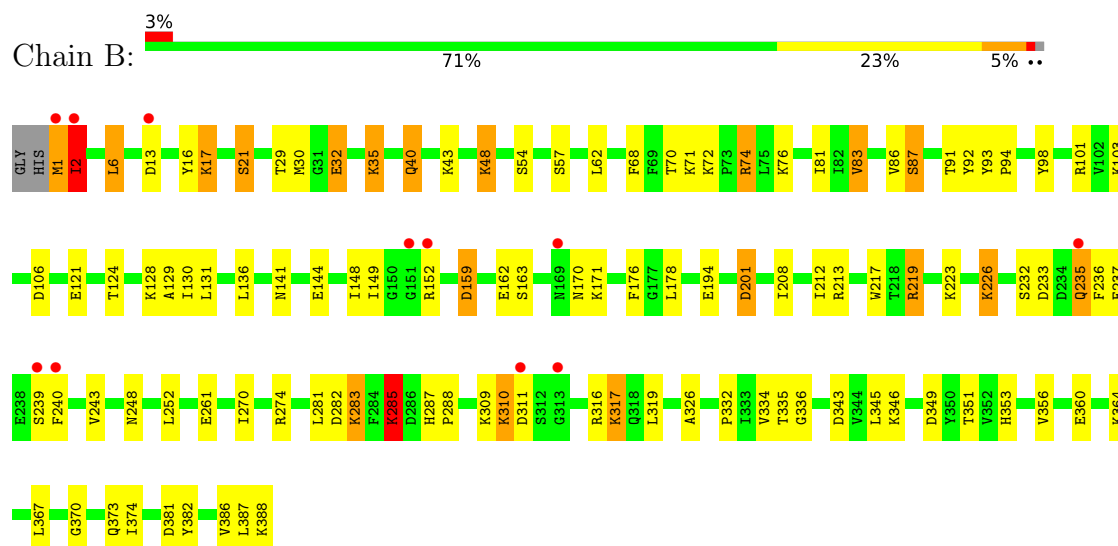
3 Residue-property plots [i](#)

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: Pyridoxamine 5-phosphate-dependent dehydrase



- Molecule 1: Pyridoxamine 5-phosphate-dependent dehydrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.41Å 98.12Å 119.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-1.70) 92.4 (30.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.82 (at 1.70Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.173 , 0.260 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 87.8	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	0.96	EDS
Total number of atoms	7020	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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: EDO, NA, G4M

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	0.83	0/3182	1.25	20/4297 (0.5%)
1	B	0.81	0/3201	1.26	23/4322 (0.5%)
All	All	0.82	0/6383	1.25	43/8619 (0.5%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	ILE	N-CA-C	11.97	123.38	108.06
1	B	243	VAL	N-CA-C	10.89	124.20	113.53
1	A	312	SER	N-CA-C	-8.48	101.79	112.90
1	B	92	TYR	N-CA-C	7.96	121.48	111.69
1	B	370	GLY	N-CA-C	7.47	123.13	112.82
1	A	91	THR	N-CA-C	-7.24	102.79	111.69
1	A	32	GLU	N-CA-C	6.95	118.50	111.07
1	B	194	GLU	N-CA-C	-6.93	98.78	109.24
1	B	285	LYS	N-CA-C	6.83	118.73	111.28
1	B	91	THR	N-CA-C	-6.72	104.04	111.36
1	B	6	LEU	N-CA-C	6.58	118.45	111.28
1	A	336	GLY	N-CA-C	-6.44	100.30	111.50
1	B	201	ASP	N-CA-C	-6.28	105.56	113.72
1	B	83	VAL	CB-CA-C	-6.19	103.21	109.89
1	A	110	ASN	N-CA-C	6.17	118.93	111.40
1	A	313	GLY	N-CA-C	-6.13	107.78	115.08
1	A	201	ASP	N-CA-C	-6.08	104.50	113.61
1	A	135	LEU	N-CA-C	6.03	119.35	109.76
1	A	370	GLY	N-CA-C	6.01	119.89	112.14
1	A	108	ASP	N-CA-C	-5.95	99.04	108.73
1	A	69	PHE	N-CA-C	5.94	121.26	113.30
1	A	194	GLU	N-CA-C	-5.86	100.40	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	GLU	N-CA-C	5.79	117.59	111.28
1	A	334	VAL	N-CA-C	5.63	121.05	109.34
1	B	72	LYS	N-CA-C	-5.59	98.63	108.69
1	B	159	ASP	N-CA-C	-5.57	97.40	107.75
1	B	336	GLY	N-CA-C	-5.57	101.67	112.02
1	A	59	ALA	N-CA-C	-5.55	105.15	111.14
1	B	261	GLU	N-CA-C	-5.54	105.33	111.36
1	B	219	ARG	N-CA-C	5.53	117.30	111.28
1	B	332	PRO	N-CA-C	-5.52	103.49	111.22
1	A	332	PRO	N-CA-C	-5.44	103.60	111.22
1	A	10	THR	N-CA-C	-5.39	105.92	112.88
1	B	381	ASP	N-CA-C	-5.39	105.40	111.28
1	B	283	LYS	N-CA-C	5.39	119.03	112.23
1	A	295	GLU	N-CA-C	5.34	117.97	109.96
1	A	163	SER	N-CA-C	5.29	117.66	110.88
1	B	163	SER	N-CA-C	5.16	117.48	110.88
1	B	178	LEU	N-CA-C	-5.15	105.66	111.28
1	B	54	SER	N-CA-C	5.11	117.59	111.71
1	B	94	PRO	N-CA-C	-5.10	107.21	113.84
1	A	349	ASP	CA-C-N	-5.03	114.32	122.36
1	A	349	ASP	C-N-CA	-5.03	114.32	122.36

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	3105	0	3083	71	0
1	B	3124	0	3108	84	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	53	0	31	4	0
3	B	53	0	31	1	0
4	A	12	0	18	3	0
5	A	330	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	335	0	0	10	0
All	All	7020	0	6271	148	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 12.

All (148) 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:6:LEU:HD11	1:A:331:ARG:HD2	1.21	1.08
1:A:331:ARG:HH21	1:B:219:ARG:HH22	1.18	0.90
1:A:6:LEU:HD11	1:A:331:ARG:CD	2.04	0.87
1:A:331:ARG:HH21	1:B:219:ARG:NH2	1.76	0.83
1:A:315:ILE:HD11	1:A:317:LYS:HB2	1.61	0.81
1:A:6:LEU:CD1	1:A:331:ARG:HD2	2.06	0.80
1:B:2:ILE:HG23	1:B:382:TYR:CD2	2.18	0.78
1:B:2:ILE:HG23	1:B:382:TYR:CE2	2.19	0.77
1:A:343:ASP:O	1:A:346:LYS:HB2	1.84	0.76
1:B:149:ILE:O	1:B:152:ARG:HG3	1.87	0.74
1:A:315:ILE:HD13	1:A:318:GLN:H	1.54	0.73
1:B:1:MET:HA	1:B:382:TYR:OH	1.89	0.71
1:A:70:THR:HG21	1:A:74:ARG:NE	2.07	0.70
1:A:331:ARG:NH2	3:A:500:G4M:O4P	2.24	0.70
1:B:87:SER:O	1:B:335:THR:HG23	1.92	0.70
1:B:360:GLU:O	1:B:364:LYS:HD2	1.93	0.69
1:A:315:ILE:HD11	1:A:317:LYS:CB	2.22	0.69
1:A:36:GLN:HG2	5:A:983:HOH:O	1.95	0.67
1:A:223:LYS:HE3	1:A:233:ASP:OD1	1.95	0.66
1:B:287:HIS:O	1:B:309:LYS:NZ	2.28	0.66
1:A:343:ASP:HB2	5:A:777:HOH:O	1.96	0.66
1:A:331:ARG:NH2	1:B:219:ARG:HH22	1.94	0.65
1:A:170:ASN:ND2	5:A:935:HOH:O	2.28	0.65
1:A:223:LYS:HE2	1:A:231:LYS:O	1.97	0.65
1:A:15:GLU:CD	1:A:265:LYS:HZ2	2.04	0.65
1:A:40:GLN:NE2	5:A:974:HOH:O	2.30	0.65
1:A:70:THR:HG21	1:A:74:ARG:HE	1.62	0.65
1:B:101:ARG:HH11	1:B:101:ARG:HG2	1.62	0.62
1:A:331:ARG:NH2	1:B:219:ARG:NH2	2.47	0.62
1:B:1:MET:C	1:B:2:ILE:HG22	2.25	0.61
1:A:289:TYR:C	1:A:309:LYS:HG3	2.25	0.61
1:B:223:LYS:HE2	1:B:233:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:NE2	5:A:876:HOH:O	2.31	0.60
1:B:40:GLN:HE22	1:B:43:LYS:HE2	1.67	0.59
1:A:367:LEU:HD22	1:A:367:LEU:C	2.28	0.59
1:A:15:GLU:OE1	1:A:265:LYS:NZ	2.36	0.58
1:B:101:ARG:HD3	1:B:349:ASP:CG	2.28	0.58
1:B:281:LEU:O	1:B:285:LYS:HB3	2.04	0.58
3:A:500:G4M:O4P	3:A:500:G4M:O1P	2.22	0.57
1:B:81:ILE:HD12	1:B:129:ALA:HB3	1.87	0.57
1:A:191:ALA:H	1:A:262:GLN:HE21	1.52	0.57
1:B:13:ASP:HB2	1:B:17:LYS:HE3	1.86	0.56
1:B:121:GLU:HB3	1:B:353:HIS:NE2	2.20	0.56
1:A:48:LYS:HE2	5:A:931:HOH:O	2.06	0.56
1:A:57:SER:HB2	1:B:248:ASN:HB3	1.88	0.55
1:A:364:LYS:NZ	5:A:998:HOH:O	2.40	0.55
1:A:252:LEU:HD12	1:B:252:LEU:HD12	1.89	0.55
1:A:248:ASN:HB3	1:B:57:SER:HB2	1.89	0.55
1:B:101:ARG:HG2	1:B:101:ARG:NH1	2.23	0.54
1:B:309:LYS:HE2	5:B:967:HOH:O	2.06	0.54
1:A:149:ILE:O	1:A:152:ARG:HG3	2.08	0.54
1:B:351:THR:HG22	5:B:710:HOH:O	2.08	0.54
1:A:23:LEU:HD22	1:B:16:TYR:CE2	2.44	0.53
1:B:101:ARG:HG3	5:B:710:HOH:O	2.09	0.53
1:B:101:ARG:HD3	1:B:349:ASP:OD1	2.10	0.52
1:B:48:LYS:HG3	1:B:201:ASP:OD1	2.10	0.52
1:A:373:GLN:NE2	1:A:374:ILE:HD12	2.25	0.51
1:B:1:MET:O	1:B:2:ILE:HG22	2.10	0.51
1:B:382:TYR:O	1:B:386:VAL:HG23	2.11	0.50
1:B:373:GLN:NE2	1:B:374:ILE:CD1	2.75	0.49
1:B:68:PHE:CZ	1:B:98:TYR:HB3	2.47	0.49
1:B:74:ARG:HD2	5:B:939:HOH:O	2.12	0.49
1:B:373:GLN:NE2	1:B:374:ILE:HD11	2.27	0.49
1:B:141:ASN:OD1	1:B:141:ASN:C	2.56	0.49
1:B:208:ILE:O	1:B:212:ILE:HG12	2.13	0.49
1:B:81:ILE:HD12	1:B:129:ALA:CB	2.43	0.48
1:A:101:ARG:HE	4:A:676:EDO:H21	1.78	0.48
1:B:17:LYS:O	1:B:21:SER:OG	2.31	0.48
1:A:245:PRO:HA	1:B:93:TYR:CD1	2.49	0.48
1:B:219:ARG:NH2	1:B:240:PHE:CE1	2.81	0.48
1:A:312:SER:OG	1:A:314:VAL:HG23	2.14	0.48
1:B:235:GLN:O	1:B:239:SER:N	2.46	0.48
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:TYR:CD2	1:A:379:GLU:HB3	2.48	0.48
1:A:235:GLN:NE2	5:A:1001:HOH:O	2.46	0.47
1:A:115:ASP:OD2	1:A:118:SER:OG	2.29	0.47
1:B:319:LEU:HD22	1:B:387:LEU:CD2	2.45	0.47
1:A:375:GLU:CG	1:A:377:PHE:CE2	2.98	0.47
1:B:121:GLU:HB3	1:B:353:HIS:HE2	1.79	0.47
1:B:171:LYS:HB3	1:B:176:PHE:CZ	2.48	0.47
1:A:372:HIS:CD2	1:A:376:LEU:HD11	2.49	0.47
1:A:13:ASP:O	1:A:17:LYS:HG3	2.15	0.47
1:A:29:THR:O	1:A:30:MET:C	2.59	0.46
1:A:101:ARG:HG2	4:A:676:EDO:H22	1.97	0.46
1:B:388:LYS:HD3	1:B:388:LYS:OXT	2.15	0.46
1:A:111:THR:O	1:A:112:LEU:HB2	2.16	0.46
1:A:317:LYS:HE3	1:A:317:LYS:HB3	1.58	0.46
1:A:10:THR:C	4:A:675:EDO:H21	2.40	0.46
1:A:315:ILE:HG23	1:A:318:GLN:HB3	1.98	0.45
1:A:234:ASP:O	1:A:237:GLU:HB3	2.16	0.45
1:B:282:ASP:O	1:B:285:LYS:HD3	2.17	0.45
1:A:40:GLN:HG2	5:A:975:HOH:O	2.16	0.45
1:B:76:LYS:HE2	5:B:941:HOH:O	2.17	0.45
1:B:316:ARG:O	1:B:317:LYS:C	2.59	0.45
1:A:281:LEU:HD23	1:A:292:VAL:HG21	1.98	0.45
1:A:281:LEU:CD2	1:A:292:VAL:HG21	2.47	0.44
1:A:289:TYR:CD1	1:A:314:VAL:HG21	2.52	0.44
1:A:337:ASN:O	1:A:340:LYS:HE2	2.16	0.44
1:B:121:GLU:HB3	1:B:353:HIS:CE1	2.52	0.44
1:B:343:ASP:N	1:B:343:ASP:OD1	2.50	0.44
1:B:162:GLU:OE2	3:B:500:G4M:O3L	2.36	0.44
1:B:326:ALA:HB1	1:B:382:TYR:CZ	2.53	0.44
1:B:32:GLU:CD	1:B:35:LYS:HZ1	2.26	0.44
1:B:144:GLU:O	1:B:148:ILE:HG13	2.18	0.43
3:A:500:G4M:H4G	5:A:817:HOH:O	2.18	0.43
1:B:32:GLU:OE2	1:B:35:LYS:HE3	2.18	0.43
1:A:29:THR:O	1:A:253:GLU:HG2	2.19	0.43
1:B:310:LYS:O	1:B:311:ASP:HB2	2.18	0.43
1:B:248:ASN:OD1	1:B:248:ASN:C	2.61	0.43
1:B:83:VAL:HG12	1:B:131:LEU:HB3	2.01	0.43
1:A:372:HIS:HD2	1:A:376:LEU:HD11	1.84	0.43
1:A:12:ASP:OD1	1:A:265:LYS:NZ	2.46	0.43
1:A:80:GLU:HA	1:A:101:ARG:O	2.19	0.42
1:A:337:ASN:O	1:A:340:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HA	1:A:97:GLN:HE21	1.83	0.42
1:B:388:LYS:HD3	5:B:832:HOH:O	2.19	0.42
1:B:71:LYS:HE2	5:B:741:HOH:O	2.18	0.42
1:B:287:HIS:CG	1:B:288:PRO:HD2	2.54	0.42
1:B:1:MET:HB3	5:B:994:HOH:O	2.19	0.42
1:B:364:LYS:HE3	5:B:896:HOH:O	2.20	0.42
1:A:238:GLU:OE2	1:A:241:LYS:NZ	2.47	0.42
1:B:48:LYS:HD2	1:B:201:ASP:HB3	2.02	0.42
1:B:70:THR:HA	1:B:208:ILE:HD11	2.02	0.42
1:A:275:LYS:HB3	1:A:275:LYS:HE2	1.58	0.42
3:A:500:G4M:H4A1	3:A:500:G4M:H3G	1.80	0.42
1:A:317:LYS:O	1:A:321:GLU:HG3	2.20	0.41
1:B:29:THR:O	1:B:30:MET:C	2.63	0.41
1:A:108:ASP:OD1	1:A:108:ASP:C	2.63	0.41
1:B:62:LEU:HD11	1:B:213:ARG:HA	2.03	0.41
1:A:310:LYS:O	1:A:311:ASP:HB2	2.20	0.41
1:B:274:ARG:HG2	1:B:274:ARG:HH11	1.86	0.41
1:B:217:TRP:NE1	1:B:219:ARG:HB2	2.36	0.41
1:B:274:ARG:HG2	1:B:274:ARG:NH1	2.36	0.41
1:B:128:LYS:HA	1:B:128:LYS:HD3	1.91	0.41
1:B:159:ASP:C	1:B:159:ASP:OD1	2.64	0.41
1:B:235:GLN:O	1:B:236:PHE:C	2.61	0.41
1:A:11:TRP:CD1	1:A:15:GLU:HG2	2.56	0.41
1:B:346:LYS:HE2	5:B:785:HOH:O	2.19	0.41
1:A:4:TYR:C	1:A:4:TYR:CD1	2.99	0.41
1:A:315:ILE:CD1	1:A:317:LYS:CB	2.98	0.40
1:B:226:LYS:N	1:B:226:LYS:CD	2.84	0.40
1:B:106:ASP:CG	1:B:356:VAL:HA	2.47	0.40
1:B:70:THR:HG21	1:B:74:ARG:HH11	1.86	0.40
1:B:86:VAL:O	1:B:87:SER:HB3	2.21	0.40
1:B:103:LYS:HG3	1:B:351:THR:CG2	2.52	0.40
1:A:245:PRO:HA	1:B:93:TYR:CE1	2.56	0.40
1:B:2:ILE:HG23	1:B:382:TYR:CG	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	388/390 (100%)	368 (95%)	19 (5%)	1 (0%)	36	22
1	B	390/390 (100%)	371 (95%)	17 (4%)	2 (0%)	24	12
All	All	778/780 (100%)	739 (95%)	36 (5%)	3 (0%)	30	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	SER
1	A	334	VAL
1	B	334	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	346/345 (100%)	324 (94%)	22 (6%)	16	4
1	B	348/345 (101%)	325 (93%)	23 (7%)	15	4
All	All	694/690 (101%)	649 (94%)	45 (6%)	15	4

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	40	GLN
1	A	108	ASP

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Mol	Chain	Res	Type
1	A	121	GLU
1	A	135	LEU
1	A	152	ARG
1	A	170	ASN
1	A	217	TRP
1	A	223	LYS
1	A	224	LYS
1	A	235	GLN
1	A	239	SER
1	A	275	LYS
1	A	315	ILE
1	A	317	LYS
1	A	318	GLN
1	A	340	LYS
1	A	344	VAL
1	A	367	LEU
1	A	374	ILE
1	A	375	GLU
1	A	388	LYS
1	B	1	MET
1	B	2	ILE
1	B	6	LEU
1	B	17	LYS
1	B	21	SER
1	B	35	LYS
1	B	40	GLN
1	B	48	LYS
1	B	74	ARG
1	B	124	THR
1	B	130	ILE
1	B	136	LEU
1	B	170	ASN
1	B	226	LYS
1	B	232	SER
1	B	235	GLN
1	B	237	GLU
1	B	270	ILE
1	B	283	LYS
1	B	285	LYS
1	B	310	LYS
1	B	317	LYS
1	B	367	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	97	GLN
1	A	140	ASN
1	A	220	ASN
1	A	262	GLN
1	A	294	GLN
1	A	322	ASN
1	A	365	ASN
1	B	36	GLN
1	B	40	GLN
1	B	220	ASN
1	B	322	ASN
1	B	324	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](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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
4	EDO	A	676	-	3,3,3	0.43	0	2,2,2	0.18	0
3	G4M	A	500	-	56,57,57	1.85	9 (16%)	82,88,88	1.63	15 (18%)
4	EDO	A	674	-	3,3,3	0.37	0	2,2,2	0.39	0
4	EDO	A	675	-	3,3,3	0.38	0	2,2,2	0.06	0
3	G4M	B	500	-	56,57,57	1.79	9 (16%)	82,88,88	1.86	19 (23%)

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
4	EDO	A	676	-	-	0/1/1/1	-
3	G4M	A	500	-	-	4/32/68/68	0/5/5/5
4	EDO	A	674	-	-	1/1/1/1	-
4	EDO	A	675	-	-	0/1/1/1	-
3	G4M	B	500	-	-	4/32/68/68	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	G4M	C4A-C4L	-7.69	1.40	1.52
3	B	500	G4M	C4A-C4L	-7.68	1.40	1.52
3	B	500	G4M	C4A-N4A	-5.59	1.30	1.46
3	A	500	G4M	C4G-N4A	-4.99	1.39	1.47
3	A	500	G4M	C4A-N4A	-4.62	1.33	1.46
3	B	500	G4M	PL-OP2	3.44	1.61	1.50
3	A	500	G4M	PL-OP2	3.37	1.60	1.50
3	B	500	G4M	P-O1P	3.28	1.62	1.50
3	B	500	G4M	P2-O3P	3.26	1.62	1.50
3	A	500	G4M	P-O1P	3.16	1.61	1.50
3	A	500	G4M	P2-O3P	3.12	1.61	1.50
3	B	500	G4M	C4G-N4A	-2.99	1.42	1.47
3	A	500	G4M	P-OPP	2.89	1.62	1.59
3	A	500	G4M	P2-OPP	2.54	1.62	1.59
3	B	500	G4M	C3L-C4L	2.43	1.43	1.40
3	B	500	G4M	PL-OP1	2.14	1.62	1.54
3	A	500	G4M	C6-N1	-2.07	1.35	1.38
3	B	500	G4M	P2-OPP	2.06	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	G4M	O5G-C1G-O1G	-6.09	103.40	111.36
3	B	500	G4M	C5-C4-N3	-5.38	119.83	128.39
3	A	500	G4M	C2-N3-C4	5.12	121.12	112.30
3	A	500	G4M	C5-C4-N3	-5.10	120.27	128.39
3	A	500	G4M	P2-O1G-C1G	-4.74	101.89	121.21
3	B	500	G4M	C2-N3-C4	4.68	120.37	112.30
3	A	500	G4M	N9-C4-N3	3.97	133.90	125.95
3	B	500	G4M	C8-N7-C5	3.92	111.24	104.26
3	B	500	G4M	O5G-C5G-C4G	-3.90	101.72	110.52
3	B	500	G4M	N9-C4-N3	3.78	133.51	125.95
3	B	500	G4M	C4-C5-N7	-3.52	105.10	110.67
3	A	500	G4M	C4A-N4A-C4G	3.50	120.73	114.07
3	B	500	G4M	O4P-P2-OPP	3.45	116.61	107.27
3	B	500	G4M	C6-C5-N7	3.08	135.90	130.29
3	A	500	G4M	C8-N7-C5	3.02	109.64	104.26
3	B	500	G4M	N9-C8-N7	-2.93	107.97	113.40
3	B	500	G4M	OPP-P-O1P	2.91	119.46	110.70
3	B	500	G4M	O2P-P-OPP	-2.87	99.51	107.27
3	A	500	G4M	C1G-O5G-C5G	-2.85	108.77	113.63
3	A	500	G4M	O5G-C1G-O1G	-2.83	107.67	111.36
3	A	500	G4M	N9-C8-N7	-2.82	108.17	113.40
3	A	500	G4M	C6-C5-N7	2.59	135.01	130.29
3	A	500	G4M	C6G-C5G-C4G	-2.59	108.83	113.57
3	A	500	G4M	C2-N1-C6	-2.57	120.46	125.11
3	B	500	G4M	C4A-N4A-C4G	2.55	118.92	114.07
3	B	500	G4M	C5L-C6L-N1L	-2.53	119.71	123.83
3	B	500	G4M	C2-N1-C6	-2.46	120.64	125.11
3	B	500	G4M	C6L-C5L-C4L	2.46	119.92	118.06
3	B	500	G4M	C6L-N1L-C2L	2.35	123.46	119.20
3	A	500	G4M	C4-C5-N7	-2.29	107.04	110.67
3	A	500	G4M	O4P-P2-OPP	2.18	113.17	107.27
3	B	500	G4M	C2A-C2L-C3L	-2.18	118.24	120.80
3	A	500	G4M	C5-C6-N1	2.03	118.43	113.25
3	B	500	G4M	O3L-C3L-C4L	2.01	124.00	118.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	G4M	N4A-C4A-C4L-C5L
3	A	500	G4M	C3G-C4G-N4A-C4A
3	B	500	G4M	N4A-C4A-C4L-C5L
3	B	500	G4M	C3G-C4G-N4A-C4A

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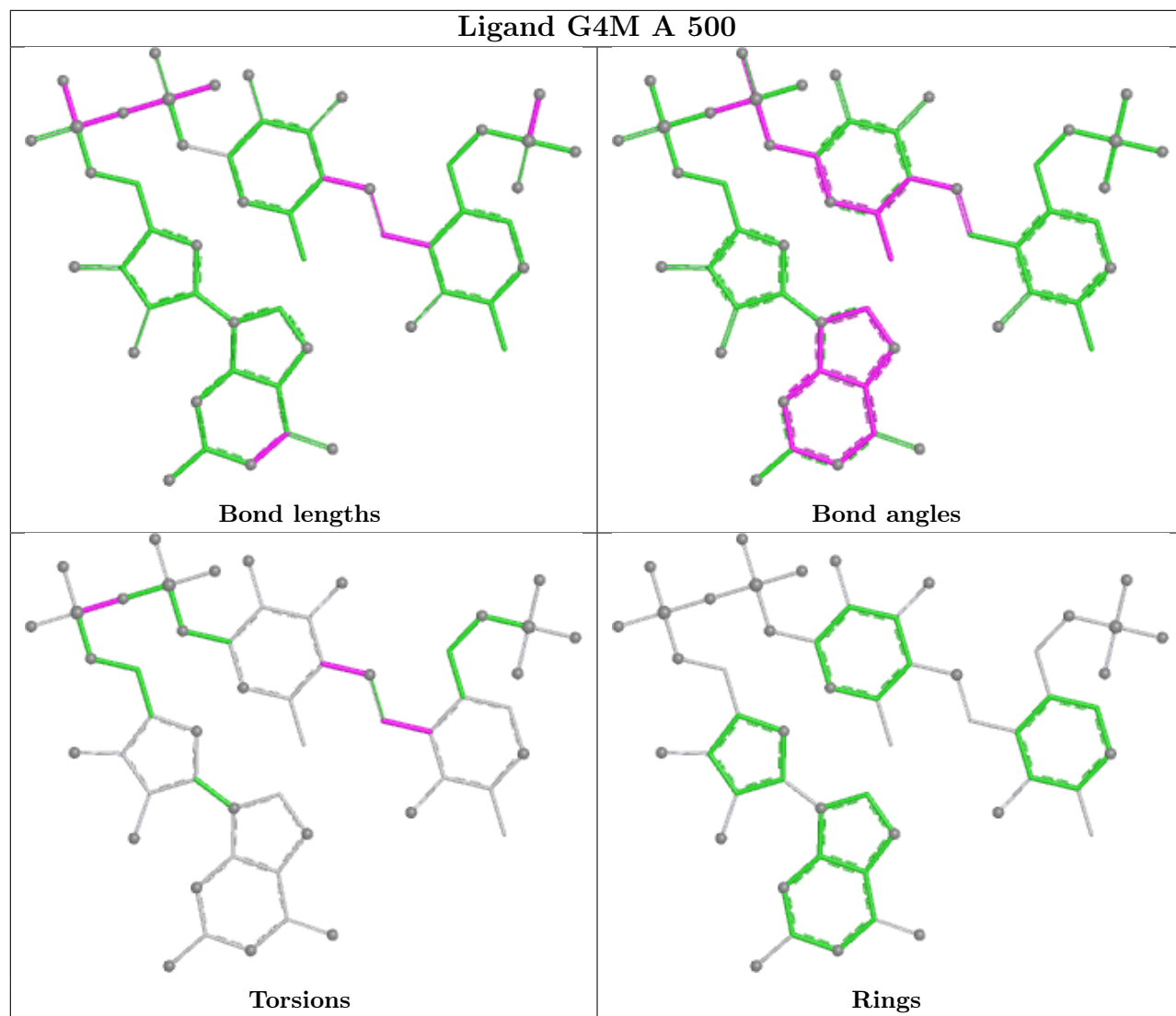
Mol	Chain	Res	Type	Atoms
3	A	500	G4M	N4A-C4A-C4L-C3L
3	B	500	G4M	N4A-C4A-C4L-C3L
3	B	500	G4M	O4'-C4'-C5'-O5'
4	A	674	EDO	O1-C1-C2-O2
3	A	500	G4M	P2-OPP-P-O2P

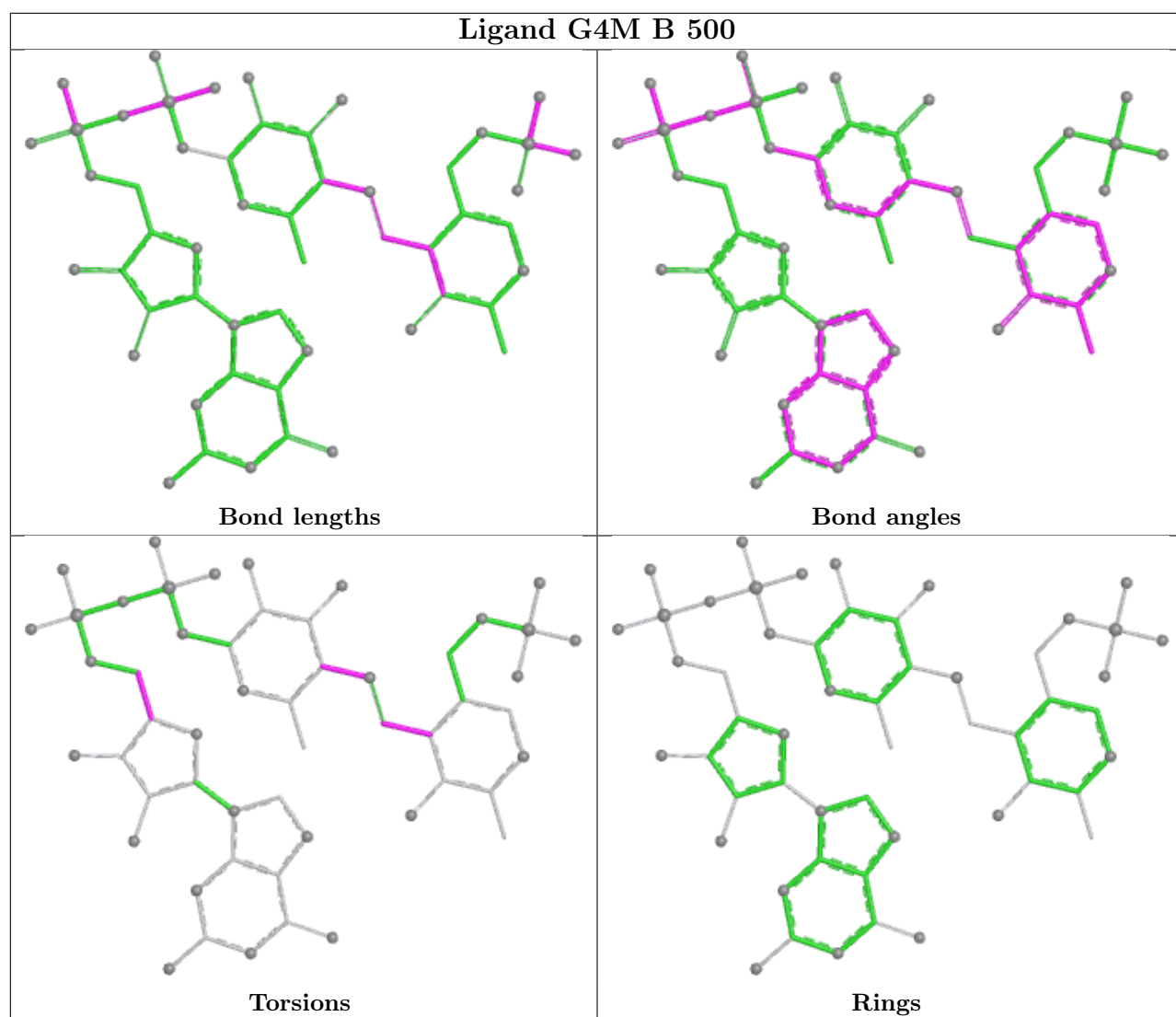
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	676	EDO	2	0
3	A	500	G4M	4	0
4	A	675	EDO	1	0
3	B	500	G4M	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	386/390 (98%)	-0.16	18 (4%)	36 40	4, 14, 46, 80	4 (1%)
1	B	388/390 (99%)	-0.07	11 (2%)	55 59	5, 16, 55, 81	4 (1%)
All	All	774/780 (99%)	-0.12	29 (3%)	45 49	4, 15, 51, 81	8 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	GLY	4.0
1	B	240	PHE	3.9
1	A	3	ASN	3.8
1	A	319	LEU	3.5
1	B	239	SER	3.2
1	A	342	THR	3.1
1	B	2	ILE	3.0
1	A	315	ILE	3.0
1	A	285	LYS	3.0
1	B	151	GLY	2.9
1	A	170	ASN	2.8
1	A	321	GLU	2.7
1	A	331	ARG	2.6
1	A	314	VAL	2.6
1	A	318	GLN	2.5
1	B	152	ARG	2.5
1	B	169	ASN	2.4
1	A	286	ASP	2.4
1	A	224	LYS	2.4
1	A	13	ASP	2.4
1	A	335	THR	2.3
1	A	310	LYS	2.3
1	B	1	MET	2.2
1	A	374	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	313	GLY	2.1
1	B	235	GLN	2.1
1	B	311	ASP	2.1
1	B	13	ASP	2.0
1	A	311	ASP	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](#)

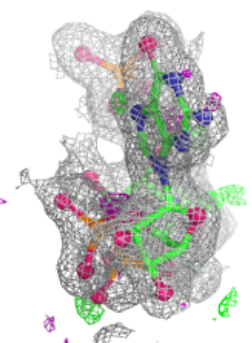
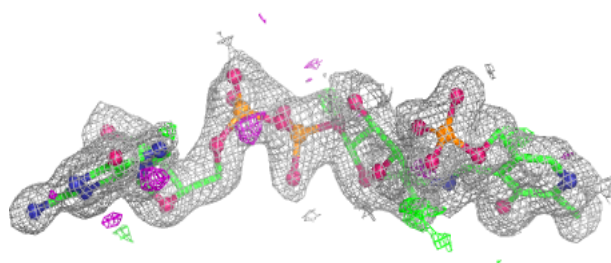
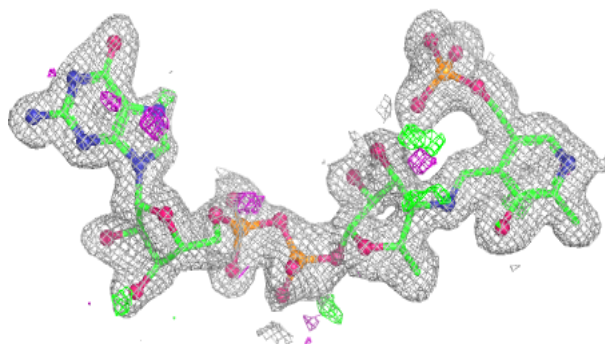
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	674	4/4	0.67	0.18	29,32,57,61	0
4	EDO	A	676	4/4	0.76	0.18	26,27,47,99	0
2	NA	B	667	1/1	0.79	0.12	43,43,43,43	0
4	EDO	A	675	4/4	0.85	0.17	31,53,60,72	0
2	NA	A	672	1/1	0.92	0.16	42,42,42,42	0
2	NA	A	673	1/1	0.94	0.17	50,50,50,50	0
2	NA	A	669	1/1	0.95	0.08	27,27,27,27	0
2	NA	A	671	1/1	0.95	0.10	32,32,32,32	0
3	G4M	A	500	53/53	0.97	0.09	4,25,94,99	0
2	NA	B	666	1/1	0.97	0.06	17,17,17,17	0
3	G4M	B	500	53/53	0.98	0.06	3,14,31,99	0
2	NA	B	670	1/1	0.98	0.05	27,27,27,27	0
2	NA	B	668	1/1	0.99	0.05	14,14,14,14	0

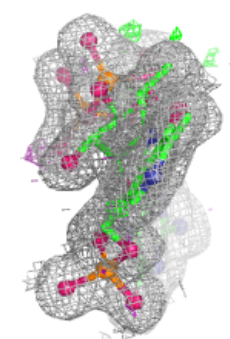
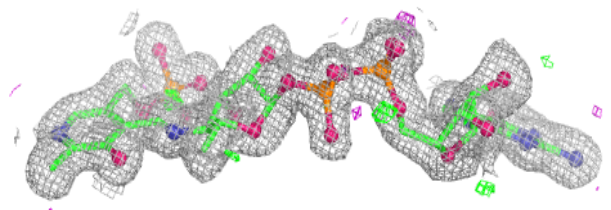
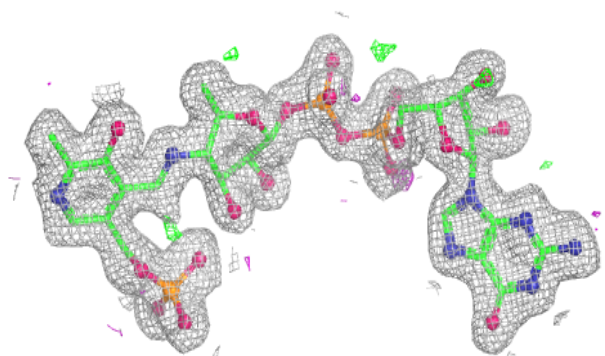
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G4M A 500:

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

**Electron density around G4M B 500:**

$2mF_o-DF_c$ (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.