



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:18 AM UTC

PDB ID : 6BW5 / pdb_00006bw5
Title : Human GPT (DPAGT1) in complex with tunicamycin
Authors : Yoo, J.; Kuk, A.C.Y.; Mashalidis, E.H.; Lee, S.-Y.
Deposited on : 2017-12-14
Resolution : 3.10 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

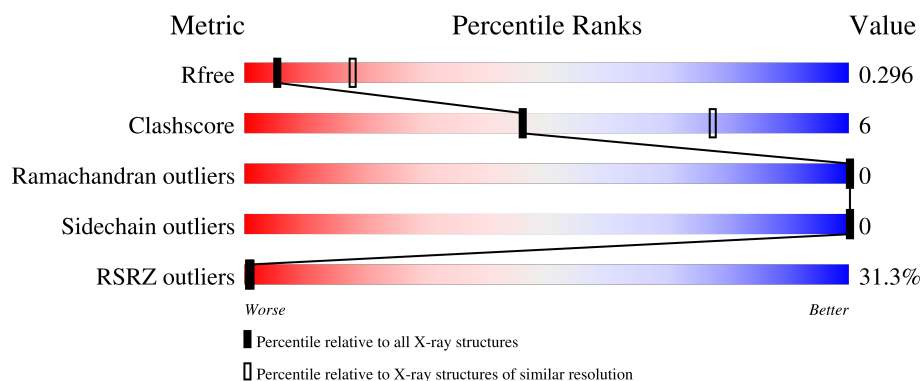
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	417	24% 79% 12% 9%
1	B	417	29% 79% 10% 12%
1	C	417	28% 76% 14% 10%
1	D	417	30% 75% 12% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22942 atoms, of which 11412 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 UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminephosphotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	378	Total	C	H	N	O	S	0	0	0
			5749	1921	2874	454	480	20			
1	B	369	Total	C	H	N	O	S	0	0	0
			5367	1822	2636	429	463	17			
1	C	375	Total	C	H	N	O	S	0	0	0
			5662	1899	2820	449	475	19			
1	D	362	Total	C	H	N	O	S	0	0	0
			5390	1825	2668	417	461	19			

There are 36 discrepancies between the modelled and reference sequences:

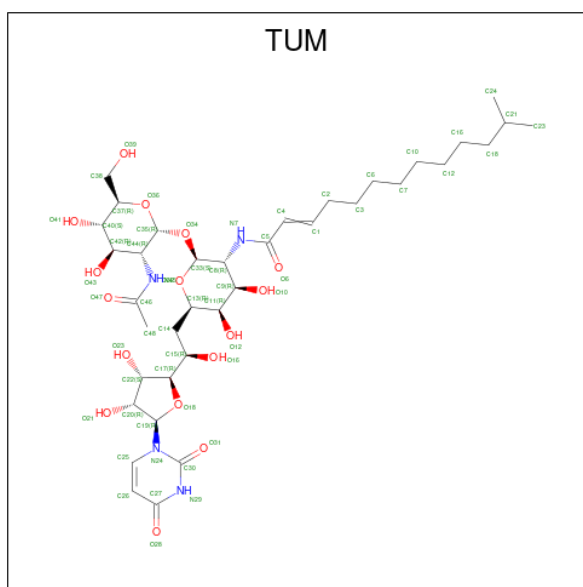
Chain	Residue	Modelled	Actual	Comment	Reference
A	409	THR	-	expression tag	UNP Q9H3H5
A	410	ASN	-	expression tag	UNP Q9H3H5
A	411	SER	-	expression tag	UNP Q9H3H5
A	412	LEU	-	expression tag	UNP Q9H3H5
A	413	GLU	-	expression tag	UNP Q9H3H5
A	414	VAL	-	expression tag	UNP Q9H3H5
A	415	LEU	-	expression tag	UNP Q9H3H5
A	416	PHE	-	expression tag	UNP Q9H3H5
A	417	GLN	-	expression tag	UNP Q9H3H5
B	409	THR	-	expression tag	UNP Q9H3H5
B	410	ASN	-	expression tag	UNP Q9H3H5
B	411	SER	-	expression tag	UNP Q9H3H5
B	412	LEU	-	expression tag	UNP Q9H3H5
B	413	GLU	-	expression tag	UNP Q9H3H5
B	414	VAL	-	expression tag	UNP Q9H3H5
B	415	LEU	-	expression tag	UNP Q9H3H5
B	416	PHE	-	expression tag	UNP Q9H3H5
B	417	GLN	-	expression tag	UNP Q9H3H5
C	409	THR	-	expression tag	UNP Q9H3H5
C	410	ASN	-	expression tag	UNP Q9H3H5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	411	SER	-	expression tag	UNP Q9H3H5
C	412	LEU	-	expression tag	UNP Q9H3H5
C	413	GLU	-	expression tag	UNP Q9H3H5
C	414	VAL	-	expression tag	UNP Q9H3H5
C	415	LEU	-	expression tag	UNP Q9H3H5
C	416	PHE	-	expression tag	UNP Q9H3H5
C	417	GLN	-	expression tag	UNP Q9H3H5
D	409	THR	-	expression tag	UNP Q9H3H5
D	410	ASN	-	expression tag	UNP Q9H3H5
D	411	SER	-	expression tag	UNP Q9H3H5
D	412	LEU	-	expression tag	UNP Q9H3H5
D	413	GLU	-	expression tag	UNP Q9H3H5
D	414	VAL	-	expression tag	UNP Q9H3H5
D	415	LEU	-	expression tag	UNP Q9H3H5
D	416	PHE	-	expression tag	UNP Q9H3H5
D	417	GLN	-	expression tag	UNP Q9H3H5

- Molecule 2 is Tunicamycin (CCD ID: TUM) (formula: $C_{37}H_{60}N_4O_{16}$) (labeled as "Ligand of Interest" by depositor).



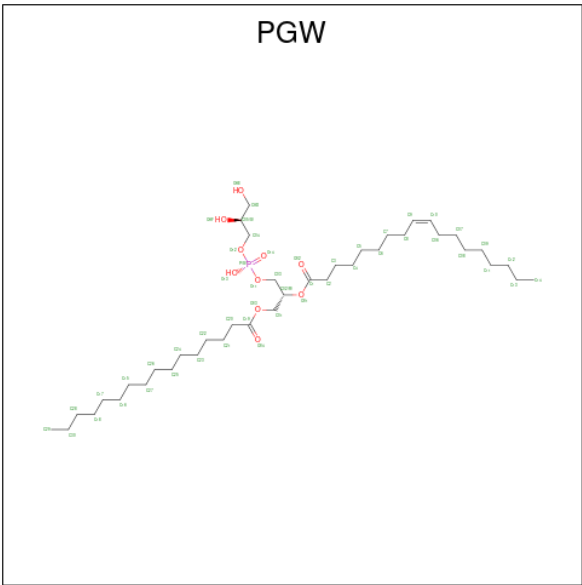
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			117	37	60	4	16		
2	B	1	Total	C	H	N	O	0	0
			117	37	60	4	16		
2	C	1	Total	C	H	N	O	0	0
			117	37	60	4	16		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	0	0
			117	37	60	4	16		

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).

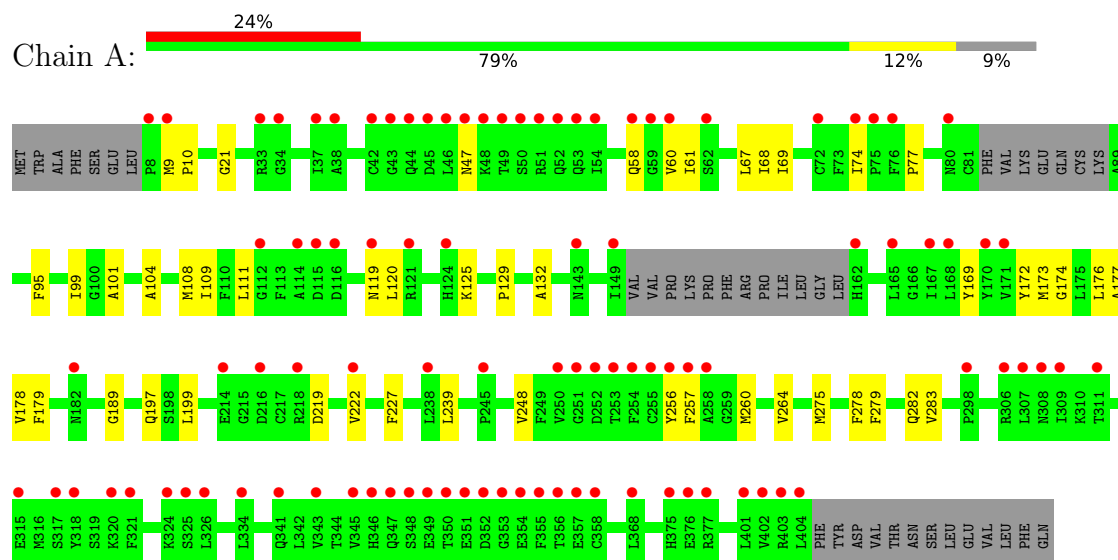


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			69	22	39	7	1		
3	B	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	C	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	D	1	Total	C	H	O	P	0	0
			79	24	45	9	1		

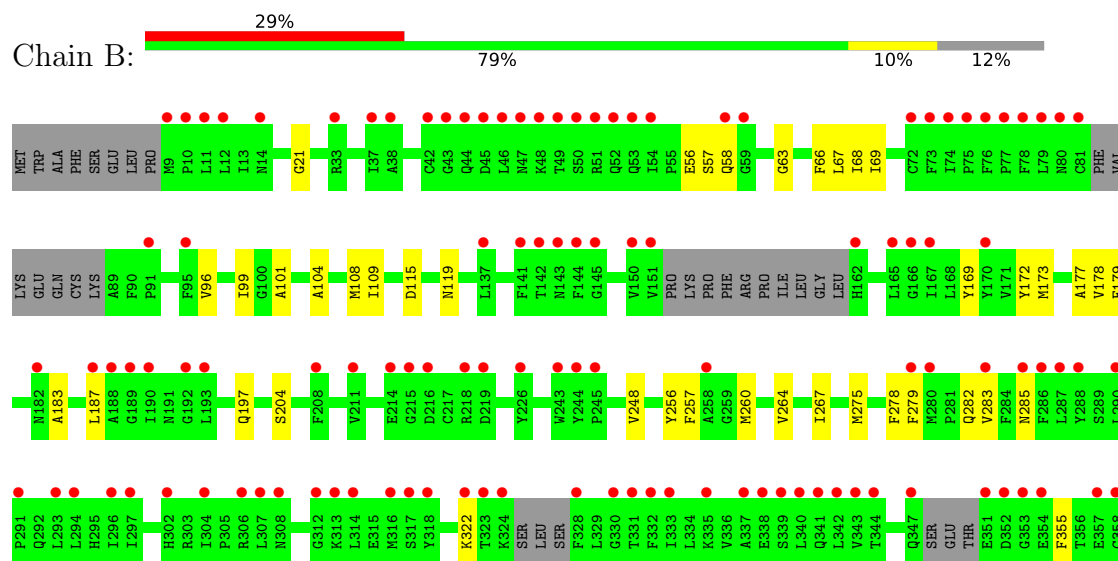
3 Residue-property plots [i](#)

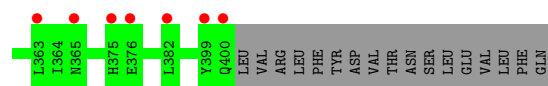
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase

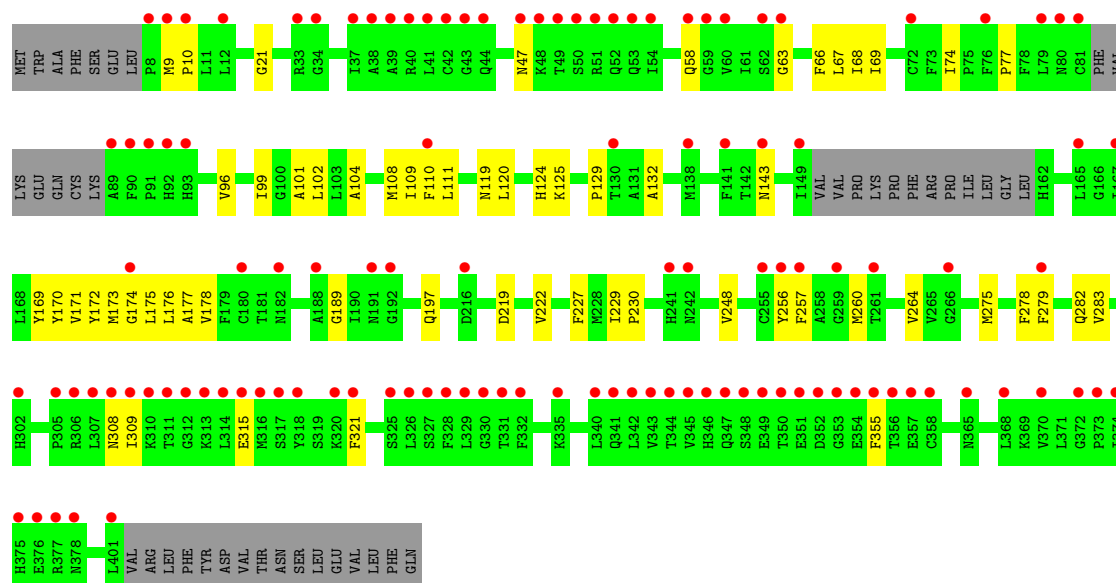
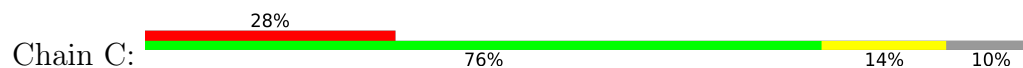


- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase

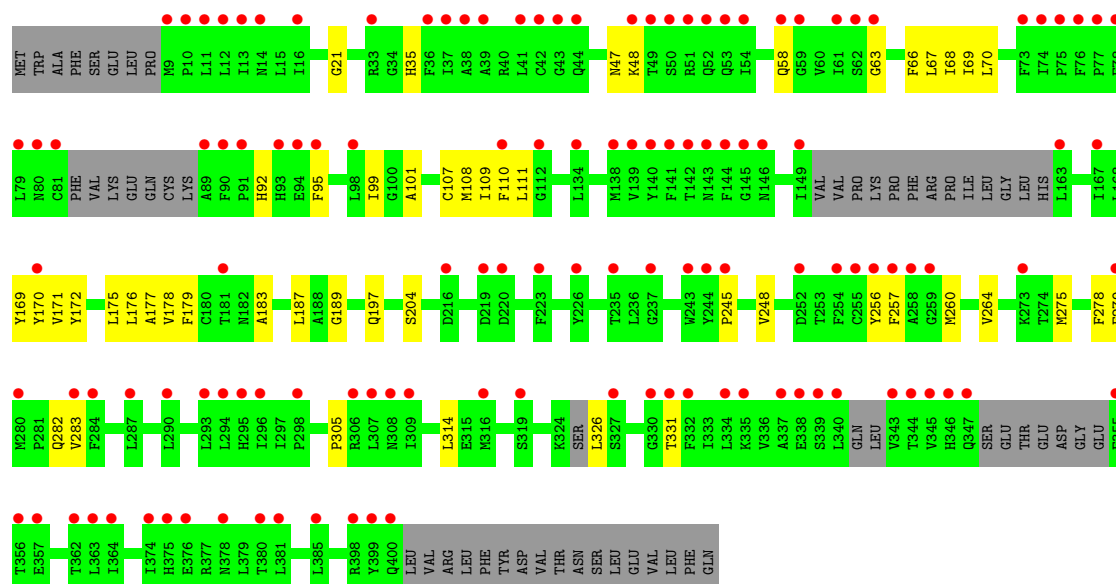
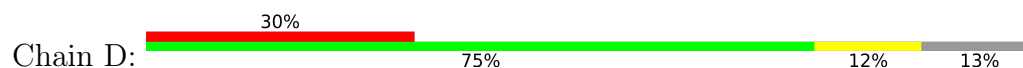




- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase



- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.27Å 105.51Å 149.39Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	83.05 – 3.10 83.05 – 3.10	Depositor EDS
% Data completeness (in resolution range)	60.1 (83.05-3.10) 56.2 (83.05-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.256 , 0.288 0.264 , 0.296	Depositor DCC
R_{free} test set	1763 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	22942	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGW, TUM

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	0.16	0/2949	0.36	0/4025
1	B	0.16	0/2799	0.35	0/3830
1	C	0.18	0/2916	0.36	0/3982
1	D	0.16	0/2791	0.34	0/3814
All	All	0.17	0/11455	0.36	0/15651

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2875	2874	2873	33	0
1	B	2731	2636	2633	27	0
1	C	2842	2820	2820	43	0
1	D	2722	2668	2666	33	0
2	A	57	60	0	1	0
2	B	57	60	0	2	0
2	C	57	60	0	1	0
2	D	57	60	0	0	0
3	A	30	39	38	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	45	45	0	0
3	C	34	45	45	5	0
3	D	34	45	45	2	0
All	All	11530	11412	11165	131	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 6.

All (131) 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:197:GLN:OE1	1:B:282:GLN:NE2	2.23	0.71
1:A:119:ASN:OD1	2:A:501:TUM:O10	2.12	0.67
1:D:197:GLN:OE1	1:D:282:GLN:NE2	2.27	0.65
1:C:108:MET:HG2	1:C:260:MET:HB2	1.78	0.65
1:A:108:MET:HG2	1:A:260:MET:HB2	1.79	0.64
1:D:47:ASN:ND2	1:D:189:GLY:O	2.31	0.64
1:B:108:MET:HG3	1:B:256:TYR:HB3	1.80	0.64
1:B:108:MET:HG2	1:B:260:MET:HB2	1.82	0.62
1:A:108:MET:HG3	1:A:256:TYR:HB3	1.82	0.61
1:C:74:ILE:HD11	1:C:102:LEU:HD12	1.83	0.61
1:C:108:MET:HG3	1:C:256:TYR:HB3	1.83	0.59
1:A:47:ASN:ND2	1:A:189:GLY:O	2.35	0.58
1:C:101:ALA:HB1	1:C:264:VAL:HG11	1.85	0.58
1:C:197:GLN:OE1	1:C:282:GLN:NE2	2.31	0.57
1:D:108:MET:HG3	1:D:256:TYR:HB3	1.87	0.57
1:D:58:GLN:HG3	1:D:248:VAL:HB	1.87	0.56
1:A:58:GLN:HG3	1:A:248:VAL:HB	1.86	0.56
1:D:107:CYS:SG	3:D:502:PGW:H12	2.45	0.56
1:A:101:ALA:HB1	1:A:264:VAL:HG11	1.90	0.54
1:A:104:ALA:HB1	1:A:260:MET:HE2	1.89	0.54
1:C:58:GLN:HG3	1:C:248:VAL:HB	1.91	0.53
1:C:47:ASN:ND2	1:C:189:GLY:O	2.40	0.52
1:B:179:PHE:O	1:B:183:ALA:N	2.38	0.52
1:D:108:MET:HG2	1:D:260:MET:HB2	1.93	0.51
1:A:197:GLN:OE1	1:A:282:GLN:NE2	2.39	0.50
1:C:109:ILE:HG12	1:C:257:PHE:HB2	1.92	0.50
1:A:120:LEU:O	1:A:125:LYS:NZ	2.42	0.50
1:B:58:GLN:HG3	1:B:248:VAL:HB	1.93	0.49
1:D:101:ALA:HB1	1:D:264:VAL:HG11	1.94	0.49
1:C:124:HIS:CE1	3:C:502:PGW:H03	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLY:HA3	1:C:69:ILE:HD11	1.95	0.48
1:B:101:ALA:HB1	1:B:264:VAL:HG11	1.95	0.48
1:C:74:ILE:HD11	1:C:102:LEU:CD1	2.44	0.47
1:A:109:ILE:HG12	1:A:257:PHE:HB2	1.95	0.47
1:C:110:PHE:HB2	1:D:110:PHE:HB2	1.96	0.47
1:B:187:LEU:HD23	1:B:197:GLN:OE1	2.13	0.47
1:C:229:ILE:HB	1:C:230:PRO:HD3	1.96	0.47
1:A:108:MET:HE1	1:A:132:ALA:HB3	1.97	0.47
1:B:21:GLY:HA3	1:B:69:ILE:HD11	1.97	0.47
3:C:502:PGW:OAF	1:D:35:HIS:NE2	2.48	0.46
1:C:108:MET:HE1	1:C:132:ALA:HB3	1.98	0.46
1:C:67:LEU:O	1:C:68:ILE:C	2.59	0.46
1:A:108:MET:HE3	1:A:260:MET:SD	2.56	0.46
1:B:119:ASN:OD1	2:B:501:TUM:O10	2.33	0.46
1:B:322:LYS:HA	1:B:355:PHE:CD1	2.51	0.46
1:A:111:LEU:HA	3:A:502:PGW:H08A	1.98	0.45
1:A:178:VAL:O	1:A:179:PHE:C	2.60	0.45
1:C:308:ASN:ND2	1:C:315:GLU:OE2	2.49	0.45
1:D:109:ILE:HG12	1:D:257:PHE:HB2	1.98	0.45
1:B:204:SER:HB3	1:B:278:PHE:CE1	2.51	0.45
1:C:124:HIS:NE2	3:C:502:PGW:H05	2.32	0.45
1:D:111:LEU:HA	3:D:502:PGW:H08A	1.97	0.45
1:C:74:ILE:O	1:C:77:PRO:HD2	2.16	0.45
1:D:204:SER:HB3	1:D:278:PHE:CE1	2.50	0.45
1:B:177:ALA:O	1:B:178:VAL:C	2.61	0.45
1:C:99:ILE:HG22	1:D:99:ILE:HG22	1.98	0.45
1:D:177:ALA:O	1:D:178:VAL:C	2.60	0.45
1:C:176:LEU:O	1:C:177:ALA:C	2.60	0.44
1:A:111:LEU:HB2	3:A:502:PGW:H08A	1.99	0.44
1:A:177:ALA:O	1:A:178:VAL:C	2.61	0.44
1:C:111:LEU:HA	3:C:502:PGW:H08A	2.00	0.44
1:D:67:LEU:O	1:D:68:ILE:C	2.61	0.44
1:A:101:ALA:HB3	1:A:227:PHE:CZ	2.53	0.44
1:D:279:PHE:O	1:D:283:VAL:HG23	2.18	0.43
1:B:104:ALA:HB1	1:B:260:MET:HE2	2.00	0.43
1:B:109:ILE:HG12	1:B:257:PHE:HB2	2.00	0.43
1:A:99:ILE:HG22	1:B:99:ILE:HG22	1.99	0.43
1:B:275:MET:HA	1:B:278:PHE:HD2	1.83	0.43
1:D:169:TYR:O	1:D:172:TYR:HB3	2.18	0.43
1:A:21:GLY:HA3	1:A:69:ILE:HD11	2.01	0.43
1:B:173:MET:SD	1:B:267:ILE:HG23	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PHE:O	1:B:283:VAL:HG23	2.17	0.43
1:C:101:ALA:HB3	1:C:227:PHE:CZ	2.54	0.43
1:B:63:GLY:O	1:B:66:PHE:HB3	2.19	0.43
1:B:115:ASP:O	1:B:119:ASN:N	2.43	0.43
1:D:21:GLY:HA3	1:D:69:ILE:HD11	2.01	0.43
1:D:275:MET:O	1:D:278:PHE:N	2.52	0.43
1:A:169:TYR:O	1:A:172:TYR:HB3	2.19	0.43
1:B:67:LEU:O	1:B:68:ILE:C	2.61	0.43
1:C:143:ASN:OD1	1:D:92:HIS:NE2	2.52	0.43
1:C:275:MET:HA	1:C:278:PHE:HD2	1.83	0.43
1:B:187:LEU:HB2	1:B:285:ASN:HD22	1.84	0.42
1:C:119:ASN:OD1	2:C:501:TUM:O10	2.37	0.42
1:A:199:LEU:HD12	1:A:239:LEU:HD22	2.01	0.42
1:C:104:ALA:HB1	1:C:260:MET:HE2	2.01	0.42
1:A:108:MET:HE1	1:A:129:PRO:HA	2.01	0.42
1:C:309:ILE:N	1:C:309:ILE:HD12	2.34	0.42
1:C:321:PHE:O	1:C:355:PHE:HB2	2.19	0.42
1:A:279:PHE:O	1:A:283:VAL:HG23	2.19	0.42
1:C:96:VAL:HG21	1:D:95:PHE:CD2	2.54	0.42
1:C:169:TYR:O	1:C:172:TYR:HB3	2.20	0.42
1:C:175:LEU:O	1:C:176:LEU:C	2.62	0.42
1:D:63:GLY:O	1:D:66:PHE:HB3	2.19	0.42
1:C:177:ALA:O	1:C:178:VAL:C	2.62	0.42
1:A:219:ASP:O	1:A:222:VAL:HG12	2.20	0.41
1:C:63:GLY:O	1:C:66:PHE:HB3	2.20	0.41
1:B:56:GLU:HG3	1:B:57:SER:N	2.35	0.41
1:C:129:PRO:HB2	1:C:178:VAL:HG22	2.02	0.41
1:D:176:LEU:O	1:D:177:ALA:C	2.61	0.41
1:A:95:PHE:CD2	1:B:96:VAL:HG21	2.55	0.41
1:D:275:MET:HA	1:D:278:PHE:HD2	1.85	0.41
1:A:67:LEU:O	1:A:68:ILE:C	2.63	0.41
1:C:120:LEU:O	1:C:125:LYS:NZ	2.51	0.41
1:C:219:ASP:O	1:C:222:VAL:HG12	2.20	0.41
1:D:66:PHE:CZ	1:D:70:LEU:HD11	2.56	0.41
1:A:60:VAL:HG13	1:A:61:ILE:N	2.35	0.41
1:A:74:ILE:O	1:A:77:PRO:HD2	2.20	0.41
1:B:275:MET:O	1:B:278:PHE:N	2.53	0.41
1:D:179:PHE:O	1:D:183:ALA:N	2.41	0.41
1:A:173:MET:O	1:A:174:GLY:C	2.64	0.41
1:A:275:MET:HA	1:A:278:PHE:HD2	1.85	0.41
1:B:169:TYR:O	1:B:172:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:PRO:HB2	1:D:314:LEU:HB3	2.03	0.41
1:A:176:LEU:O	1:A:177:ALA:C	2.63	0.41
2:B:501:TUM:O41	2:B:501:TUM:O39	2.38	0.41
1:C:104:ALA:HB1	1:C:260:MET:CE	2.51	0.41
1:C:111:LEU:HB2	3:C:502:PGW:H08A	2.03	0.41
1:C:173:MET:O	1:C:174:GLY:C	2.64	0.41
1:D:48:LYS:NZ	1:D:245:PRO:HB3	2.36	0.41
1:D:326:LEU:HD23	1:D:331:THR:HG22	2.02	0.41
1:C:9:MET:N	1:C:10:PRO:CD	2.84	0.41
1:C:170:TYR:O	1:C:171:VAL:C	2.64	0.41
1:C:279:PHE:O	1:C:283:VAL:HG23	2.20	0.41
1:D:175:LEU:O	1:D:176:LEU:C	2.64	0.41
1:D:178:VAL:O	1:D:179:PHE:C	2.64	0.41
1:D:187:LEU:HD23	1:D:197:GLN:OE1	2.21	0.40
1:A:9:MET:N	1:A:10:PRO:CD	2.84	0.40
1:B:178:VAL:O	1:B:179:PHE:C	2.63	0.40
1:C:173:MET:O	1:C:176:LEU:HB3	2.21	0.40
1:D:170:TYR:O	1:D:171:VAL:C	2.65	0.40
1:A:60:VAL:CG1	1:A:61:ILE:N	2.84	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	372/417 (89%)	361 (97%)	11 (3%)	0	100	100
1	B	359/417 (86%)	343 (96%)	16 (4%)	0	100	100
1	C	369/417 (88%)	357 (97%)	12 (3%)	0	100	100
1	D	350/417 (84%)	338 (97%)	12 (3%)	0	100	100
All	All	1450/1668 (87%)	1399 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	303/370 (82%)	303 (100%)	0	100	100
1	B	273/370 (74%)	273 (100%)	0	100	100
1	C	296/370 (80%)	296 (100%)	0	100	100
1	D	282/370 (76%)	282 (100%)	0	100	100
All	All	1154/1480 (78%)	1154 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	119	ASN
1	B	53	GLN
1	B	359	ASN
1	C	35	HIS
1	C	359	ASN
1	C	375	HIS
1	D	124	HIS
1	D	375	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

8 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$
3	PGW	C	502	-	33,33,50	0.92	2 (6%)	35,38,56	0.87	1 (2%)
3	PGW	D	502	-	33,33,50	0.89	2 (6%)	35,38,56	0.91	1 (2%)
2	TUM	A	501	-	60,60,60	1.77	13 (21%)	83,84,84	1.57	17 (20%)
3	PGW	A	502	-	29,29,50	0.92	2 (6%)	31,33,56	0.98	1 (3%)
2	TUM	B	501	-	60,60,60	1.77	13 (21%)	83,84,84	1.60	17 (20%)
2	TUM	C	501	-	60,60,60	1.75	13 (21%)	83,84,84	1.53	12 (14%)
2	TUM	D	501	-	60,60,60	1.75	14 (23%)	83,84,84	1.53	15 (18%)
3	PGW	B	502	-	33,33,50	0.89	2 (6%)	35,38,56	0.90	1 (2%)

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	PGW	C	502	-	-	14/37/37/55	-
3	PGW	D	502	-	-	7/37/37/55	-
2	TUM	A	501	-	-	12/39/95/95	0/4/4/4
3	PGW	A	502	-	-	11/32/32/55	-
2	TUM	B	501	-	-	13/39/95/95	0/4/4/4
2	TUM	C	501	-	-	10/39/95/95	0/4/4/4
2	TUM	D	501	-	-	10/39/95/95	0/4/4/4
3	PGW	B	502	-	-	15/37/37/55	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TUM	C5-N7	6.33	1.48	1.34
2	A	501	TUM	C5-N7	6.24	1.48	1.34
2	C	501	TUM	C5-N7	6.21	1.47	1.34
2	D	501	TUM	C5-N7	6.12	1.47	1.34
2	B	501	TUM	O18-C17	3.98	1.50	1.44
2	A	501	TUM	O18-C17	3.88	1.49	1.44
2	A	501	TUM	C26-C27	-3.87	1.35	1.43
2	C	501	TUM	C26-C27	-3.86	1.35	1.43
2	D	501	TUM	C26-C27	-3.85	1.35	1.43
2	B	501	TUM	C26-C27	-3.78	1.35	1.43
2	C	501	TUM	O18-C17	3.74	1.49	1.44
2	D	501	TUM	O18-C17	3.73	1.49	1.44
2	B	501	TUM	O18-C19	3.72	1.50	1.42
2	A	501	TUM	O18-C19	3.69	1.50	1.42
2	D	501	TUM	O18-C19	3.64	1.50	1.42
2	B	501	TUM	C27-N29	-3.63	1.32	1.38
2	C	501	TUM	O18-C19	3.60	1.50	1.42
2	C	501	TUM	C27-N29	-3.57	1.32	1.38
2	A	501	TUM	C27-N29	-3.56	1.32	1.38
2	D	501	TUM	C27-N29	-3.54	1.32	1.38
2	B	501	TUM	C46-N45	3.32	1.45	1.34
2	D	501	TUM	C46-N45	3.30	1.45	1.34
2	A	501	TUM	C46-N45	3.26	1.44	1.34
2	C	501	TUM	C46-N45	3.20	1.44	1.34
2	A	501	TUM	C4-C5	3.11	1.54	1.48
2	C	501	TUM	C4-C5	3.03	1.54	1.48
2	B	501	TUM	C4-C5	2.95	1.54	1.48
2	A	501	TUM	O6-C5	-2.94	1.18	1.24
2	D	501	TUM	O6-C5	-2.93	1.18	1.24
2	C	501	TUM	O6-C5	-2.91	1.18	1.24
2	B	501	TUM	O6-C5	-2.86	1.18	1.24
2	D	501	TUM	C4-C5	2.78	1.54	1.48
2	C	501	TUM	O28-C27	-2.78	1.19	1.24
2	B	501	TUM	O28-C27	-2.76	1.19	1.24
2	D	501	TUM	O28-C27	-2.75	1.19	1.24
2	A	501	TUM	O28-C27	-2.72	1.19	1.24
3	A	502	PGW	O01-C02	-2.63	1.40	1.46
2	A	501	TUM	C22-C20	-2.62	1.46	1.53
2	D	501	TUM	C22-C20	-2.54	1.46	1.53
2	A	501	TUM	C25-N24	-2.52	1.32	1.38
3	D	502	PGW	O01-C02	-2.52	1.40	1.46
2	C	501	TUM	C22-C20	-2.50	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	TUM	C25-N24	-2.50	1.32	1.38
3	C	502	PGW	O01-C02	-2.47	1.40	1.46
3	B	502	PGW	O01-C02	-2.46	1.40	1.46
2	B	501	TUM	C22-C20	-2.45	1.46	1.53
2	D	501	TUM	C25-N24	-2.41	1.32	1.38
3	C	502	PGW	O01-C1	2.39	1.41	1.34
2	B	501	TUM	C25-N24	-2.30	1.32	1.38
3	B	502	PGW	O01-C1	2.25	1.40	1.34
2	D	501	TUM	O31-C30	-2.25	1.19	1.23
2	C	501	TUM	O47-C46	-2.24	1.18	1.23
2	B	501	TUM	O31-C30	-2.24	1.19	1.23
2	D	501	TUM	O47-C46	-2.24	1.18	1.23
2	A	501	TUM	O47-C46	-2.23	1.18	1.23
2	B	501	TUM	O47-C46	-2.23	1.18	1.23
3	D	502	PGW	O01-C1	2.22	1.40	1.34
2	C	501	TUM	O31-C30	-2.15	1.19	1.23
2	A	501	TUM	O31-C30	-2.14	1.19	1.23
3	A	502	PGW	O01-C1	2.12	1.40	1.34
2	D	501	TUM	C22-C17	-2.08	1.48	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	TUM	C27-N29-C30	-5.32	120.00	126.61
2	C	501	TUM	C27-N29-C30	-5.26	120.08	126.61
2	D	501	TUM	C27-N29-C30	-5.22	120.14	126.61
2	A	501	TUM	C27-N29-C30	-5.10	120.28	126.61
2	B	501	TUM	N29-C30-N24	4.29	120.47	114.89
2	B	501	TUM	C2-C1-C4	-4.09	117.41	125.92
3	B	502	PGW	O01-C1-C2	4.05	120.25	111.48
2	D	501	TUM	C15-C17-C22	-3.97	110.25	115.95
2	D	501	TUM	N29-C30-N24	3.91	119.98	114.89
3	D	502	PGW	O01-C1-C2	3.90	119.92	111.48
2	C	501	TUM	N29-C30-N24	3.87	119.93	114.89
2	A	501	TUM	N29-C30-N24	3.87	119.92	114.89
3	A	502	PGW	O01-C1-C2	3.86	119.83	111.48
3	C	502	PGW	O01-C1-C2	3.78	119.67	111.48
2	C	501	TUM	C26-C27-N29	3.64	119.89	114.80
2	D	501	TUM	C26-C27-N29	3.61	119.86	114.80
2	B	501	TUM	C26-C27-N29	3.54	119.75	114.80
2	D	501	TUM	C2-C1-C4	-3.54	118.56	125.92
2	A	501	TUM	C26-C27-N29	3.51	119.71	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TUM	C15-C17-C22	-3.49	110.93	115.95
2	C	501	TUM	C15-C17-C22	-3.48	110.95	115.95
2	C	501	TUM	C14-C13-C11	-3.35	108.04	113.47
2	C	501	TUM	C2-C1-C4	-3.27	119.11	125.92
2	B	501	TUM	C40-C42-C44	-3.25	105.66	110.40
2	C	501	TUM	O28-C27-C26	-3.09	119.83	125.16
2	B	501	TUM	C22-C20-C19	3.03	107.20	101.46
2	D	501	TUM	O28-C27-C26	-3.02	119.95	125.16
2	A	501	TUM	C2-C1-C4	-3.02	119.64	125.92
2	A	501	TUM	O28-C27-C26	-3.00	119.99	125.16
2	C	501	TUM	C22-C20-C19	2.96	107.07	101.46
2	B	501	TUM	C48-C46-N45	2.96	121.02	116.12
2	C	501	TUM	C20-C22-C17	2.91	106.48	102.35
2	B	501	TUM	O28-C27-C26	-2.87	120.22	125.16
2	D	501	TUM	C22-C20-C19	2.84	106.83	101.46
2	A	501	TUM	C22-C20-C19	2.74	106.65	101.46
2	D	501	TUM	C20-C22-C17	2.69	106.18	102.35
2	A	501	TUM	C4-C5-N7	2.67	119.18	114.61
2	A	501	TUM	C35-O36-C37	2.64	118.87	113.72
2	A	501	TUM	C48-C46-N45	2.60	120.44	116.12
2	B	501	TUM	C15-C17-C22	-2.56	112.28	115.95
2	B	501	TUM	O31-C30-N24	-2.56	119.47	122.80
2	A	501	TUM	C14-C13-C11	-2.55	109.33	113.47
2	A	501	TUM	C19-N24-C30	2.49	122.06	117.59
2	B	501	TUM	C20-C22-C17	2.48	105.87	102.35
2	B	501	TUM	C17-O18-C19	-2.46	102.82	108.37
2	D	501	TUM	C48-C46-N45	2.36	120.03	116.12
2	A	501	TUM	C38-C37-C40	-2.29	107.41	113.02
2	A	501	TUM	C40-C42-C44	-2.29	107.07	110.40
2	C	501	TUM	C11-C9-C8	-2.27	107.09	110.40
2	B	501	TUM	O18-C19-N24	2.25	113.45	108.36
2	D	501	TUM	O32-C33-C8	-2.23	106.39	110.59
2	A	501	TUM	C11-C9-C8	-2.20	107.20	110.40
2	B	501	TUM	O32-C33-C8	-2.19	106.45	110.59
2	A	501	TUM	C44-N45-C46	-2.19	117.99	123.11
2	D	501	TUM	C4-C5-N7	2.18	118.34	114.61
2	D	501	TUM	O31-C30-N24	-2.14	120.01	122.80
2	D	501	TUM	C38-C37-C40	-2.12	107.81	113.02
2	C	501	TUM	O31-C30-N24	-2.12	120.04	122.80
2	A	501	TUM	O31-C30-N24	-2.09	120.07	122.80
2	C	501	TUM	C40-C42-C44	-2.07	107.39	110.40
2	B	501	TUM	C44-N45-C46	-2.06	118.29	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	TUM	C42-C40-C37	-2.05	106.52	110.23
2	D	501	TUM	C19-N24-C30	2.03	121.23	117.59
2	B	501	TUM	C35-O34-C33	-2.02	110.71	114.33
2	D	501	TUM	C14-C13-C11	-2.01	110.21	113.47

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TUM	C33-C8-N7-C5
2	A	501	TUM	C35-C44-N45-C46
2	B	501	TUM	C33-C8-N7-C5
2	C	501	TUM	C33-C8-N7-C5
2	D	501	TUM	C33-C8-N7-C5
3	A	502	PGW	C03-O11-P-O12
3	A	502	PGW	C03-O11-P-O13
3	A	502	PGW	C03-O11-P-O14
3	B	502	PGW	C04-O12-P-O11
3	B	502	PGW	C04-O12-P-O13
3	B	502	PGW	C04-O12-P-O14
3	B	502	PGW	O03-C01-C02-O01
3	B	502	PGW	O03-C01-C02-C03
3	C	502	PGW	C03-O11-P-O12
3	C	502	PGW	C03-O11-P-O13
3	C	502	PGW	C03-O11-P-O14
3	C	502	PGW	O03-C01-C02-O01
3	C	502	PGW	O03-C01-C02-C03
3	D	502	PGW	C04-O12-P-O11
2	B	501	TUM	C40-C37-C38-O39
2	B	501	TUM	O36-C37-C38-O39
2	A	501	TUM	C1-C4-C5-N7
3	B	502	PGW	C1-C2-C3-C4
3	C	502	PGW	C1-C2-C3-C4
3	B	502	PGW	O12-C04-C05-OAF
3	C	502	PGW	O12-C04-C05-OAF
2	A	501	TUM	C1-C4-C5-O6
3	C	502	PGW	O12-C04-C05-CAD
2	D	501	TUM	C16-C18-C21-C24
2	C	501	TUM	C16-C18-C21-C23
2	D	501	TUM	C16-C18-C21-C23
2	C	501	TUM	C16-C18-C21-C24
3	B	502	PGW	O12-C04-C05-CAD

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Mol	Chain	Res	Type	Atoms
2	B	501	TUM	C2-C3-C6-C7
2	B	501	TUM	C35-C44-N45-C46
3	B	502	PGW	C2-C1-O01-C02
3	A	502	PGW	C1-C2-C3-C4
2	B	501	TUM	C16-C18-C21-C23
3	D	502	PGW	C1-C2-C3-C4
2	D	501	TUM	C2-C3-C6-C7
3	A	502	PGW	C07-C08-C09-C11
3	B	502	PGW	C06-C07-C08-C09
3	B	502	PGW	C07-C08-C09-C11
2	B	501	TUM	C16-C18-C21-C24
3	B	502	PGW	C2-C3-C4-C5
3	B	502	PGW	C4-C5-C6-C7
2	D	501	TUM	C1-C2-C3-C6
3	B	502	PGW	O02-C1-O01-C02
3	A	502	PGW	O01-C02-C03-O11
2	A	501	TUM	C2-C3-C6-C7
3	D	502	PGW	C4-C5-C6-C7
3	A	502	PGW	C01-C02-C03-O11
3	C	502	PGW	C5-C6-C7-C8
3	C	502	PGW	C7-C8-C9-C10
2	B	501	TUM	C1-C4-C5-O6
3	C	502	PGW	C4-C5-C6-C7
2	D	501	TUM	C4-C1-C2-C3
3	D	502	PGW	C09-C11-C12-C13
3	C	502	PGW	C2-C3-C4-C5
2	B	501	TUM	C1-C4-C5-N7
3	C	502	PGW	C6-C7-C8-C9
2	C	501	TUM	C4-C1-C2-C3
2	A	501	TUM	C3-C6-C7-C10
2	A	501	TUM	C7-C10-C12-C16
2	C	501	TUM	C14-C15-C17-C22
2	A	501	TUM	C4-C1-C2-C3
3	D	502	PGW	C07-C08-C09-C11
3	A	502	PGW	C02-C03-O11-P
2	A	501	TUM	C16-C18-C21-C23
2	C	501	TUM	C1-C4-C5-O6
2	D	501	TUM	C12-C10-C7-C6
2	D	501	TUM	C7-C10-C12-C16
3	A	502	PGW	C06-C07-C08-C09
2	C	501	TUM	O36-C37-C38-O39
2	D	501	TUM	C9-C8-N7-C5

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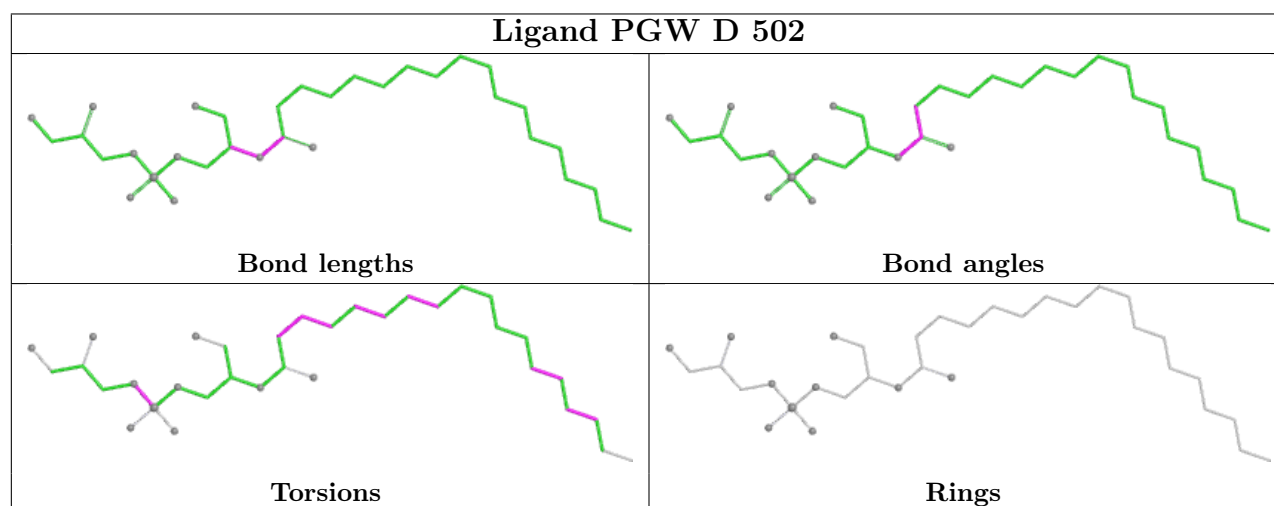
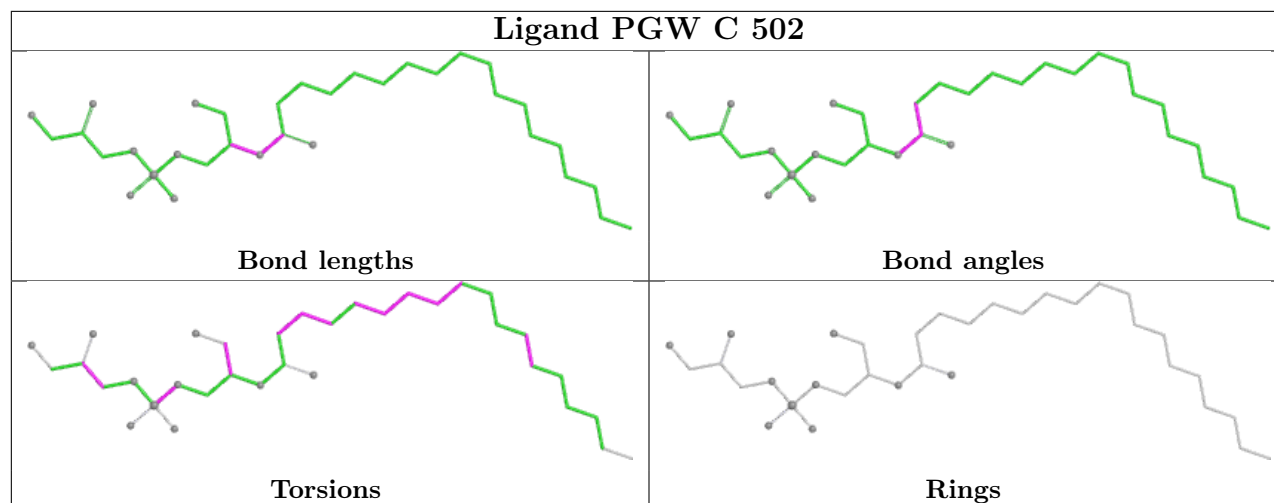
Mol	Chain	Res	Type	Atoms
3	A	502	PGW	C10-C06-C07-C08
2	A	501	TUM	C16-C18-C21-C24
3	C	502	PGW	C06-C07-C08-C09
2	C	501	TUM	C1-C4-C5-N7
3	D	502	PGW	C2-C3-C4-C5
3	D	502	PGW	C6-C7-C8-C9
3	A	502	PGW	C7-C8-C9-C10
2	B	501	TUM	C4-C1-C2-C3
2	C	501	TUM	C14-C15-C17-O18
3	B	502	PGW	O01-C02-C03-O11
2	A	501	TUM	C9-C8-N7-C5
2	A	501	TUM	C42-C44-N45-C46
2	D	501	TUM	O36-C37-C38-O39
2	B	501	TUM	C3-C6-C7-C10
2	B	501	TUM	C9-C8-N7-C5
2	B	501	TUM	C42-C44-N45-C46
2	C	501	TUM	C9-C8-N7-C5

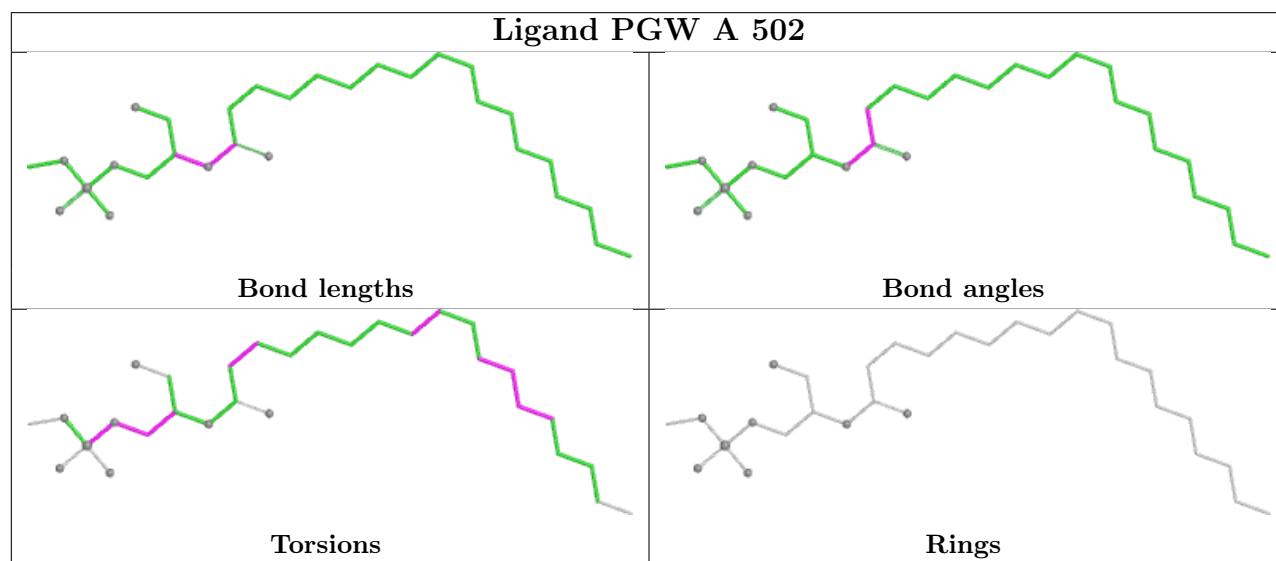
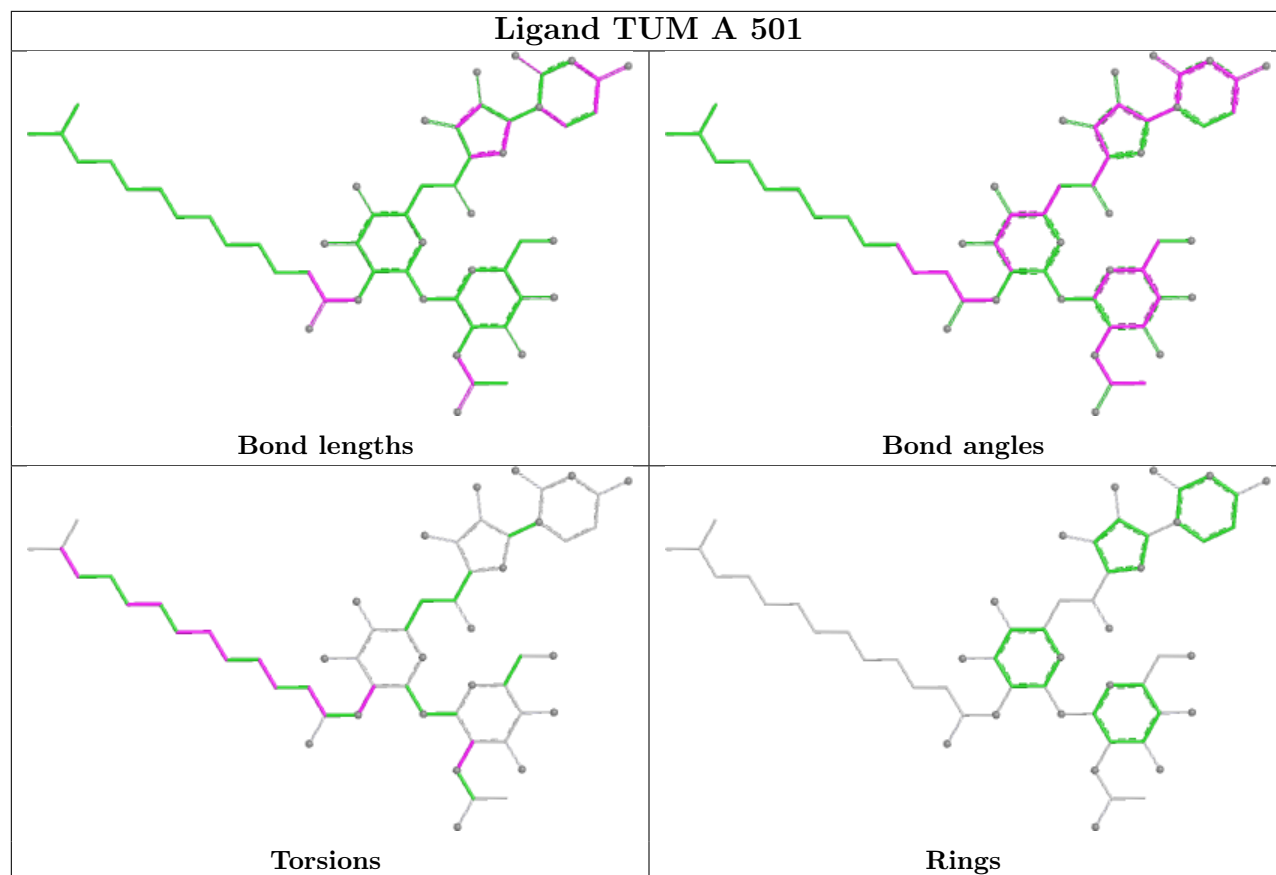
There are no ring outliers.

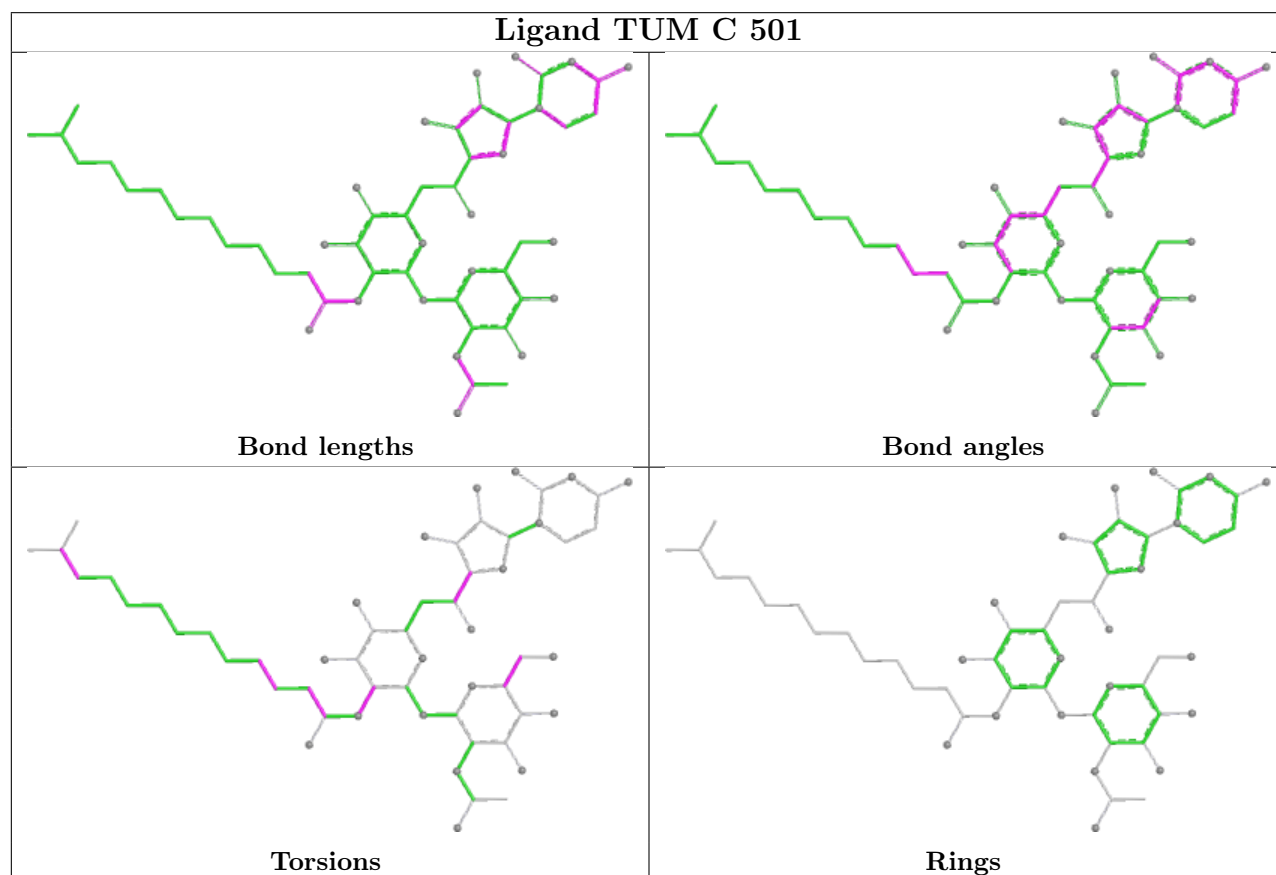
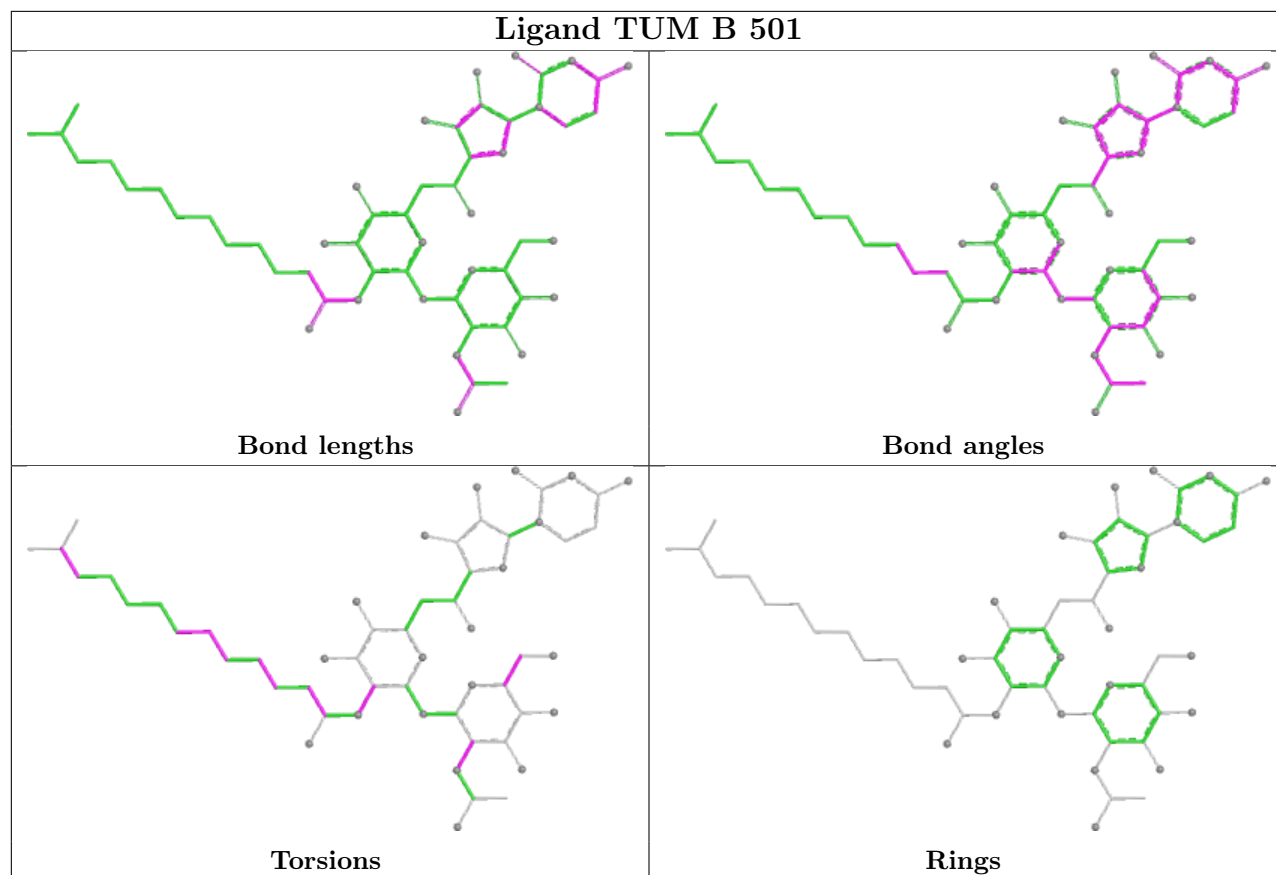
6 monomers are involved in 13 short contacts:

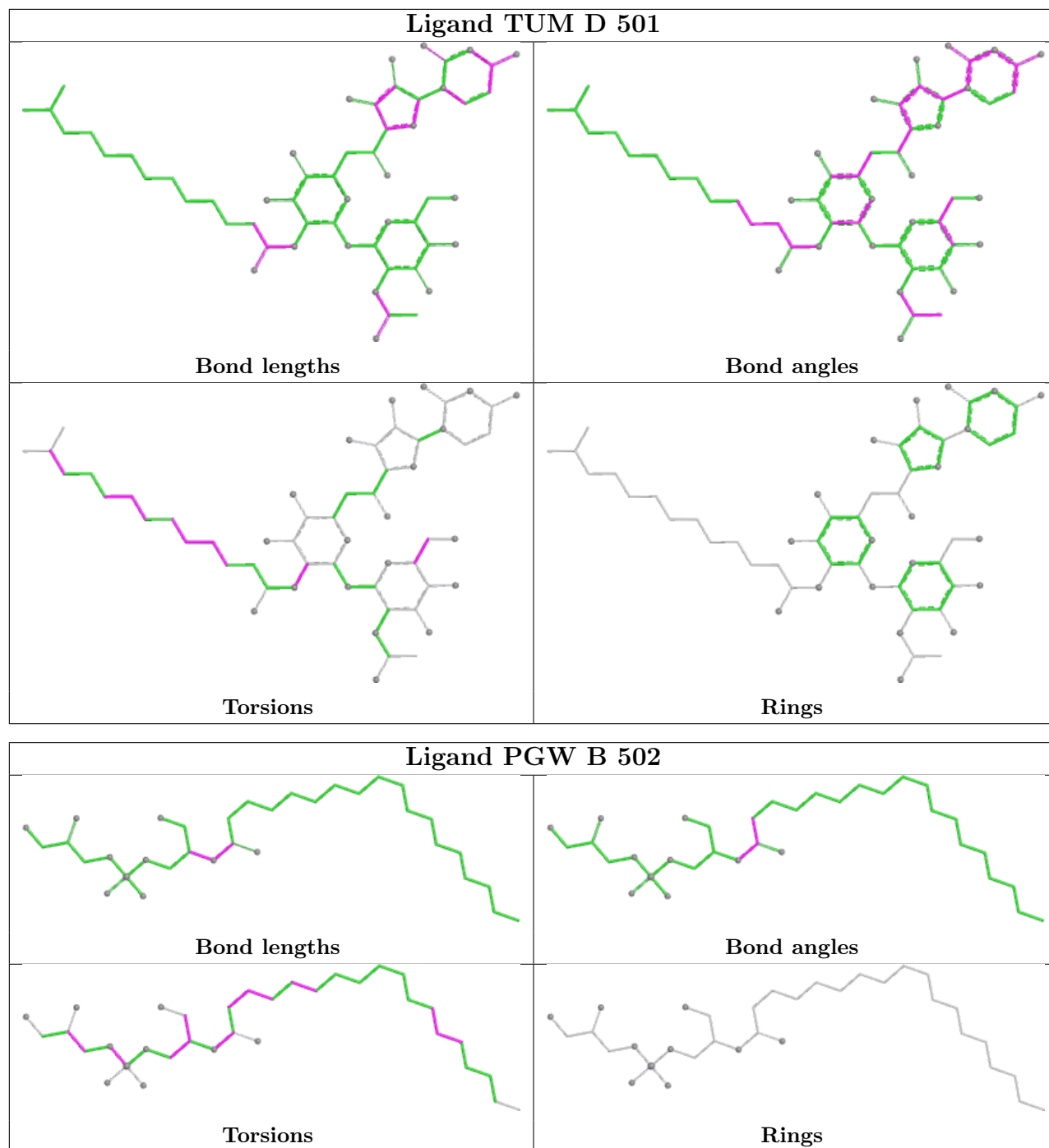
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	PGW	5	0
3	D	502	PGW	2	0
2	A	501	TUM	1	0
3	A	502	PGW	2	0
2	B	501	TUM	2	0
2	C	501	TUM	1	0

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	378/417 (90%)	1.36	98 (25%) 1 1	4, 33, 84, 132	0
1	B	369/417 (88%)	1.81	122 (33%) 1 0	10, 55, 109, 135	0
1	C	375/417 (89%)	2.01	117 (31%) 1 1	7, 42, 117, 133	0
1	D	362/417 (86%)	2.15	127 (35%) 1 0	7, 48, 93, 137	0
All	All	1484/1668 (88%)	1.83	464 (31%) 1 1	4, 44, 105, 137	0

All (464) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	PRO	16.7
1	A	52	GLN	15.9
1	D	9	MET	15.5
1	D	51	ARG	15.3
1	C	53	GLN	14.3
1	C	52	GLN	13.7
1	A	53	GLN	13.3
1	D	52	GLN	12.9
1	D	53	GLN	12.8
1	D	49	THR	12.7
1	C	311	THR	12.3
1	C	348	SER	11.8
1	C	49	THR	11.7
1	C	308	ASN	11.5
1	C	312	GLY	11.5
1	B	52	GLN	11.5
1	C	44	GLN	11.5
1	C	313	LYS	11.2
1	D	76	PHE	11.0
1	D	44	GLN	10.9
1	A	51	ARG	10.4

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Mol	Chain	Res	Type	RSRZ
1	C	309	ILE	10.4
1	A	348	SER	10.3
1	D	42	CYS	9.9
1	A	306	ARG	9.7
1	C	51	ARG	9.3
1	C	347	GLN	9.3
1	D	79	LEU	9.1
1	B	400	GLN	9.1
1	B	307	LEU	9.1
1	B	76	PHE	9.0
1	C	315	GLU	9.0
1	D	78	PHE	8.9
1	D	145	GLY	8.8
1	D	77	PRO	8.7
1	B	50	SER	8.7
1	C	37	ILE	8.6
1	A	355	PHE	8.5
1	D	12	LEU	8.3
1	D	343	VAL	8.1
1	C	307	LEU	8.0
1	B	72	CYS	7.9
1	C	80	ASN	7.9
1	C	355	PHE	7.9
1	C	368	LEU	7.9
1	D	11	LEU	7.8
1	D	149	ILE	7.8
1	D	38	ALA	7.7
1	D	80	ASN	7.5
1	D	81	CYS	7.5
1	C	72	CYS	7.4
1	B	12	LEU	7.3
1	D	143	ASN	7.2
1	D	13	ILE	7.1
1	C	373	PRO	7.1
1	C	310	LYS	7.0
1	B	51	ARG	7.0
1	D	91	PRO	7.0
1	B	53	GLN	6.9
1	C	327	SER	6.9
1	B	46	LEU	6.9
1	A	357	GLU	6.9
1	B	47	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	44	GLN	6.8
1	B	79	LEU	6.8
1	D	75	PRO	6.7
1	C	318	TYR	6.7
1	A	50	SER	6.6
1	D	376	GLU	6.6
1	C	401	LEU	6.6
1	D	37	ILE	6.3
1	B	75	PRO	6.3
1	B	188	ALA	6.2
1	B	80	ASN	6.1
1	A	49	THR	6.1
1	C	357	GLU	6.1
1	D	50	SER	6.1
1	B	324	LYS	6.1
1	D	400	GLN	6.1
1	D	138	MET	6.0
1	B	43	GLY	6.0
1	B	10	PRO	6.0
1	B	9	MET	6.0
1	C	349	GLU	6.0
1	A	404	LEU	5.9
1	C	306	ARG	5.8
1	C	375	HIS	5.8
1	D	144	PHE	5.8
1	C	42	CYS	5.8
1	D	347	GLN	5.7
1	D	142	THR	5.7
1	C	12	LEU	5.7
1	D	337	ALA	5.6
1	B	339	SER	5.6
1	D	355	PHE	5.6
1	C	81	CYS	5.6
1	C	321	PHE	5.6
1	C	76	PHE	5.5
1	C	376	GLU	5.4
1	A	37	ILE	5.4
1	C	38	ALA	5.4
1	B	328	PHE	5.4
1	D	356	THR	5.3
1	A	354	GLU	5.3
1	A	352	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	94	GLU	5.2
1	B	48	LYS	5.2
1	D	39	ALA	5.2
1	C	91	PRO	5.2
1	B	342	LEU	5.2
1	B	347	GLN	5.2
1	D	54	ILE	5.1
1	A	149	ILE	5.1
1	C	354	GLU	5.1
1	A	74	ILE	5.1
1	A	356	THR	5.1
1	A	349	GLU	5.1
1	D	141	PHE	5.1
1	B	151	VAL	5.1
1	D	33	ARG	5.0
1	B	308	ASN	5.0
1	C	320	LYS	5.0
1	D	89	ALA	5.0
1	B	338	GLU	5.0
1	B	351	GLU	4.9
1	C	316	MET	4.9
1	A	307	LEU	4.9
1	D	334	LEU	4.9
1	A	353	GLY	4.9
1	A	112	GLY	4.9
1	D	309	ILE	4.8
1	C	89	ALA	4.8
1	A	168	LEU	4.8
1	A	38	ALA	4.8
1	C	365	ASN	4.8
1	D	48	LYS	4.8
1	C	346	HIS	4.7
1	B	219	ASP	4.7
1	C	378	ASN	4.7
1	D	357	GLU	4.7
1	D	307	LEU	4.7
1	C	328	PHE	4.7
1	C	351	GLU	4.7
1	B	304	ILE	4.7
1	A	76	PHE	4.6
1	D	59	GLY	4.6
1	D	90	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	74	ILE	4.5
1	B	341	GLN	4.5
1	D	340	LEU	4.4
1	A	72	CYS	4.4
1	C	358	CYS	4.4
1	A	320	LYS	4.4
1	B	216	ASP	4.4
1	C	8	PRO	4.3
1	C	350	THR	4.3
1	A	44	GLN	4.2
1	C	9	MET	4.2
1	B	189	GLY	4.2
1	B	37	ILE	4.2
1	B	376	GLU	4.2
1	B	363	LEU	4.1
1	B	286	PHE	4.1
1	C	149	ILE	4.1
1	C	43	GLY	4.1
1	A	358	CYS	4.1
1	B	354	GLU	4.1
1	C	352	ASP	4.1
1	B	312	GLY	4.1
1	A	321	PHE	4.0
1	C	329	LEU	4.0
1	B	352	ASP	4.0
1	C	90	PHE	4.0
1	D	255	CYS	4.0
1	D	163	LEU	4.0
1	B	245	PRO	4.0
1	A	43	GLY	4.0
1	A	251	GLY	3.9
1	A	308	ASN	3.9
1	A	167	ILE	3.9
1	A	33	ARG	3.9
1	B	45	ASP	3.9
1	C	374	ILE	3.9
1	D	95	PHE	3.9
1	D	93	HIS	3.9
1	A	311	THR	3.8
1	C	143	ASN	3.8
1	D	335	LYS	3.8
1	B	287	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	3.8
1	D	167	ILE	3.8
1	B	78	PHE	3.8
1	B	331	THR	3.8
1	C	341	GLN	3.8
1	C	305	PRO	3.8
1	B	226	TYR	3.8
1	D	344	THR	3.8
1	A	75	PRO	3.7
1	A	254	PHE	3.7
1	B	279	PHE	3.7
1	B	332	PHE	3.7
1	A	42	CYS	3.7
1	A	162	HIS	3.7
1	A	325	SER	3.7
1	B	73	PHE	3.7
1	C	356	THR	3.7
1	C	10	PRO	3.7
1	B	150	VAL	3.7
1	D	287	LEU	3.7
1	C	50	SER	3.6
1	A	54	ILE	3.6
1	D	74	ILE	3.6
1	D	346	HIS	3.6
1	C	59	GLY	3.6
1	D	398	ARG	3.6
1	D	283	VAL	3.6
1	A	318	TYR	3.6
1	D	375	HIS	3.6
1	C	372	GLY	3.6
1	D	381	LEU	3.6
1	A	59	GLY	3.5
1	D	140	TYR	3.5
1	B	54	ILE	3.5
1	D	98	LEU	3.5
1	D	399	TYR	3.5
1	C	353	GLY	3.5
1	D	244	TYR	3.5
1	A	253	THR	3.5
1	C	79	LEU	3.5
1	A	403	ARG	3.5
1	D	339	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	306	ARG	3.4
1	D	295	HIS	3.4
1	B	77	PRO	3.4
1	B	49	THR	3.4
1	B	42	CYS	3.4
1	D	139	VAL	3.4
1	C	256	TYR	3.4
1	D	146	ASN	3.3
1	A	402	VAL	3.3
1	C	377	ARG	3.3
1	B	145	GLY	3.3
1	B	190	ILE	3.3
1	B	353	GLY	3.3
1	C	39	ALA	3.3
1	C	342	LEU	3.3
1	D	62	SER	3.3
1	B	166	GLY	3.3
1	D	243	TRP	3.2
1	A	46	LEU	3.2
1	D	280	MET	3.2
1	A	326	LEU	3.2
1	B	14	ASN	3.2
1	D	294	LEU	3.2
1	D	338	GLU	3.2
1	C	93	HIS	3.2
1	B	316	MET	3.2
1	C	174	GLY	3.1
1	A	401	LEU	3.1
1	C	259	GLY	3.1
1	A	48	LYS	3.1
1	B	302	HIS	3.1
1	C	325	SER	3.1
1	C	255	CYS	3.1
1	C	332	PHE	3.1
1	D	14	ASN	3.1
1	C	92	HIS	3.1
1	C	48	LYS	3.1
1	D	219	ASP	3.1
1	A	347	GLN	3.0
1	D	226	TYR	3.0
1	B	81	CYS	3.0
1	B	313	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	40	ARG	3.0
1	A	116	ASP	3.0
1	C	344	THR	3.0
1	B	11	LEU	3.0
1	A	256	TYR	3.0
1	C	335	LYS	3.0
1	D	256	TYR	3.0
1	A	252	ASP	3.0
1	C	326	LEU	2.9
1	C	62	SER	2.9
1	D	327	SER	2.9
1	C	257	PHE	2.9
1	A	47	ASN	2.9
1	A	255	CYS	2.9
1	D	319	SER	2.9
1	B	243	TRP	2.9
1	B	162	HIS	2.9
1	B	344	THR	2.9
1	B	144	PHE	2.9
1	D	43	GLY	2.9
1	B	323	THR	2.8
1	A	214	GLU	2.8
1	C	182	ASN	2.8
1	B	340	LEU	2.8
1	C	33	ARG	2.8
1	C	343	VAL	2.8
1	C	34	GLY	2.8
1	A	9	MET	2.8
1	B	399	TYR	2.8
1	C	58	GLN	2.8
1	A	171	VAL	2.8
1	C	317	SER	2.8
1	C	192	GLY	2.7
1	B	170	TYR	2.7
1	B	322	LYS	2.7
1	A	341	GLN	2.7
1	D	279	PHE	2.7
1	D	296	ILE	2.7
1	C	302	HIS	2.7
1	D	363	LEU	2.7
1	B	297	ILE	2.7
1	D	332	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	62	SER	2.7
1	A	182	ASN	2.7
1	D	290	LEU	2.7
1	D	245	PRO	2.7
1	A	34	GLY	2.7
1	B	192	GLY	2.7
1	B	375	HIS	2.7
1	B	59	GLY	2.7
1	C	180	CYS	2.7
1	D	330	GLY	2.7
1	C	188	ALA	2.7
1	B	382	LEU	2.7
1	B	182	ASN	2.7
1	A	377	ARG	2.6
1	D	73	PHE	2.6
1	C	167	ILE	2.6
1	C	331	THR	2.6
1	B	244	TYR	2.6
1	B	95	PHE	2.6
1	D	254	PHE	2.6
1	C	345	VAL	2.6
1	C	261	THR	2.6
1	B	290	LEU	2.6
1	B	357	GLU	2.6
1	B	33	ARG	2.6
1	B	283	VAL	2.6
1	A	170	TYR	2.5
1	B	318	TYR	2.5
1	B	215	GLY	2.5
1	A	334	LEU	2.5
1	A	368	LEU	2.5
1	D	41	LEU	2.5
1	D	380	THR	2.5
1	D	308	ASN	2.5
1	D	378	ASN	2.5
1	D	181	THR	2.5
1	C	165	LEU	2.5
1	C	370	VAL	2.5
1	A	257	PHE	2.5
1	A	350	THR	2.5
1	B	330	GLY	2.5
1	B	58	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	110	PHE	2.5
1	B	143	ASN	2.4
1	B	285	ASN	2.4
1	D	252	ASP	2.4
1	D	170	TYR	2.4
1	D	258	ALA	2.4
1	A	218	ARG	2.4
1	A	324	LYS	2.4
1	C	47	ASN	2.4
1	A	245	PRO	2.4
1	A	114	ALA	2.4
1	C	141	PHE	2.4
1	B	294	LEU	2.4
1	B	211	VAL	2.4
1	D	345	VAL	2.4
1	D	16	ILE	2.4
1	C	314	LEU	2.4
1	A	60	VAL	2.4
1	A	343	VAL	2.4
1	D	216	ASP	2.4
1	A	298	PRO	2.4
1	C	266	GLY	2.3
1	C	330	GLY	2.3
1	A	309	ILE	2.3
1	A	376	GLU	2.3
1	D	362	THR	2.3
1	A	124	HIS	2.3
1	B	280	MET	2.3
1	B	214	GLU	2.3
1	B	38	ALA	2.3
1	A	80	ASN	2.3
1	B	137	LEU	2.3
1	B	314	LEU	2.3
1	C	242	ASN	2.3
1	A	45	ASP	2.3
1	C	60	VAL	2.3
1	D	63	GLY	2.3
1	B	293	LEU	2.3
1	A	143	ASN	2.3
1	B	358	CYS	2.3
1	A	351	GLU	2.3
1	C	54	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	258	ALA	2.3
1	A	165	LEU	2.3
1	A	216	ASP	2.3
1	D	220	ASP	2.3
1	B	296	ILE	2.2
1	B	165	LEU	2.2
1	C	41	LEU	2.2
1	D	385	LEU	2.2
1	A	346	HIS	2.2
1	D	223	PHE	2.2
1	D	235	THR	2.2
1	B	365	ASN	2.2
1	B	167	ILE	2.2
1	D	298	PRO	2.2
1	A	375	HIS	2.2
1	B	142	THR	2.2
1	C	241	HIS	2.2
1	C	191	ASN	2.2
1	D	364	ILE	2.2
1	A	115	ASP	2.2
1	C	216	ASP	2.2
1	D	134	LEU	2.2
1	D	284	PHE	2.2
1	D	331	THR	2.2
1	B	187	LEU	2.2
1	D	257	PHE	2.2
1	A	238	LEU	2.2
1	D	306	ARG	2.2
1	B	141	PHE	2.2
1	C	279	PHE	2.2
1	D	374	ILE	2.1
1	D	316	MET	2.1
1	A	8	PRO	2.1
1	D	237	GLY	2.1
1	A	345	VAL	2.1
1	B	288	TYR	2.1
1	C	138	MET	2.1
1	B	208	PHE	2.1
1	B	193	LEU	2.1
1	D	110	PHE	2.1
1	D	273	LYS	2.1
1	C	340	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	61	ILE	2.1
1	B	218	ARG	2.1
1	C	130	THR	2.1
1	B	337	ALA	2.1
1	A	315	GLU	2.1
1	D	36	PHE	2.1
1	A	317	SER	2.1
1	A	121	ARG	2.1
1	D	293	LEU	2.1
1	A	258	ALA	2.1
1	C	63	GLY	2.1
1	B	333	ILE	2.0
1	A	58	GLN	2.0
1	D	58	GLN	2.0
1	D	112	GLY	2.0
1	D	259	GLY	2.0
1	B	91	PRO	2.0
1	B	335	LYS	2.0
1	B	317	SER	2.0
1	A	119	ASN	2.0
1	B	291	PRO	2.0
1	A	222	VAL	2.0
1	A	250	VAL	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](#)

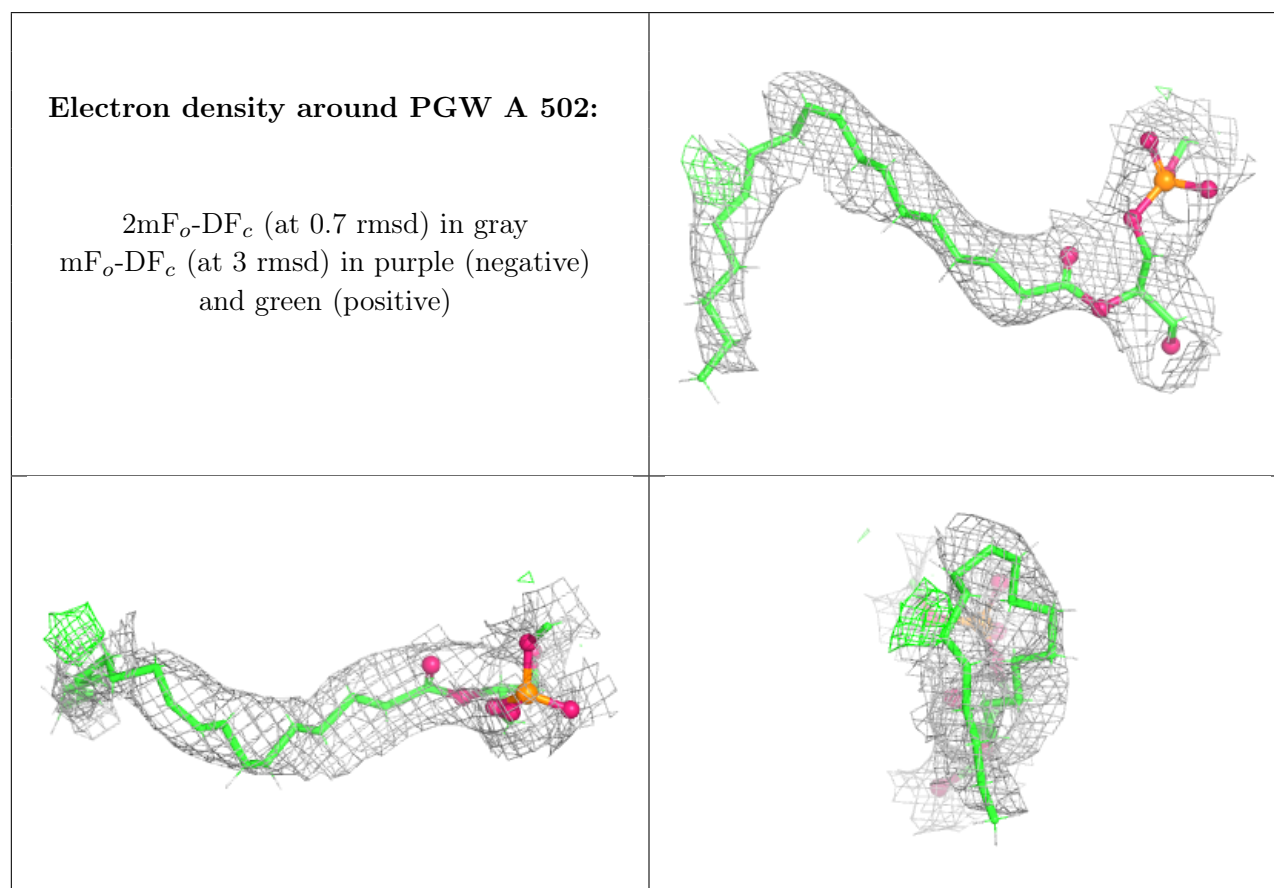
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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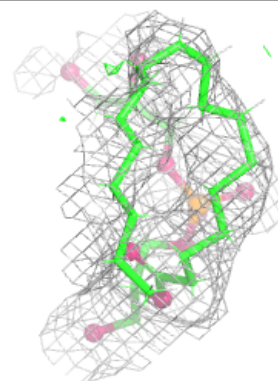
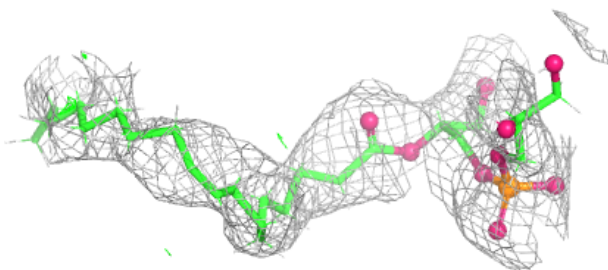
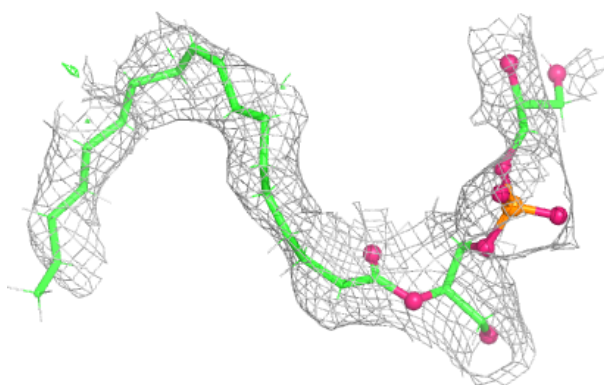
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PGW	A	502	30/51	0.79	0.25	23,49,139,159	0
3	PGW	C	502	34/51	0.80	0.25	19,63,122,128	0
3	PGW	B	502	34/51	0.81	0.22	19,48,118,128	0
3	PGW	D	502	34/51	0.85	0.19	14,42,106,118	0
2	TUM	B	501	57/57	0.87	0.15	25,59,82,92	0
2	TUM	C	501	57/57	0.88	0.14	16,40,65,78	0
2	TUM	D	501	57/57	0.89	0.18	25,58,89,116	0
2	TUM	A	501	57/57	0.91	0.14	8,29,47,53	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.

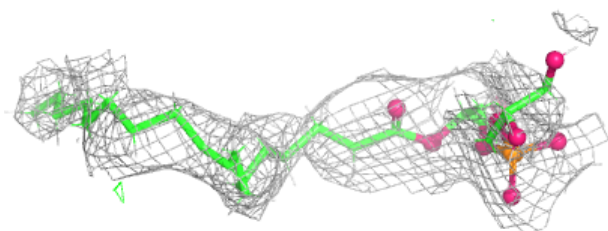
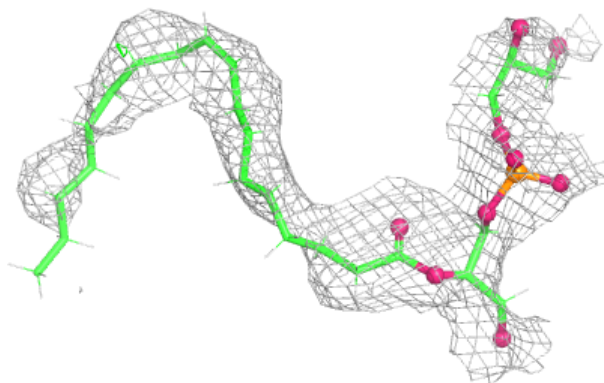


Electron density around PGW C 502:

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

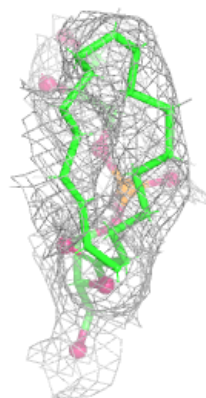
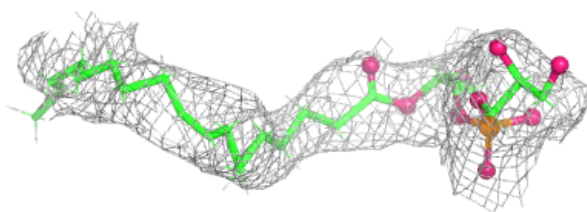
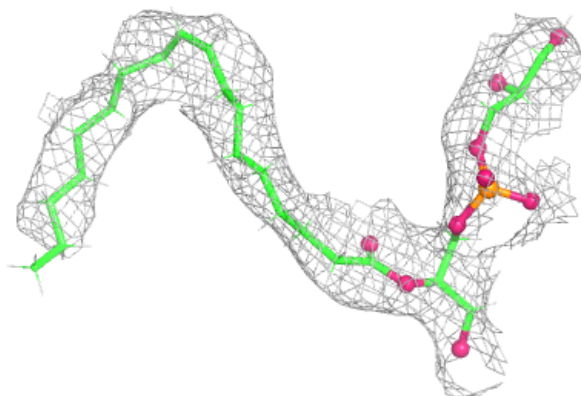
**Electron density around PGW B 502:**

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

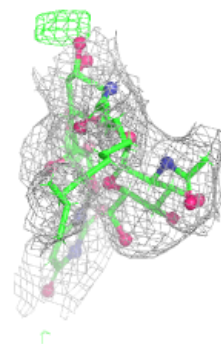
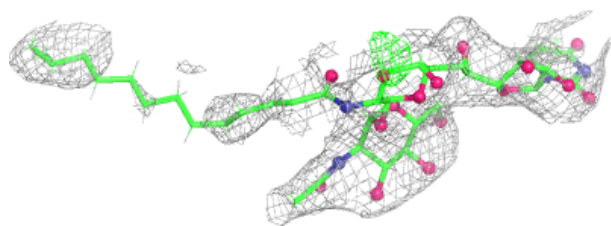
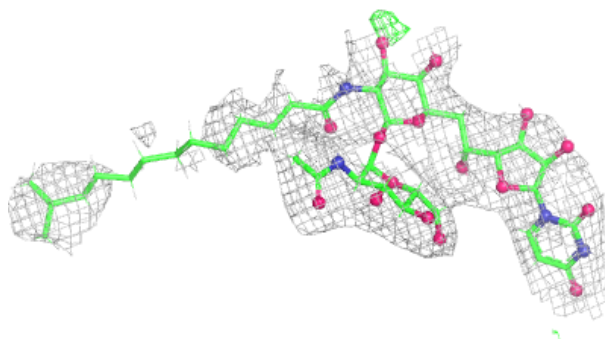


Electron density around PGW D 502:

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

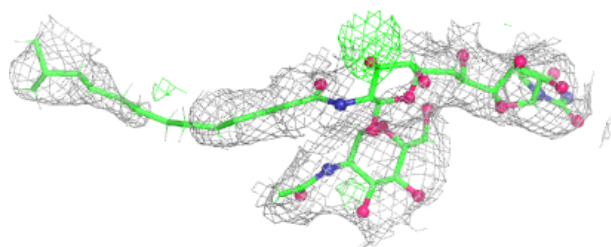
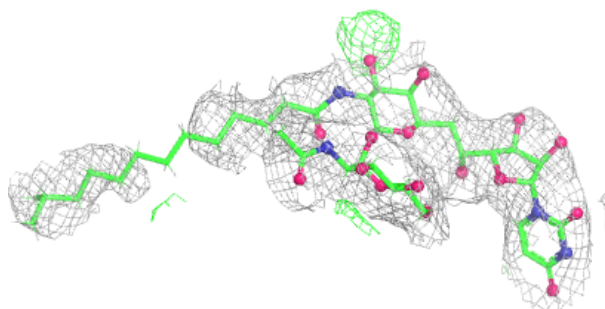
**Electron density around TUM B 501:**

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

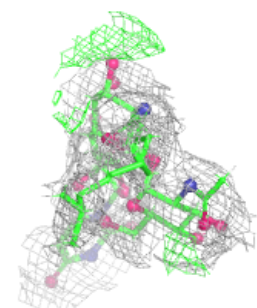
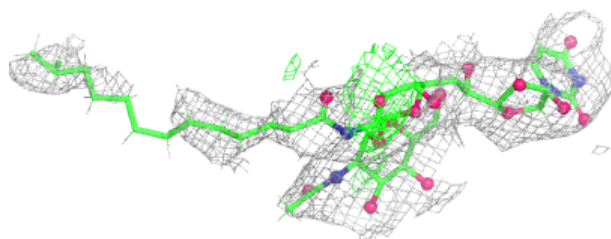
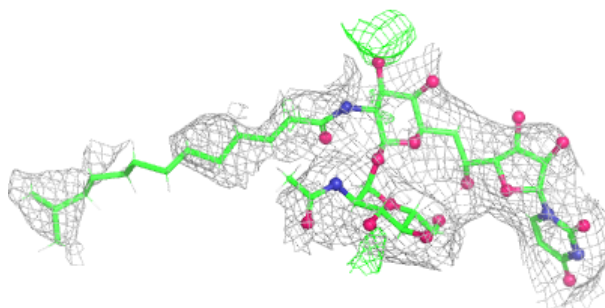


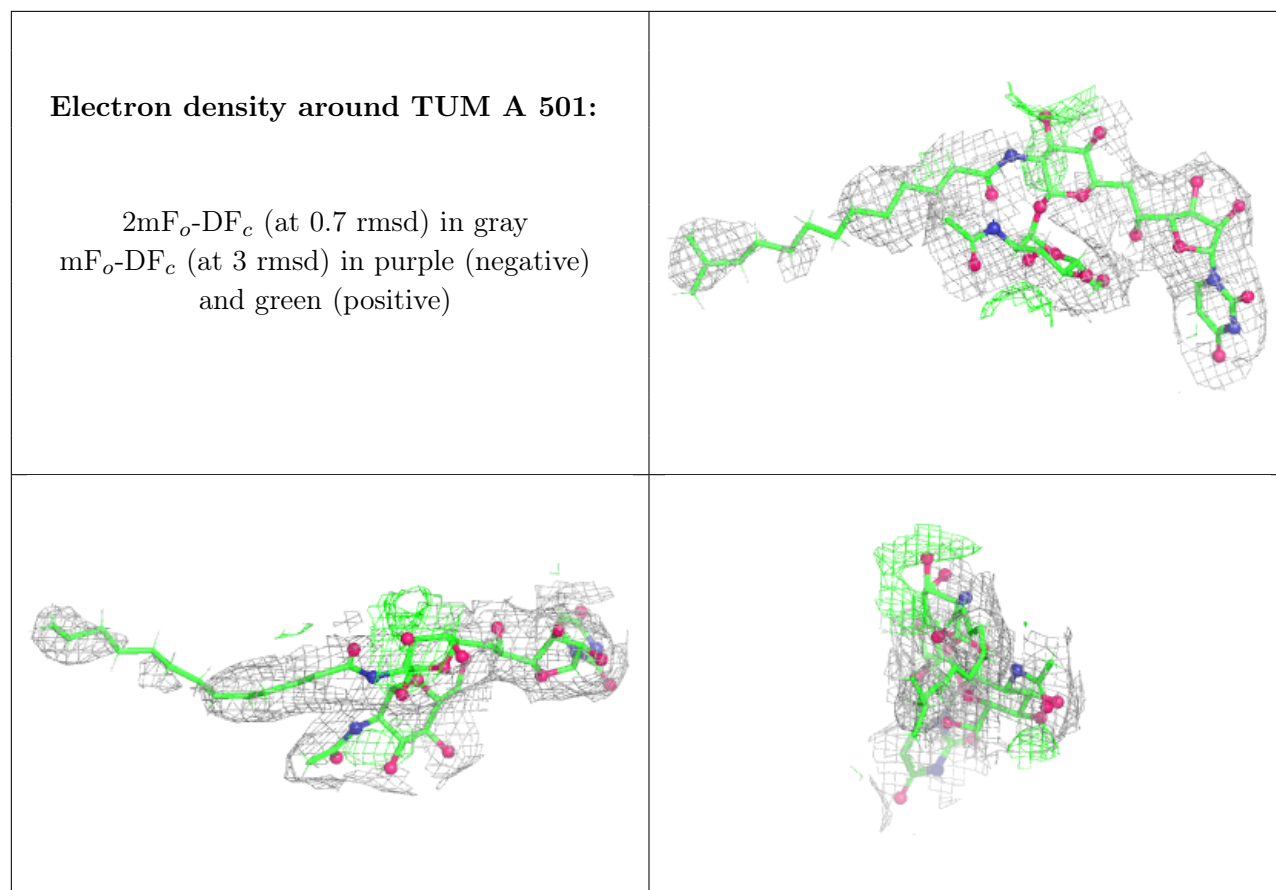
Electron density around TUM C 501:

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

**Electron density around TUM D 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.