



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:24 PM UTC

PDB ID : 6BW6 / pdb_00006bw6
Title : Human GPT (DPAGT1) H129 variant in complex with tunicamycin
Authors : Yoo, J.; Kuk, A.C.Y.; Mashalidis, E.H.; Lee, S.-Y.
Deposited on : 2017-12-14
Resolution : 2.95 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

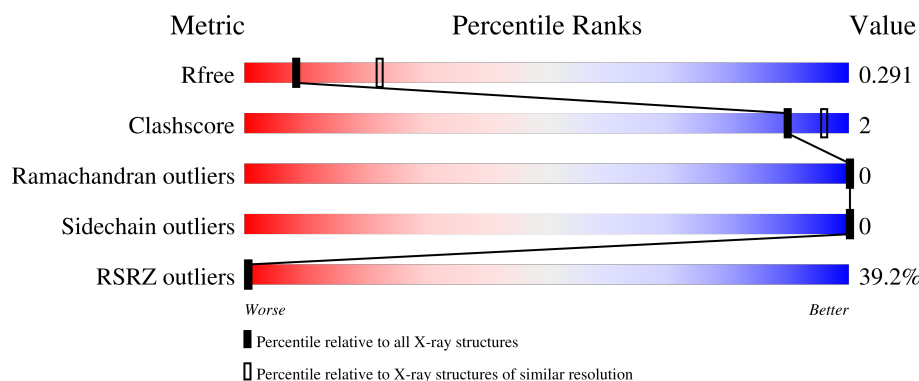
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	41% 82% 6% 12%
1	B	417	27% 86% • 10%
1	C	417	41% 83% • 12%
1	D	417	29% 84% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23372 atoms, of which 11728 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	368	Total	C	H	N	O	S	0	0	0
			5574	1876	2777	430	471	20			
1	B	374	Total	C	H	N	O	S	0	0	0
			5769	1917	2901	455	475	21			
1	C	365	Total	C	H	N	O	S	0	0	0
			5607	1876	2806	438	467	20			
1	D	369	Total	C	H	N	O	S	0	0	0
			5638	1885	2824	441	468	20			

There are 40 discrepancies between the modelled and reference sequences:

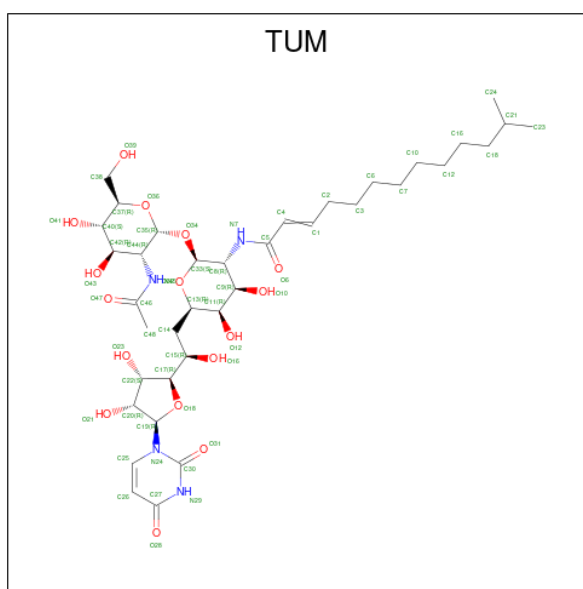
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	HIS	PRO	variant	UNP Q9H3H5
A	409	THR	-	expression tag	UNP Q9H3H5
A	410	ASN	-	expression tag	UNP Q9H3H5
A	411	SER	-	expression tag	UNP Q9H3H5
A	412	LEU	-	expression tag	UNP Q9H3H5
A	413	GLU	-	expression tag	UNP Q9H3H5
A	414	VAL	-	expression tag	UNP Q9H3H5
A	415	LEU	-	expression tag	UNP Q9H3H5
A	416	PHE	-	expression tag	UNP Q9H3H5
A	417	GLN	-	expression tag	UNP Q9H3H5
B	129	HIS	PRO	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	129	HIS	PRO	variant	UNP Q9H3H5
C	409	THR	-	expression tag	UNP Q9H3H5
C	410	ASN	-	expression tag	UNP Q9H3H5
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	129	HIS	PRO	variant	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).



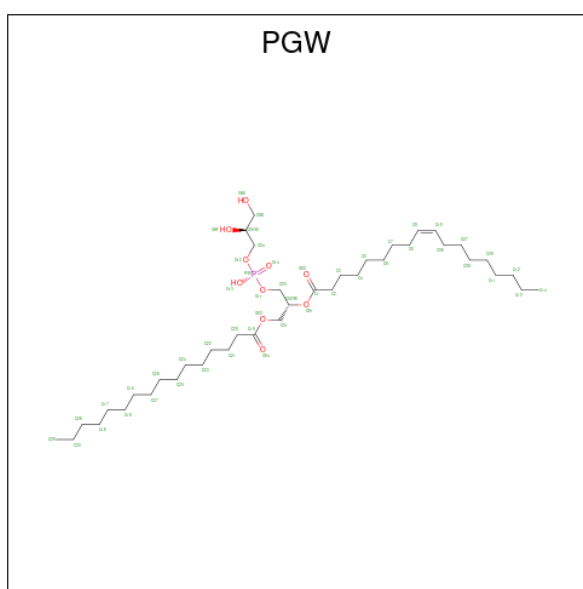
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			117	37	60	4	16		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
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).

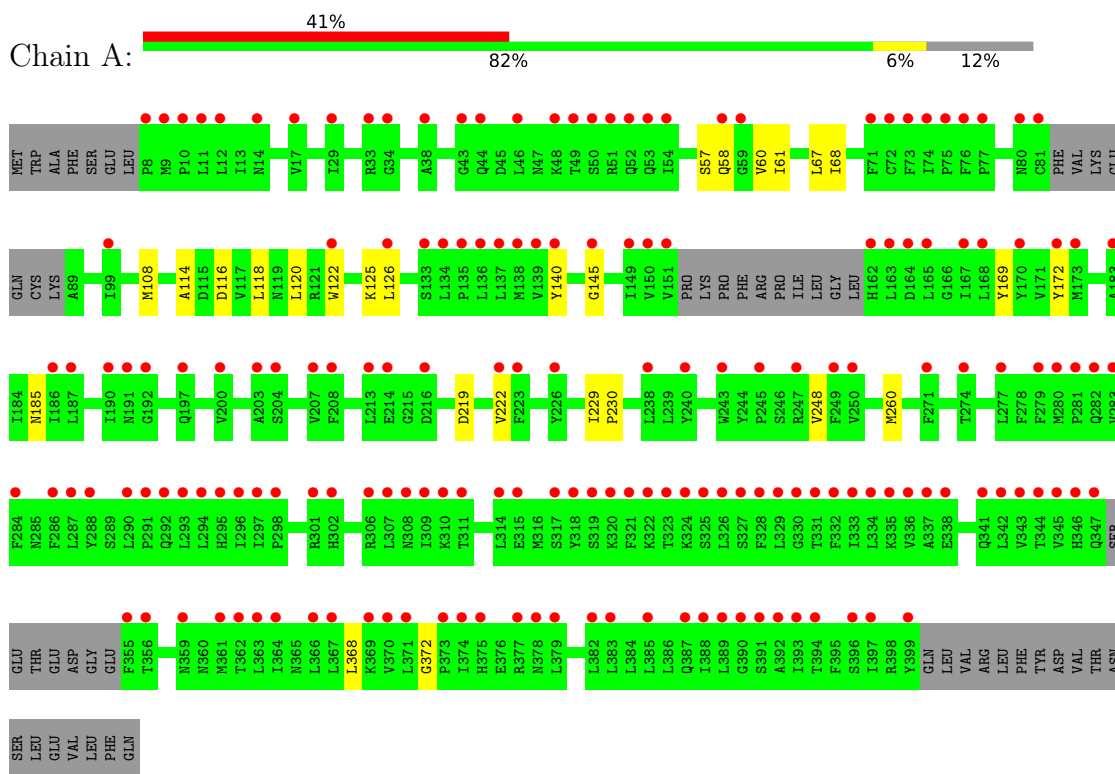


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	B	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	C	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	C	1	Total	C	H	O	P	0	0
			79	24	45	9	1		

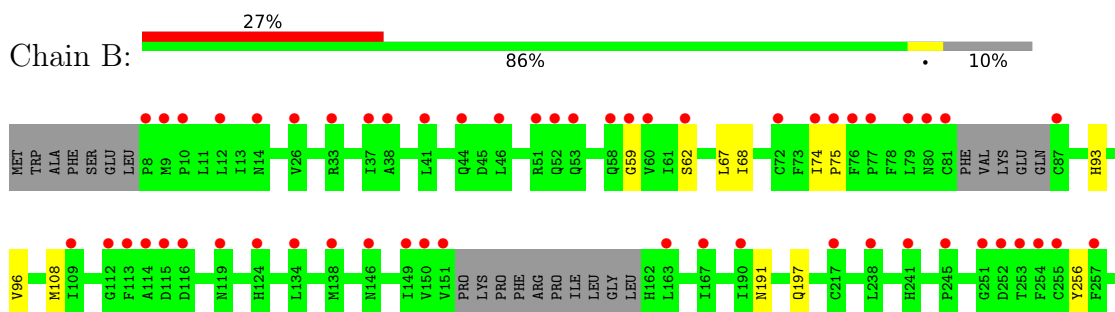
3 Residue-property plots [i](#)

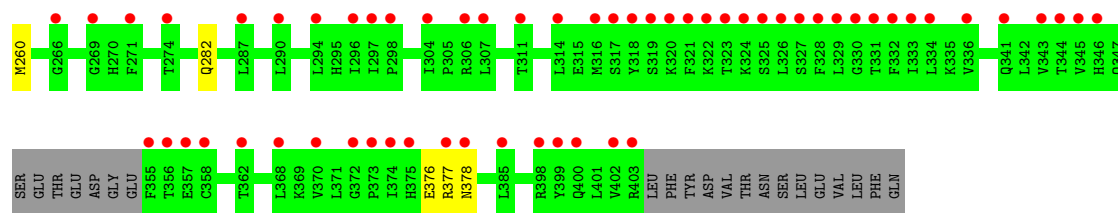
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

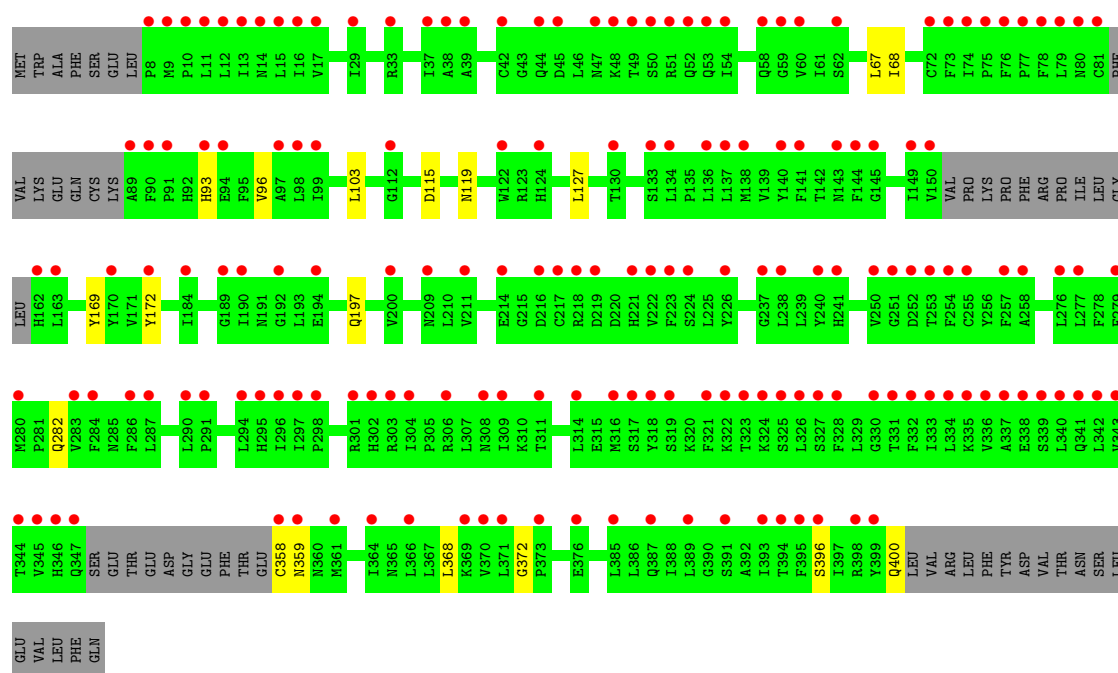
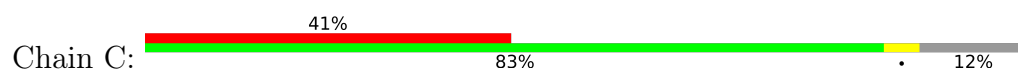


- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase

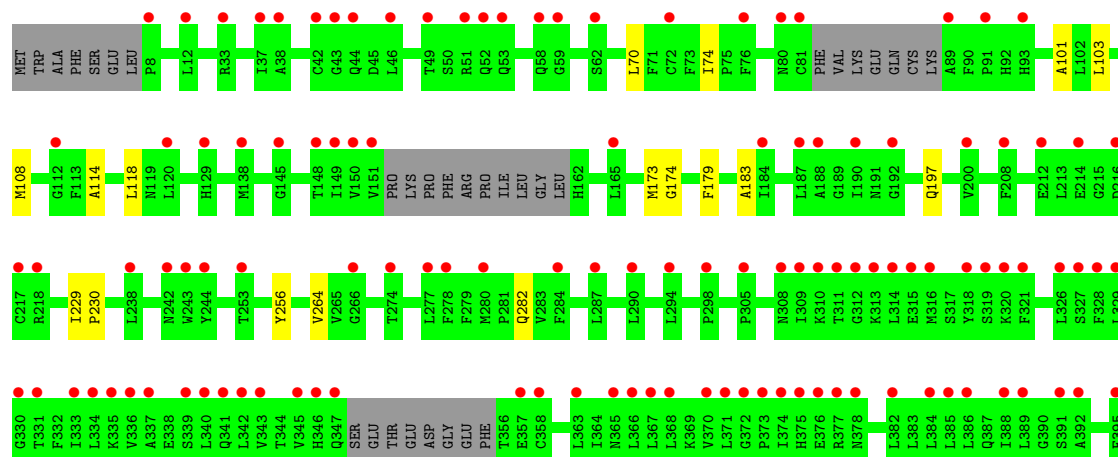
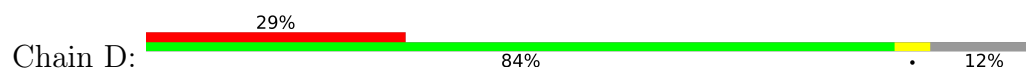




• Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminephosphotransferase



• Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminephosphotransferase



Y399	VAL
Q400	ARG
L401	LEU
	PHE
	TYR
	ASP
	VAL
	THR
	ASN
	SER
	LEU
	GLU
	VAL
	LEU
	PHE
	GLN

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.62Å 105.36Å 148.08Å 90.00° 103.49° 90.00°	Depositor
Resolution (Å)	94.51 – 2.95 94.51 – 2.95	Depositor EDS
% Data completeness (in resolution range)	55.3 (94.51-2.95) 51.5 (94.51-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.260 , 0.291 0.260 , 0.291	Depositor DCC
R_{free} test set	1832 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	23372	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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	0.15	0/2870	0.31	0/3923
1	B	0.16	0/2940	0.30	0/4009
1	C	0.15	0/2874	0.30	0/3922
1	D	0.15	0/2886	0.29	0/3939
All	All	0.15	0/11570	0.30	0/15793

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	2797	2777	2777	14	0
1	B	2868	2901	2901	9	0
1	C	2801	2806	2806	10	0
1	D	2814	2824	2824	9	0
2	A	57	60	0	1	0
2	B	57	60	0	0	0
2	C	57	60	0	0	0
2	D	57	60	0	0	0
3	A	34	45	45	0	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	68	90	90	0	0
All	All	11644	11728	11488	41	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 2.

All (41) 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:C:358:CYS:SG	1:C:359:ASN:N	2.76	0.57
1:C:396:SER:O	1:C:400:GLN:N	2.38	0.56
1:B:108:MET:HG3	1:B:256:TYR:HB3	1.88	0.55
1:B:191:ASN:ND2	1:B:376:GLU:OE2	2.42	0.53
1:C:115:ASP:O	1:C:119:ASN:N	2.39	0.51
1:A:57:SER:OG	1:A:116:ASP:OD2	2.29	0.50
1:A:185:ASN:ND2	2:A:501:TUM:O6	2.45	0.49
1:A:114:ALA:O	1:A:118:LEU:HG	2.12	0.49
1:D:197:GLN:OE1	1:D:282:GLN:NE2	2.46	0.49
1:A:58:GLN:HG3	1:A:248:VAL:HB	1.96	0.48
1:A:120:LEU:O	1:A:125:LYS:NZ	2.46	0.48
1:C:368:LEU:O	1:C:372:GLY:N	2.47	0.47
1:D:114:ALA:O	1:D:118:LEU:HG	2.14	0.47
1:B:197:GLN:OE1	1:B:282:GLN:NE2	2.41	0.47
1:A:368:LEU:O	1:A:372:GLY:N	2.47	0.47
1:D:101:ALA:HB1	1:D:264:VAL:HG11	1.98	0.46
1:B:377:ARG:NH2	1:B:378:ASN:OD1	2.49	0.46
1:C:197:GLN:OE1	1:C:282:GLN:NE2	2.43	0.46
1:C:169:TYR:O	1:C:172:TYR:HB3	2.16	0.46
1:A:140:TYR:O	1:A:145:GLY:N	2.49	0.45
1:B:93:HIS:O	1:B:96:VAL:HG12	2.16	0.45
1:D:229:ILE:HB	1:D:230:PRO:HD3	1.99	0.45
1:C:103:LEU:HA	1:D:103:LEU:HD13	1.99	0.45
1:D:70:LEU:O	1:D:74:ILE:HG13	2.17	0.45
1:D:108:MET:HG3	1:D:256:TYR:HB3	2.00	0.43
1:A:67:LEU:O	1:A:68:ILE:C	2.61	0.43
1:A:229:ILE:HB	1:A:230:PRO:HD3	2.01	0.42
1:B:67:LEU:O	1:B:68:ILE:C	2.61	0.42
1:C:67:LEU:O	1:C:68:ILE:C	2.63	0.42
1:C:127:LEU:C	1:C:127:LEU:HD23	2.45	0.42
1:D:179:PHE:O	1:D:183:ALA:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG13	1:A:61:ILE:N	2.35	0.42
1:A:122:TRP:O	1:A:126:LEU:HG	2.20	0.41
1:A:219:ASP:HA	1:A:222:VAL:HG12	2.03	0.41
1:A:108:MET:HG2	1:A:260:MET:HB2	2.03	0.41
1:B:108:MET:HG2	1:B:260:MET:HB2	2.03	0.41
1:B:59:GLY:O	1:B:62:SER:OG	2.39	0.40
1:A:169:TYR:O	1:A:172:TYR:HB3	2.21	0.40
1:B:74:ILE:N	1:B:75:PRO:CD	2.85	0.40
1:D:173:MET:O	1:D:174:GLY:C	2.65	0.40
1:C:93:HIS:O	1:C:96:VAL:HG12	2.21	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	360/417 (86%)	352 (98%)	8 (2%)	0	100	100
1	B	366/417 (88%)	355 (97%)	11 (3%)	0	100	100
1	C	357/417 (86%)	342 (96%)	15 (4%)	0	100	100
1	D	361/417 (87%)	354 (98%)	7 (2%)	0	100	100
All	All	1444/1668 (87%)	1403 (97%)	41 (3%)	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	296/370 (80%)	296 (100%)	0	100	100
1	B	307/370 (83%)	307 (100%)	0	100	100
1	C	298/370 (80%)	298 (100%)	0	100	100
1	D	298/370 (80%)	298 (100%)	0	100	100
All	All	1199/1480 (81%)	1199 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	92	HIS
1	B	143	ASN
1	B	292	GLN
1	B	359	ASN
1	C	92	HIS
1	C	124	HIS
1	D	124	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	502	-	33,33,50	0.89	2 (6%)	35,38,56	0.82	1 (2%)
2	TUM	C	501	-	60,60,60	1.72	14 (23%)	83,84,84	1.58	16 (19%)
3	PGW	C	502	-	33,33,50	0.90	2 (6%)	35,38,56	0.81	1 (2%)
3	PGW	C	503	-	33,33,50	0.90	2 (6%)	35,38,56	0.85	1 (2%)
2	TUM	B	502	-	60,60,60	1.73	14 (23%)	83,84,84	1.56	14 (16%)
3	PGW	B	501	-	33,33,50	0.90	2 (6%)	35,38,56	0.81	1 (2%)
2	TUM	D	501	-	60,60,60	1.73	14 (23%)	83,84,84	1.68	14 (16%)
2	TUM	A	501	-	60,60,60	1.72	13 (21%)	83,84,84	1.52	12 (14%)

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	A	502	-	-	12/37/37/55	-
2	TUM	C	501	-	-	11/39/95/95	0/4/4/4
3	PGW	C	502	-	-	20/37/37/55	-
3	PGW	C	503	-	-	11/37/37/55	-
2	TUM	B	502	-	-	10/39/95/95	0/4/4/4
3	PGW	B	501	-	-	14/37/37/55	-
2	TUM	D	501	-	-	10/39/95/95	0/4/4/4
2	TUM	A	501	-	-	3/39/95/95	0/4/4/4

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	TUM	C5-N7	5.91	1.47	1.34
2	D	501	TUM	C5-N7	5.90	1.47	1.34
2	C	501	TUM	C5-N7	5.87	1.47	1.34
2	A	501	TUM	C5-N7	5.83	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TUM	O18-C17	4.11	1.50	1.44
2	C	501	TUM	O18-C17	3.91	1.49	1.44
2	B	502	TUM	O18-C17	3.86	1.49	1.44
2	D	501	TUM	O18-C17	3.85	1.49	1.44
2	A	501	TUM	O18-C19	3.68	1.50	1.42
2	B	502	TUM	O18-C19	3.59	1.50	1.42
2	C	501	TUM	O18-C19	3.59	1.50	1.42
2	B	502	TUM	C26-C27	-3.57	1.36	1.43
2	D	501	TUM	O18-C19	3.54	1.50	1.42
2	D	501	TUM	C26-C27	-3.50	1.36	1.43
2	A	501	TUM	C26-C27	-3.50	1.36	1.43
2	C	501	TUM	C27-N29	-3.48	1.32	1.38
2	B	502	TUM	C27-N29	-3.47	1.32	1.38
2	A	501	TUM	C27-N29	-3.47	1.32	1.38
2	C	501	TUM	C26-C27	-3.47	1.36	1.43
2	D	501	TUM	C27-N29	-3.36	1.32	1.38
2	C	501	TUM	C46-N45	3.26	1.44	1.34
2	A	501	TUM	C46-N45	3.26	1.44	1.34
2	B	502	TUM	C46-N45	3.21	1.44	1.34
2	D	501	TUM	C46-N45	3.19	1.44	1.34
2	B	502	TUM	O28-C27	-3.01	1.18	1.24
2	C	501	TUM	O28-C27	-2.95	1.18	1.24
2	D	501	TUM	O6-C5	-2.91	1.18	1.24
2	C	501	TUM	O6-C5	-2.91	1.18	1.24
2	B	502	TUM	C4-C5	2.89	1.54	1.48
2	D	501	TUM	O28-C27	-2.88	1.18	1.24
2	A	501	TUM	O28-C27	-2.87	1.18	1.24
2	B	502	TUM	O6-C5	-2.83	1.19	1.24
2	A	501	TUM	O6-C5	-2.83	1.19	1.24
2	A	501	TUM	C4-C5	2.78	1.54	1.48
2	C	501	TUM	C4-C5	2.74	1.54	1.48
3	B	501	PGW	O01-C02	-2.71	1.40	1.46
2	D	501	TUM	C4-C5	2.71	1.54	1.48
3	C	502	PGW	O01-C02	-2.70	1.40	1.46
3	C	503	PGW	O01-C02	-2.69	1.40	1.46
2	C	501	TUM	C22-C20	-2.62	1.46	1.53
3	A	502	PGW	O01-C02	-2.58	1.40	1.46
2	B	502	TUM	C22-C20	-2.57	1.46	1.53
2	A	501	TUM	C22-C20	-2.56	1.46	1.53
2	D	501	TUM	C22-C20	-2.49	1.46	1.53
2	D	501	TUM	C25-N24	-2.48	1.32	1.38
2	C	501	TUM	O31-C30	-2.34	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	TUM	O31-C30	-2.33	1.18	1.23
2	B	502	TUM	C25-N24	-2.32	1.32	1.38
2	B	502	TUM	O31-C30	-2.32	1.19	1.23
2	C	501	TUM	C25-N24	-2.30	1.32	1.38
2	A	501	TUM	C25-N24	-2.30	1.32	1.38
2	A	501	TUM	O31-C30	-2.27	1.19	1.23
3	A	502	PGW	O01-C1	2.27	1.40	1.34
2	C	501	TUM	O47-C46	-2.26	1.18	1.23
2	B	502	TUM	O47-C46	-2.25	1.18	1.23
2	D	501	TUM	O47-C46	-2.22	1.18	1.23
2	A	501	TUM	O47-C46	-2.20	1.18	1.23
3	C	503	PGW	O01-C1	2.15	1.40	1.34
3	C	502	PGW	O01-C1	2.12	1.40	1.34
3	B	501	PGW	O01-C1	2.11	1.40	1.34
2	D	501	TUM	C19-N24	-2.09	1.41	1.47
2	C	501	TUM	C19-N24	-2.07	1.41	1.47
2	B	502	TUM	C19-N24	-2.05	1.41	1.47

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	TUM	C27-N29-C30	-5.65	119.60	126.61
2	B	502	TUM	C27-N29-C30	-5.56	119.71	126.61
2	C	501	TUM	C27-N29-C30	-5.54	119.74	126.61
2	A	501	TUM	C27-N29-C30	-5.51	119.77	126.61
2	D	501	TUM	C33-O32-C13	4.61	122.72	113.72
2	B	502	TUM	C26-C27-N29	4.06	120.49	114.80
2	C	501	TUM	C26-C27-N29	4.05	120.47	114.80
2	D	501	TUM	O32-C13-C11	4.02	116.94	109.70
2	A	501	TUM	N29-C30-N24	4.00	120.10	114.89
2	A	501	TUM	C26-C27-N29	3.94	120.33	114.80
2	D	501	TUM	N29-C30-N24	3.92	120.00	114.89
2	D	501	TUM	C26-C27-N29	3.89	120.25	114.80
2	B	502	TUM	N29-C30-N24	3.81	119.84	114.89
2	C	501	TUM	N29-C30-N24	3.80	119.84	114.89
3	C	503	PGW	O01-C1-C2	3.64	119.36	111.48
3	A	502	PGW	O01-C1-C2	3.62	119.31	111.48
2	A	501	TUM	C15-C17-C22	-3.62	110.76	115.95
3	B	501	PGW	O01-C1-C2	3.33	118.69	111.48
2	B	502	TUM	O28-C27-C26	-3.27	119.53	125.16
2	B	502	TUM	C15-C17-C22	-3.26	111.28	115.95
2	D	501	TUM	O28-C27-C26	-3.23	119.60	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TUM	O28-C27-C26	-3.15	119.72	125.16
2	D	501	TUM	C22-C20-C19	3.14	107.40	101.46
2	C	501	TUM	O28-C27-C26	-3.13	119.77	125.16
2	D	501	TUM	C9-C8-N7	3.12	116.37	110.62
2	A	501	TUM	C22-C20-C19	3.12	107.36	101.46
3	C	502	PGW	O01-C1-C2	3.11	118.20	111.48
2	C	501	TUM	C22-C20-C19	3.08	107.28	101.46
2	B	502	TUM	C22-C20-C19	3.03	107.19	101.46
2	D	501	TUM	C15-C17-C22	-2.99	111.65	115.95
2	C	501	TUM	O32-C33-C8	-2.99	104.94	110.59
2	D	501	TUM	C20-C22-C17	2.82	106.36	102.35
2	C	501	TUM	C15-C17-C22	-2.80	111.93	115.95
2	B	502	TUM	C2-C1-C4	-2.78	120.13	125.92
2	D	501	TUM	C2-C1-C4	-2.75	120.19	125.92
2	A	501	TUM	C2-C1-C4	-2.72	120.26	125.92
2	C	501	TUM	C20-C22-C17	2.72	106.21	102.35
2	A	501	TUM	C33-O32-C13	2.71	119.02	113.72
2	B	502	TUM	C33-O32-C13	2.62	118.84	113.72
2	B	502	TUM	C14-C13-C11	-2.62	109.22	113.47
2	A	501	TUM	C20-C22-C17	2.60	106.05	102.35
2	C	501	TUM	C2-C1-C4	-2.55	120.62	125.92
2	B	502	TUM	C20-C22-C17	2.49	105.89	102.35
2	D	501	TUM	O31-C30-N24	-2.42	119.65	122.80
2	C	501	TUM	C11-C9-C8	-2.36	106.96	110.40
2	B	502	TUM	O32-C13-C11	2.29	113.82	109.70
2	A	501	TUM	C48-C46-N45	2.28	119.90	116.12
2	C	501	TUM	C14-C13-C11	-2.28	109.77	113.47
2	A	501	TUM	O32-C13-C11	2.25	113.76	109.70
2	C	501	TUM	C33-O32-C13	2.23	118.08	113.72
2	B	502	TUM	C4-C5-N7	2.20	118.37	114.61
2	C	501	TUM	C4-C5-N7	2.19	118.36	114.61
2	B	502	TUM	O31-C30-N24	-2.19	119.95	122.80
2	A	501	TUM	C4-C5-N7	2.16	118.30	114.61
2	B	502	TUM	C11-C9-C8	-2.14	107.29	110.40
2	D	501	TUM	C48-C46-N45	2.08	119.56	116.12
2	C	501	TUM	O31-C30-N24	-2.06	120.12	122.80
2	D	501	TUM	C19-N24-C30	2.05	121.28	117.59
2	C	501	TUM	C48-C46-N45	2.04	119.50	116.12
2	C	501	TUM	C33-C8-N7	2.03	114.32	110.92

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TUM	C9-C8-N7-C5
2	B	502	TUM	C33-C8-N7-C5
2	B	502	TUM	C14-C15-C17-O18
2	B	502	TUM	O16-C15-C17-O18
2	C	501	TUM	C33-C8-N7-C5
2	C	501	TUM	O16-C15-C17-O18
2	D	501	TUM	C9-C8-N7-C5
2	D	501	TUM	O16-C15-C17-O18
3	A	502	PGW	O12-C04-C05-CAD
3	B	501	PGW	C03-O11-P-O12
3	B	501	PGW	C03-O11-P-O13
3	B	501	PGW	O12-C04-C05-CAD
3	C	502	PGW	C03-O11-P-O12
3	C	502	PGW	C03-O11-P-O14
3	C	502	PGW	C04-O12-P-O14
3	C	503	PGW	C03-O11-P-O12
3	C	503	PGW	C03-O11-P-O14
3	B	501	PGW	C05-C04-O12-P
3	B	501	PGW	O12-C04-C05-OAF
3	A	502	PGW	C05-C04-O12-P
3	A	502	PGW	O12-C04-C05-OAF
3	C	502	PGW	O12-C04-C05-OAF
3	C	503	PGW	O12-C04-C05-OAF
3	C	502	PGW	C1-C2-C3-C4
2	D	501	TUM	C1-C4-C5-O6
3	C	502	PGW	O12-C04-C05-CAD
3	C	503	PGW	O12-C04-C05-CAD
2	D	501	TUM	C1-C4-C5-N7
3	B	501	PGW	C5-C6-C7-C8
3	C	503	PGW	C1-C2-C3-C4
2	B	502	TUM	O16-C15-C17-C22
2	C	501	TUM	O16-C15-C17-C22
2	D	501	TUM	O16-C15-C17-C22
3	B	501	PGW	C1-C2-C3-C4
3	B	501	PGW	C2-C1-O01-C02
3	A	502	PGW	C3-C4-C5-C6
3	B	501	PGW	C06-C07-C08-C09
2	B	502	TUM	C14-C15-C17-C22
2	C	501	TUM	C14-C15-C17-C22
2	D	501	TUM	C14-C15-C17-C22
2	C	501	TUM	C14-C15-C17-O18
2	D	501	TUM	C14-C15-C17-O18
3	A	502	PGW	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
3	B	501	PGW	O02-C1-O01-C02
3	C	502	PGW	C4-C5-C6-C7
2	D	501	TUM	O36-C37-C38-O39
2	B	502	TUM	O36-C37-C38-O39
2	A	501	TUM	O36-C37-C38-O39
3	C	503	PGW	C06-C07-C08-C09
3	C	502	PGW	C06-C07-C08-C09
3	C	502	PGW	C6-C7-C8-C9
3	C	503	PGW	C01-C02-C03-O11
3	A	502	PGW	C5-C6-C7-C8
3	C	503	PGW	C6-C7-C8-C9
2	C	501	TUM	O36-C37-C38-O39
2	B	502	TUM	C1-C2-C3-C6
2	C	501	TUM	C12-C10-C7-C6
3	C	502	PGW	C01-C02-C03-O11
3	A	502	PGW	C6-C7-C8-C9
2	D	501	TUM	C12-C10-C7-C6
3	C	502	PGW	O01-C02-C03-O11
2	D	501	TUM	C1-C2-C3-C6
3	C	502	PGW	C09-C11-C12-C13
3	C	503	PGW	O01-C02-C03-O11
3	B	501	PGW	C03-O11-P-O14
3	B	501	PGW	C04-O12-P-O11
3	C	502	PGW	C03-O11-P-O13
3	C	502	PGW	C04-O12-P-O11
3	A	502	PGW	C2-C3-C4-C5
2	C	501	TUM	C2-C3-C6-C7
3	A	502	PGW	C08-C09-C11-C12
3	B	501	PGW	C09-C11-C12-C13
3	C	502	PGW	C2-C3-C4-C5
3	C	502	PGW	C08-C09-C11-C12
3	C	503	PGW	C7-C8-C9-C10
3	A	502	PGW	C10-C06-C07-C08
2	B	502	TUM	C12-C10-C7-C6
3	C	502	PGW	C01-C02-O01-C1
3	B	501	PGW	O03-C01-C02-O01
2	B	502	TUM	C9-C8-N7-C5
3	C	502	PGW	C03-C02-O01-C1
2	C	501	TUM	C4-C1-C2-C3
2	B	502	TUM	C4-C1-C2-C3
3	C	503	PGW	C4-C5-C6-C7
3	A	502	PGW	O01-C02-C03-O11

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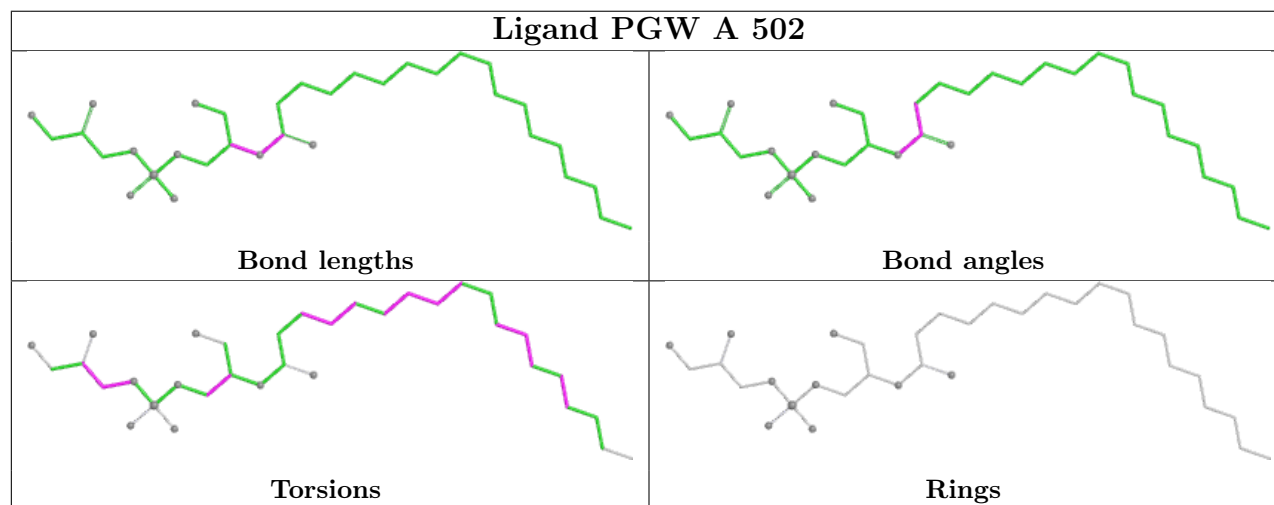
Mol	Chain	Res	Type	Atoms
3	A	502	PGW	C7-C8-C9-C10
3	C	502	PGW	C7-C8-C9-C10
2	C	501	TUM	O36-C35-O34-C33
2	C	501	TUM	C9-C8-N7-C5
3	C	502	PGW	O02-C1-O01-C02
2	A	501	TUM	C3-C6-C7-C10

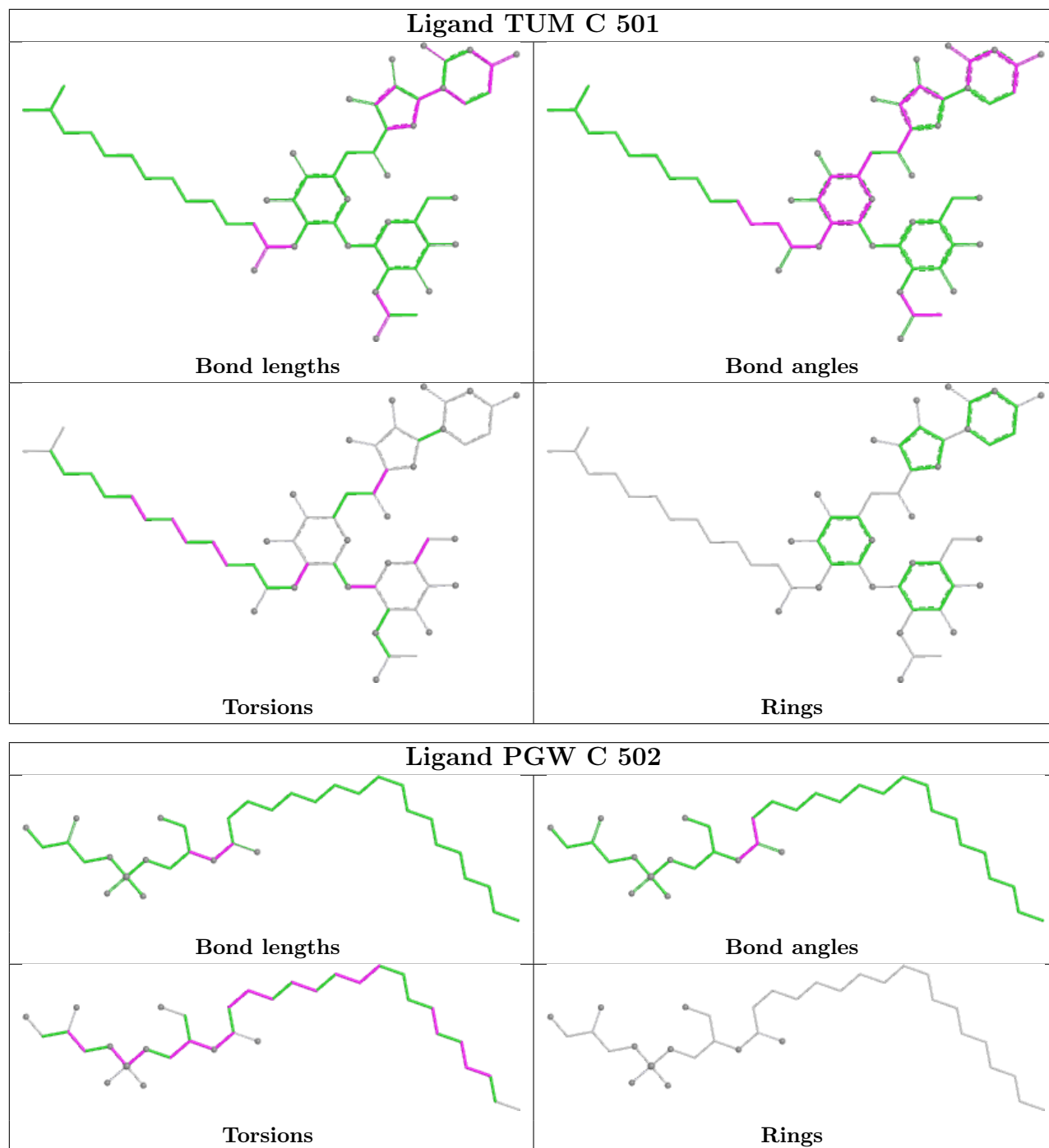
There are no ring outliers.

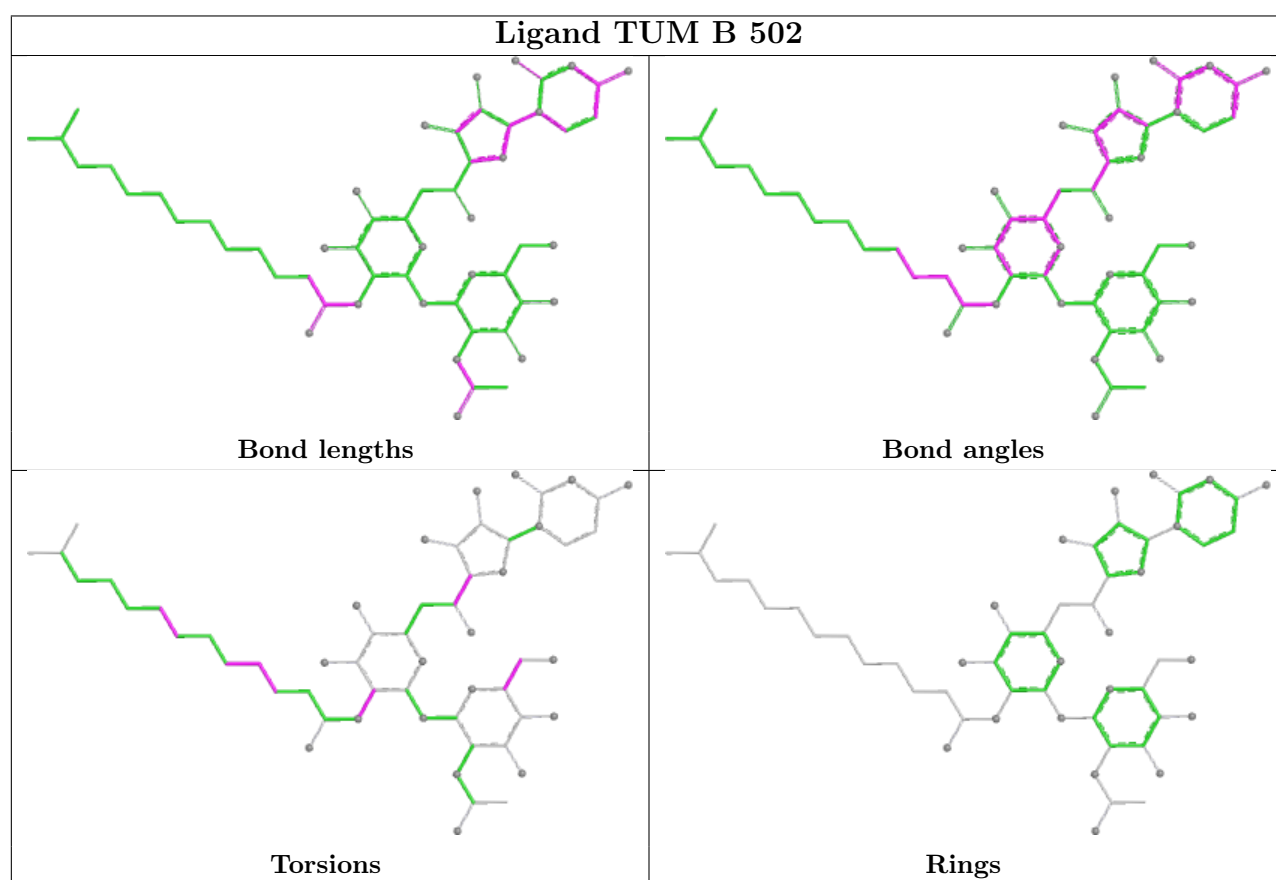
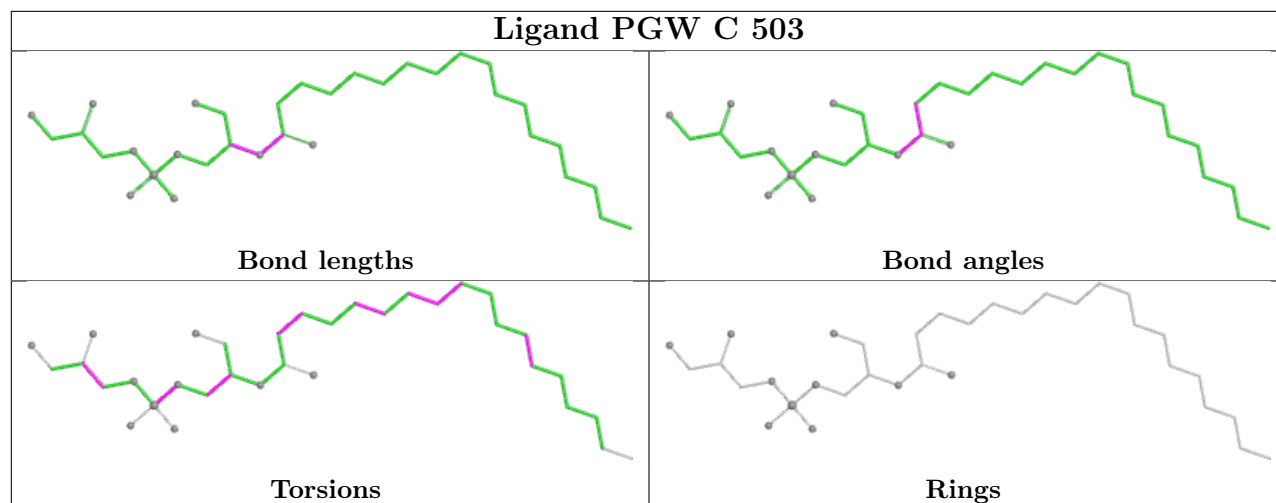
1 monomer is involved in 1 short contact:

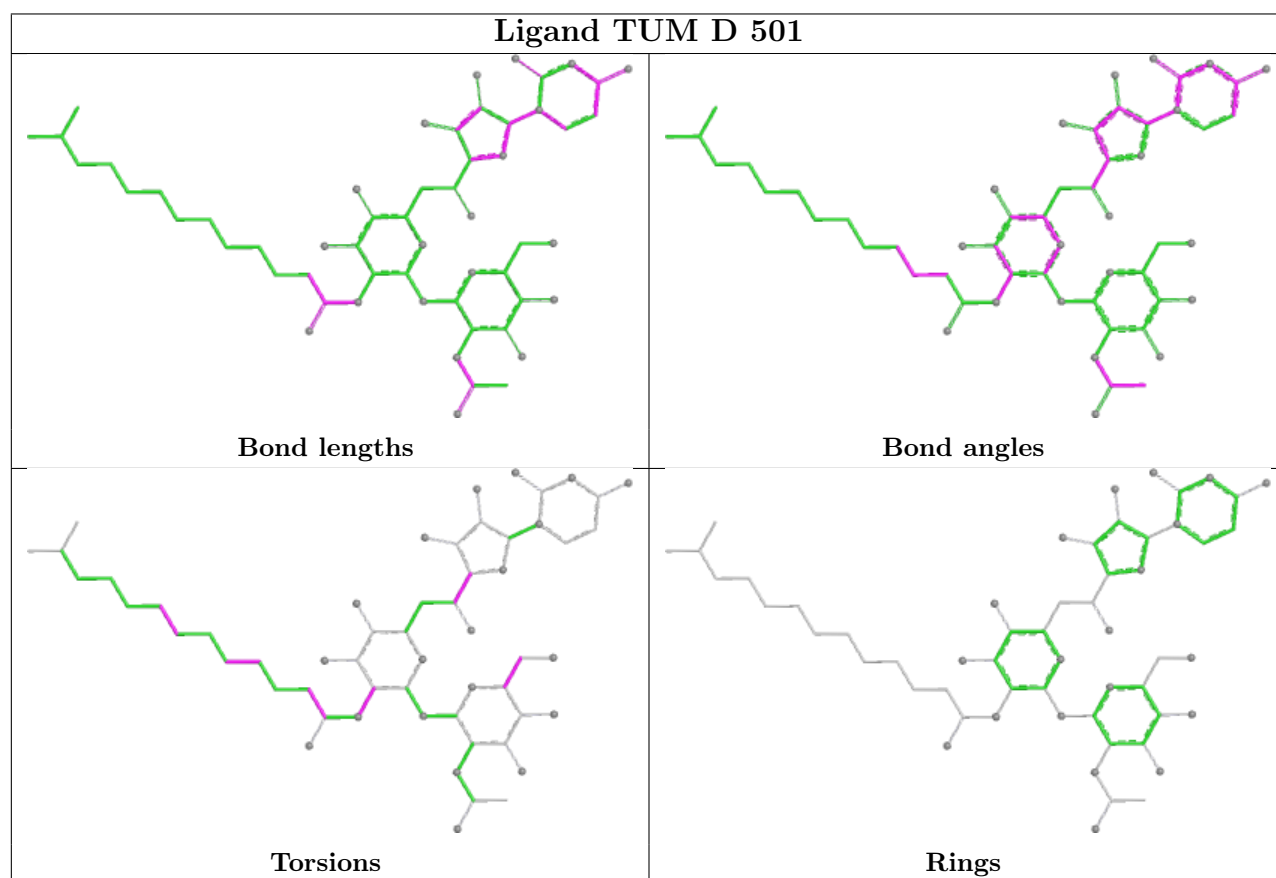
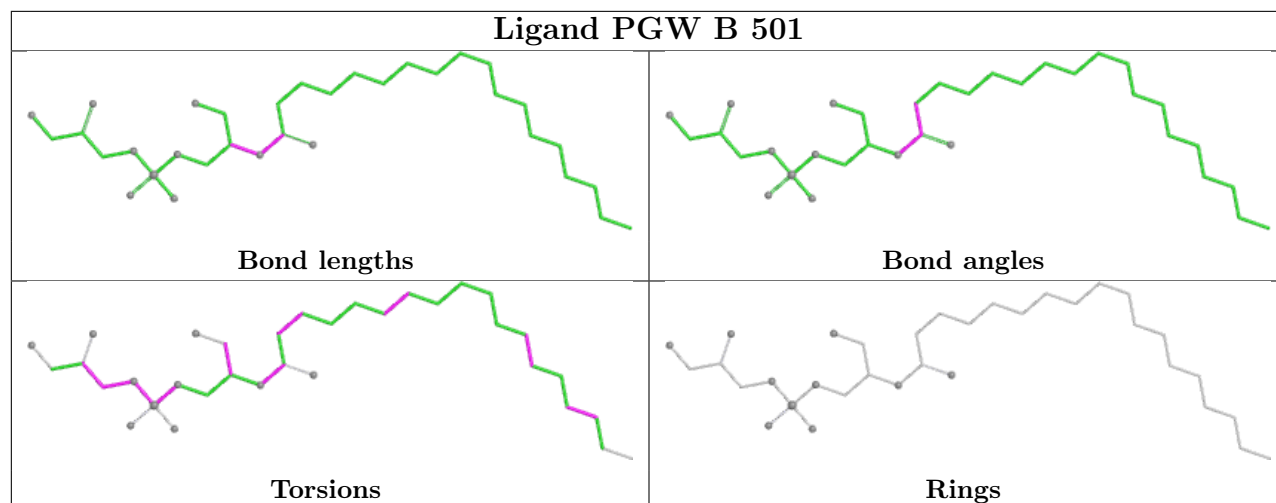
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TUM	1	0

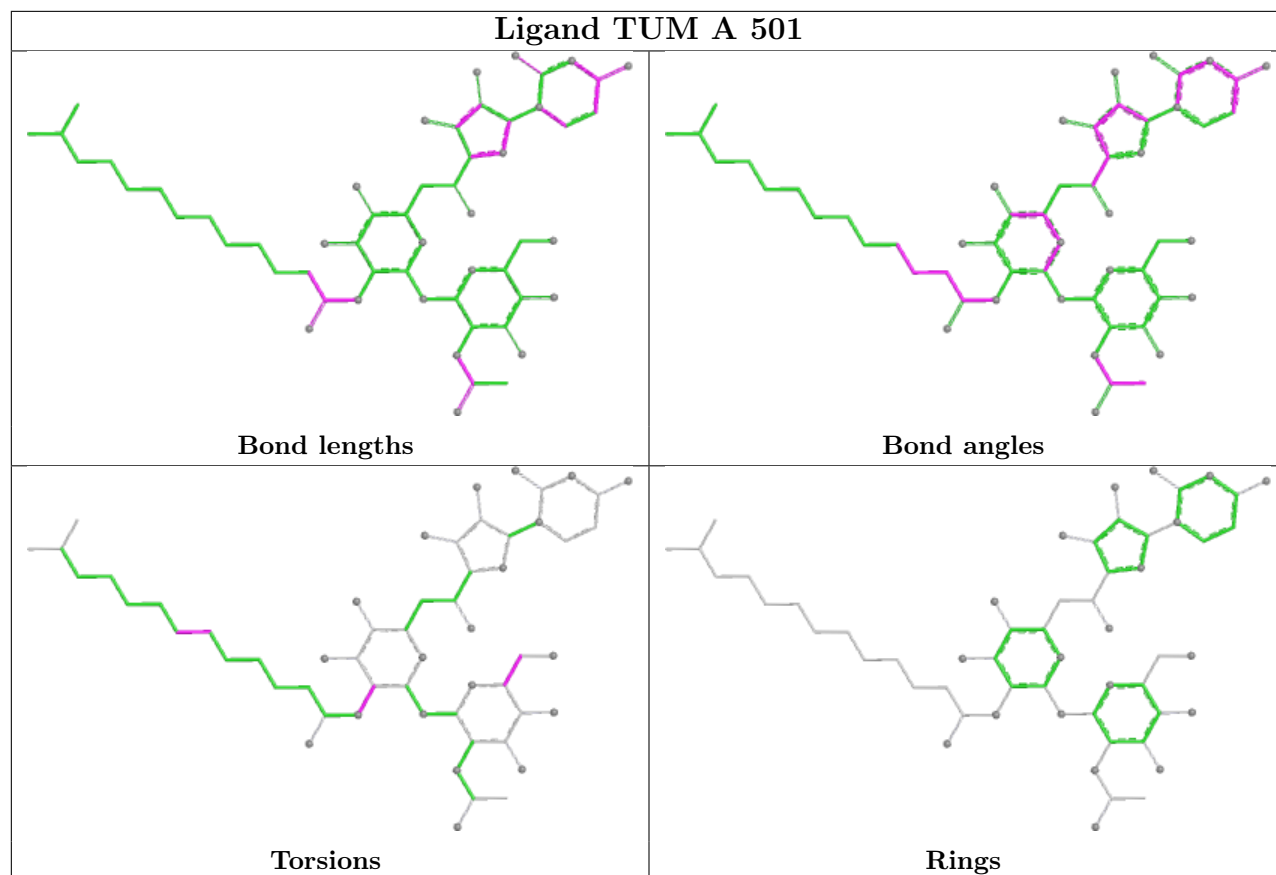
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	368/417 (88%)	2.25	173 (47%) 0 0	11, 58, 95, 120	0
1	B	374/417 (89%)	1.57	114 (30%) 1 1	8, 32, 72, 88	0
1	C	365/417 (87%)	2.45	172 (47%) 0 0	10, 46, 90, 107	0
1	D	369/417 (88%)	1.72	120 (32%) 1 1	7, 38, 79, 100	0
All	All	1476/1668 (88%)	2.00	579 (39%) 1 0	7, 42, 86, 120	0

All (579) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	MET	19.3
1	C	10	PRO	18.4
1	C	8	PRO	16.9
1	C	12	LEU	14.6
1	C	52	GLN	13.2
1	C	51	ARG	11.8
1	B	52	GLN	11.4
1	B	357	GLU	10.3
1	C	49	THR	10.2
1	C	76	PHE	10.1
1	C	81	CYS	9.4
1	A	72	CYS	8.8
1	A	389	LEU	8.6
1	B	306	ARG	8.6
1	C	13	ILE	8.6
1	C	53	GLN	8.5
1	D	53	GLN	8.4
1	C	341	GLN	8.3
1	C	283	VAL	8.2
1	D	313	LYS	8.2
1	A	138	MET	8.0

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Mol	Chain	Res	Type	RSRZ
1	B	53	GLN	7.9
1	A	347	GLN	7.7
1	D	318	TYR	7.6
1	B	326	LEU	7.6
1	B	345	VAL	7.5
1	B	74	ILE	7.3
1	D	389	LEU	7.2
1	B	356	THR	7.1
1	D	375	HIS	7.0
1	C	11	LEU	7.0
1	C	75	PRO	6.9
1	D	309	ILE	6.7
1	A	391	SER	6.6
1	D	311	THR	6.6
1	A	137	LEU	6.6
1	D	52	GLN	6.5
1	A	287	LEU	6.5
1	C	394	THR	6.4
1	A	325	SER	6.4
1	D	312	GLY	6.4
1	C	74	ILE	6.3
1	D	368	LEU	6.3
1	A	328	PHE	6.3
1	A	277	LEU	6.2
1	D	372	GLY	6.1
1	C	287	LEU	6.1
1	B	321	PHE	6.0
1	C	337	ALA	6.0
1	C	343	VAL	6.0
1	C	223	PHE	5.9
1	B	402	VAL	5.9
1	C	309	ILE	5.8
1	C	297	ILE	5.8
1	A	280	MET	5.8
1	D	327	SER	5.8
1	B	72	CYS	5.8
1	D	374	ILE	5.8
1	C	224	SER	5.7
1	D	49	THR	5.7
1	A	309	ILE	5.7
1	A	168	LEU	5.7
1	A	322	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	75	PRO	5.7
1	D	370	VAL	5.7
1	C	44	GLN	5.6
1	B	318	TYR	5.6
1	B	76	PHE	5.6
1	A	8	PRO	5.6
1	C	335	LYS	5.5
1	A	286	PHE	5.5
1	A	294	LEU	5.5
1	A	52	GLN	5.5
1	C	327	SER	5.5
1	C	145	GLY	5.4
1	A	170	TYR	5.4
1	A	226	TYR	5.4
1	C	277	LEU	5.4
1	A	321	PHE	5.3
1	C	144	PHE	5.3
1	B	44	GLN	5.3
1	C	79	LEU	5.3
1	A	295	HIS	5.3
1	D	378	ASN	5.2
1	C	325	SER	5.2
1	C	50	SER	5.2
1	A	49	THR	5.2
1	C	339	SER	5.2
1	B	320	LYS	5.2
1	C	59	GLY	5.2
1	C	226	TYR	5.2
1	D	81	CYS	5.1
1	C	15	LEU	5.1
1	A	76	PHE	5.1
1	C	78	PHE	5.1
1	A	165	LEU	5.1
1	C	276	LEU	5.1
1	B	51	ARG	5.1
1	B	372	GLY	5.0
1	D	59	GLY	5.0
1	A	334	LEU	5.0
1	B	59	GLY	5.0
1	A	216	ASP	5.0
1	A	200	VAL	5.0
1	A	290	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	323	THR	4.9
1	C	42	CYS	4.9
1	B	343	VAL	4.9
1	A	17	VAL	4.8
1	A	284	PHE	4.8
1	D	357	GLU	4.8
1	B	37	ILE	4.8
1	C	14	ASN	4.8
1	A	387	GLN	4.8
1	C	98	LEU	4.7
1	C	138	MET	4.7
1	A	388	ILE	4.7
1	C	359	ASN	4.7
1	C	219	ASP	4.7
1	D	308	ASN	4.7
1	D	51	ARG	4.7
1	B	112	GLY	4.6
1	B	358	CYS	4.6
1	C	334	LEU	4.5
1	C	358	CYS	4.5
1	A	296	ILE	4.5
1	A	335	LYS	4.5
1	D	377	ARG	4.5
1	A	145	GLY	4.5
1	D	401	LEU	4.5
1	A	172	TYR	4.5
1	A	74	ILE	4.5
1	A	392	ALA	4.5
1	A	341	GLN	4.5
1	C	280	MET	4.4
1	B	116	ASP	4.4
1	A	393	ILE	4.4
1	A	396	SER	4.4
1	C	344	THR	4.4
1	A	297	ILE	4.4
1	D	151	VAL	4.4
1	D	376	GLU	4.4
1	D	336	VAL	4.4
1	C	290	LEU	4.4
1	A	337	ALA	4.3
1	A	377	ARG	4.3
1	B	325	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	4.3
1	A	378	ASN	4.3
1	A	9	MET	4.3
1	D	331	THR	4.2
1	C	301	ARG	4.2
1	A	344	THR	4.2
1	C	80	ASN	4.2
1	D	385	LEU	4.2
1	C	322	LYS	4.2
1	A	75	PRO	4.2
1	C	222	VAL	4.2
1	C	255	CYS	4.1
1	D	244	TYR	4.1
1	C	37	ILE	4.1
1	C	328	PHE	4.1
1	C	338	GLU	4.1
1	A	53	GLN	4.1
1	C	347	GLN	4.1
1	D	341	GLN	4.1
1	A	204	SER	4.1
1	A	326	LEU	4.0
1	C	291	PRO	4.0
1	C	39	ALA	4.0
1	A	164	ASP	4.0
1	A	12	LEU	4.0
1	C	342	LEU	4.0
1	C	389	LEU	4.0
1	C	254	PHE	4.0
1	D	371	LEU	4.0
1	D	382	LEU	4.0
1	D	345	VAL	4.0
1	A	362	THR	4.0
1	A	149	ILE	3.9
1	A	14	ASN	3.9
1	B	344	THR	3.9
1	D	290	LEU	3.9
1	C	324	LYS	3.9
1	C	318	TYR	3.9
1	D	42	CYS	3.9
1	A	355	PHE	3.9
1	A	385	LEU	3.9
1	C	332	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	3.9
1	B	377	ARG	3.9
1	C	77	PRO	3.9
1	A	192	GLY	3.8
1	A	324	LYS	3.8
1	B	9	MET	3.8
1	A	44	GLN	3.8
1	A	133	SER	3.8
1	B	327	SER	3.8
1	A	10	PRO	3.8
1	D	315	GLU	3.8
1	D	72	CYS	3.8
1	B	290	LEU	3.8
1	A	167	ILE	3.8
1	B	287	LEU	3.8
1	A	50	SER	3.7
1	D	266	GLY	3.7
1	A	319	SER	3.7
1	C	38	ALA	3.7
1	D	340	LEU	3.7
1	C	16	ILE	3.7
1	C	345	VAL	3.7
1	C	393	ILE	3.7
1	B	375	HIS	3.7
1	D	44	GLN	3.7
1	A	363	LEU	3.7
1	D	284	PHE	3.7
1	A	29	ILE	3.7
1	B	12	LEU	3.7
1	A	331	THR	3.7
1	A	374	ILE	3.7
1	C	150	VAL	3.7
1	A	342	LEU	3.6
1	D	138	MET	3.6
1	C	284	PHE	3.6
1	A	371	LEU	3.6
1	B	77	PRO	3.6
1	C	134	LEU	3.6
1	D	310	LYS	3.6
1	A	345	VAL	3.6
1	B	151	VAL	3.6
1	D	305	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	391	SER	3.6
1	B	253	THR	3.6
1	C	311	THR	3.6
1	A	306	ARG	3.6
1	C	250	VAL	3.6
1	C	340	LEU	3.6
1	B	355	PHE	3.5
1	C	211	VAL	3.5
1	A	150	VAL	3.5
1	D	373	PRO	3.5
1	A	222	VAL	3.5
1	C	306	ARG	3.5
1	D	367	LEU	3.5
1	D	62	SER	3.5
1	B	298	PRO	3.5
1	D	399	TYR	3.5
1	D	38	ALA	3.5
1	B	374	ILE	3.4
1	A	151	VAL	3.4
1	C	72	CYS	3.4
1	A	288	TYR	3.4
1	B	81	CYS	3.4
1	C	143	ASN	3.4
1	C	286	PHE	3.4
1	D	316	MET	3.4
1	C	366	LEU	3.4
1	C	33	ARG	3.4
1	A	329	LEU	3.4
1	D	43	GLY	3.4
1	A	51	ARG	3.4
1	A	279	PHE	3.4
1	D	358	CYS	3.3
1	D	37	ILE	3.3
1	D	287	LEU	3.3
1	C	326	LEU	3.3
1	B	150	VAL	3.3
1	C	94	GLU	3.3
1	A	163	LEU	3.3
1	C	279	PHE	3.3
1	D	76	PHE	3.3
1	B	311	THR	3.3
1	A	298	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	11	LEU	3.3
1	D	391	SER	3.3
1	C	298	PRO	3.2
1	B	124	HIS	3.2
1	A	58	GLN	3.2
1	D	58	GLN	3.2
1	B	324	LYS	3.2
1	A	361	MET	3.2
1	C	385	LEU	3.2
1	A	292	GLN	3.2
1	C	48	LYS	3.2
1	C	323	THR	3.2
1	C	54	ILE	3.2
1	C	251	GLY	3.2
1	C	376	GLU	3.2
1	B	149	ILE	3.2
1	B	80	ASN	3.2
1	B	294	LEU	3.2
1	D	294	LEU	3.2
1	D	386	LEU	3.2
1	B	38	ALA	3.2
1	B	346	HIS	3.2
1	A	283	VAL	3.2
1	A	191	ASN	3.1
1	A	223	PHE	3.1
1	C	364	ILE	3.1
1	A	139	VAL	3.1
1	B	254	PHE	3.1
1	D	298	PRO	3.1
1	A	48	LYS	3.1
1	C	17	VAL	3.1
1	D	319	SER	3.1
1	A	238	LEU	3.1
1	A	369	LYS	3.1
1	C	369	LYS	3.1
1	A	73	PHE	3.0
1	C	295	HIS	3.0
1	B	252	ASP	3.0
1	A	81	CYS	3.0
1	D	314	LEU	3.0
1	C	331	THR	3.0
1	A	183	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	162	HIS	3.0
1	B	296	ILE	3.0
1	A	187	LEU	3.0
1	B	238	LEU	3.0
1	A	315	GLU	3.0
1	C	237	GLY	3.0
1	D	80	ASN	3.0
1	A	126	LEU	3.0
1	A	356	THR	3.0
1	A	343	VAL	3.0
1	C	302	HIS	3.0
1	A	122	TRP	3.0
1	A	282	GLN	3.0
1	B	79	LEU	3.0
1	B	341	GLN	3.0
1	B	331	THR	3.0
1	A	314	LEU	2.9
1	B	251	GLY	2.9
1	C	58	GLN	2.9
1	D	337	ALA	2.9
1	C	140	TYR	2.9
1	D	145	GLY	2.9
1	B	328	PHE	2.9
1	D	395	PHE	2.9
1	D	346	HIS	2.9
1	A	367	LEU	2.9
1	D	363	LEU	2.9
1	B	266	GLY	2.9
1	B	10	PRO	2.9
1	C	214	GLU	2.9
1	C	319	SER	2.9
1	B	60	VAL	2.9
1	A	186	ILE	2.9
1	B	163	LEU	2.9
1	C	387	GLN	2.9
1	A	135	PRO	2.9
1	C	396	SER	2.9
1	C	112	GLY	2.8
1	B	373	PRO	2.8
1	D	216	ASP	2.8
1	A	327	SER	2.8
1	B	319	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	62	SER	2.8
1	A	333	ILE	2.8
1	A	366	LEU	2.8
1	C	371	LEU	2.8
1	A	71	PHE	2.8
1	C	90	PHE	2.8
1	A	308	ASN	2.8
1	A	291	PRO	2.8
1	C	200	VAL	2.8
1	C	163	LEU	2.8
1	C	241	HIS	2.8
1	C	314	LEU	2.8
1	B	317	SER	2.8
1	D	339	SER	2.8
1	D	33	ARG	2.8
1	A	99	ILE	2.8
1	C	29	ILE	2.8
1	C	99	ILE	2.8
1	C	184	ILE	2.8
1	C	252	ASP	2.8
1	A	390	GLY	2.8
1	A	281	PRO	2.8
1	B	217	CYS	2.7
1	D	328	PHE	2.7
1	B	41	LEU	2.7
1	B	14	ASN	2.7
1	C	133	SER	2.7
1	C	73	PHE	2.7
1	D	320	LYS	2.7
1	C	216	ASP	2.7
1	D	149	ILE	2.7
1	D	188	ALA	2.7
1	C	93	HIS	2.7
1	A	34	GLY	2.7
1	A	43	GLY	2.7
1	A	330	GLY	2.7
1	B	323	THR	2.7
1	A	373	PRO	2.7
1	D	150	VAL	2.7
1	C	172	TYR	2.7
1	A	247	ARG	2.7
1	C	218	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	26	VAL	2.7
1	D	200	VAL	2.7
1	C	330	GLY	2.6
1	D	278	PHE	2.6
1	C	399	TYR	2.6
1	A	213	LEU	2.6
1	C	194	GLU	2.6
1	D	89	ALA	2.6
1	C	189	GLY	2.6
1	A	364	ILE	2.6
1	A	370	VAL	2.6
1	A	382	LEU	2.6
1	C	294	LEU	2.6
1	A	173	MET	2.6
1	B	115	ASP	2.6
1	C	192	GLY	2.6
1	C	370	VAL	2.6
1	D	217	CYS	2.6
1	D	347	GLN	2.6
1	D	365	ASN	2.6
1	A	379	LEU	2.5
1	A	59	GLY	2.5
1	A	383	LEU	2.5
1	C	91	PRO	2.5
1	D	238	LEU	2.5
1	C	149	ILE	2.5
1	B	58	GLN	2.5
1	C	130	THR	2.5
1	B	403	ARG	2.5
1	B	62	SER	2.5
1	B	385	LEU	2.5
1	D	12	LEU	2.5
1	A	240	TYR	2.5
1	A	214	GLU	2.5
1	B	322	LYS	2.5
1	A	302	HIS	2.5
1	B	307	LEU	2.5
1	B	316	MET	2.5
1	A	346	HIS	2.5
1	B	138	MET	2.4
1	C	137	LEU	2.4
1	D	366	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	384	LEU	2.4
1	A	332	PHE	2.4
1	C	257	PHE	2.4
1	D	208	PHE	2.4
1	B	399	TYR	2.4
1	B	274	THR	2.4
1	D	274	THR	2.4
1	D	165	LEU	2.4
1	A	397	ILE	2.4
1	B	113	PHE	2.4
1	D	321	PHE	2.4
1	D	253	THR	2.4
1	A	359	ASN	2.4
1	B	245	PRO	2.4
1	D	388	ILE	2.4
1	C	336	VAL	2.4
1	D	330	GLY	2.4
1	A	33	ARG	2.4
1	B	398	ARG	2.4
1	C	303	ARG	2.4
1	B	257	PHE	2.4
1	D	243	TRP	2.4
1	A	399	TYR	2.4
1	A	375	HIS	2.4
1	C	346	HIS	2.4
1	A	134	LEU	2.4
1	D	333	ILE	2.4
1	B	119	ASN	2.4
1	C	308	ASN	2.4
1	B	255	CYS	2.4
1	C	253	THR	2.4
1	C	238	LEU	2.4
1	A	80	ASN	2.3
1	A	271	PHE	2.3
1	A	338	GLU	2.3
1	C	162	HIS	2.3
1	A	190	ILE	2.3
1	C	333	ILE	2.3
1	A	245	PRO	2.3
1	B	370	VAL	2.3
1	B	314	LEU	2.3
1	A	243	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	304	ILE	2.3
1	B	8	PRO	2.3
1	D	343	VAL	2.3
1	B	330	GLY	2.3
1	D	242	ASN	2.3
1	A	203	ALA	2.3
1	B	87	CYS	2.3
1	C	221	HIS	2.3
1	D	93	HIS	2.3
1	A	301	ARG	2.3
1	D	8	PRO	2.3
1	B	269	GLY	2.3
1	A	38	ALA	2.3
1	B	114	ALA	2.3
1	C	258	ALA	2.3
1	C	136	LEU	2.3
1	D	329	LEU	2.3
1	B	297	ILE	2.3
1	A	394	THR	2.3
1	C	122	TRP	2.3
1	D	218	ARG	2.3
1	A	77	PRO	2.3
1	B	271	PHE	2.2
1	C	361	MET	2.2
1	D	214	GLU	2.2
1	A	197	GLN	2.2
1	B	241	HIS	2.2
1	C	217	CYS	2.2
1	A	249	PHE	2.2
1	D	120	LEU	2.2
1	D	212	GLU	2.2
1	D	392	ALA	2.2
1	A	320	LYS	2.2
1	B	378	ASN	2.2
1	A	318	TYR	2.2
1	B	368	LEU	2.2
1	D	46	LEU	2.2
1	D	334	LEU	2.2
1	D	335	LYS	2.2
1	D	342	LEU	2.2
1	C	209	ASN	2.2
1	B	304	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	190	ILE	2.2
1	A	274	THR	2.2
1	A	311	THR	2.2
1	A	208	PHE	2.2
1	A	136	LEU	2.2
1	C	97	ALA	2.2
1	B	109	ILE	2.2
1	B	167	ILE	2.2
1	D	184	ILE	2.2
1	C	47	ASN	2.2
1	B	46	LEU	2.2
1	B	336	VAL	2.1
1	C	373	PRO	2.1
1	D	91	PRO	2.1
1	D	192	GLY	2.1
1	C	141	PHE	2.1
1	C	170	TYR	2.1
1	B	333	ILE	2.1
1	B	146	ASN	2.1
1	A	336	VAL	2.1
1	C	60	VAL	2.1
1	C	316	MET	2.1
1	C	321	PHE	2.1
1	B	33	ARG	2.1
1	C	240	TYR	2.1
1	C	190	ILE	2.1
1	D	326	LEU	2.1
1	C	395	PHE	2.1
1	B	190	ILE	2.1
1	C	296	ILE	2.1
1	C	124	HIS	2.1
1	D	277	LEU	2.1
1	B	362	THR	2.1
1	C	45	ASP	2.1
1	C	317	SER	2.0
1	B	400	GLN	2.0
1	D	129	HIS	2.0
1	A	293	LEU	2.0
1	A	307	LEU	2.0
1	D	187	LEU	2.0
1	A	54	ILE	2.0
1	A	140	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	310	LYS	2.0
1	D	280	MET	2.0
1	A	317	SER	2.0
1	A	46	LEU	2.0
1	B	134	LEU	2.0
1	B	329	LEU	2.0
1	C	398	ARG	2.0
1	B	332	PHE	2.0
1	D	112	GLY	2.0
1	C	89	ALA	2.0
1	D	148	THR	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.

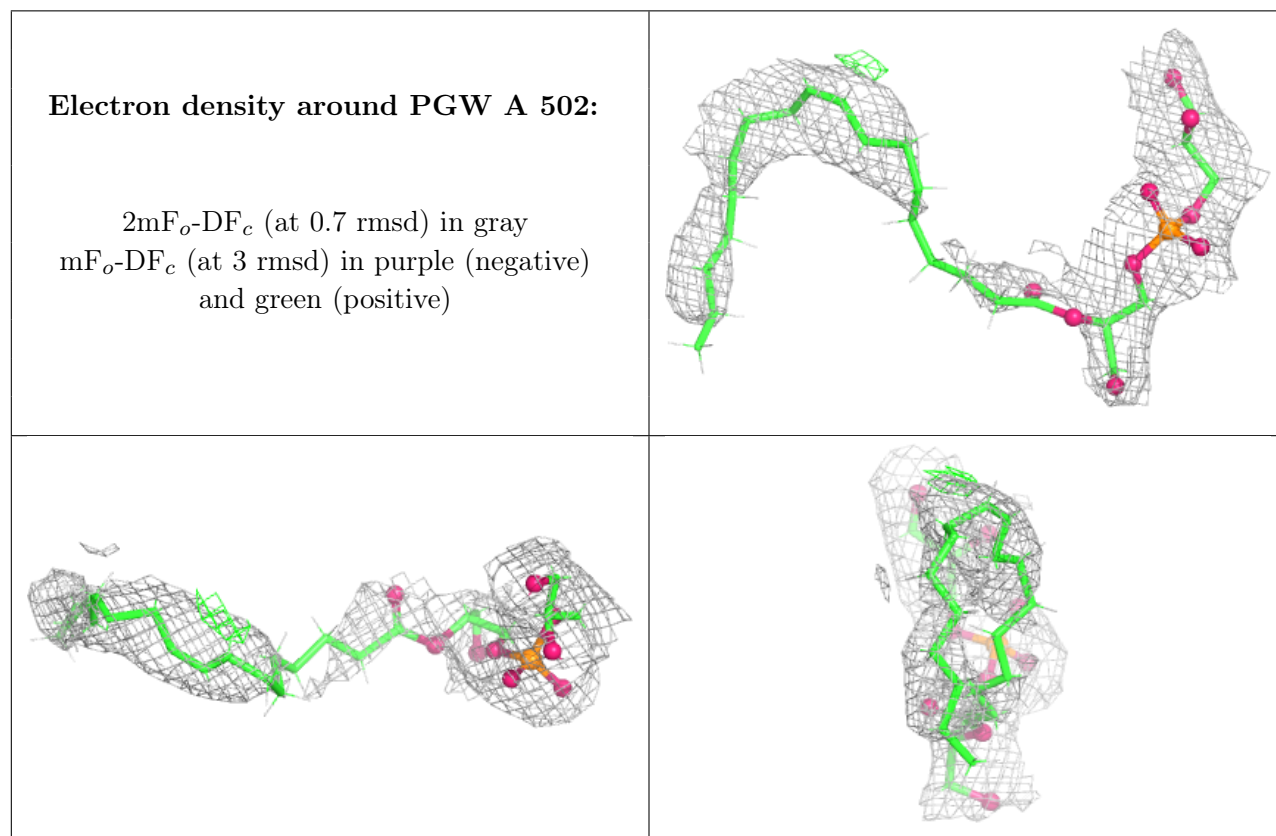
6.4 Ligands [i](#)

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PGW	A	502	34/51	0.79	0.23	18,64,92,110	0
3	PGW	C	502	34/51	0.79	0.21	9,40,93,100	0
3	PGW	C	503	34/51	0.79	0.20	9,43,91,119	0
3	PGW	B	501	34/51	0.83	0.19	14,41,80,87	0
2	TUM	A	501	57/57	0.87	0.15	28,49,69,81	0
2	TUM	D	501	57/57	0.88	0.17	15,34,58,69	0
2	TUM	C	501	57/57	0.89	0.18	27,45,69,83	0
2	TUM	B	502	57/57	0.90	0.22	45,57,75,84	0

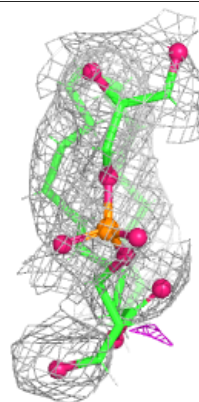
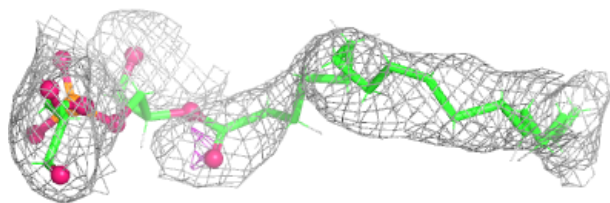
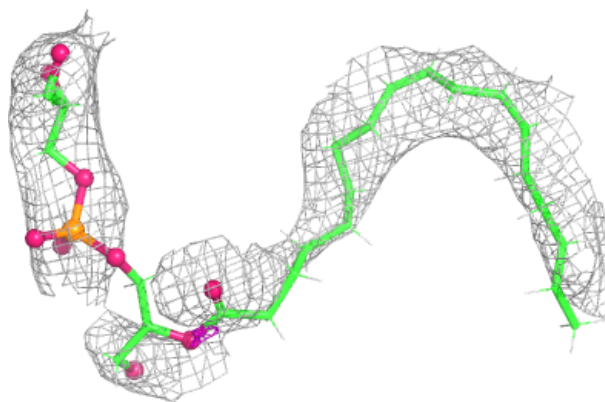
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

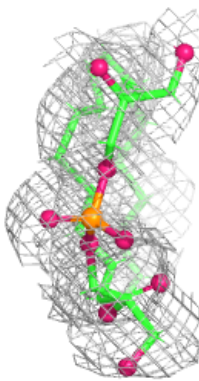
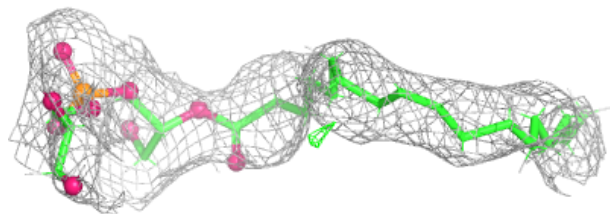


Electron density around PGW C 502:

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

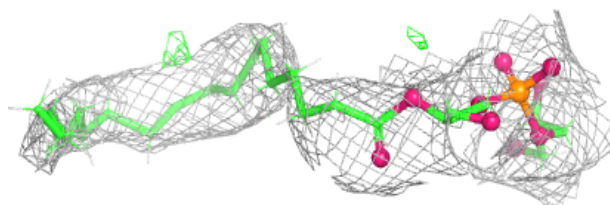
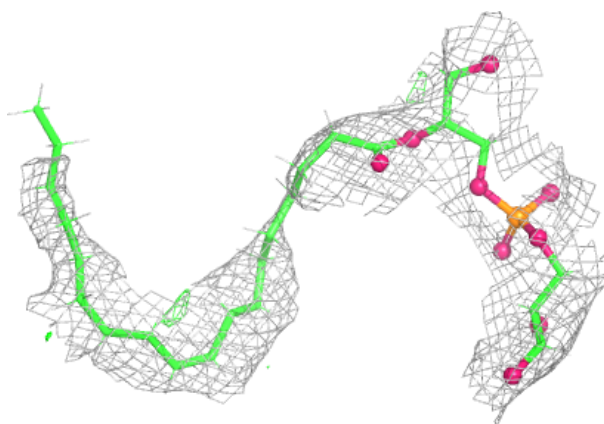
**Electron density around PGW C 503:**

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

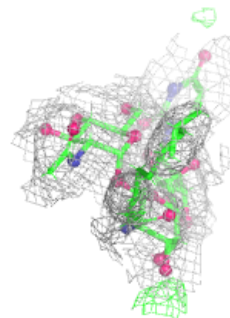
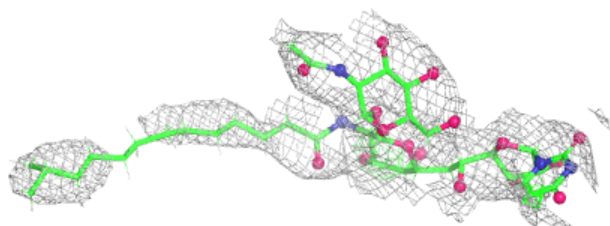
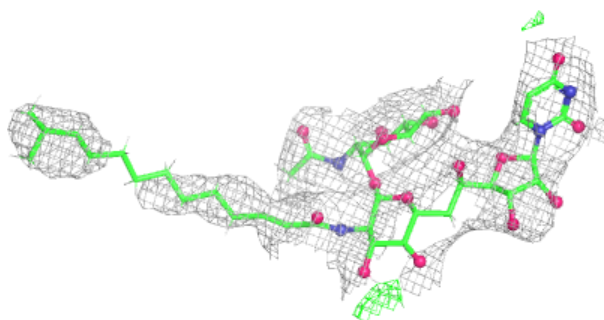


Electron density around PGW B 501:

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

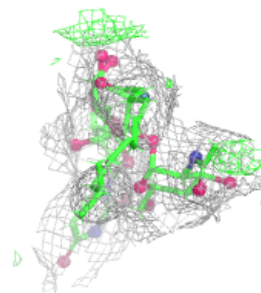
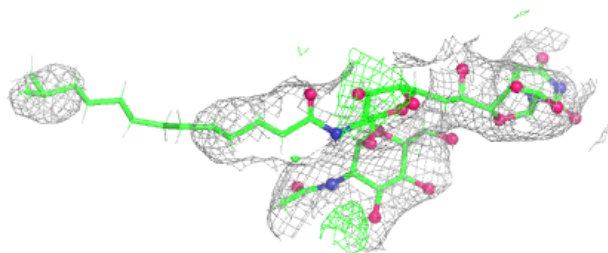
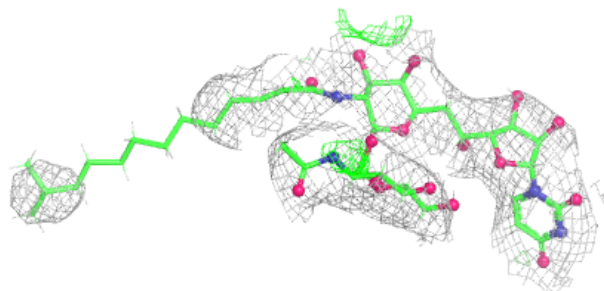
**Electron density around TUM A 501:**

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

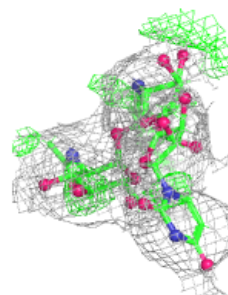
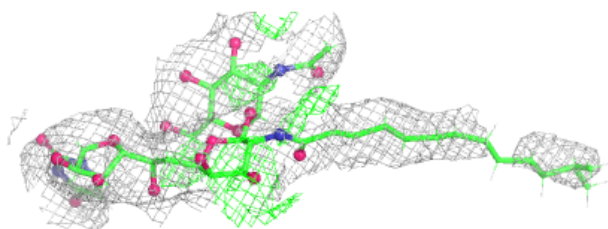
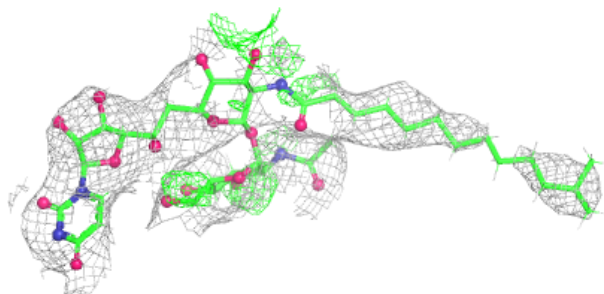


Electron density around TUM D 501:

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

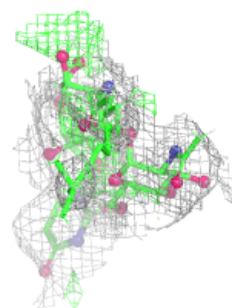
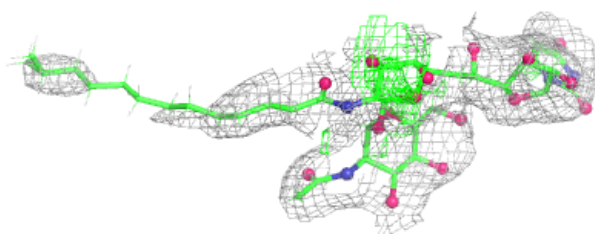
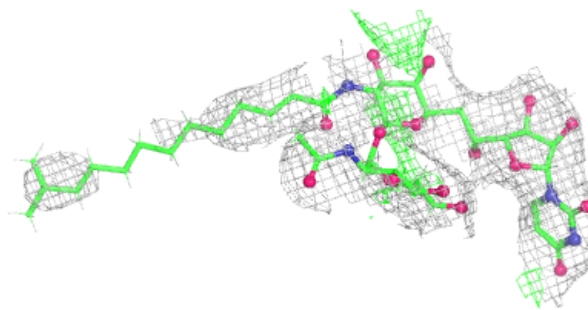
**Electron density around TUM C 501:**

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



Electron density around TUM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.