



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 01:33 PM EST

PDB ID : 6BW5
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

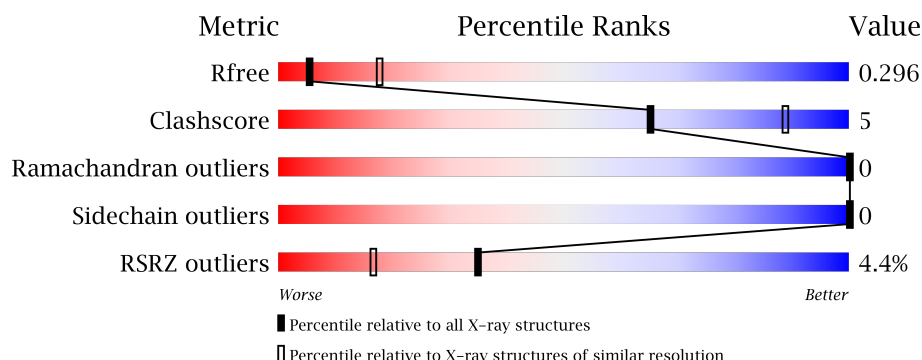
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>81% 10% 9%</div> </div>
1	B	417	<div> <div>4%</div> <div>80% 9% 12%</div> </div>
1	C	417	<div> <div>4%</div> <div>77% 13% 10%</div> </div>
1	D	417	<div> <div>4%</div> <div>77% 10% 13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGW	A	502	-	-	-	X
3	PGW	C	502	-	-	-	X

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:

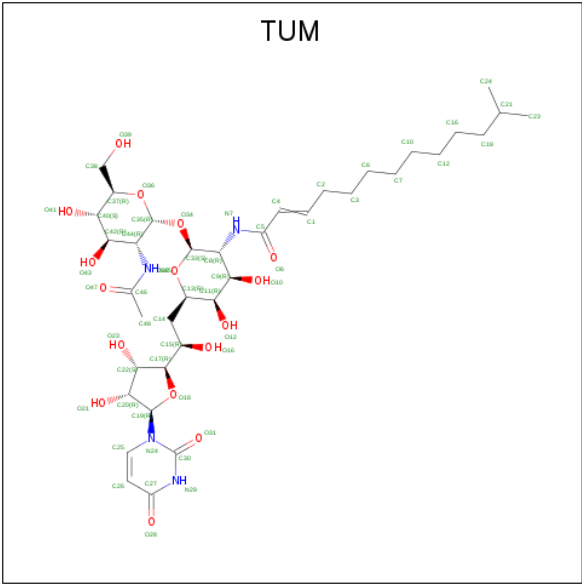
Chain	Residue	Modelled	Actual	Comment	Reference
A	409	THR	-	expression tag	UNP Q9H3H5
A	410	ASN	-	expression tag	UNP Q9H3H5
A	411	SER	-	expression tag	UNP Q9H3H5
A	412	LEU	-	expression tag	UNP Q9H3H5
A	413	GLU	-	expression tag	UNP Q9H3H5
A	414	VAL	-	expression tag	UNP Q9H3H5
A	415	LEU	-	expression tag	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 (three-letter code: TUM) (formula: C₃₇H₆₀N₄O₁₆).



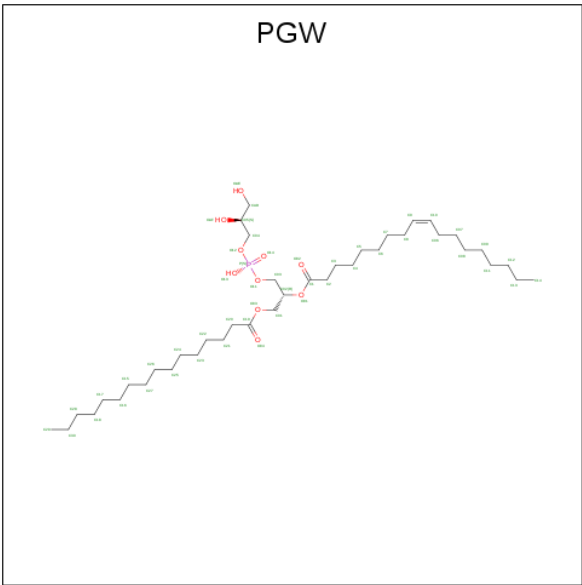
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			117	37	60	4	16		
2	B	1	Total	C	H	N	O	0	0
			117	37	60	4	16		
2	C	1	Total	C	H	N	O	0	0
			117	37	60	4	16		

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

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

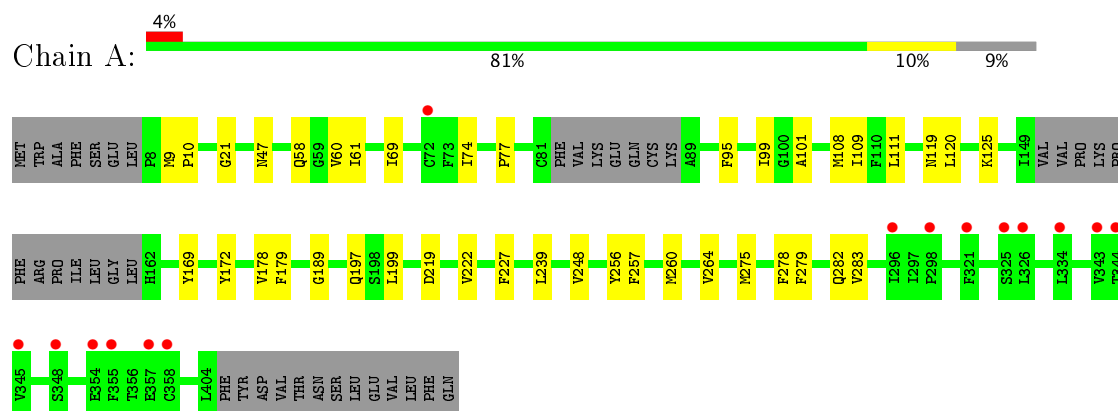


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
3	A	1	69	22	39	7	1	0	0
3	B	1	79	24	45	9	1	0	0
3	C	1	79	24	45	9	1	0	0
3	D	1	79	24	45	9	1	0	0

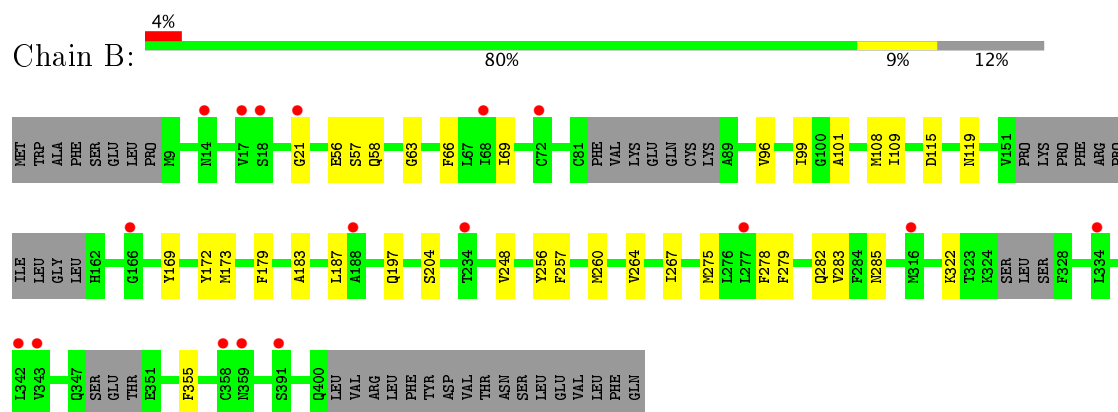
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

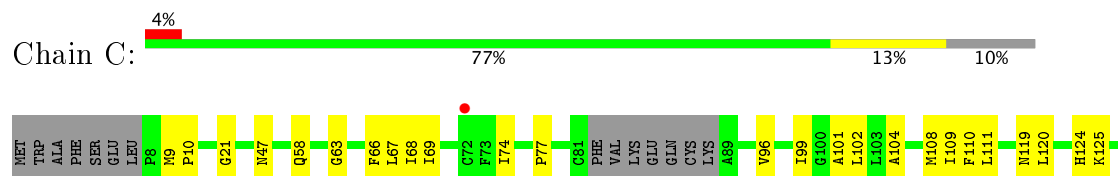
- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase

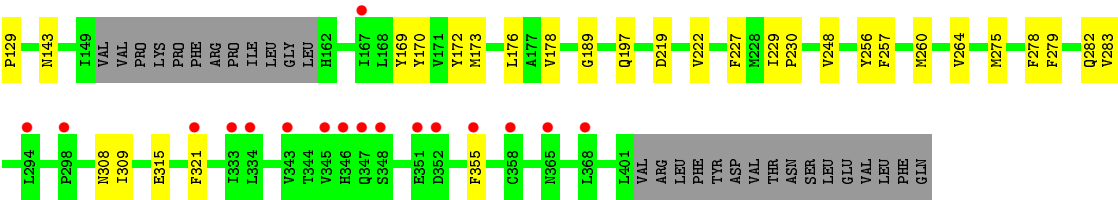


- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase

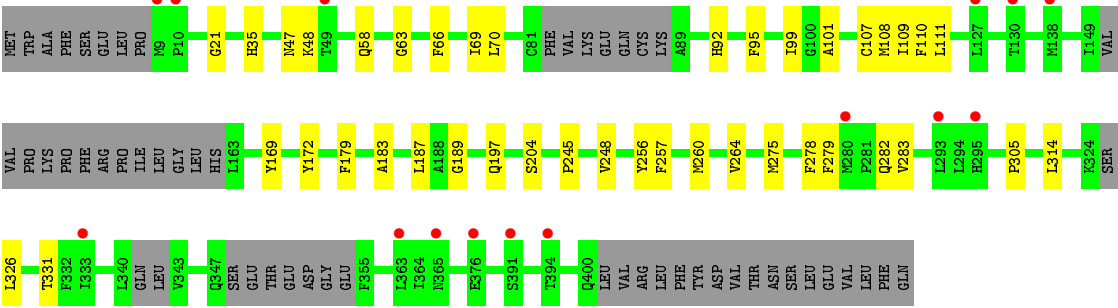
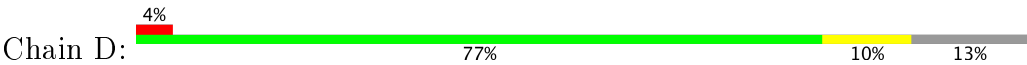


- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase





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



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 95.30 – 3.10	Depositor EDS
% Data completeness (in resolution range)	60.1 (83.05-3.10) 56.2 (95.30-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.256 , 0.288 0.261 , 0.296	Depositor DCC
R_{free} test set	1648 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 4.92% 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	0.27	0/2949	0.46	0/4025
1	B	0.27	0/2799	0.43	0/3830
1	C	0.29	0/2916	0.45	0/3982
1	D	0.28	0/2791	0.44	0/3814
All	All	0.28	0/11455	0.45	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	25	0
1	B	2731	2636	2633	23	0
1	C	2842	2820	2820	37	0
1	D	2722	2668	2666	27	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	107	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 5.

All (107) 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: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
1:C:21:GLY:HA3	1:C:69:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:99:ILE:HG22	1:D:99:ILE:HG22	1.98	0.45
1:A:111:LEU:HB2	3:A:502:PGW:H08A	1.99	0.44
1:C:170:TYR:HA	1:C:173:MET:HE2	1.99	0.44
1:C:111:LEU:HA	3:C:502:PGW:H08A	2.00	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:109:ILE:HG12	1:B:257:PHE:HB2	2.00	0.43
1:B:275:MET:HA	1:B:278:PHE:HD2	1.83	0.43
1:A:99:ILE:HG22	1:B:99:ILE:HG22	1.99	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
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:115:ASP:O	1:B:119:ASN:N	2.43	0.43
1:B:63:GLY:O	1:B:66:PHE:HB3	2.19	0.43
1:D:275:MET:O	1:D:278:PHE:N	2.52	0.43
1:D:21:GLY:HA3	1:D:69:ILE:HD11	2.01	0.43
1:A:169:TYR:O	1:A:172:TYR:HB3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD12	1:A:239:LEU:HD22	2.01	0.42
1:C:309:ILE:HD12	1:C:309:ILE:N	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:169:TYR:O	1:C:172:TYR:HB3	2.20	0.42
1:C:96:VAL:HG21	1:D:95:PHE:CD2	2.54	0.42
1:D:63:GLY:O	1:D:66:PHE:HB3	2.19	0.42
1:A:60:VAL:HG13	1:A:61:ILE:N	2.35	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: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: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:C:67:LEU:O	1:C:68:ILE:C	2.59	0.41
1:D:66:PHE:CZ	1:D:70:LEU:HD11	2.56	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: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
1:D:305:PRO:HB2	1:D:314:LEU:HB3	2.03	0.41
2:B:501:TUM:O41	2:B:501:TUM:O39	2.38	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:A:178:VAL:O	1:A:179:PHE:C	2.60	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:9:MET:N	1:C:10:PRO:CD	2.84	0.41
1:C:279:PHE:O	1:C:283:VAL:HG23	2.20	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:C:173:MET:O	1:C:176:LEU:HB3	2.21	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.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
2	TUM	A	501	-	55,60,60	1.81	12 (21%)	66,84,84	1.30	10 (15%)
3	PGW	A	502	-	29,29,50	0.86	2 (6%)	30,33,56	1.01	1 (3%)
2	TUM	B	501	-	55,60,60	1.79	12 (21%)	66,84,84	1.36	10 (15%)
3	PGW	B	502	-	33,33,50	0.86	2 (6%)	33,38,56	0.93	1 (3%)
2	TUM	C	501	-	55,60,60	1.78	12 (21%)	66,84,84	1.25	5 (7%)
3	PGW	C	502	-	33,33,50	0.89	2 (6%)	33,38,56	0.90	1 (3%)
2	TUM	D	501	-	55,60,60	1.77	13 (23%)	66,84,84	1.25	6 (9%)
3	PGW	D	502	-	33,33,50	0.85	2 (6%)	33,38,56	0.94	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TUM	A	501	-	-	0/35/95/95	0/4/4/4
3	PGW	A	502	-	-	0/32/32/55	0/0/0/0
2	TUM	B	501	-	-	0/35/95/95	0/4/4/4
3	PGW	B	502	-	-	0/37/37/55	0/0/0/0
2	TUM	C	501	-	-	0/35/95/95	0/4/4/4
3	PGW	C	502	-	-	0/37/37/55	0/0/0/0
2	TUM	D	501	-	-	0/35/95/95	0/4/4/4
3	PGW	D	502	-	-	0/37/37/55	0/0/0/0

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TUM	C27-N29	-3.13	1.32	1.36
2	C	501	TUM	C27-N29	-3.05	1.32	1.36
2	A	501	TUM	C27-N29	-3.05	1.32	1.36
2	D	501	TUM	C27-N29	-3.01	1.32	1.36
2	A	501	TUM	O6-C5	-2.96	1.18	1.24
2	A	501	TUM	C20-C19	-2.95	1.48	1.53
2	D	501	TUM	C20-C19	-2.94	1.49	1.53
2	D	501	TUM	O6-C5	-2.94	1.18	1.24
2	C	501	TUM	C20-C19	-2.93	1.49	1.53
2	C	501	TUM	O6-C5	-2.93	1.18	1.24
2	B	501	TUM	O6-C5	-2.87	1.18	1.24
2	B	501	TUM	C20-C19	-2.74	1.49	1.53
2	A	501	TUM	C25-N24	-2.73	1.32	1.35
2	C	501	TUM	C25-N24	-2.70	1.32	1.35
2	A	501	TUM	C20-C22	-2.70	1.46	1.53
2	D	501	TUM	C20-C22	-2.62	1.46	1.53
2	C	501	TUM	C20-C22	-2.58	1.46	1.53
2	D	501	TUM	C25-N24	-2.54	1.32	1.35
2	B	501	TUM	C20-C22	-2.53	1.46	1.53
3	A	502	PGW	O01-C02	-2.37	1.40	1.46
2	B	501	TUM	C25-N24	-2.35	1.32	1.35
3	D	502	PGW	O01-C02	-2.27	1.40	1.46
3	C	502	PGW	O01-C02	-2.22	1.40	1.46
3	B	502	PGW	O01-C02	-2.21	1.40	1.46
2	C	501	TUM	O28-C27	-2.20	1.19	1.24
2	B	501	TUM	O28-C27	-2.18	1.19	1.24
2	D	501	TUM	O28-C27	-2.17	1.19	1.24
2	C	501	TUM	O47-C46	-2.14	1.18	1.23
2	D	501	TUM	O47-C46	-2.14	1.18	1.23
2	A	501	TUM	O28-C27	-2.14	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TUM	O47-C46	-2.13	1.18	1.23
2	B	501	TUM	O47-C46	-2.13	1.18	1.23
2	D	501	TUM	C22-C17	-2.05	1.48	1.53
3	A	502	PGW	O01-C1	2.06	1.40	1.34
3	D	502	PGW	O01-C1	2.16	1.40	1.34
3	B	502	PGW	O01-C1	2.19	1.40	1.34
3	C	502	PGW	O01-C1	2.33	1.41	1.34
2	C	501	TUM	C46-N45	2.81	1.44	1.34
2	A	501	TUM	C46-N45	2.86	1.44	1.34
2	D	501	TUM	C46-N45	2.90	1.45	1.34
2	B	501	TUM	C46-N45	2.91	1.45	1.34
2	D	501	TUM	C4-C5	3.12	1.54	1.48
2	B	501	TUM	C4-C5	3.31	1.54	1.48
2	C	501	TUM	C4-C5	3.40	1.54	1.48
2	A	501	TUM	C4-C5	3.49	1.54	1.48
2	D	501	TUM	O18-C17	3.63	1.49	1.44
2	C	501	TUM	O18-C17	3.65	1.49	1.44
2	A	501	TUM	O18-C17	3.78	1.49	1.44
2	B	501	TUM	O18-C17	3.89	1.50	1.44
2	D	501	TUM	C5-N7	4.88	1.47	1.34
2	C	501	TUM	C5-N7	4.95	1.47	1.34
2	A	501	TUM	C5-N7	4.97	1.48	1.34
2	B	501	TUM	C5-N7	5.05	1.48	1.34
2	C	501	TUM	O18-C19	6.56	1.50	1.41
2	D	501	TUM	O18-C19	6.62	1.50	1.41
2	A	501	TUM	O18-C19	6.70	1.50	1.41
2	B	501	TUM	O18-C19	6.75	1.50	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	TUM	C15-C17-C22	-4.19	110.25	115.86
2	B	501	TUM	C2-C1-C4	-3.94	117.41	125.88
2	A	501	TUM	C15-C17-C22	-3.69	110.93	115.86
2	C	501	TUM	C15-C17-C22	-3.67	110.95	115.86
2	D	501	TUM	C2-C1-C4	-3.40	118.56	125.88
2	C	501	TUM	C14-C13-C11	-3.23	108.04	113.48
2	B	501	TUM	C40-C42-C44	-3.15	105.66	110.33
2	C	501	TUM	C2-C1-C4	-3.14	119.11	125.88
2	A	501	TUM	C2-C1-C4	-2.90	119.64	125.88
2	B	501	TUM	C15-C17-C22	-2.68	112.28	115.86
2	A	501	TUM	C14-C13-C11	-2.47	109.33	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	TUM	C17-O18-C19	-2.46	102.82	108.28
2	A	501	TUM	C38-C37-C40	-2.39	107.41	113.00
2	D	501	TUM	C38-C37-C40	-2.22	107.81	113.00
2	A	501	TUM	C40-C42-C44	-2.19	107.07	110.33
2	C	501	TUM	C11-C9-C8	-2.18	107.09	110.33
2	A	501	TUM	C11-C9-C8	-2.11	107.20	110.33
2	B	501	TUM	C42-C40-C37	-2.10	106.52	110.22
2	D	501	TUM	O32-C33-C8	-2.08	106.39	110.65
2	A	501	TUM	C44-N45-C46	-2.05	117.99	123.19
2	B	501	TUM	O32-C33-C8	-2.05	106.45	110.65
2	B	501	TUM	C35-O34-C33	-2.03	110.71	114.37
2	D	501	TUM	C48-C46-N45	2.17	120.03	116.11
2	B	501	TUM	C20-C22-C17	2.37	105.87	102.45
2	A	501	TUM	C4-C5-N7	2.39	119.18	114.43
2	A	501	TUM	C48-C46-N45	2.40	120.44	116.11
2	D	501	TUM	C20-C22-C17	2.58	106.18	102.45
2	B	501	TUM	O18-C19-N24	2.68	113.45	108.08
2	B	501	TUM	C48-C46-N45	2.72	121.02	116.11
2	A	501	TUM	C35-O36-C37	2.74	118.87	113.72
2	C	501	TUM	C20-C22-C17	2.79	106.48	102.45
3	C	502	PGW	O01-C1-C2	3.91	119.67	111.55
3	A	502	PGW	O01-C1-C2	3.99	119.83	111.55
3	D	502	PGW	O01-C1-C2	4.03	119.92	111.55
3	B	502	PGW	O01-C1-C2	4.19	120.25	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/417 (90%)	0.12	15 (3%) 39 19	4, 31, 79, 121	0
1	B	369/417 (88%)	0.20	17 (4%) 33 15	10, 51, 103, 127	0
1	C	375/417 (89%)	0.19	18 (4%) 31 14	6, 38, 109, 127	0
1	D	362/417 (86%)	0.26	15 (4%) 38 18	7, 44, 89, 123	0
All	All	1484/1668 (88%)	0.19	65 (4%) 35 17	4, 40, 97, 127	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	CYS	6.8
1	B	358	CYS	6.5
1	C	358	CYS	4.8
1	B	343	VAL	4.6
1	C	348	SER	4.2
1	C	72	CYS	4.1
1	C	343	VAL	4.1
1	A	348	SER	3.8
1	D	9	MET	3.8
1	D	10	PRO	3.6
1	A	357	GLU	3.5
1	C	334	LEU	3.5
1	B	72	CYS	3.5
1	A	326	LEU	3.5
1	A	355	PHE	3.4
1	A	334	LEU	3.2
1	B	21	GLY	3.2
1	C	347	GLN	3.2
1	D	365	ASN	3.0
1	C	333	ILE	3.0
1	B	342	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	316	MET	3.0
1	A	296	ILE	2.9
1	A	345	VAL	2.8
1	D	391	SER	2.8
1	D	280	MET	2.7
1	D	394	THR	2.7
1	D	49	THR	2.7
1	A	343	VAL	2.7
1	D	295	HIS	2.7
1	A	298	PRO	2.6
1	B	188	ALA	2.5
1	B	18	SER	2.5
1	B	359	ASN	2.5
1	C	352	ASP	2.5
1	C	351	GLU	2.5
1	B	391	SER	2.4
1	A	321	PHE	2.4
1	D	376	GLU	2.4
1	A	344	THR	2.4
1	C	167	ILE	2.3
1	C	298	PRO	2.3
1	D	363	LEU	2.3
1	C	345	VAL	2.3
1	D	293	LEU	2.2
1	B	17	VAL	2.2
1	C	368	LEU	2.2
1	B	68	ILE	2.2
1	D	138	MET	2.2
1	C	294	LEU	2.2
1	C	321	PHE	2.2
1	A	72	CYS	2.2
1	A	325	SER	2.2
1	B	166	GLY	2.2
1	B	277	LEU	2.1
1	A	354	GLU	2.1
1	B	14	ASN	2.1
1	B	234	THR	2.1
1	C	346	HIS	2.1
1	C	355	PHE	2.1
1	D	127	LEU	2.0
1	B	334	LEU	2.0
1	C	365	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	333	ILE	2.0
1	D	130	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PGW	C	502	34/51	0.81	0.45	4.29	19,63,122,128	0
3	PGW	A	502	30/51	0.88	0.48	2.68	23,49,139,159	0
3	PGW	B	502	34/51	0.87	0.34	1.76	19,48,118,128	0
3	PGW	D	502	34/51	0.87	0.36	1.42	14,42,106,118	0
2	TUM	C	501	57/57	0.92	0.27	0.70	16,40,65,78	0
2	TUM	D	501	57/57	0.91	0.27	0.32	25,58,89,116	0
2	TUM	A	501	57/57	0.92	0.23	0.30	8,29,47,53	0
2	TUM	B	501	57/57	0.91	0.23	-0.32	25,59,82,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.