



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:19 PM UTC

PDB ID : 2R0T / pdb_00002r0t
Title : Crystal structure of GDP-4-keto-6-deoxymannose-3-dehydratase with a trapped PLP-glutamate geminal diamine
Authors : Cook, P.D.; Holden, H.M.
Deposited on : 2007-08-21
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

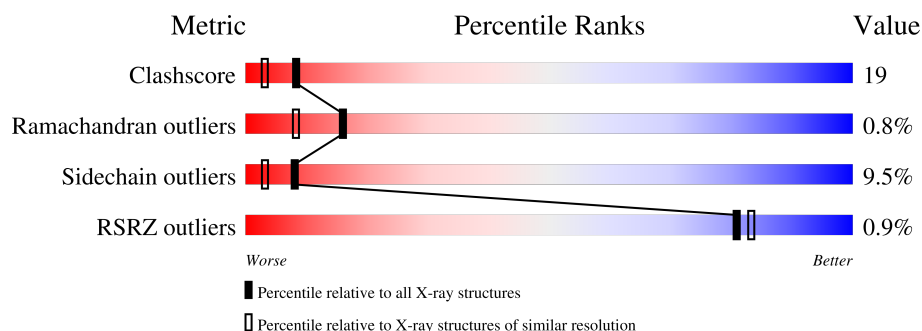
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	% 55% 38% 5% ..
1	B	390	% 57% 33% 8% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6494 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

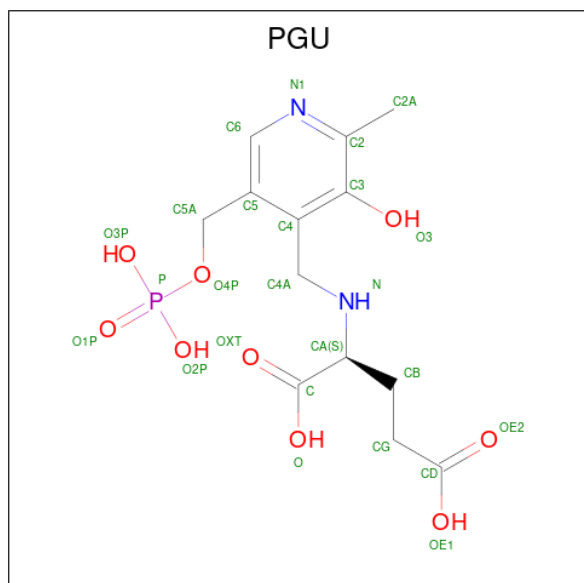
- Molecule 1 is a protein called Pyridoxamine 5-phosphate-dependent dehydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	1	0
			3093	1985	506	588	14			
1	B	386	Total	C	N	O	S	0	2	0
			3093	1985	506	588	14			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)-L-glutamic acid (CCD ID: PGU) (formula: C₁₃H₁₉N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

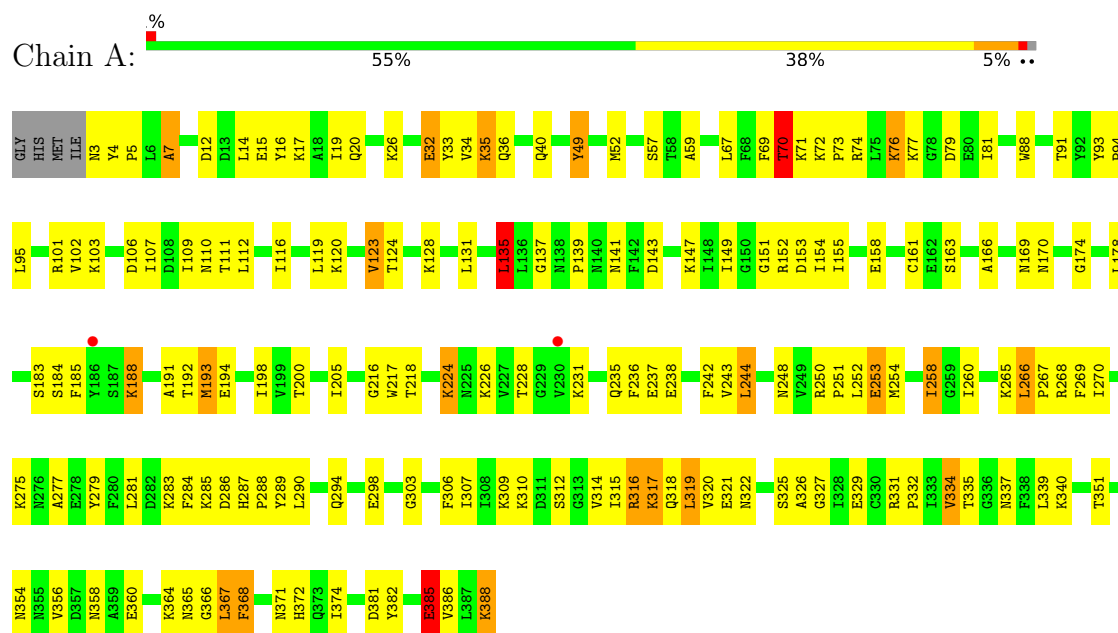
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		
3	B	124	Total	O	0	0
			124	124		

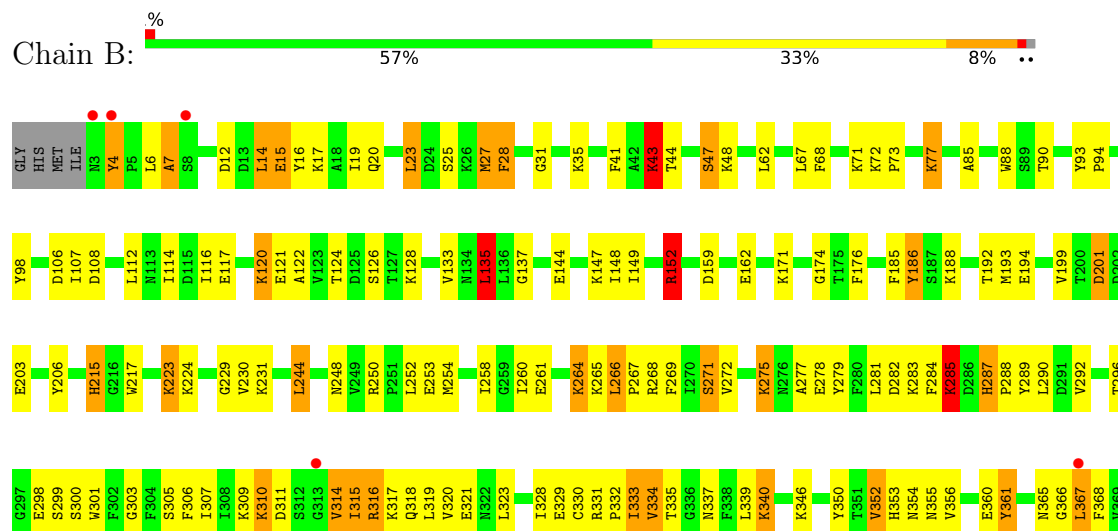
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pyridoxamine 5-phosphate-dependent dehydrase



- Molecule 1: Pyridoxamine 5-phosphate-dependent dehydrase



G370	D378
N371	E379
H372	I380
Q373	D381
I374	Y382
	L383
	R384
	E385
	V386
	L387
	K388

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.91Å 72.91Å 86.96Å 90.00° 107.94° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.90) 92.8 (30.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 1.91Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.183 , 0.255 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 138.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6494	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.94	2/3163 (0.1%)	1.49	33/4271 (0.8%)
1	B	0.97	2/3163 (0.1%)	1.51	34/4271 (0.8%)
All	All	0.95	4/6326 (0.1%)	1.50	67/8542 (0.8%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	27	MET	SD-CE	6.22	1.95	1.79
1	A	193	MET	SD-CE	5.79	1.94	1.79
1	B	193	MET	SD-CE	5.31	1.92	1.79
1	A	198	ILE	CA-CB	5.13	1.61	1.54

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	SER	N-CA-C	-9.32	101.60	113.72
1	B	300	SER	N-CA-C	-8.15	102.90	113.17
1	A	59	ALA	N-CA-C	-8.03	102.61	111.36
1	A	91	THR	N-CA-C	-7.15	103.22	112.23
1	A	365	ASN	N-CA-C	7.14	123.01	112.94
1	A	385	GLU	N-CA-C	-7.14	102.91	111.69
1	A	275	LYS	N-CA-C	-6.86	103.73	111.14
1	B	28	PHE	N-CA-C	6.78	121.63	113.23
1	A	123	VAL	N-CA-C	6.77	118.41	109.21
1	B	352	VAL	CB-CA-C	-6.63	100.75	110.62
1	A	7	ALA	N-CA-C	6.44	119.65	108.76
1	A	95	LEU	N-CA-C	-6.38	104.41	111.36
1	B	192	THR	N-CA-C	-6.34	102.93	111.87
1	B	266	LEU	N-CA-C	6.34	121.49	113.25
1	B	174	GLY	N-CA-C	-6.29	107.20	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ILE	CB-CA-C	-6.27	102.44	112.16
1	A	107	ILE	CB-CA-C	-6.23	102.37	112.03
1	B	296	THR	N-CA-C	-6.20	99.30	109.40
1	A	371	ASN	N-CA-C	-6.17	99.75	109.50
1	B	116	ILE	N-CA-C	6.12	116.86	110.62
1	B	114	ILE	CA-C-N	-6.09	112.47	121.24
1	B	114	ILE	C-N-CA	-6.09	112.47	121.24
1	A	244	LEU	O-C-N	6.08	126.20	121.88
1	B	194	GLU	N-CA-C	-6.08	99.90	109.50
1	A	224	LYS	N-CA-C	-6.05	99.34	109.07
1	A	316	ARG	N-CA-C	6.03	118.62	111.33
1	B	361	TYR	N-CA-C	-5.97	104.69	111.14
1	B	7	ALA	N-CA-C	5.92	118.85	109.50
1	B	15	GLU	N-CA-C	-5.86	105.03	111.82
1	A	284	PHE	N-CA-C	5.84	121.12	113.30
1	A	243	VAL	N-CA-C	5.83	119.24	113.53
1	A	188	LYS	N-CA-C	5.79	118.82	109.79
1	B	314	VAL	N-CA-C	5.74	116.56	108.36
1	B	201	ASP	N-CA-C	-5.73	106.33	113.38
1	A	70	THR	N-CA-C	-5.69	102.47	110.50
1	A	135	LEU	N-CA-C	5.67	118.78	109.76
1	A	124	THR	N-CA-C	5.67	115.76	108.34
1	B	41	PHE	N-CA-C	5.54	117.76	111.11
1	A	319	LEU	N-CA-C	-5.54	105.24	111.28
1	B	266	LEU	CA-C-N	5.54	125.00	119.24
1	B	266	LEU	C-N-CA	5.54	125.00	119.24
1	B	350	TYR	N-CA-C	5.52	117.37	109.14
1	B	287	HIS	CA-C-N	5.43	125.77	119.47
1	B	287	HIS	C-N-CA	5.43	125.77	119.47
1	B	379	GLU	N-CA-C	-5.36	105.44	111.28
1	B	72	LYS	N-CA-C	-5.35	97.72	109.11
1	B	215	HIS	N-CA-CB	-5.34	105.80	113.65
1	A	116	ILE	N-CA-C	5.34	116.11	110.72
1	A	266	LEU	N-CA-C	5.33	121.59	109.81
1	A	367	LEU	N-CA-C	-5.30	101.06	108.96
1	A	318	GLN	N-CA-C	5.29	116.73	111.07
1	B	133	VAL	N-CA-C	-5.28	100.52	108.12
1	B	4	TYR	C-N-CD	-5.27	103.39	125.00
1	B	152	ARG	CB-CG-CD	-5.20	99.34	111.30
1	A	67	LEU	N-CA-C	5.19	118.71	112.38
1	A	253	GLU	CA-C-N	5.17	127.47	120.38
1	A	253	GLU	C-N-CA	5.17	127.47	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	TRP	N-CA-C	5.16	118.44	111.17
1	B	43	LYS	N-CA-C	-5.15	105.56	111.07
1	B	135	LEU	N-CA-C	5.10	117.86	109.76
1	B	23	LEU	N-CA-C	-5.09	105.82	111.36
1	A	49	TYR	N-CA-C	5.07	117.52	109.50
1	A	107	ILE	O-C-N	5.07	126.84	122.12
1	A	102	VAL	N-CA-C	5.06	115.26	108.17
1	A	258	ILE	CA-C-N	5.06	125.59	119.98
1	A	258	ILE	C-N-CA	5.06	125.59	119.98
1	B	244	LEU	N-CA-C	-5.05	100.28	108.82

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	3093	0	3066	108	0
1	B	3093	0	3064	137	0
2	A	25	0	13	2	0
2	B	25	0	13	4	0
3	A	134	0	0	4	0
3	B	124	0	0	5	0
All	All	6494	0	6156	238	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 19.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD21	1:A:205:ILE:HD11	1.41	0.99
1:B:315:ILE:N	1:B:315:ILE:HD13	1.84	0.92
1:A:360:GLU:HB3	1:A:364:LYS:HZ1	1.35	0.91
1:A:339:LEU:HD12	1:A:356:VAL:HG21	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HG	1:B:329:GLU:HG2	1.59	0.81
1:B:47:SER:HB2	3:B:658:HOH:O	1.78	0.81
1:A:119:LEU:O	1:A:123:VAL:HG23	1.82	0.79
1:B:6:LEU:CD1	1:B:329:GLU:HG2	2.12	0.79
1:B:128:LYS:HE2	1:B:128:LYS:HA	1.64	0.78
1:A:360:GLU:CB	1:A:364:LYS:HZ1	1.94	0.78
1:A:32:GLU:O	1:A:36:GLN:HG3	1.83	0.78
1:B:314:VAL:C	1:B:315:ILE:HD13	2.11	0.76
1:A:128:LYS:O	1:A:155:ILE:HD12	1.87	0.75
1:B:149:ILE:O	1:B:152:ARG:HG2	1.86	0.75
1:A:3:ASN:HB3	1:A:327:GLY:O	1.87	0.75
1:A:149:ILE:O	1:A:152:ARG:HG3	1.86	0.74
1:A:360:GLU:HB3	1:A:364:LYS:NZ	2.02	0.74
1:A:178:LEU:HD21	1:A:205:ILE:CD1	2.16	0.73
1:A:317:LYS:O	1:A:321:GLU:HG3	1.89	0.72
1:B:25:SER:O	1:B:27:MET:HE2	1.90	0.72
1:B:6:LEU:CG	1:B:329:GLU:HG2	2.19	0.72
1:B:382:TYR:O	1:B:386:VAL:HG23	1.89	0.71
1:B:271:SER:O	1:B:275:LYS:HD3	1.90	0.71
1:B:331:ARG:HG3	1:B:368:PHE:HD2	1.57	0.70
1:B:331:ARG:HD3	1:B:368:PHE:CE2	2.28	0.69
1:B:287:HIS:HE1	1:B:289:TYR:CE2	2.11	0.69
1:B:307:ILE:CD1	1:B:366:GLY:HA2	2.24	0.68
1:B:331:ARG:HB2	1:B:332:PRO:HD2	1.75	0.68
1:A:26:LYS:NZ	3:A:548:HOH:O	2.27	0.67
1:B:279:TYR:CD2	1:B:380:ILE:HG21	2.29	0.67
1:B:306:PHE:O	1:B:307:ILE:HD13	1.95	0.66
1:B:320:VAL:O	1:B:321:GLU:C	2.39	0.65
1:B:307:ILE:HD13	1:B:366:GLY:HA2	1.78	0.64
1:A:15:GLU:OE2	1:A:265:LYS:NZ	2.27	0.64
1:B:106:ASP:CG	1:B:356:VAL:HA	2.23	0.64
1:A:93:TYR:HB2	1:A:94:PRO:HD3	1.80	0.64
1:B:303:GLY:HA3	1:B:368:PHE:CE1	2.33	0.63
1:A:283:LYS:HE3	1:A:381:ASP:OD1	1.99	0.63
1:B:261:GLU:OE1	1:B:264:LYS:NZ	2.28	0.62
1:B:287:HIS:HE1	1:B:289:TYR:CD2	2.17	0.62
1:A:19:ILE:HD11	1:A:258:ILE:HD11	1.82	0.61
1:A:253:GLU:HA	1:A:253:GLU:OE1	2.00	0.61
1:B:331:ARG:HD3	1:B:368:PHE:HE2	1.64	0.61
1:B:7:ALA:HA	1:B:372:HIS:HE1	1.66	0.61
1:B:287:HIS:CE1	1:B:290:LEU:HD12	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:HB2	1:B:248:ASN:HB3	1.84	0.60
1:B:306:PHE:HB2	1:B:367:LEU:HD23	1.82	0.60
1:B:355:ASN:C	1:B:355:ASN:OD1	2.45	0.59
1:B:260:ILE:O	1:B:264:LYS:HG3	2.02	0.59
1:B:135:LEU:HD11	1:B:334:VAL:HG21	1.85	0.59
1:A:106:ASP:OD1	1:A:358:ASN:HB2	2.03	0.58
1:B:328:ILE:HD13	1:B:383:LEU:HD13	1.85	0.58
1:A:287:HIS:O	1:A:309:LYS:NZ	2.26	0.58
1:A:339:LEU:CD1	1:A:356:VAL:HG21	2.32	0.58
1:B:171:LYS:HD3	1:B:176:PHE:CE2	2.39	0.58
1:B:287:HIS:O	1:B:309:LYS:NZ	2.36	0.57
1:B:31:GLY:N	1:B:253:GLU:OE2	2.34	0.57
1:B:303:GLY:HA3	1:B:368:PHE:HE1	1.66	0.57
1:A:14:LEU:N	1:A:14:LEU:HD23	2.18	0.57
1:A:106:ASP:CG	1:A:358:ASN:HB2	2.30	0.57
1:A:32:GLU:OE1	1:A:32:GLU:HA	2.04	0.56
1:A:319:LEU:N	1:A:319:LEU:HD12	2.21	0.56
1:B:6:LEU:HD12	1:B:329:GLU:HG2	1.85	0.56
1:B:117:GLU:HA	1:B:120:LYS:HD2	1.87	0.56
1:B:93:TYR:HB2	1:B:94:PRO:HD3	1.87	0.56
1:B:217:TRP:HB2	3:B:613:HOH:O	2.06	0.56
1:B:4:TYR:HB2	1:B:328:ILE:HA	1.88	0.56
1:A:184:SER:O	1:A:191:ALA:HA	2.06	0.55
1:A:331:ARG:HB2	1:A:332:PRO:HD2	1.87	0.55
1:B:268:ARG:O	1:B:272:VAL:HG23	2.06	0.55
1:A:235:GLN:O	1:A:236:PHE:C	2.49	0.55
1:A:218:THR:O	1:A:231:LYS:HE3	2.06	0.54
1:B:266:LEU:HB3	1:B:267:PRO:HD3	1.89	0.54
1:B:287:HIS:CE1	1:B:289:TYR:CE2	2.93	0.54
1:B:384:ARG:HD2	1:B:384:ARG:C	2.33	0.53
1:A:141:ASN:OD1	1:A:141:ASN:C	2.51	0.53
1:A:111:THR:O	1:A:112:LEU:HB2	2.08	0.53
1:B:6:LEU:HG	1:B:329:GLU:CG	2.36	0.53
1:A:382:TYR:O	1:A:386:VAL:HG23	2.08	0.53
1:B:279:TYR:HD2	1:B:380:ILE:HG21	1.72	0.53
1:B:384:ARG:HD2	1:B:384:ARG:O	2.09	0.53
1:A:319:LEU:O	1:A:322:ASN:HB2	2.08	0.53
1:B:88:TRP:CD1	1:B:90:THR:HG1	2.26	0.53
1:B:277:ALA:O	1:B:281:LEU:HG	2.09	0.53
1:A:35:LYS:HD2	1:A:35:LYS:O	2.09	0.53
1:B:88:TRP:HD1	1:B:90:THR:HG1	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HG3	1:A:238:GLU:N	2.23	0.53
1:A:135:LEU:HD11	1:A:334:VAL:HG21	1.91	0.52
1:B:284:PHE:CZ	1:B:384:ARG:HD3	2.44	0.52
1:B:320:VAL:O	1:B:323:LEU:N	2.43	0.52
1:B:12:ASP:OD1	1:B:12:ASP:C	2.50	0.52
1:B:287:HIS:CE1	1:B:289:TYR:CD2	2.97	0.52
1:B:112:LEU:HD23	1:B:112:LEU:N	2.25	0.52
1:B:373:GLN:CD	1:B:373:GLN:H	2.18	0.52
1:A:326:ALA:HB1	1:A:382:TYR:OH	2.11	0.51
1:A:252:LEU:HD12	1:B:252:LEU:HD12	1.93	0.51
1:A:319:LEU:N	1:A:319:LEU:CD1	2.73	0.51
1:A:192:THR:O	1:A:193:MET:HB2	2.11	0.50
1:A:337:ASN:O	1:A:340:LYS:HG2	2.12	0.50
1:B:224:LYS:HG3	1:B:230:VAL:HG22	1.93	0.50
1:B:188:LYS:HE3	2:B:500:PGU:HA	1.93	0.50
1:A:217:TRP:CD1	1:A:217:TRP:C	2.89	0.50
1:A:141:ASN:OD1	1:A:143:ASP:HB2	2.11	0.50
1:A:161:CYS:HB2	2:A:500:PGU:C2	2.42	0.50
1:B:171:LYS:HB3	1:B:176:PHE:CZ	2.46	0.50
1:A:242:PHE:CE1	1:B:335:THR:HG21	2.46	0.50
1:B:331:ARG:HB2	1:B:332:PRO:CD	2.39	0.50
1:B:353:HIS:ND1	3:B:664:HOH:O	2.33	0.50
1:A:152:ARG:O	1:A:154:ILE:N	2.45	0.49
1:A:285:LYS:O	1:A:286:ASP:HB2	2.11	0.49
1:B:188:LYS:CE	2:B:500:PGU:HA	2.42	0.49
1:B:331:ARG:CG	1:B:368:PHE:HD2	2.25	0.48
1:A:12:ASP:OD1	1:A:14:LEU:HG	2.13	0.48
1:A:12:ASP:O	1:A:16:TYR:HD1	1.97	0.48
1:A:285:LYS:O	1:A:285:LYS:HG3	2.13	0.48
1:B:4:TYR:CD1	1:B:328:ILE:HG12	2.48	0.48
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.47	0.48
1:B:278:GLU:O	1:B:281:LEU:HB2	2.14	0.48
1:A:306:PHE:O	1:A:366:GLY:HA2	2.13	0.47
1:A:183:SER:HB3	1:A:188:LYS:HD2	1.97	0.47
1:B:162:GLU:HG3	2:B:500:PGU:O3	2.15	0.47
1:A:4:TYR:C	1:A:4:TYR:CD2	2.93	0.47
1:A:52:MET:HG2	1:A:251:PRO:HG3	1.96	0.47
1:A:279:TYR:OH	1:A:381:ASP:OD1	2.32	0.47
1:A:287:HIS:CG	1:A:288:PRO:HD2	2.48	0.47
1:A:248:ASN:OD1	1:A:248:ASN:C	2.57	0.47
1:A:385:GLU:O	1:A:388:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:O	1:B:206:TYR:HB3	2.15	0.47
1:B:266:LEU:N	1:B:267:PRO:CD	2.77	0.47
1:B:278:GLU:O	1:B:279:TYR:C	2.57	0.47
1:B:284:PHE:CZ	1:B:384:ARG:HA	2.50	0.47
1:B:371:ASN:OD1	1:B:372:HIS:N	2.48	0.47
1:A:14:LEU:HD23	1:A:17:LYS:HE3	1.97	0.46
1:A:88:TRP:HE1	1:B:215:HIS:CE1	2.32	0.46
1:A:70:THR:OG1	1:A:73:PRO:HA	2.16	0.46
1:A:314:VAL:CG1	1:A:319:LEU:HD11	2.45	0.46
2:A:500:PGU:O2P	2:A:500:PGU:OE2	2.34	0.46
1:B:137:GLY:O	1:B:299:SER:HA	2.15	0.46
1:B:287:HIS:CD2	1:B:384:ARG:CZ	2.98	0.46
1:B:287:HIS:HA	1:B:288:PRO:HD2	1.76	0.46
1:B:337:ASN:ND2	1:B:360:GLU:HG3	2.31	0.46
1:B:47:SER:OG	1:B:199:VAL:HB	2.16	0.46
1:A:385:GLU:OE2	1:A:385:GLU:HA	2.16	0.46
1:A:15:GLU:CD	1:A:265:LYS:HZ2	2.22	0.45
1:B:320:VAL:HG13	1:B:330:CYS:SG	2.57	0.45
1:A:5:PRO:HA	1:A:329:GLU:CD	2.41	0.45
1:B:307:ILE:CD1	1:B:366:GLY:CA	2.95	0.45
1:B:319:LEU:H	1:B:319:LEU:HG	1.56	0.45
1:B:67:LEU:HA	1:B:67:LEU:HD23	1.76	0.45
1:A:360:GLU:O	1:A:364:LYS:HD2	2.17	0.45
1:B:120:LYS:HG2	1:B:148:ILE:HD11	1.98	0.45
1:B:374:ILE:O	1:B:374:ILE:HG12	2.15	0.45
1:A:266:LEU:N	1:A:267:PRO:CD	2.80	0.45
1:A:303:GLY:HA3	1:A:368:PHE:CE1	2.51	0.45
1:B:15:GLU:OE2	1:B:265:LYS:HE3	2.16	0.45
1:B:122:ALA:O	1:B:124:THR:HG23	2.17	0.45
1:A:155:ILE:HD12	1:A:155:ILE:H	1.82	0.44
1:A:335:THR:OG1	3:A:599:HOH:O	2.21	0.44
1:B:305:SER:HB2	1:B:333:ILE:CD1	2.47	0.44
1:B:331:ARG:O	1:B:368:PHE:N	2.50	0.44
1:A:19:ILE:HG12	1:A:254:MET:HG2	1.99	0.44
1:A:141:ASN:OD1	1:A:143:ASP:N	2.47	0.44
1:B:12:ASP:O	1:B:16:TYR:HD1	2.00	0.44
1:A:93:TYR:N	1:A:94:PRO:CD	2.80	0.44
1:B:85:ALA:HB1	1:B:339:LEU:HD12	2.00	0.44
1:A:33:TYR:O	1:A:34:VAL:C	2.60	0.44
1:B:43:LYS:CG	1:B:44:THR:N	2.80	0.44
1:A:388:LYS:HB3	1:A:388:LYS:HE2	1.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:TYR:HB3	1:B:379:GLU:OE1	2.18	0.43
1:B:284:PHE:CE1	1:B:384:ARG:HD3	2.53	0.43
1:B:287:HIS:CG	1:B:288:PRO:HD2	2.53	0.43
1:B:310:LYS:O	1:B:311:ASP:HB2	2.18	0.43
1:A:193:MET:HE2	1:A:258:ILE:HD12	2.00	0.43
1:A:289:TYR:HA	1:A:309:LYS:HD2	2.01	0.43
1:B:88:TRP:HD1	1:B:90:THR:OG1	2.02	0.43
1:B:310:LYS:HB2	1:B:310:LYS:HE2	1.46	0.43
1:A:321:GLU:O	1:A:322:ASN:C	2.61	0.43
1:B:224:LYS:HA	1:B:229:GLY:O	2.18	0.43
1:A:228:THR:HG21	3:A:620:HOH:O	2.18	0.43
1:A:266:LEU:O	1:A:270:ILE:HG12	2.19	0.43
1:B:340:LYS:HZ2	1:B:340:LYS:HG2	1.54	0.43
1:A:266:LEU:O	1:A:269:PHE:HB2	2.18	0.42
1:B:68:PHE:CZ	1:B:98:TYR:HB3	2.54	0.42
1:B:352:VAL:HG12	1:B:353:HIS:N	2.34	0.42
1:B:217:TRP:CD1	1:B:217:TRP:C	2.96	0.42
1:B:287:HIS:HD2	1:B:384:ARG:CZ	2.32	0.42
1:B:361:TYR:CE1	1:B:365:ASN:ND2	2.87	0.42
1:B:93:TYR:N	1:B:94:PRO:CD	2.82	0.42
1:A:7:ALA:HA	1:A:372:HIS:HE1	1.82	0.42
1:A:242:PHE:HE1	1:B:335:THR:CG2	2.31	0.42
1:B:17:LYS:O	1:B:20:GLN:HB3	2.18	0.42
1:A:110:ASN:HB3	1:A:294:GLN:NE2	2.35	0.42
1:B:108:ASP:C	1:B:108:ASP:OD1	2.61	0.42
1:A:74:ARG:O	3:A:607:HOH:O	2.21	0.42
1:A:139:PRO:HD3	1:A:166:ALA:HB1	2.01	0.42
1:A:316:ARG:O	1:A:320:VAL:HG23	2.20	0.42
1:A:20:GLN:OE1	1:A:20:GLN:HA	2.19	0.42
1:B:331:ARG:HD3	1:B:368:PHE:CD2	2.53	0.42
1:A:277:ALA:O	1:A:281:LEU:HG	2.19	0.42
1:A:314:VAL:HG12	1:A:319:LEU:HD11	2.02	0.42
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.89	0.42
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.89	0.42
1:B:23:LEU:HA	1:B:28:PHE:HE2	1.84	0.42
1:B:264:LYS:HB2	3:B:704:HOH:O	2.19	0.42
1:B:340:LYS:NZ	3:B:623:HOH:O	2.48	0.42
1:A:250:ARG:NH2	2:B:500:PGU:OE1	2.48	0.41
1:B:281:LEU:O	1:B:285:LYS:N	2.53	0.41
1:A:216:GLY:HA3	1:A:244:LEU:O	2.20	0.41
1:B:117:GLU:O	1:B:120:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PHE:CE1	1:B:335:THR:CG2	3.03	0.41
1:A:5:PRO:HB3	1:A:329:GLU:OE2	2.21	0.41
1:B:77:LYS:HB3	1:B:77:LYS:HE3	1.81	0.41
1:B:290:LEU:HD22	1:B:306:PHE:HB3	2.02	0.41
1:B:185:PHE:O	1:B:186:TYR:C	2.63	0.41
1:B:317:LYS:O	1:B:318:GLN:C	2.62	0.41
1:B:353:HIS:O	1:B:354:ASN:HB3	2.21	0.41
1:A:169:ASN:O	1:A:170:ASN:HB2	2.21	0.41
1:B:223:LYS:HE2	1:B:231:LYS:O	2.20	0.41
1:B:305:SER:CB	1:B:333:ILE:CD1	2.98	0.41
1:A:76:LYS:HG3	1:A:79:ASP:OD2	2.20	0.41
1:A:103:LYS:HG3	1:A:351:THR:HG23	2.03	0.41
1:B:282:ASP:HA	1:B:285:LYS:HB2	2.03	0.41
1:B:384:ARG:HD3	1:B:384:ARG:HA	1.75	0.41
1:A:69:PHE:CG	1:A:244:LEU:HD22	2.56	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.68	0.41
1:B:269:PHE:HA	1:B:373:GLN:HB2	2.03	0.40
1:B:315:ILE:O	1:B:316:ARG:C	2.63	0.40
1:A:5:PRO:HA	1:A:329:GLU:OE2	2.22	0.40
1:A:137:GLY:HA2	1:A:163:SER:HA	2.03	0.40
1:A:194:GLU:CD	1:B:250:ARG:HH21	2.29	0.40
1:B:152:ARG:HG2	1:B:152:ARG:H	1.72	0.40
1:A:49:TYR:HB2	1:A:200:THR:O	2.22	0.40
1:A:71:LYS:HA	1:A:71:LYS:HD3	1.93	0.40
1:A:185:PHE:CE1	1:B:250:ARG:NH2	2.90	0.40
1:B:48:LYS:HB2	1:B:201:ASP:HA	2.03	0.40
1:A:158:GLU:CD	1:A:174:GLY:H	2.28	0.40
1:B:6:LEU:HD23	1:B:370:GLY:H	1.86	0.40
1:B:159:ASP:C	1:B:159:ASP:OD1	2.64	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	385/390 (99%)	365 (95%)	17 (4%)	3 (1%)	16	8
1	B	385/390 (99%)	365 (95%)	17 (4%)	3 (1%)	16	8
All	All	770/780 (99%)	730 (95%)	34 (4%)	6 (1%)	16	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLY
1	A	354	ASN
1	B	186	TYR
1	B	334	VAL
1	A	334	VAL
1	B	285	LYS

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	343/345 (99%)	313 (91%)	30 (9%)	9	4
1	B	343/345 (99%)	308 (90%)	35 (10%)	7	2
All	All	686/690 (99%)	621 (90%)	65 (10%)	8	3

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	35	LYS
1	A	40	GLN
1	A	70	THR
1	A	72	LYS
1	A	76	LYS
1	A	77	LYS
1	A	81	ILE
1	A	101	ARG
1	A	109	ILE

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Mol	Chain	Res	Type
1	A	120	LYS
1	A	131	LEU
1	A	135	LEU
1	A	147	LYS
1	A	153	ASP
1	A	224	LYS
1	A	226	LYS
1	A	260	ILE
1	A	268	ARG
1	A	298	GLU
1	A	307	ILE
1	A	310	LYS
1	A	315	ILE
1	A	317	LYS
1	A	325	SER
1	A	367	LEU
1	A	368	PHE
1	A	374	ILE
1	A	385	GLU
1	A	388	LYS
1	B	14	LEU
1	B	19	ILE
1	B	35	LYS
1	B	43	LYS
1	B	47	SER
1	B	62	LEU
1	B	71	LYS
1	B	73	PRO
1	B	77	LYS
1	B	107	ILE
1	B	120	LYS
1	B	121	GLU
1	B	126	SER
1	B	135	LEU
1	B	144	GLU
1	B	147	LYS
1	B	152	ARG
1	B	223	LYS
1	B	254	MET
1	B	264	LYS
1	B	271	SER
1	B	275	LYS

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Mol	Chain	Res	Type
1	B	283	LYS
1	B	285	LYS
1	B	292	VAL
1	B	298	GLU
1	B	310	LYS
1	B	315	ILE
1	B	316	ARG
1	B	333	ILE
1	B	340	LYS
1	B	346	LYS
1	B	367	LEU
1	B	374	ILE
1	B	378	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	20	GLN
1	A	170	ASN
1	A	294	GLN
1	A	322	ASN
1	A	353	HIS
1	A	372	HIS
1	B	3	ASN
1	B	134	ASN
1	B	140	ASN
1	B	365	ASN
1	B	372	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PGU	A	500	1	25,25,25	1.31	3 (12%)	31,35,35	1.36	5 (16%)
2	PGU	B	500	1	25,25,25	2.14	6 (24%)	31,35,35	2.35	6 (19%)

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	PGU	A	500	1	-	6/20/20/20	0/1/1/1
2	PGU	B	500	1	-	7/20/20/20	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	PGU	CA-N	-7.26	1.30	1.46
2	B	500	PGU	C5-C4	4.08	1.46	1.40
2	B	500	PGU	P-O1P	3.62	1.61	1.50
2	A	500	PGU	P-O1P	3.12	1.60	1.50
2	B	500	PGU	C4A-C4	3.03	1.56	1.52
2	A	500	PGU	OE2-CD	2.79	1.31	1.22
2	A	500	PGU	OXT-C	2.55	1.29	1.22
2	B	500	PGU	OXT-C	2.25	1.28	1.22
2	B	500	PGU	P-O2P	2.08	1.62	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PGU	C4A-C4-C5	7.39	127.79	119.75
2	B	500	PGU	C3-C4-C5	-6.72	112.64	118.73
2	B	500	PGU	C6-C5-C4	4.79	121.68	118.06
2	B	500	PGU	C5A-C5-C6	-3.19	114.17	119.36
2	A	500	PGU	C4A-C4-C5	2.74	122.73	119.75
2	B	500	PGU	C2A-C2-C3	-2.68	117.66	120.80
2	A	500	PGU	CG-CB-CA	-2.55	108.46	113.16
2	A	500	PGU	C3-C4-C5	-2.45	116.50	118.73
2	A	500	PGU	O3-C3-C2	2.36	122.46	117.58
2	A	500	PGU	C6-C5-C4	2.30	119.80	118.06
2	B	500	PGU	CG-CB-CA	-2.18	109.14	113.16

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	PGU	C4-C5-C5A-O4P
2	B	500	PGU	N-CA-CB-CG
2	A	500	PGU	N-CA-CB-CG
2	A	500	PGU	C-CA-CB-CG
2	B	500	PGU	C-CA-CB-CG
2	A	500	PGU	CB-CA-N-C4A
2	B	500	PGU	CB-CA-N-C4A
2	A	500	PGU	C-CA-N-C4A
2	B	500	PGU	C-CA-N-C4A
2	B	500	PGU	OE1-CD-CG-CB
2	A	500	PGU	OE1-CD-CG-CB
2	A	500	PGU	OE2-CD-CG-CB
2	B	500	PGU	OE2-CD-CG-CB

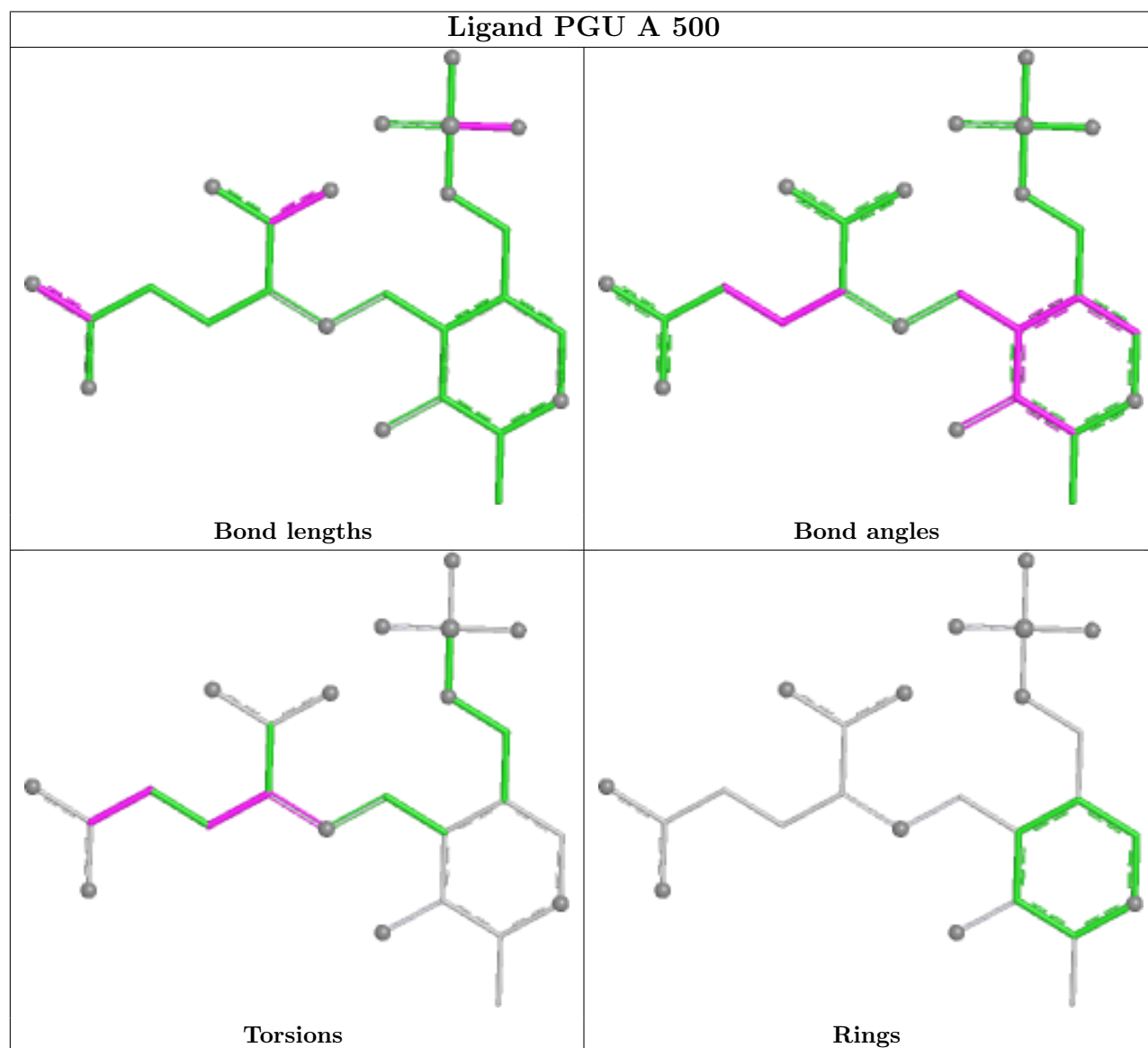
There are no ring outliers.

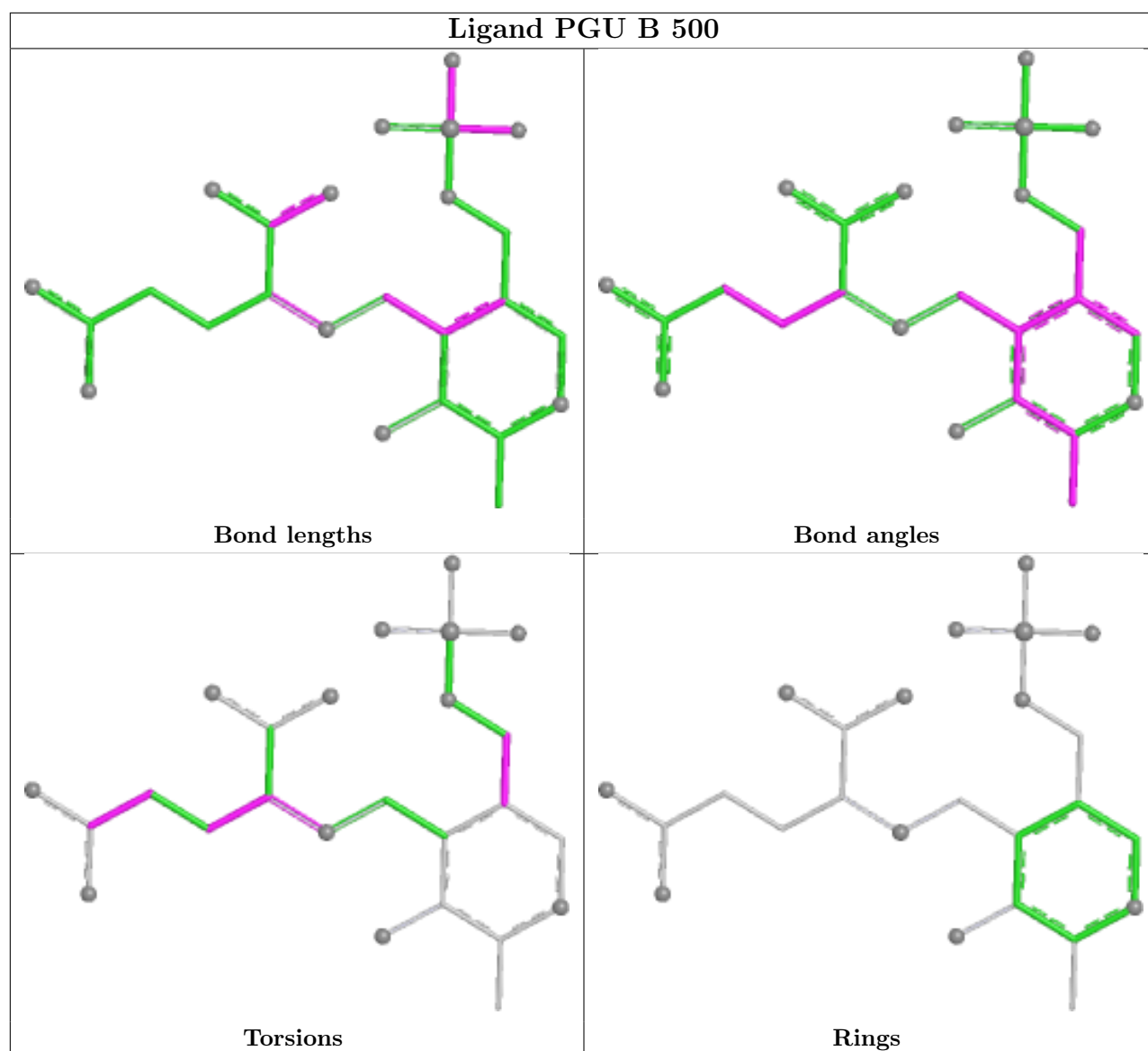
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PGU	2	0
2	B	500	PGU	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/390 (98%)	-0.28	2 (0%) 87 89	15, 34, 71, 95	1 (0%)
1	B	386/390 (98%)	-0.19	5 (1%) 75 78	16, 36, 74, 100	1 (0%)
All	All	772/780 (98%)	-0.23	7 (0%) 81 83	15, 35, 74, 100	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	TYR	3.2
1	A	186	TYR	2.5
1	B	3	ASN	2.4
1	B	313	GLY	2.3
1	A	230	VAL	2.2
1	B	8	SER	2.1
1	B	367	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

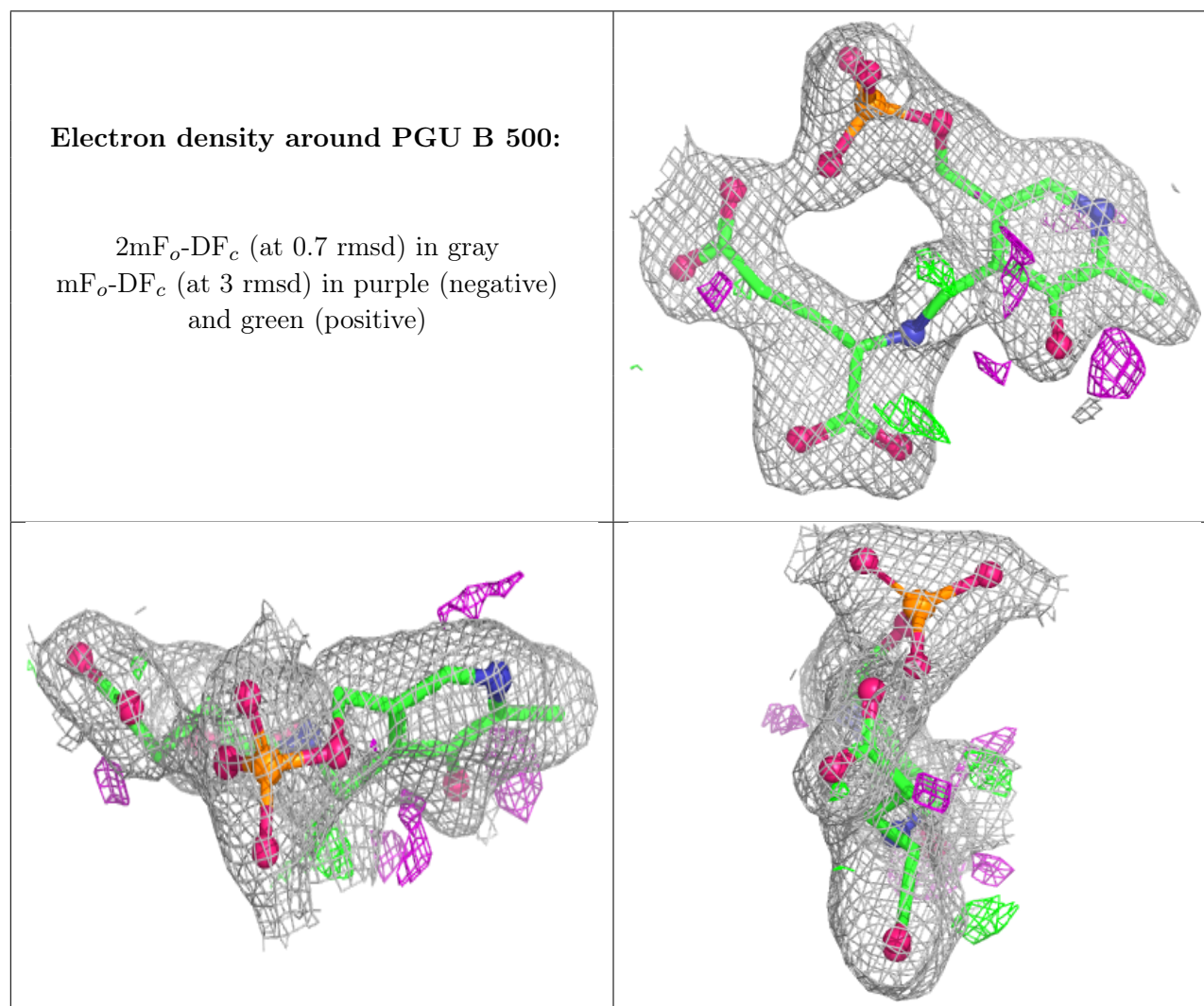
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

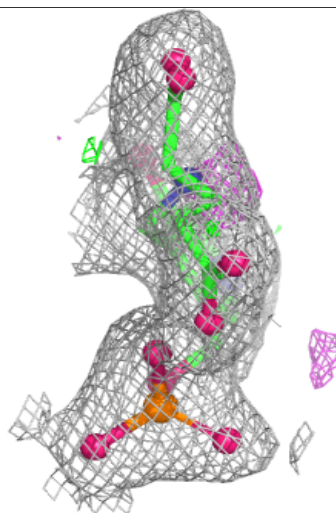
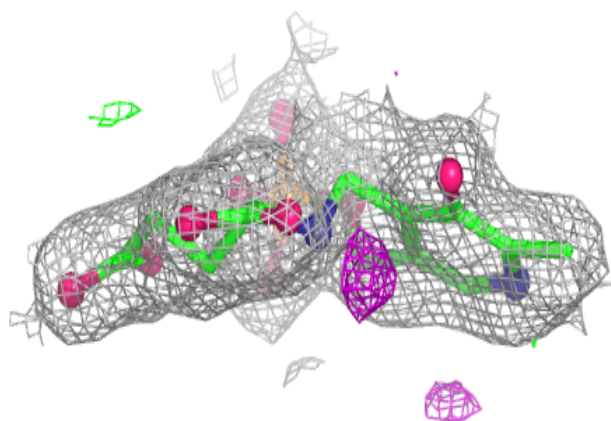
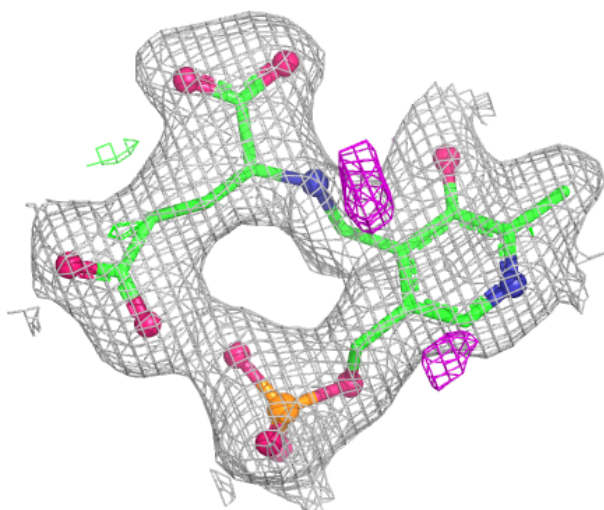
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PGU	B	500	25/25	0.97	0.09	18,41,99,99	0
2	PGU	A	500	25/25	0.98	0.06	10,26,57,71	0

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 PGU A 500:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.