



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:28 PM UTC

PDB ID : 2NZ4 / pdb_00002nz4
Title : Structural investigation of the GlmS ribozyme bound to its catalytic cofactor
Authors : Cochrane, J.C.
Deposited on : 2006-11-22
Resolution : 2.50 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

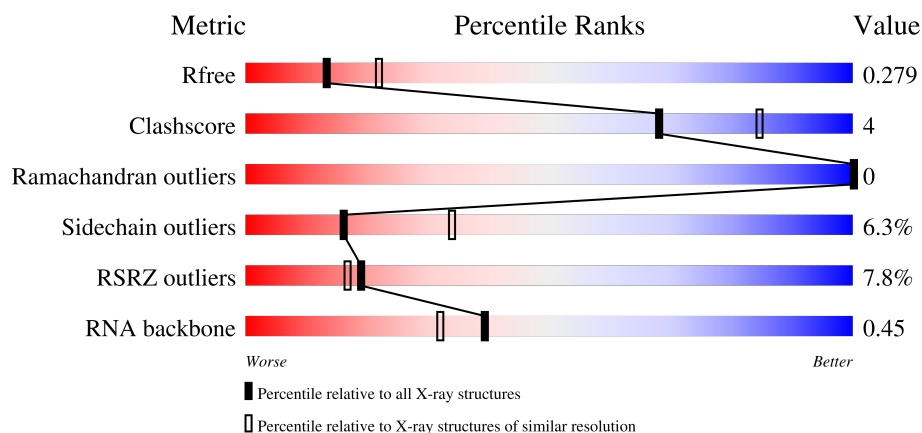
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	E	13	85% 8% 8%
1	F	13	77% 15% 8%
1	G	13	62% 15% 23%
1	H	13	77% 15% 8%

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Mol	Chain	Length	Quality of chain
2	P	141	
2	Q	141	
2	R	141	
2	S	141	
3	A	94	
3	B	94	
3	C	94	
3	D	94	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	F	9011	-	-	-	X
5	MG	G	9013	-	-	-	X
5	MG	H	9015	-	-	-	X
5	MG	S	9003	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16274 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 RNA chain called substrate strand RNA 13-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			263	120	47	84	12			
1	F	13	Total	C	N	O	P	0	0	0
			277	126	54	85	12			
1	G	13	Total	C	N	O	P	0	0	0
			277	126	54	85	12			
1	H	13	Total	C	N	O	P	0	0	0
			267	121	49	85	12			

- Molecule 2 is a RNA chain called GlmS ribozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	141	Total	C	N	O	P	0	0	0
			2979	1324	523	989	143			
2	Q	141	Total	C	N	O	P	0	0	0
			3003	1336	530	994	143			
2	R	141	Total	C	N	O	P	0	0	0
			3011	1340	532	996	143			
2	S	141	Total	C	N	O	P	0	0	0
			3003	1336	531	993	143			

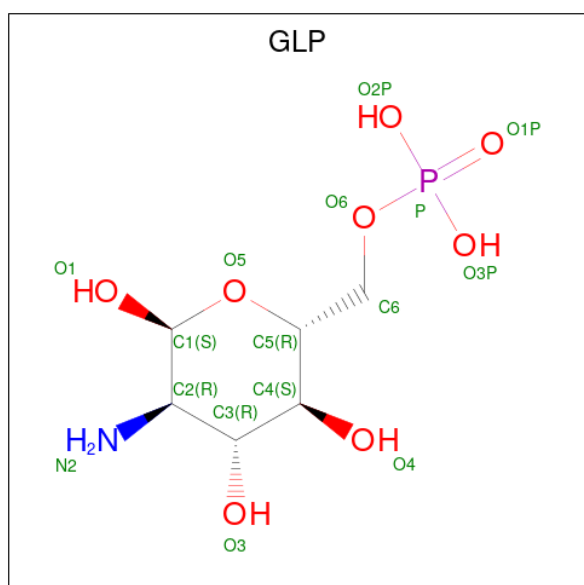
- Molecule 3 is a protein called U1 Small Nuclear Ribonucleoprotein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	90	Total	C	N	O	S	0	0	0
			720	462	126	129	3			
3	B	94	Total	C	N	O	S	0	0	0
			749	480	131	134	4			
3	C	90	Total	C	N	O	S	0	0	0
			723	464	126	129	4			
3	D	90	Total	C	N	O	S	0	0	0
			716	459	125	129	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	HIS	TYR	engineered mutation	UNP P09012
A	36	ARG	GLN	engineered mutation	UNP P09012
B	31	HIS	TYR	engineered mutation	UNP P09012
B	36	ARG	GLN	engineered mutation	UNP P09012
C	31	HIS	TYR	engineered mutation	UNP P09012
C	36	ARG	GLN	engineered mutation	UNP P09012
D	31	HIS	TYR	engineered mutation	UNP P09012
D	36	ARG	GLN	engineered mutation	UNP P09012

- Molecule 4 is 2-amino-2-deoxy-6-O-phosphono-alpha-D-glucopyranose (CCD ID: GLP) (formula: $C_6H_{14}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	P	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	F	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	G	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	H	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	4	Total Mg 4 4	0	0
5	F	1	Total Mg 1 1	0	0
5	Q	3	Total Mg 3 3	0	0
5	G	1	Total Mg 1 1	0	0
5	R	3	Total Mg 3 3	0	0
5	H	2	Total Mg 2 2	0	0
5	S	2	Total Mg 2 2	0	0

- Molecule 6 is water.

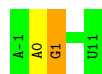
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	6	Total O 6 6	0	0
6	P	40	Total O 40 40	0	0
6	F	9	Total O 9 9	0	0
6	Q	43	Total O 43 43	0	0
6	G	10	Total O 10 10	0	0
6	R	43	Total O 43 43	0	0
6	H	10	Total O 10 10	0	0
6	S	30	Total O 30 30	0	0
6	A	2	Total O 2 2	0	0
6	B	7	Total O 7 7	0	0
6	C	3	Total O 3 3	0	0
6	D	3	Total O 3 3	0	0

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.

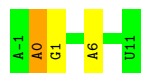
- Molecule 1: substrate strand RNA 13-mer

Chain E: 



- Molecule 1: substrate strand RNA 13-mer

Chain F: 



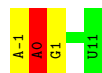
- Molecule 1: substrate strand RNA 13-mer

Chain G: 



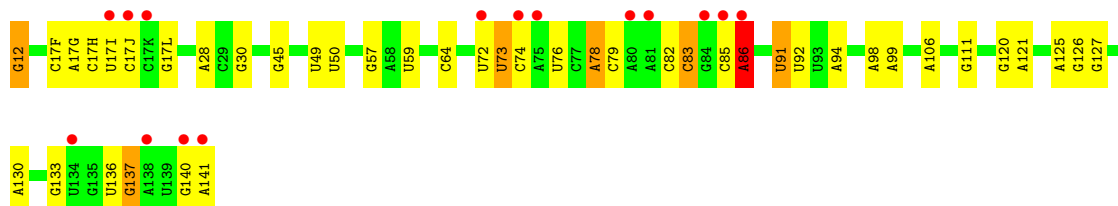
- Molecule 1: substrate strand RNA 13-mer

Chain H: 

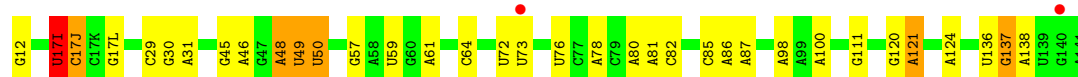
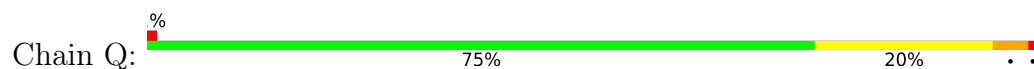


- Molecule 2: GlnS ribozyme

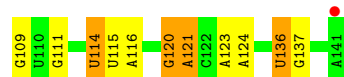
Chain P: 



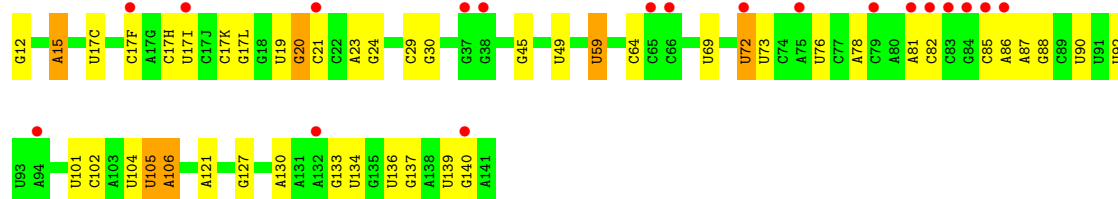
- Molecule 2: GlmS ribozyme



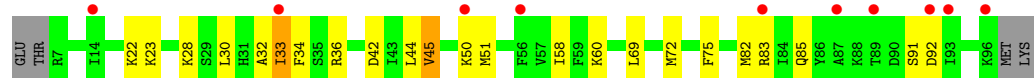
- Molecule 2: GlmS ribozyme



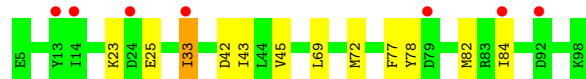
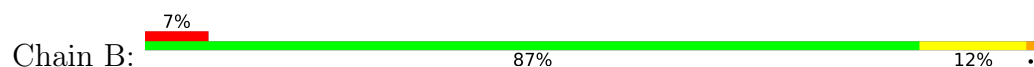
- Molecule 2: GlmS ribozyme



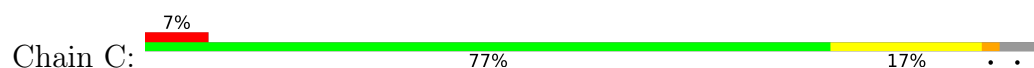
- Molecule 3: U1 Small Nuclear Ribonucleoprotein A



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● Molecule 3: U1 Small Nuclear Ribonucleoprotein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.13Å 234.16Å 105.00Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	34.94 – 2.50 34.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.94-2.50) 99.3 (34.94-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.269 0.255 , 0.279	Depositor DCC
R_{free} test set	3987 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.095 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16274	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: GTP, GLP, A2M, MG

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	E	0.63	0/267	1.08	0/412
1	F	0.60	0/284	1.18	1/441 (0.2%)
1	G	0.67	0/284	1.26	3/441 (0.7%)
1	H	0.65	1/272 (0.4%)	1.21	4/422 (0.9%)
2	P	0.54	0/3295	1.03	6/5134 (0.1%)
2	Q	0.59	0/3322	1.12	12/5176 (0.2%)
2	R	0.60	1/3331 (0.0%)	1.11	7/5190 (0.1%)
2	S	0.55	0/3322	1.04	2/5176 (0.0%)
3	A	1.48	1/733 (0.1%)	0.78	1/984 (0.1%)
3	B	0.56	0/762	0.77	1/1022 (0.1%)
3	C	0.55	0/736	0.74	0/986
3	D	0.56	0/729	0.75	0/979
All	All	0.64	3/17337 (0.0%)	1.04	37/26363 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	92	ASP	C-N	-37.29	0.91	1.33
1	H	0	A2M	O3'-P	5.15	1.61	1.56
2	R	49	U	C4-O4	5.05	1.33	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	0	A2M	P-O3'-C3'	8.52	129.93	119.70
2	Q	17(I)	U	P-O3'-C3'	7.42	128.60	119.70
1	H	-1	A	C1'-O4'-C4'	-7.09	102.61	109.70
2	S	72	U	O4'-C4'-C3'	-6.97	99.13	106.10
1	G	-1	A	C1'-O4'-C4'	-6.74	102.96	109.70
1	F	0	A2M	P-O3'-C3'	6.68	127.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	0	A2M	P-O3'-C3'	6.67	127.71	119.70
1	H	-1	A	O4'-C4'-C3'	-6.51	99.59	106.10
2	P	57	G	O5'-C5'-C4'	-6.36	101.96	111.50
2	Q	111	G	N9-C1'-C2'	6.32	121.48	112.00
3	A	92	ASP	O-C-N	6.22	130.77	122.43
2	R	114	U	C4'-C3'-C2'	-6.12	96.48	102.60
2	P	111	G	N9-C1'-C2'	6.11	121.17	112.00
2	R	121	A	C4'-C3'-C2'	-6.08	96.52	102.60
2	P	73	U	N1-C1'-C2'	5.97	120.96	112.00
2	Q	48	A	N9-C1'-C2'	-5.87	105.19	114.00
2	R	114	U	C3'-C2'-C1'	-5.85	95.45	101.30
3	B	33	ILE	CB-CA-C	-5.81	103.46	111.65
1	G	-1	A	O4'-C4'-C3'	-5.79	100.31	106.10
2	P	91	U	P-O3'-C3'	5.70	128.76	120.20
2	Q	121	A	C4'-C3'-C2'	-5.68	96.92	102.60
2	P	73	U	O4'-C1'-C2'	-5.66	101.94	107.60
2	R	83	C	N1-C1'-C2'	5.64	120.45	112.00
2	P	86	A	O4'-C1'-C2'	-5.60	102.00	107.60
2	Q	45	G	P-O5'-C5'	5.54	129.21	120.90
2	R	111	G	N9-C1'-C2'	5.50	120.25	112.00
2	Q	48	A	O4'-C1'-N9	5.41	116.32	108.20
2	S	134	U	O4'-C1'-C2'	-5.33	102.27	107.60
2	Q	17(I)	U	N1-C1'-C2'	5.33	119.99	112.00
2	Q	98	A	N9-C1'-C2'	5.30	119.96	112.00
2	Q	17(I)	U	O4'-C1'-C2'	-5.23	102.37	107.60
2	R	120	G	C4'-C3'-C2'	-5.21	97.39	102.60
2	Q	61	A	N9-C1'-C2'	5.20	119.80	112.00
1	H	-1	A	C5'-C4'-C3'	5.13	122.89	115.20
2	R	114	U	C3'-C2'-O2'	5.06	118.29	110.70
2	Q	137	G	C2'-C3'-O3'	5.06	121.29	113.70
2	Q	50	U	O4'-C4'-C3'	-5.03	101.07	106.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	263	0	135	2	0
1	F	277	0	146	0	0
1	G	277	0	146	4	0
1	H	267	0	141	2	0
2	P	2979	0	1492	11	0
2	Q	3003	0	1505	7	0
2	R	3011	0	1509	15	0
2	S	3003	0	1506	10	0
3	A	720	0	730	13	0
3	B	749	0	762	12	0
3	C	723	0	739	12	0
3	D	716	0	721	18	0
4	F	16	0	12	0	0
4	G	16	0	12	0	0
4	H	16	0	12	0	0
4	P	16	0	12	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	P	4	0	0	0	0
5	Q	3	0	0	0	0
5	R	3	0	0	0	0
5	S	2	0	0	0	0
6	A	2	0	0	0	0
6	B	7	0	0	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
6	E	6	0	0	0	0
6	F	9	0	0	0	0
6	G	10	0	0	1	0
6	H	10	0	0	0	0
6	P	40	0	0	1	0
6	Q	43	0	0	1	0
6	R	43	0	0	0	0
6	S	30	0	0	2	0
All	All	16274	0	9580	93	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 4.

All (93) 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:E:1:G:C2	1:E:1:G:C4	2.19	1.21
2:Q:48:A:O2'	2:Q:49:U:OP2	1.96	0.83
3:D:9:ASN:HD22	3:D:87:ALA:HB3	1.49	0.78
2:Q:46:A:OP2	6:Q:9029:HOH:O	2.06	0.74
3:D:9:ASN:ND2	3:D:87:ALA:HB3	2.05	0.72
3:C:75:PHE:HB3	3:C:82:MET:HE2	1.72	0.71
3:D:41:LEU:HD12	3:D:58:ILE:HG22	1.77	0.65
2:S:17(C):U:O4	6:S:9033:HOH:O	2.13	0.64
2:R:120:G:H2'	2:R:121:A:O4'	1.98	0.63
3:C:15:ASN:ND2	3:C:83:ARG:HB3	2.14	0.62
3:B:33:ILE:HD11	3:B:77:PHE:CE1	2.34	0.62
3:D:33:ILE:HG23	3:D:72:MET:HE2	1.81	0.61
3:A:42:ASP:HB3	3:A:58:ILE:HD12	1.83	0.61
3:B:82:MET:HE3	3:B:84:ILE:HD11	1.83	0.60
3:D:33:ILE:CG2	3:D:72:MET:HE2	2.32	0.60
3:B:23:LYS:HG3	3:B:45:VAL:HG12	1.84	0.58
3:D:72:MET:HE3	3:D:75:PHE:CG	2.39	0.57
3:A:33:ILE:CG2	3:A:34:PHE:CD2	2.87	0.57
2:Q:81:A:H2'	2:Q:82:C:O4'	2.05	0.57
2:R:17(C):U:O2	2:R:17(E):G:N2	2.40	0.55
3:B:33:ILE:HG21	3:B:72:MET:CE	2.37	0.53
3:A:28:LYS:HD3	3:B:25:GLU:HG3	1.91	0.52
2:Q:120:G:H2'	2:Q:121:A:O4'	2.08	0.52
3:D:17:LEU:HD21	3:D:82:MET:HG2	1.90	0.52
3:D:11:THR:HG23	3:D:57:VAL:C	2.36	0.51
2:P:126:G:H2'	2:P:127:G:O4'	2.11	0.50
2:P:82:C:H5''	6:P:9027:HOH:O	2.10	0.50
3:C:26:LEU:HD23	3:C:45:VAL:HG11	1.94	0.50
3:C:69:LEU:C	3:C:69:LEU:HD23	2.37	0.50
3:D:41:LEU:HD12	3:D:58:ILE:CG2	2.42	0.50
2:P:17(F):C:H41	3:A:85:GLN:NE2	2.10	0.49
2:P:83:C:O2'	2:P:86:A:N3	2.43	0.48
3:A:23:LYS:HG3	3:A:45:VAL:HG12	1.93	0.48
3:A:69:LEU:C	3:A:69:LEU:HD23	2.37	0.48
2:P:125:A:H2'	2:P:126:G:O4'	2.12	0.48
3:D:72:MET:CE	3:D:75:PHE:CG	2.97	0.48
2:R:51:U:H4'	2:R:52:C:OP2	2.13	0.48
1:G:11:U:H6	1:G:11:U:H5''	1.79	0.48
3:D:34:PHE:CZ	3:D:82:MET:HE1	2.49	0.47
1:G:-1:A:H1'	6:G:9021:HOH:O	2.14	0.47
3:C:15:ASN:HD21	3:C:83:ARG:HB3	1.79	0.47
3:A:75:PHE:HB3	3:A:82:MET:HE2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:17(F):C:H41	3:C:85:GLN:NE2	2.14	0.46
2:R:81:A:H2'	2:R:82:C:O4'	2.15	0.46
3:A:72:MET:HB3	3:A:82:MET:HE3	1.98	0.46
3:B:33:ILE:HG21	3:B:72:MET:HE1	1.97	0.46
3:D:72:MET:HE1	3:D:75:PHE:CD2	2.51	0.46
2:S:106:A:N7	6:S:9032:HOH:O	2.36	0.46
2:R:63:U:H2'	2:R:64:C:C6	2.51	0.46
3:B:33:ILE:CG2	3:B:72:MET:HE2	2.46	0.45
2:S:105:U:O2'	2:S:106:A:O5'	2.28	0.45
3:B:42:ASP:OD1	3:B:43:ILE:N	2.49	0.45
3:C:15:ASN:HD22	3:C:15:ASN:N	2.15	0.45
2:S:15:A:H61	2:S:19:U:H3	1.64	0.44
2:P:17(H):C:N3	3:A:91:SER:HA	2.33	0.44
2:Q:80:A:H2'	2:Q:81:A:C8	2.53	0.44
2:P:120:G:H2'	2:P:121:A:O4'	2.18	0.44
3:C:76:PRO:HG2	3:D:36:ARG:HD3	1.99	0.44
3:A:33:ILE:HG22	3:A:34:PHE:CD2	2.51	0.44
3:B:33:ILE:HG21	3:B:72:MET:HE2	1.99	0.44
2:Q:17(I):U:H4'	2:Q:17(J):C:OP1	2.18	0.44
2:S:69:U:H1'	2:S:87:A:C4	2.52	0.44
2:R:106:A:C2	2:R:116:A:C2	3.06	0.43
2:S:15:A:C2	2:S:20:G:C2	3.06	0.43
2:S:101:U:C5	2:S:102:C:C5	3.06	0.43
1:G:0:A2M:HM'1	2:R:58:A:O2'	2.19	0.43
3:D:58:ILE:HD13	3:D:93:ILE:CG2	2.49	0.43
2:P:17(G):A:H4'	3:A:51:MET:HE3	2.01	0.43
2:R:15:A:C2	2:R:20:G:C2	3.06	0.42
3:C:37:PHE:CZ	3:C:72:MET:HE2	2.53	0.42
1:E:1:G:C6	2:P:28:A:C6	3.08	0.42
2:S:20:G:C2	2:S:21:C:C2	3.07	0.42
3:A:30:LEU:O	3:A:33:ILE:HG22	2.19	0.42
3:B:33:ILE:CG2	3:B:72:MET:CE	2.97	0.42
2:R:136:U:H5'	2:R:136:U:H6	1.85	0.42
1:H:0:A2M:N9	1:H:0:A2M:HM'3	2.35	0.42
1:H:0:A2M:HM'2	2:S:59:U:C4	2.55	0.42
2:P:78:A:C2	2:P:137:G:C2	3.07	0.42
3:D:34:PHE:CE1	3:D:72:MET:HG3	2.55	0.42
2:R:17(H):C:N3	3:C:91:SER:HA	2.35	0.41
3:C:33:ILE:HD12	3:C:77:PHE:CE1	2.54	0.41
3:D:31:HIS:O	3:D:35:SER:OG	2.36	0.41
2:R:123:A:H2'	2:R:124:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:31:A:H1'	2:Q:124:A:N1	2.35	0.41
2:S:23:A:H2'	2:S:24:G:O4'	2.20	0.41
3:B:69:LEU:C	3:B:69:LEU:HD23	2.46	0.41
1:G:11:U:C2	2:R:24:G:N2	2.88	0.41
3:D:66:THR:HG23	3:D:86:TYR:OH	2.20	0.41
2:R:29:C:O2'	2:R:99:A:N3	2.51	0.41
2:R:93:U:H2'	2:R:94:A:C8	2.56	0.40
2:P:98:A:C6	2:P:99:A:C6	3.09	0.40
3:A:32:ALA:HB2	3:B:78:TYR:CZ	2.57	0.40
3:C:32:ALA:HB2	3:D:78:TYR:CZ	2.57	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	
3	A	88/94 (94%)	85 (97%)	3 (3%)	0	100	100
3	B	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
3	C	88/94 (94%)	84 (96%)	4 (4%)	0	100	100
3	D	88/94 (94%)	85 (97%)	3 (3%)	0	100	100
All	All	356/376 (95%)	345 (97%)	11 (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	
3	A	78/85 (92%)	70 (90%)	8 (10%)	7	14
3	B	81/85 (95%)	81 (100%)	0	100	100
3	C	79/85 (93%)	74 (94%)	5 (6%)	16	34
3	D	77/85 (91%)	70 (91%)	7 (9%)	9	19
All	All	315/340 (93%)	295 (94%)	20 (6%)	16	34

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	22	LYS
3	A	33	ILE
3	A	36	ARG
3	A	44	LEU
3	A	45	VAL
3	A	50	LYS
3	A	60	LYS
3	A	83	ARG
3	C	15	ASN
3	C	25	GLU
3	C	28	LYS
3	C	36	ARG
3	C	83	ARG
3	D	12	ILE
3	D	24	ASP
3	D	35	SER
3	D	36	ARG
3	D	47	ARG
3	D	50	LYS
3	D	63	SER

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

Mol	Chain	Res	Type
3	A	31	HIS
3	A	54	GLN
3	A	85	GLN
3	B	31	HIS
3	B	85	GLN

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Mol	Chain	Res	Type
3	C	15	ASN
3	C	85	GLN
3	D	9	ASN
3	D	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	11/13 (84%)	1 (9%)	0
1	F	12/13 (92%)	3 (25%)	0
1	G	12/13 (92%)	3 (25%)	0
1	H	12/13 (92%)	2 (16%)	0
2	P	140/141 (99%)	27 (19%)	5 (3%)
2	Q	139/141 (98%)	20 (14%)	6 (4%)
2	R	139/141 (98%)	23 (16%)	6 (4%)
2	S	139/141 (98%)	34 (24%)	5 (3%)
All	All	604/616 (98%)	113 (18%)	22 (3%)

All (113) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	1	G
2	P	17(I)	U
2	P	17(J)	C
2	P	17(L)	G
2	P	30	G
2	P	45	G
2	P	49	U
2	P	50	U
2	P	59	U
2	P	64	C
2	P	72	U
2	P	73	U
2	P	74	C
2	P	76	U
2	P	78	A
2	P	79	C
2	P	83	C
2	P	85	C
2	P	86	A
2	P	91	U

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Mol	Chain	Res	Type
2	P	92	U
2	P	94	A
2	P	106	A
2	P	130	A
2	P	133	G
2	P	137	G
2	P	140	G
2	P	141	A
1	F	0	A2M
1	F	1	G
1	F	6	A
2	Q	17(I)	U
2	Q	17(J)	C
2	Q	17(L)	G
2	Q	29	C
2	Q	30	G
2	Q	49	U
2	Q	50	U
2	Q	57	G
2	Q	59	U
2	Q	64	C
2	Q	72	U
2	Q	73	U
2	Q	76	U
2	Q	78	A
2	Q	85	C
2	Q	86	A
2	Q	87	A
2	Q	100	A
2	Q	137	G
2	Q	138	A
1	G	1	G
1	G	6	A
1	G	11	U
2	R	14	C
2	R	15	A
2	R	17(A)	C
2	R	17(I)	U
2	R	17(J)	C
2	R	17(K)	C
2	R	17(L)	G
2	R	21	C

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Mol	Chain	Res	Type
2	R	29	C
2	R	45	G
2	R	49	U
2	R	50	U
2	R	59	U
2	R	72	U
2	R	73	U
2	R	77	C
2	R	85	C
2	R	87	A
2	R	95	C
2	R	109	G
2	R	115	U
2	R	136	U
2	R	137	G
1	H	0	A2M
1	H	1	G
2	S	15	A
2	S	17(F)	C
2	S	17(H)	C
2	S	17(I)	U
2	S	17(K)	C
2	S	17(L)	G
2	S	20	G
2	S	29	C
2	S	30	G
2	S	45	G
2	S	49	U
2	S	59	U
2	S	64	C
2	S	72	U
2	S	73	U
2	S	76	U
2	S	78	A
2	S	81	A
2	S	82	C
2	S	85	C
2	S	86	A
2	S	88	G
2	S	90	U
2	S	92	U
2	S	104	U

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Mol	Chain	Res	Type
2	S	105	U
2	S	106	A
2	S	121	A
2	S	127	G
2	S	130	A
2	S	133	G
2	S	137	G
2	S	139	U
2	S	140	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	P	12	GTP
2	P	49	U
2	P	72	U
2	P	73	U
2	P	136	U
2	Q	17(I)	U
2	Q	50	U
2	Q	72	U
2	Q	86	A
2	Q	136	U
2	Q	137	G
2	R	17(I)	U
2	R	49	U
2	R	72	U
2	R	86	A
2	R	114	U
2	R	136	U
2	S	15	A
2	S	17(H)	C
2	S	72	U
2	S	85	C
2	S	136	U

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

8 non-standard protein/DNA/RNA residues 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	GTP	P	12	2	33,34,34	1.04	2 (6%)	50,54,54	1.59	9 (18%)
2	GTP	S	12	2	33,34,34	1.16	5 (15%)	50,54,54	1.57	9 (18%)
2	GTP	R	12	2	33,34,34	1.23	4 (12%)	50,54,54	1.53	7 (14%)
1	A2M	F	0	2,5,1	22,25,26	1.02	2 (9%)	30,36,39	2.06	7 (23%)
1	A2M	E	0	2,1	22,25,26	1.08	4 (18%)	30,36,39	2.08	9 (30%)
2	GTP	Q	12	2	33,34,34	1.56	5 (15%)	50,54,54	1.53	9 (18%)
1	A2M	H	0	2,1	22,25,26	1.08	4 (18%)	30,36,39	2.14	9 (30%)
1	A2M	G	0	2,1	22,25,26	1.10	2 (9%)	30,36,39	2.34	10 (33%)

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	GTP	P	12	2	-	6/22/38/38	0/3/3/3
2	GTP	S	12	2	-	3/22/38/38	0/3/3/3
2	GTP	R	12	2	-	4/22/38/38	0/3/3/3
1	A2M	F	0	2,5,1	-	0/9/27/28	0/3/3/3
1	A2M	E	0	2,1	-	0/9/27/28	0/3/3/3
2	GTP	Q	12	2	-	3/22/38/38	0/3/3/3
1	A2M	H	0	2,1	-	2/9/27/28	0/3/3/3
1	A2M	G	0	2,1	-	0/9/27/28	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	12	GTP	PB-O3A	5.12	1.65	1.59
2	Q	12	GTP	PA-O3A	4.47	1.64	1.59
2	R	12	GTP	PB-O3A	3.36	1.63	1.59
2	Q	12	GTP	PB-O3B	3.06	1.62	1.59
1	F	0	A2M	C4-N9	-3.04	1.31	1.37
1	G	0	A2M	C8-N9	-2.96	1.32	1.37
2	S	12	GTP	PB-O3B	2.91	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	12	GTP	PA-O3A	2.84	1.62	1.59
2	R	12	GTP	PA-O3A	2.78	1.62	1.59
2	P	12	GTP	PB-O3B	2.74	1.62	1.59
1	E	0	A2M	C4-N9	-2.55	1.32	1.37
2	R	12	GTP	PB-O3B	2.53	1.62	1.59
1	H	0	A2M	C8-N7	2.43	1.36	1.31
1	H	0	A2M	C5-N7	-2.40	1.34	1.39
1	E	0	A2M	C8-N9	-2.34	1.33	1.37
1	F	0	A2M	C8-N9	-2.34	1.33	1.37
1	G	0	A2M	C5-N7	-2.27	1.34	1.39
1	E	0	A2M	C5-N7	-2.27	1.34	1.39
1	H	0	A2M	C4-N9	-2.22	1.33	1.37
2	S	12	GTP	PB-O3A	2.17	1.61	1.59
1	E	0	A2M	C8-N7	2.08	1.35	1.31
2	S	12	GTP	C5-N7	-2.05	1.35	1.39
2	S	12	GTP	C4-N9	-2.05	1.32	1.38
2	R	12	GTP	C5-N7	-2.04	1.35	1.39
2	Q	12	GTP	C4-N9	-2.03	1.32	1.38
1	H	0	A2M	C8-N9	-2.03	1.34	1.37
2	Q	12	GTP	C5-N7	-2.02	1.35	1.39
2	P	12	GTP	C5-N7	-2.01	1.35	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	0	A2M	C5-C4-N3	-5.78	118.76	126.72
1	G	0	A2M	C5-C4-N3	-5.67	118.90	126.72
2	P	12	GTP	C5-C4-N3	-5.13	120.22	128.39
1	E	0	A2M	C5-C4-N3	-4.86	120.03	126.72
2	R	12	GTP	C5-C4-N3	-4.85	120.68	128.39
1	F	0	A2M	C5-C4-N3	-4.84	120.05	126.72
1	F	0	A2M	N3-C2-N1	-4.79	121.33	128.58
2	S	12	GTP	C5-C4-N3	-4.74	120.84	128.39
1	G	0	A2M	N3-C2-N1	-4.74	121.41	128.58
2	Q	12	GTP	C5-C4-N3	-4.65	120.99	128.39
2	P	12	GTP	C2-N3-C4	4.65	120.30	112.30
1	H	0	A2M	N3-C2-N1	-4.61	121.60	128.58
2	S	12	GTP	C2-N3-C4	4.55	120.14	112.30
1	E	0	A2M	N3-C2-N1	-4.53	121.72	128.58
2	R	12	GTP	C2-N3-C4	4.41	119.89	112.30
2	Q	12	GTP	C2-N3-C4	4.31	119.72	112.30
1	G	0	A2M	N9-C8-N7	-3.98	108.30	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	0	A2M	N3-C4-N9	3.71	133.48	127.17
1	G	0	A2M	C2-N3-C4	3.63	120.70	111.83
1	H	0	A2M	N3-C4-N9	3.62	133.33	127.17
1	F	0	A2M	N3-C4-N9	3.61	133.31	127.17
1	H	0	A2M	C2-N3-C4	3.52	120.44	111.83
1	E	0	A2M	N9-C8-N7	-3.47	109.02	113.94
1	E	0	A2M	N3-C4-N9	3.44	133.02	127.17
1	G	0	A2M	C4-C5-N7	-3.43	106.66	110.58
1	F	0	A2M	C4-N9-C8	3.41	109.32	105.74
1	E	0	A2M	C4-N9-C8	3.39	109.30	105.74
1	H	0	A2M	O4'-C1'-N9	3.33	114.49	108.09
1	F	0	A2M	C2-N3-C4	3.25	119.77	111.83
1	G	0	A2M	O4'-C1'-N9	3.18	114.20	108.09
1	G	0	A2M	C4-N9-C8	3.18	109.08	105.74
2	R	12	GTP	O6-C6-C5	-3.14	118.24	126.53
1	G	0	A2M	C5-N7-C8	3.12	108.35	103.45
2	R	12	GTP	N9-C4-N3	3.11	132.18	125.95
1	E	0	A2M	C2-N3-C4	3.05	119.27	111.83
1	H	0	A2M	N9-C8-N7	-2.99	109.70	113.94
1	F	0	A2M	O4'-C1'-N9	2.98	113.82	108.09
1	E	0	A2M	O4'-C1'-N9	2.93	113.72	108.09
1	F	0	A2M	N9-C8-N7	-2.91	109.81	113.94
2	Q	12	GTP	O6-C6-C5	-2.84	119.02	126.53
2	P	12	GTP	N9-C4-N3	2.76	131.47	125.95
2	S	12	GTP	O6-C6-C5	-2.66	119.51	126.53
2	Q	12	GTP	N9-C4-N3	2.66	131.26	125.95
2	S	12	GTP	N9-C4-N3	2.60	131.16	125.95
2	P	12	GTP	O6-C6-C5	-2.58	119.72	126.53
2	S	12	GTP	C5-C6-N1	2.49	119.58	113.25
1	H	0	A2M	C4-C5-N7	-2.45	107.78	110.58
2	P	12	GTP	C2-N1-C6	-2.44	120.69	125.11
2	R	12	GTP	N9-C8-N7	-2.40	108.95	113.40
2	P	12	GTP	C5-C6-N1	2.40	119.36	113.25
2	R	12	GTP	C5-C6-N1	2.35	119.23	113.25
2	Q	12	GTP	C5'-C4'-C3'	-2.35	106.77	115.21
2	P	12	GTP	N2-C2-N1	2.35	121.71	116.76
2	R	12	GTP	C2-N1-C6	-2.33	120.88	125.11
2	S	12	GTP	C2-N1-C6	-2.33	120.88	125.11
2	S	12	GTP	N9-C8-N7	-2.30	109.13	113.40
1	G	0	A2M	CM'-O2'-C2'	-2.30	108.58	114.47
2	Q	12	GTP	C5-C6-N1	2.26	119.02	113.25
1	E	0	A2M	C4-C5-N7	-2.20	108.06	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	12	GTP	N2-C2-N1	2.19	121.38	116.76
2	P	12	GTP	C4-C5-N7	-2.18	107.21	110.67
2	Q	12	GTP	N9-C8-N7	-2.16	109.39	113.40
1	H	0	A2M	C4-N9-C8	2.16	108.00	105.74
2	P	12	GTP	N9-C8-N7	-2.14	109.43	113.40
2	S	12	GTP	N2-C2-N1	2.10	121.19	116.76
2	Q	12	GTP	C2-N1-C6	-2.09	121.33	125.11
1	E	0	A2M	C5-N7-C8	2.05	106.67	103.45
2	S	12	GTP	C6-C5-N7	2.01	133.95	130.29
1	H	0	A2M	C5-N7-C8	2.00	106.60	103.45

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	12	GTP	C5'-O5'-PA-O3A
2	P	12	GTP	C5'-O5'-PA-O1A
2	P	12	GTP	C5'-O5'-PA-O2A
2	P	12	GTP	O4'-C4'-C5'-O5'
2	R	12	GTP	O4'-C4'-C5'-O5'
2	S	12	GTP	PB-O3A-PA-O5'
2	P	12	GTP	C3'-C4'-C5'-O5'
2	R	12	GTP	C3'-C4'-C5'-O5'
2	Q	12	GTP	PB-O3B-PG-O1G
1	H	0	A2M	O4'-C4'-C5'-O5'
2	S	12	GTP	O4'-C4'-C5'-O5'
2	R	12	GTP	PB-O3A-PA-O5'
1	H	0	A2M	C3'-C4'-C5'-O5'
2	P	12	GTP	PB-O3B-PG-O3G
2	R	12	GTP	PB-O3A-PA-O1A
2	Q	12	GTP	PA-O3A-PB-O3B
2	Q	12	GTP	PA-O3A-PB-O1B
2	S	12	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	0	A2M	2	0
1	G	0	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GLP	G	5003	-	16,16,16	0.82	1 (6%)	22,24,24	1.19	2 (9%)
4	GLP	H	5004	-	16,16,16	0.79	0	22,24,24	1.16	2 (9%)
4	GLP	P	5001	-	16,16,16	0.58	0	22,24,24	1.11	2 (9%)
4	GLP	F	5002	-	16,16,16	0.77	0	22,24,24	1.18	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLP	G	5003	-	-	0/6/26/26	0/1/1/1
4	GLP	H	5004	-	-	0/6/26/26	0/1/1/1
4	GLP	P	5001	-	-	0/6/26/26	0/1/1/1
4	GLP	F	5002	-	-	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5003	GLP	C3-C2	-2.02	1.51	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5002	GLP	O3P-P-O2P	3.14	119.59	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	5001	GLP	O5-C1-C2	2.86	112.85	109.51
4	H	5004	GLP	O6-P-O1P	-2.75	99.02	106.44
4	G	5003	GLP	O5-C1-C2	2.71	112.67	109.51
4	F	5002	GLP	O2P-P-O6	-2.43	100.34	106.67
4	H	5004	GLP	O5-C1-C2	2.39	112.30	109.51
4	G	5003	GLP	O3P-P-O2P	2.19	116.01	107.80
4	P	5001	GLP	C4-C3-C2	-2.11	107.49	110.99
4	F	5002	GLP	O3-C3-C4	-2.06	105.52	110.38

There are no chirality outliers.

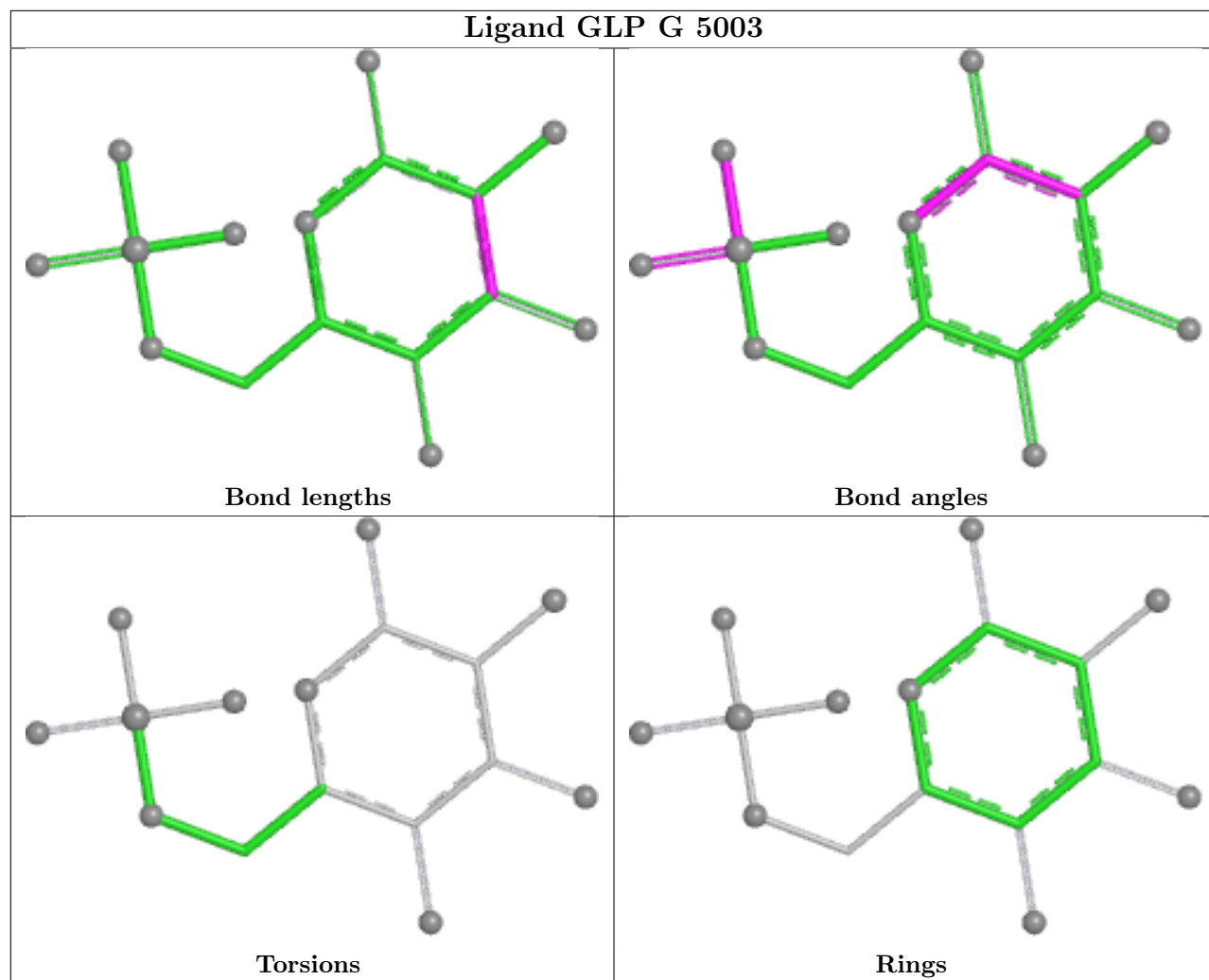
There are no torsion outliers.

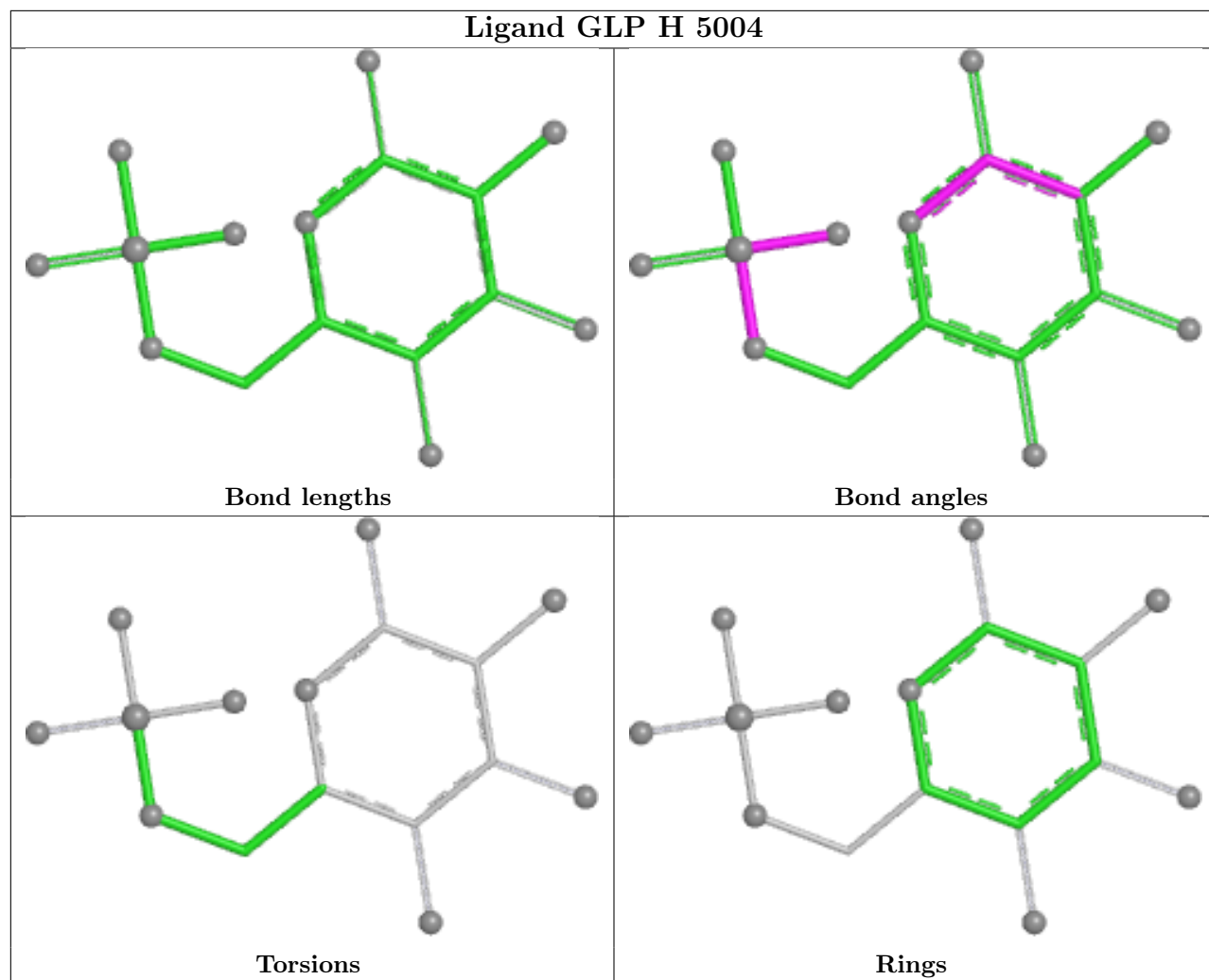
There are no ring outliers.

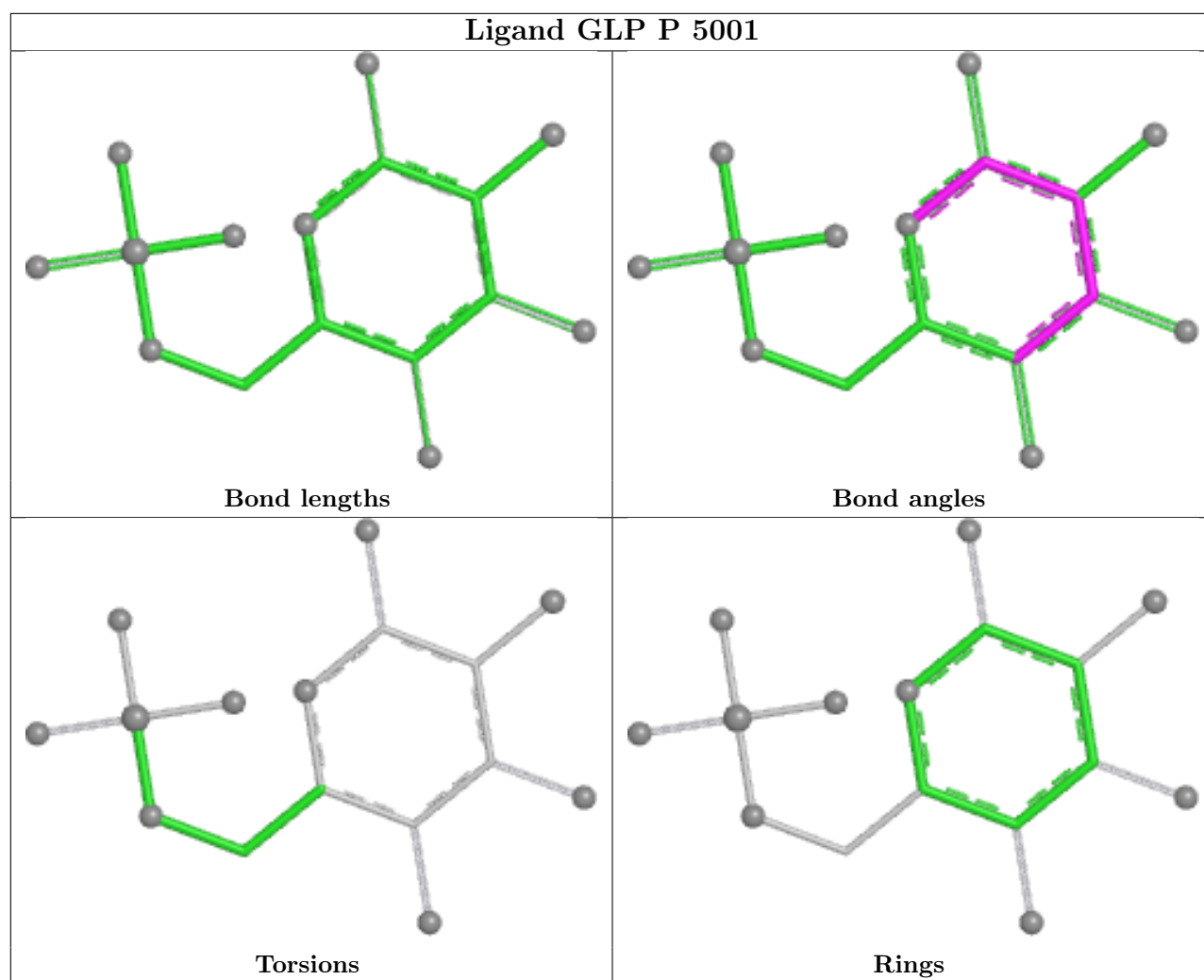
No monomer is involved in short contacts.

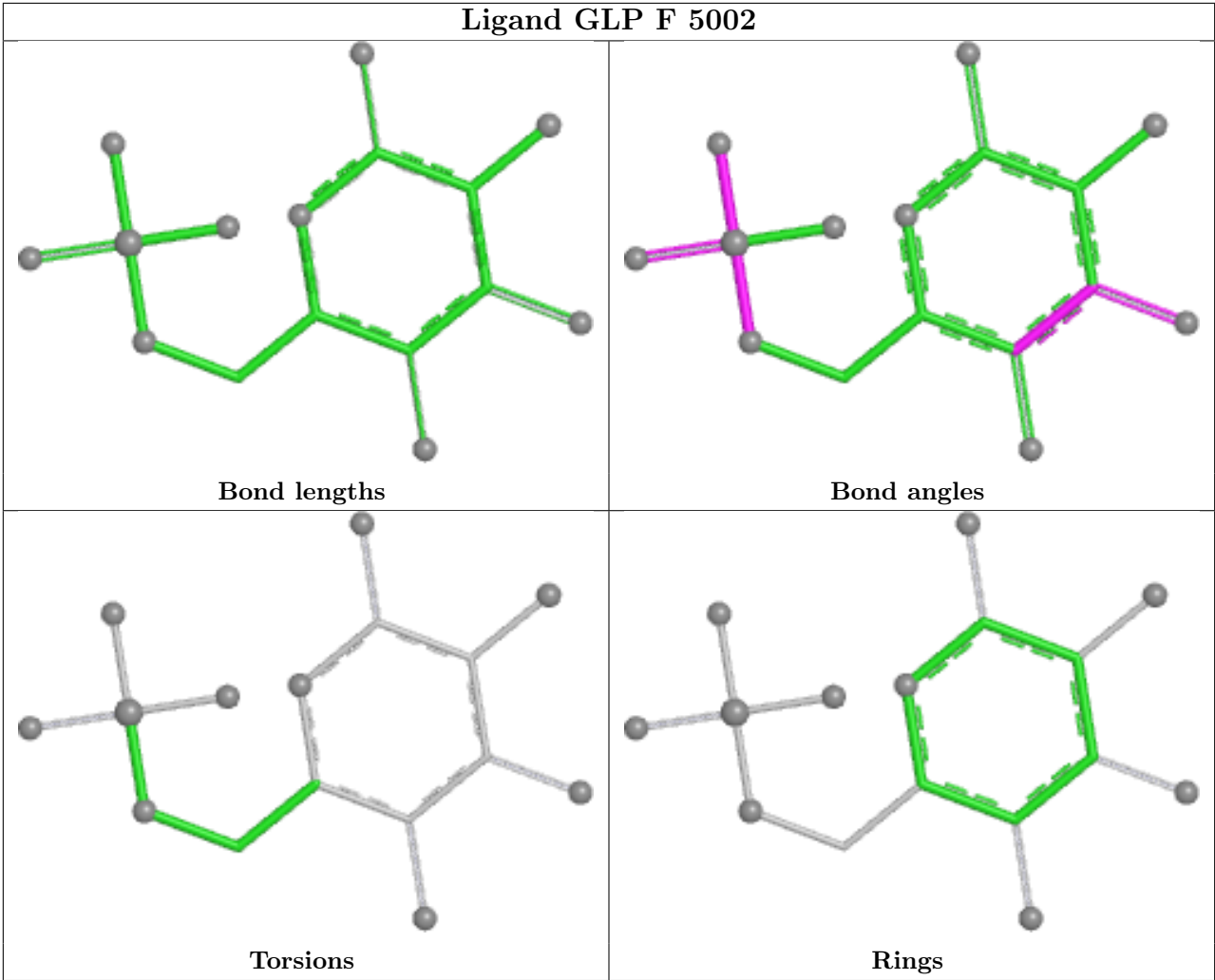
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand GLP G 5003









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	92:ASP	C	93:ILE	N	0.91

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	E	12/13 (92%)	0.09	0 100 100	33, 51, 61, 62	0
1	F	12/13 (92%)	0.09	0 100 100	25, 46, 51, 60	0
1	G	12/13 (92%)	0.24	0 100 100	25, 46, 51, 60	0
1	H	12/13 (92%)	0.15	0 100 100	34, 51, 61, 61	0
2	P	140/141 (99%)	0.78	15 (10%) 11 9	38, 61, 103, 117	0
2	Q	140/141 (99%)	0.22	2 (1%) 73 70	28, 49, 73, 79	0
2	R	140/141 (99%)	0.33	4 (2%) 53 49	28, 49, 73, 79	0
2	S	140/141 (99%)	0.98	19 (13%) 7 5	37, 61, 102, 117	0
3	A	90/94 (95%)	0.97	10 (11%) 10 8	42, 59, 69, 99	0
3	B	94/94 (100%)	0.64	7 (7%) 20 18	40, 47, 68, 78	0
3	C	90/94 (95%)	0.81	7 (7%) 19 17	40, 47, 68, 70	0
3	D	90/94 (95%)	1.18	12 (13%) 7 6	42, 60, 69, 99	0
All	All	972/992 (97%)	0.67	76 (7%) 19 17	25, 55, 95, 117	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	59	PHE	6.4
2	S	85	C	4.8
2	R	72	U	4.2
3	D	57	VAL	3.9
3	A	50	LYS	3.6
3	D	40	ILE	3.6
2	P	140	G	3.4
2	P	72	U	3.4
3	B	84	ILE	3.4
3	D	85	GLN	3.3
2	P	85	C	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	56	PHE	3.2
2	P	17(J)	C	3.2
3	D	56	PHE	3.1
3	A	83	ARG	3.1
2	S	83	C	3.0
3	D	87	ALA	2.9
2	S	82	C	2.9
2	S	86	A	2.9
2	P	17(K)	C	2.9
2	P	141	A	2.9
3	C	11	THR	2.8
2	P	75	A	2.8
3	A	93	ILE	2.8
3	A	89	THR	2.8
3	C	33	ILE	2.7
2	P	17(I)	U	2.7
2	R	21	C	2.7
3	C	17	LEU	2.7
3	B	92	ASP	2.7
3	A	14	ILE	2.7
2	S	65	C	2.7
3	B	33	ILE	2.6
2	S	94	A	2.6
2	S	79	C	2.5
2	S	38	G	2.5
2	S	81	A	2.5
2	P	84	G	2.5
3	A	92	ASP	2.4
2	P	81	A	2.4
3	D	65	ALA	2.4
3	D	30	LEU	2.4
2	S	140	G	2.4
3	A	96	LYS	2.3
2	P	138	A	2.3
2	S	132	A	2.3
3	B	14	ILE	2.3
2	S	17(F)	C	2.3
3	C	56	PHE	2.3
2	P	86	A	2.3
2	P	134	U	2.3
2	S	72	U	2.2
3	B	13	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	93	ILE	2.2
3	D	33	ILE	2.2
2	Q	73	U	2.2
2	S	37	G	2.2
2	S	75	A	2.1
3	A	87	ALA	2.1
3	A	33	ILE	2.1
3	B	79	ASP	2.1
3	C	57	VAL	2.1
3	D	15	ASN	2.1
2	P	80	A	2.1
3	B	24	ASP	2.1
2	P	74	C	2.1
2	Q	140	G	2.0
3	C	21	ILE	2.0
2	R	141	A	2.0
2	S	21	C	2.0
2	S	66	C	2.0
3	D	34	PHE	2.0
2	R	18	G	2.0
2	S	84	G	2.0
3	D	12	ILE	2.0
2	S	17(I)	U	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	GTP	S	12	32/32	0.74	0.14	69,72,85,85	0
2	GTP	P	12	32/32	0.76	0.13	69,72,84,85	0
2	GTP	R	12	32/32	0.81	0.13	41,47,66,66	0
2	GTP	Q	12	32/32	0.85	0.12	42,47,65,66	0
1	A2M	G	0	23/24	0.90	0.11	25,26,36,37	0
1	A2M	H	0	23/24	0.92	0.10	35,37,43,44	0
1	A2M	F	0	23/24	0.93	0.09	23,26,37,39	0
1	A2M	E	0	23/24	0.94	0.09	35,36,43,44	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

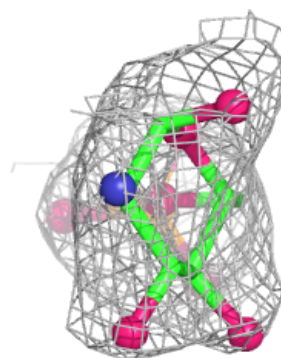
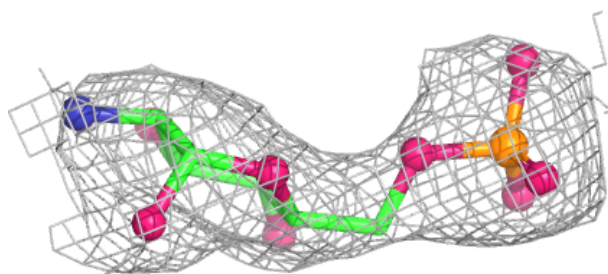
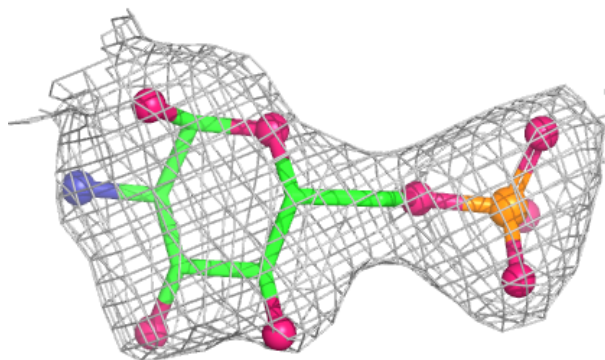
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	MG	P	9009	1/1	0.59	0.36	70,70,70,70	0
5	MG	F	9011	1/1	0.65	0.44	73,73,73,73	0
5	MG	G	9013	1/1	0.65	0.45	68,68,68,68	0
5	MG	S	9003	1/1	0.70	0.86	79,79,79,79	0
5	MG	H	9015	1/1	0.73	0.52	76,76,76,76	0
5	MG	Q	9012	1/1	0.75	0.32	56,56,56,56	0
5	MG	P	9010	1/1	0.84	0.20	49,49,49,49	0
5	MG	P	9006	1/1	0.85	0.12	59,59,59,59	0
5	MG	R	9014	1/1	0.86	0.25	51,51,51,51	0
4	GLP	H	5004	16/16	0.93	0.15	51,54,59,60	0
4	GLP	F	5002	16/16	0.95	0.14	40,45,50,51	0
4	GLP	P	5001	16/16	0.96	0.12	51,53,55,56	0
4	GLP	G	5003	16/16	0.96	0.12	41,45,48,48	0
5	MG	R	9002	1/1	0.97	0.06	47,47,47,47	0
5	MG	Q	9008	1/1	0.99	0.10	46,46,46,46	0
5	MG	P	9005	1/1	0.99	0.09	50,50,50,50	0
5	MG	Q	9007	1/1	0.99	0.09	42,42,42,42	0
5	MG	H	9016	1/1	0.99	0.12	57,57,57,57	0
5	MG	R	9001	1/1	0.99	0.12	51,51,51,51	0
5	MG	S	9004	1/1	0.99	0.08	54,54,54,54	0

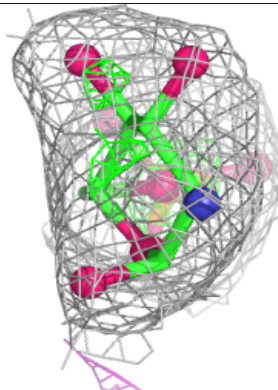
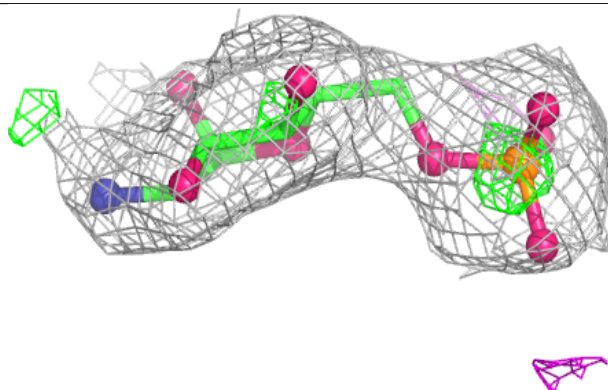
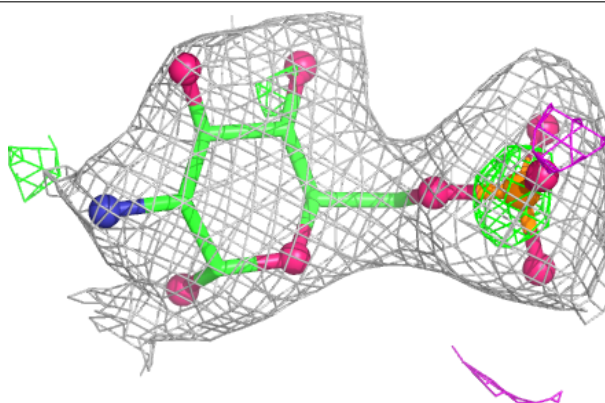
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GLP H 5004:

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

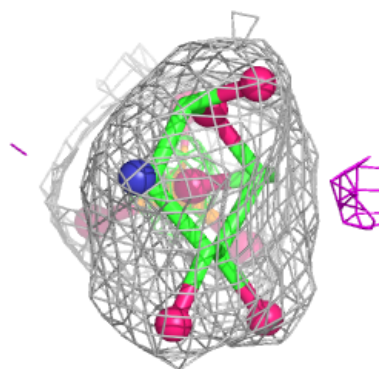
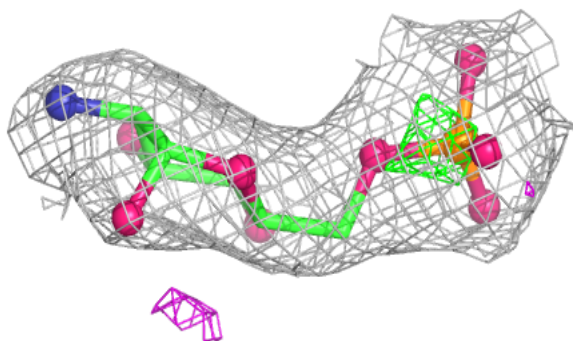
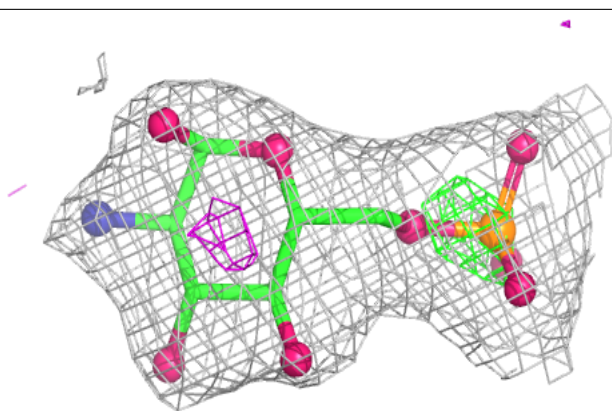
**Electron density around GLP F 5002:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

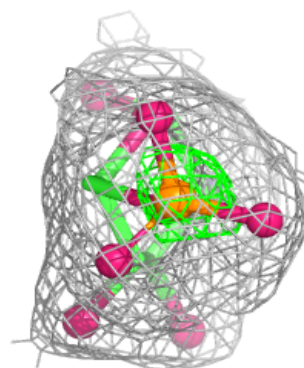
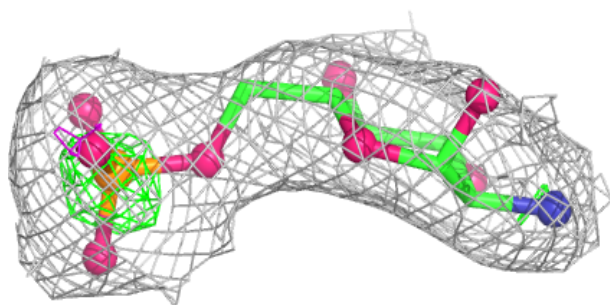
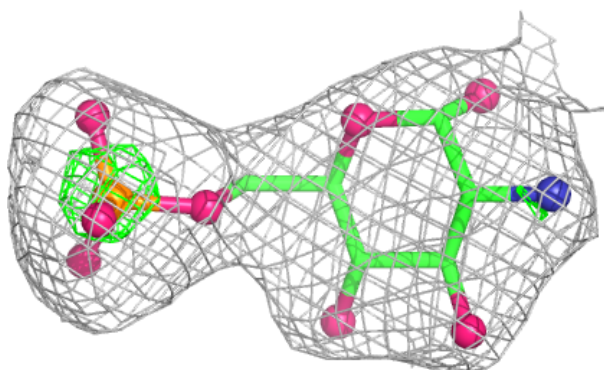


Electron density around GLP P 5001:

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

**Electron density around GLP G 5003:**

$2mF_o-DF_c$ (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.