wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 03:37 PM EDT

PDB ID	:	2NZ4
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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

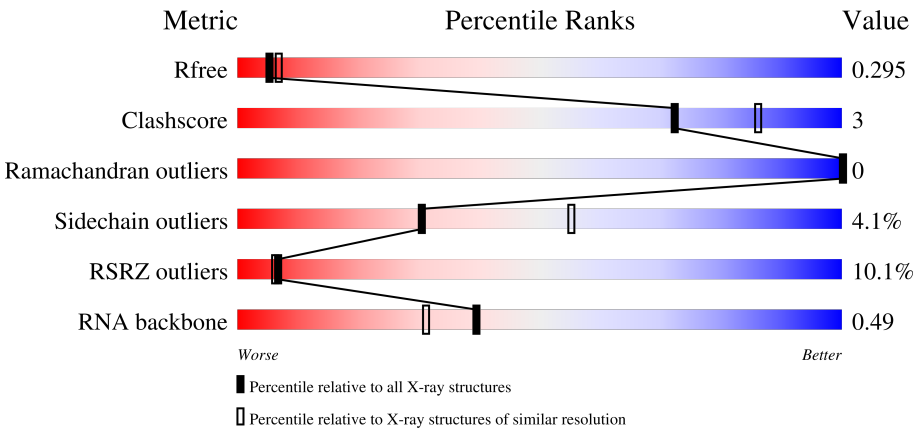
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 <=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	69% 23% 8%
1	F	13	69% 23% 8%
1	G	13	54% 15% 23% 8%
1	H	13	77% 8% 8% 8%

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Mol	Chain	Length	Quality of chain
2	P	141	8% 69% 24% 7%
2	Q	141	70% 23% 6%
2	R	141	2% 60% 33% 6%
2	S	141	10% 62% 34%
3	A	94	18% 80% 15%
3	B	94	3% 87% 13%
3	C	94	16% 81% 14%
3	D	94	37% 72% 21%

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	G	9013	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	P			
1	E	13	263	120	47	84	12	0	0	0
1	F	13	277	126	54	85	12	0	0	0
1	G	13	277	126	54	85	12	0	0	0
1	H	13	267	121	49	85	12	0	0	0

- Molecule 2 is a RNA chain called GlmS ribozyme.

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

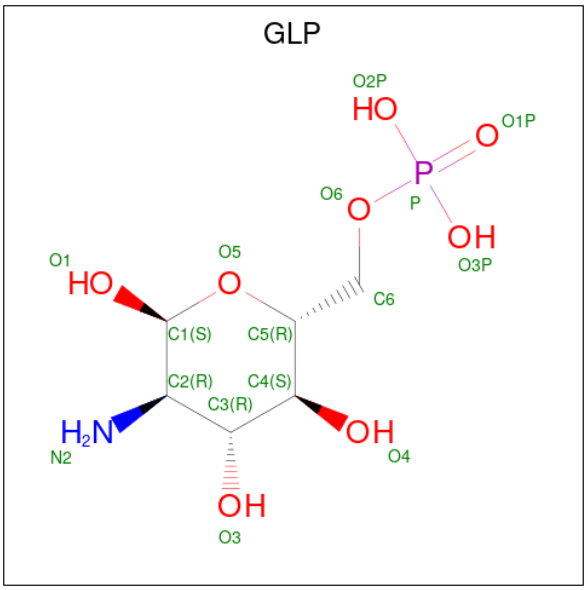
- Molecule 3 is a protein called U1 Small Nuclear Ribonucleoprotein A.

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

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 (three-letter code: GLP) (formula: $C_6H_{14}NO_8P$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

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

3 Residue-property plots (i)

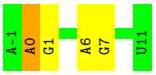
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

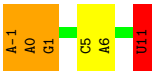
- Molecule 1: substrate strand RNA 13-mer

Chain F:



- Molecule 1: substrate strand RNA 13-mer

Chain G:

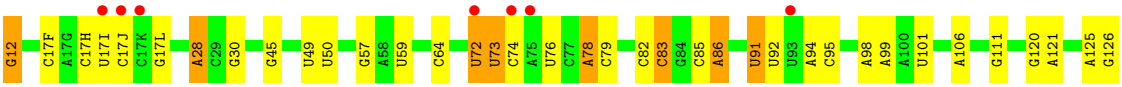


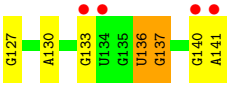
- Molecule 1: substrate strand RNA 13-mer

Chain H:

- Molecule 2: GlmS ribozyme

Chain P:



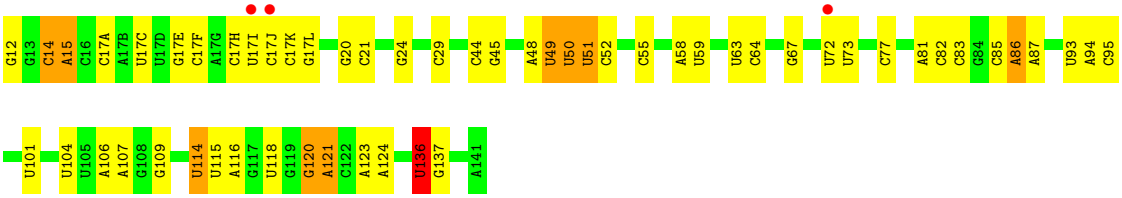


• Molecule 2: GlmS ribozyme

Chain Q:

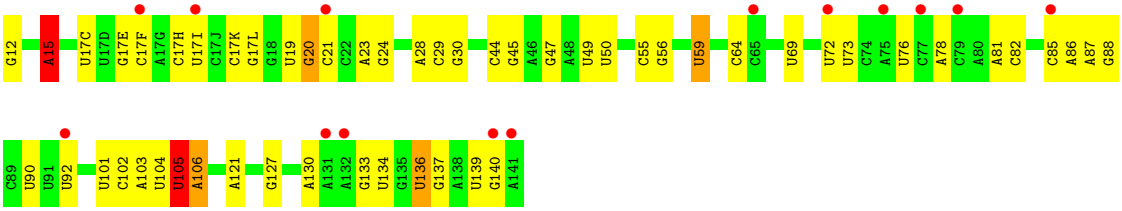
• Molecule 2: GlmS ribozyme

Chain R:



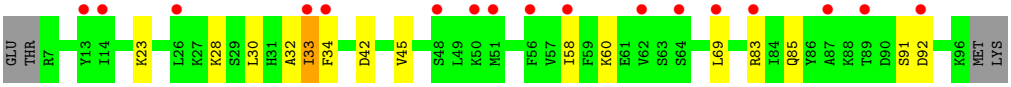
• Molecule 2: GlmS ribozyme

Chain S:



• Molecule 3: U1 Small Nuclear Ribonucleoprotein A

Chain A:

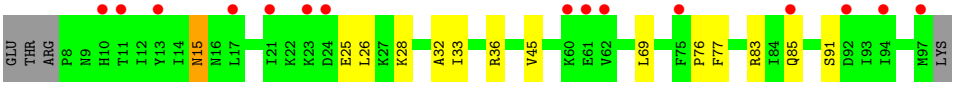


• Molecule 3: U1 Small Nuclear Ribonucleoprotein A

Chain B:

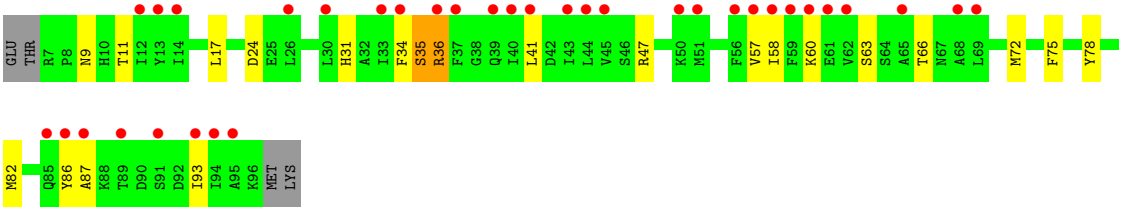
• Molecule 3: U1 Small Nuclear Ribonucleoprotein A

Chain C:



• Molecule 3: U1 Small Nuclear Ribonucleoprotein A

Chain D:



4 Data and refinement statistics (i)

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 39.08 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.94-2.50) 99.3 (39.08-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.269 0.255 , 0.295	Depositor DCC
R_{free} test set	3987 reflections (5.01%)	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 , 21.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: A2M, GLP, GTP, 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	0.85	0/267	1.47	4/412 (1.0%)
1	F	0.81	0/284	1.52	2/441 (0.5%)
1	G	0.93	0/284	1.66	8/441 (1.8%)
1	H	0.79	0/272	1.51	3/422 (0.7%)
2	P	0.68	0/3295	1.26	10/5134 (0.2%)
2	Q	0.82	2/3322 (0.1%)	1.42	23/5176 (0.4%)
2	R	0.85	1/3331 (0.0%)	1.41	27/5190 (0.5%)
2	S	0.70	0/3322	1.29	15/5176 (0.3%)
3	A	0.80	1/733 (0.1%)	0.60	1/984 (0.1%)
3	B	0.42	0/762	0.57	0/1022
3	C	0.43	0/736	0.54	0/986
3	D	0.42	0/729	0.54	0/979
All	All	0.74	4/17337 (0.0%)	1.27	93/26363 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	92	ASP	C-N	-18.71	0.91	1.34
2	R	49	U	C4-O4	12.62	1.33	1.23
2	Q	125	A	N7-C5	-6.01	1.35	1.39
2	Q	124	A	N7-C5	-5.67	1.35	1.39

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	49	U	N3-C4-C5	12.19	121.92	114.60
2	R	49	U	C2-N3-C4	-11.65	120.01	127.00
2	R	49	U	C5-C4-O4	-10.23	119.76	125.90
2	Q	48	A	O4'-C1'-N9	10.14	116.32	108.20
1	H	-1	A	C1'-O4'-C4'	-9.12	102.61	109.90

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	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	10	0
2	Q	3003	0	1505	7	0
2	R	3011	0	1509	14	0
2	S	3003	0	1506	10	0
3	A	720	0	730	10	0
3	B	749	0	762	12	0
3	C	723	0	739	10	0
3	D	716	0	721	17	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	43	0	0	0	0
6	S	30	0	0	2	0
All	All	16274	0	9580	86	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 3.

The worst 5 of 86 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:72:MET:HE3	3:D:75:PHE:CG	2.18	0.79
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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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 (i)

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%)	75 (96%)	3 (4%)	33	58
3	B	81/85 (95%)	81 (100%)	0	100	100
3	C	79/85 (93%)	75 (95%)	4 (5%)	24	45
3	D	77/85 (91%)	71 (92%)	6 (8%)	12	24
All	All	315/340 (93%)	302 (96%)	13 (4%)	30	55

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	24	ASP
3	D	35	SER
3	D	63	SER
3	D	47	ARG
3	D	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	85	GLN
3	D	9	ASN
3	D	85	GLN
3	B	85	GLN
3	A	85	GLN

5.3.3 RNA (i)

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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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%)	33 (23%)	5 (3%)
All	All	604/616 (98%)	112 (18%)	22 (3%)

5 of 112 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

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	86	A
2	S	15	A
2	R	136	U
2	S	17(H)	C
2	Q	50	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	Q	12	2	26,34,34	0.82	0	33,54,54	1.85	8 (24%)
1	A2M	G	0	1,2	18,25,26	0.85	0	18,36,39	1.55	3 (16%)
1	A2M	E	0	1,2	18,25,26	0.85	0	18,36,39	1.48	1 (5%)
2	GTP	S	12	2	26,34,34	0.76	0	33,54,54	1.81	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	A2M	H	0	1,2	18,25,26	0.89	1 (5%)	18,36,39	1.40	1 (5%)
1	A2M	F	0	2,1,5	18,25,26	0.76	0	18,36,39	1.51	1 (5%)
2	GTP	R	12	2	26,34,34	0.83	0	33,54,54	1.75	6 (18%)
2	GTP	P	12	2	26,34,34	0.78	0	33,54,54	1.86	9 (27%)

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	Q	12	2	-	3/18/38/38	0/3/3/3
1	A2M	G	0	1,2	-	0/5/27/28	0/3/3/3
1	A2M	E	0	1,2	-	0/5/27/28	0/3/3/3
2	GTP	S	12	2	-	3/18/38/38	0/3/3/3
1	A2M	H	0	1,2	-	2/5/27/28	0/3/3/3
1	A2M	F	0	2,1,5	-	0/5/27/28	0/3/3/3
2	GTP	R	12	2	-	6/18/38/38	0/3/3/3
2	GTP	P	12	2	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	0	A2M	O4'-C1'	2.12	1.44	1.41

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	12	GTP	N3-C2-N1	-5.22	120.27	127.22
2	Q	12	GTP	N3-C2-N1	-5.14	120.37	127.22
2	R	12	GTP	N3-C2-N1	-5.11	120.41	127.22
2	P	12	GTP	N3-C2-N1	-5.00	120.55	127.22
1	F	0	A2M	N3-C2-N1	-4.70	121.33	128.68

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	12	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
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'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	P	5001	-	16,16,16	0.58	0	23,24,24	1.14	2 (8%)
4	GLP	H	5004	-	16,16,16	0.78	0	23,24,24	1.16	2 (8%)
4	GLP	G	5003	-	16,16,16	0.81	1 (6%)	23,24,24	1.19	3 (13%)
4	GLP	F	5002	-	16,16,16	0.76	0	23,24,24	1.17	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	P	5001	-	-	0/6/26/26	0/1/1/1
4	GLP	H	5004	-	-	0/6/26/26	0/1/1/1
4	GLP	G	5003	-	-	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

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5002	GLP	O3P-P-O2P	3.13	119.59	107.64
4	P	5001	GLP	O5-C1-C2	2.86	112.85	109.51
4	G	5003	GLP	O5-C1-C2	2.71	112.67	109.51
4	H	5004	GLP	O6-P-O1P	-2.66	99.02	106.47
4	F	5002	GLP	O2P-P-O6	-2.40	100.34	106.73

There are no chirality outliers.

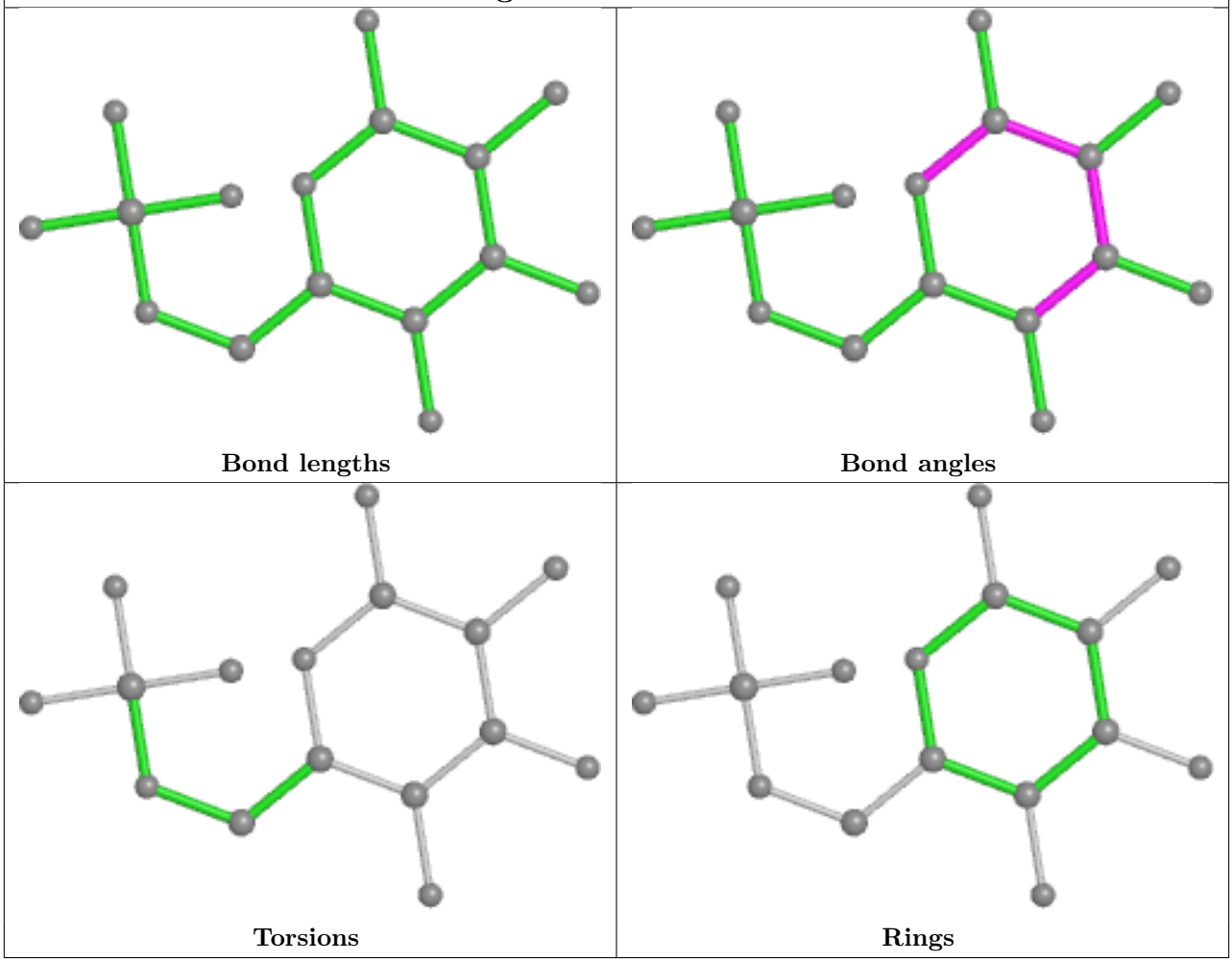
There are no torsion outliers.

There are no ring outliers.

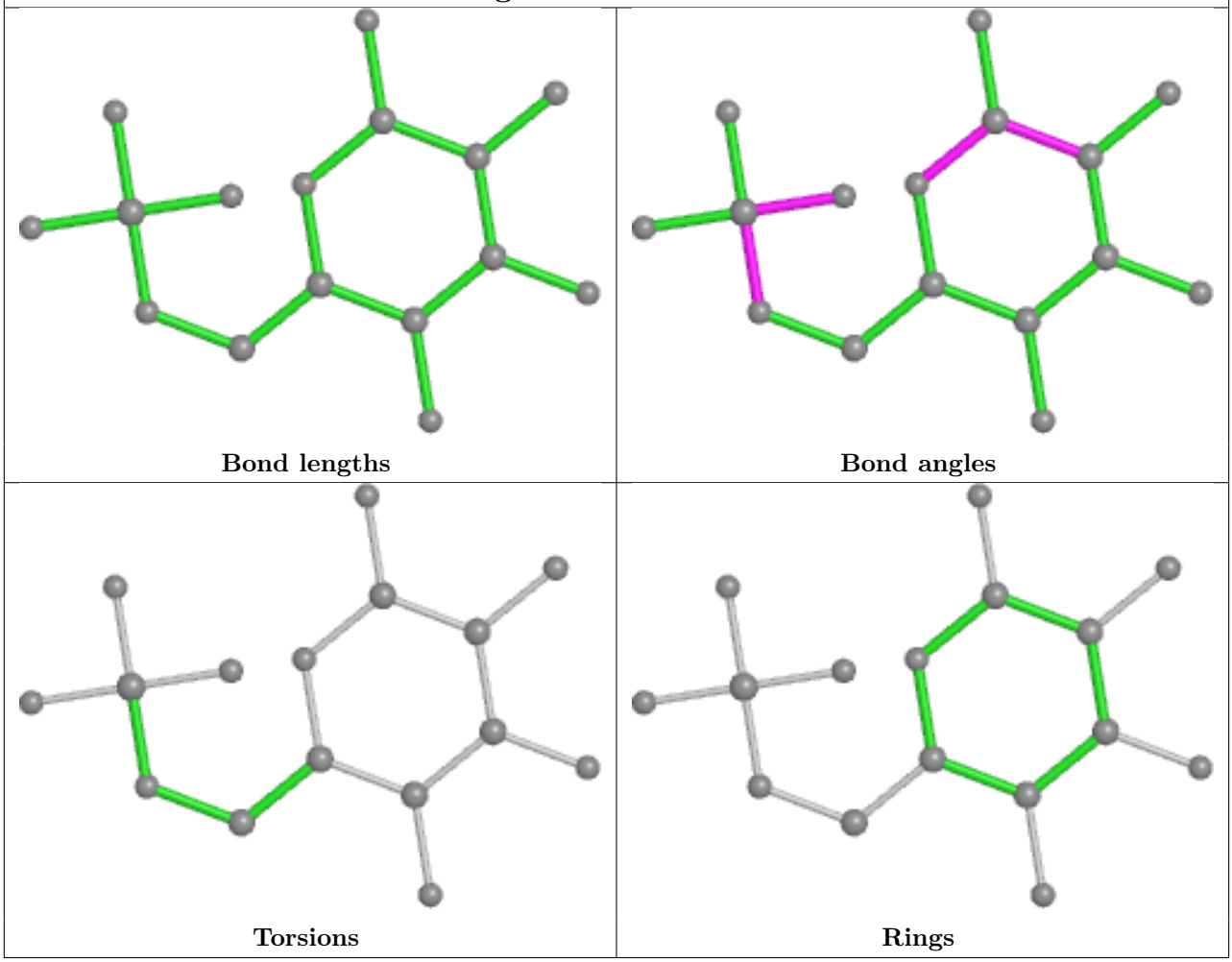
No monomer is involved in short contacts.

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 then 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.

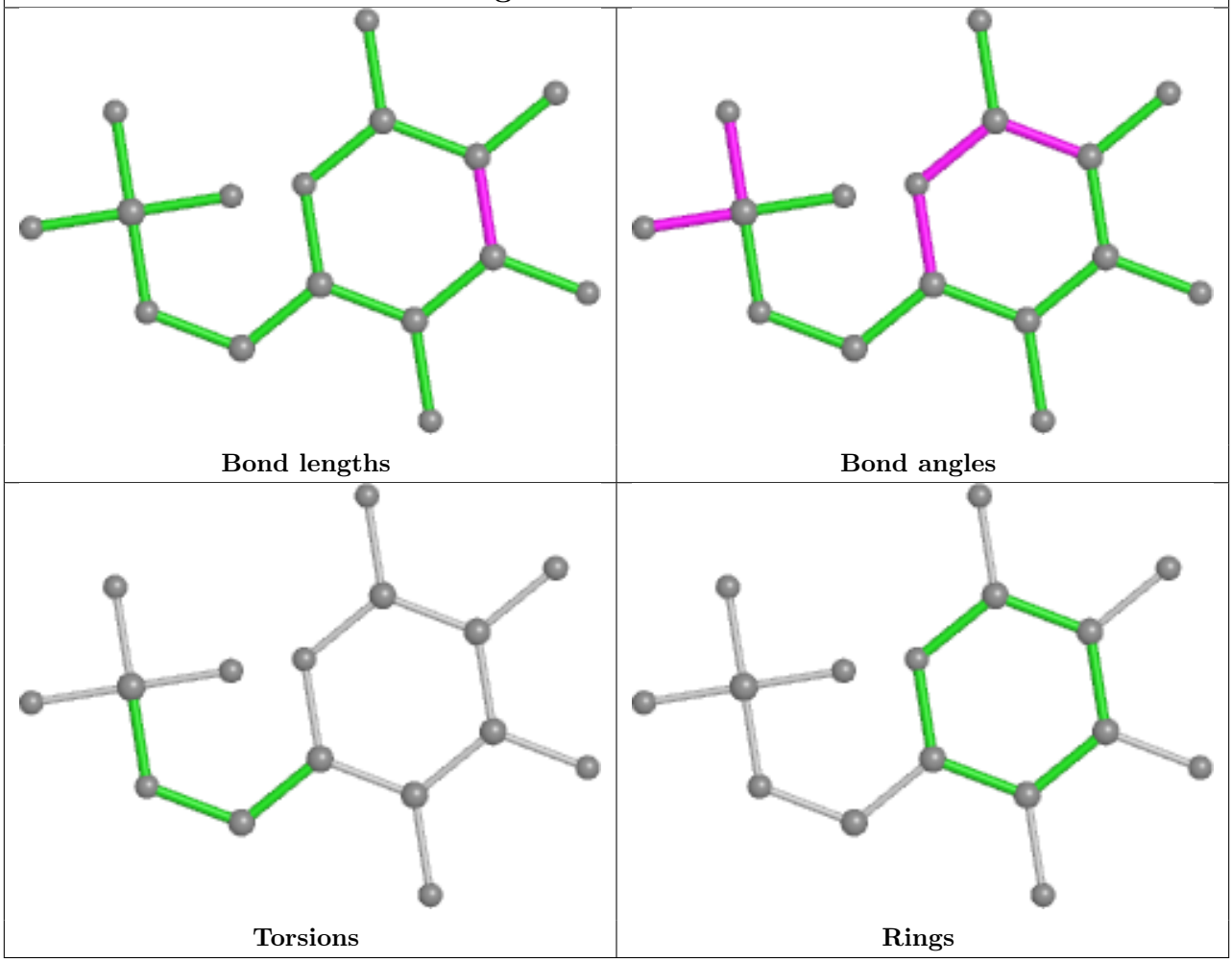
Ligand GLP P 5001



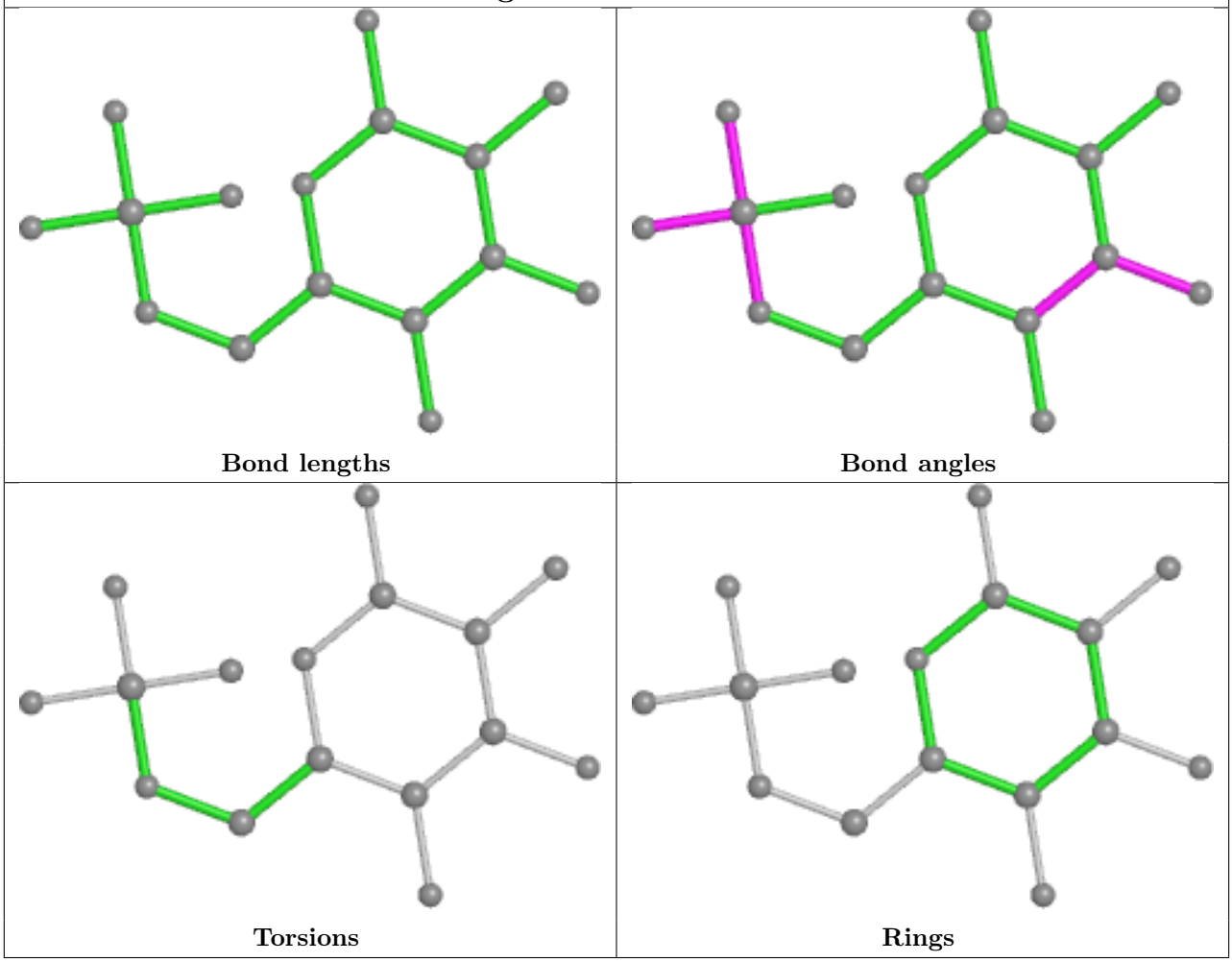
Ligand GLP H 5004



Ligand GLP G 5003



Ligand GLP F 5002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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 (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	E	12/13 (92%)	-0.54	0	100	100	33, 51, 61, 62	0
1	F	12/13 (92%)	-0.21	0	100	100	25, 46, 51, 60	0
1	G	12/13 (92%)	-0.37	0	100	100	25, 46, 51, 60	0
1	H	12/13 (92%)	-0.57	0	100	100	34, 51, 61, 61	0
2	P	140/141 (99%)	0.13	11 (7%)	12	12	38, 61, 103, 117	0
2	Q	140/141 (99%)	-0.26	0	100	100	28, 49, 73, 79	0
2	R	140/141 (99%)	-0.19	3 (2%)	63	66	28, 49, 73, 79	0
2	S	140/141 (99%)	0.29	14 (10%)	7	6	37, 61, 102, 117	0
3	A	90/94 (95%)	1.15	17 (18%)	1	1	42, 59, 69, 99	0
3	B	94/94 (100%)	0.54	3 (3%)	47	51	40, 47, 68, 78	0
3	C	90/94 (95%)	0.94	15 (16%)	1	1	40, 47, 68, 70	0
3	D	90/94 (95%)	2.12	35 (38%)	0	0	42, 60, 69, 99	0
All	All	972/992 (97%)	0.42	98 (10%)	7	6	25, 55, 95, 117	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	59	PHE	12.1
3	D	40	ILE	7.5
3	D	94	ILE	6.7
3	D	39	GLN	6.5
3	D	57	VAL	6.5

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	P	12	32/32	0.79	0.14	69,72,84,85	0
2	GTP	S	12	32/32	0.81	0.16	69,72,85,85	0
2	GTP	R	12	32/32	0.85	0.17	41,47,66,66	0
2	GTP	Q	12	32/32	0.87	0.15	42,47,65,66	0
1	A2M	G	0	23/24	0.93	0.15	25,26,36,37	0
1	A2M	H	0	23/24	0.94	0.14	35,37,43,44	0
1	A2M	F	0	23/24	0.95	0.13	23,26,37,39	0
1	A2M	E	0	23/24	0.97	0.14	35,36,43,44	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	P	9009	1/1	0.72	0.32	70,70,70,70	0
5	MG	G	9013	1/1	0.77	0.43	68,68,68,68	0
5	MG	P	9006	1/1	0.80	0.14	59,59,59,59	0
5	MG	F	9011	1/1	0.84	0.42	73,73,73,73	0
5	MG	R	9002	1/1	0.84	0.12	47,47,47,47	0
5	MG	P	9010	1/1	0.88	0.18	49,49,49,49	0
5	MG	R	9014	1/1	0.89	0.29	51,51,51,51	0
5	MG	Q	9012	1/1	0.93	0.38	56,56,56,56	0
5	MG	H	9015	1/1	0.94	0.40	76,76,76,76	0
5	MG	S	9003	1/1	0.94	0.59	79,79,79,79	0
4	GLP	H	5004	16/16	0.96	0.19	51,54,59,60	0
5	MG	R	9001	1/1	0.97	0.20	51,51,51,51	0
4	GLP	P	5001	16/16	0.97	0.18	51,53,55,56	0
5	MG	P	9005	1/1	0.97	0.15	50,50,50,50	0
4	GLP	F	5002	16/16	0.97	0.22	40,45,50,51	0
5	MG	H	9016	1/1	0.97	0.17	57,57,57,57	0
4	GLP	G	5003	16/16	0.97	0.21	41,45,48,48	0
5	MG	S	9004	1/1	0.97	0.14	54,54,54,54	0

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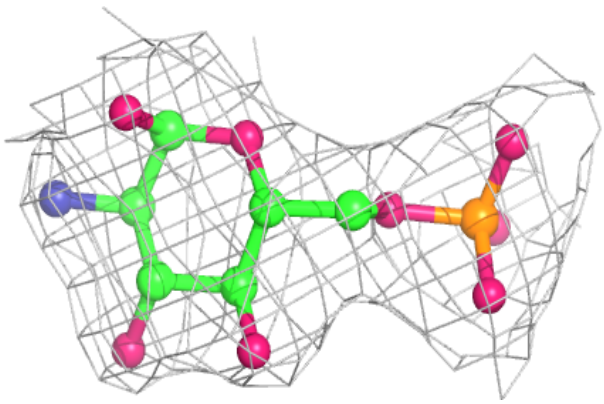
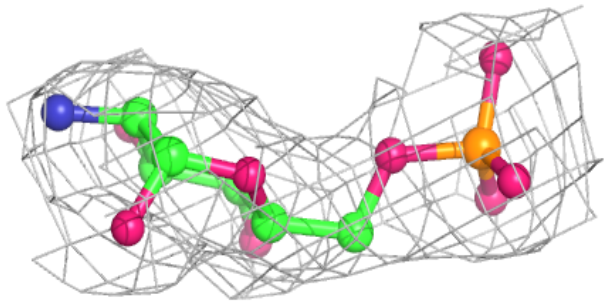
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	Q	9008	1/1	0.98	0.18	46,46,46,46	0
5	MG	Q	9007	1/1	0.99	0.14	42,42,42,42	0

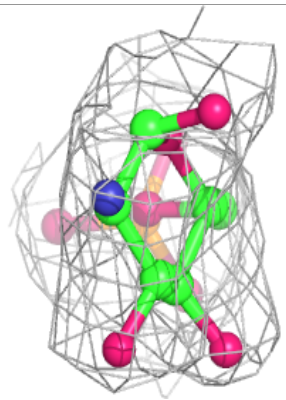
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

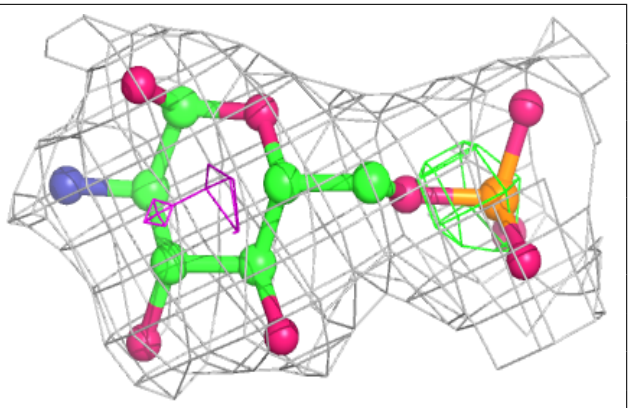


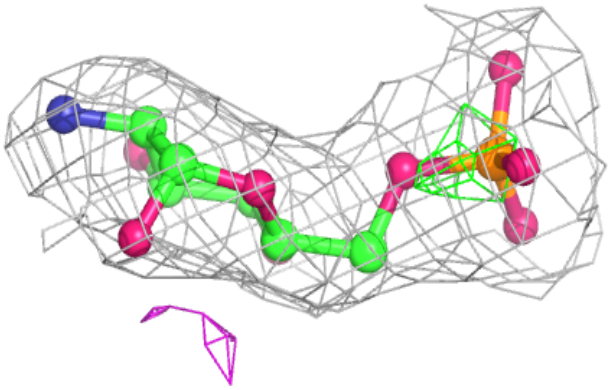


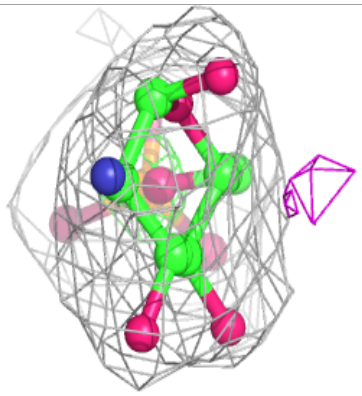


Electron density around GLP P 5001:

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

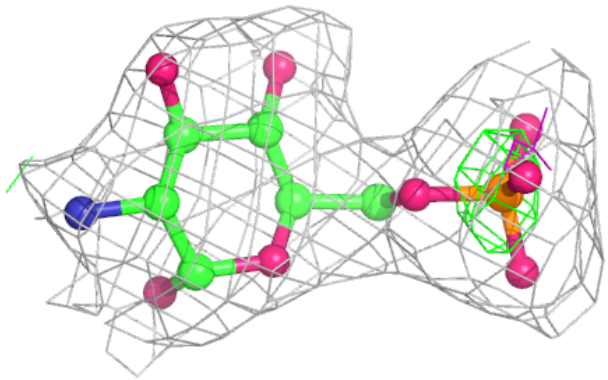


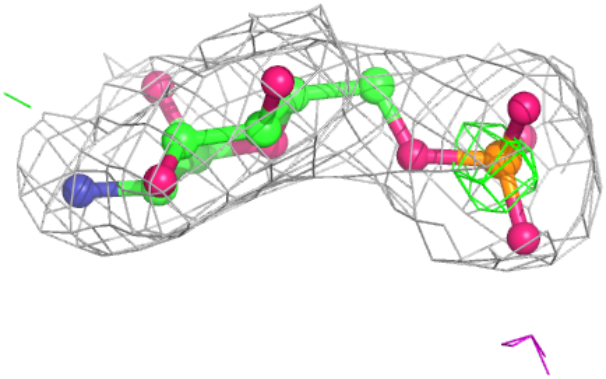


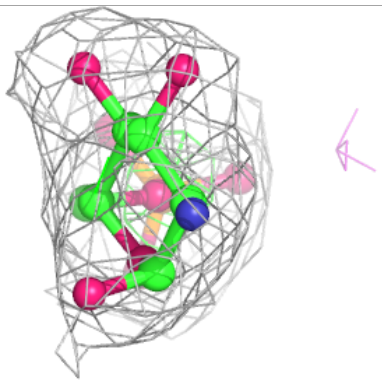


Electron density around GLP F 5002:

$2mF_o$-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:

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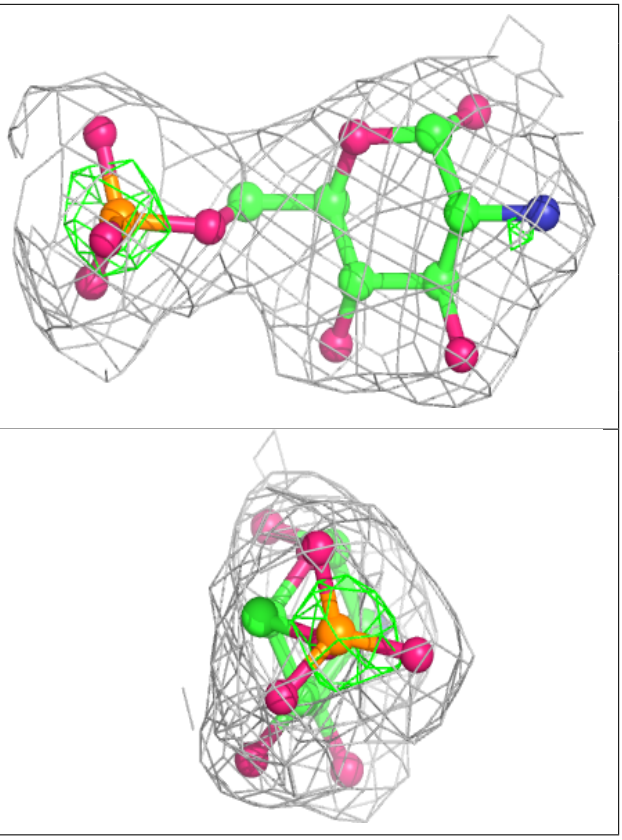
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.