



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:44 AM UTC

PDB ID : 1H7U / pdb_00001h7u
Title : hPMS2-ATPgS
Authors : Guarne, A.; Junop, M.S.; Yang, W.
Deposited on : 2001-07-10
Resolution : 2.70 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

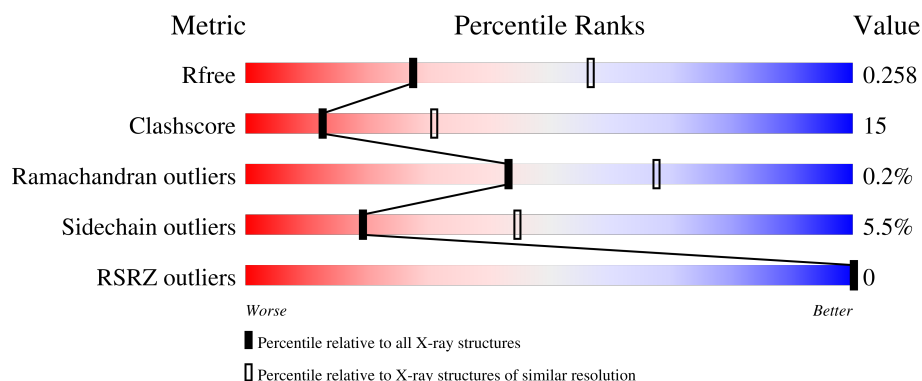
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	365	
1	B	365	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4808 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.

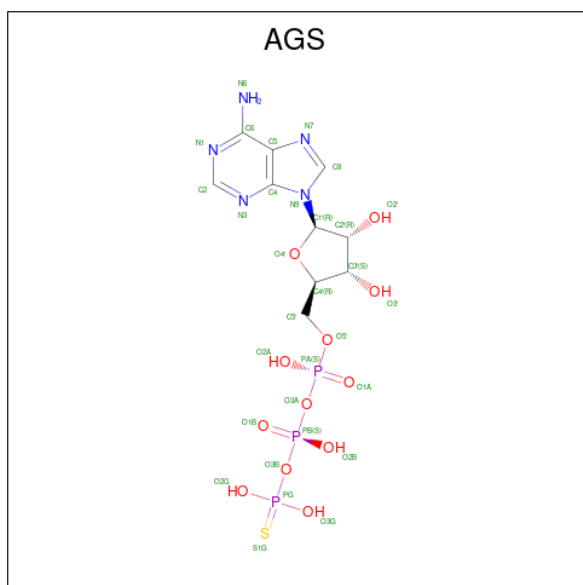
- Molecule 1 is a protein called MISMATCH REPAIR ENDONUCLEASE PMS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	1
			2379	1500	411	452	16			
1	B	302	Total	C	N	O	S	0	0	1
			2334	1472	402	444	16			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is water.

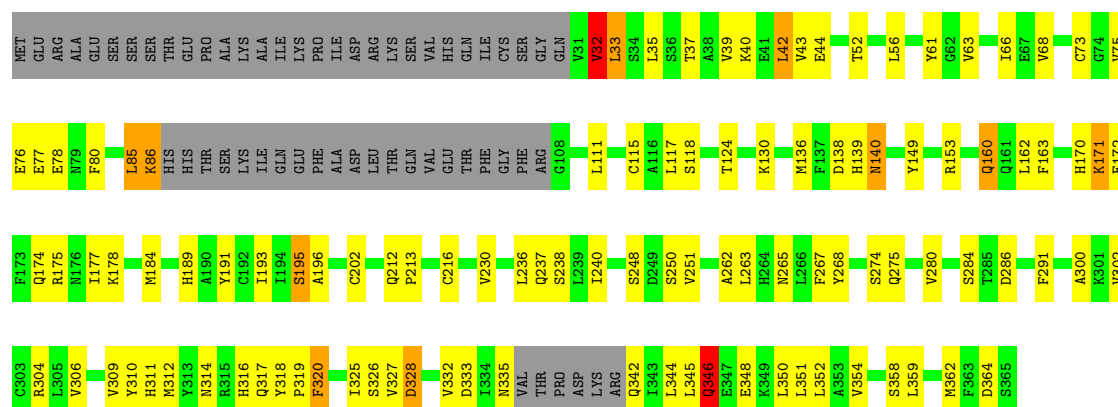
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	15	Total	O	0	0
			15	15		

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.

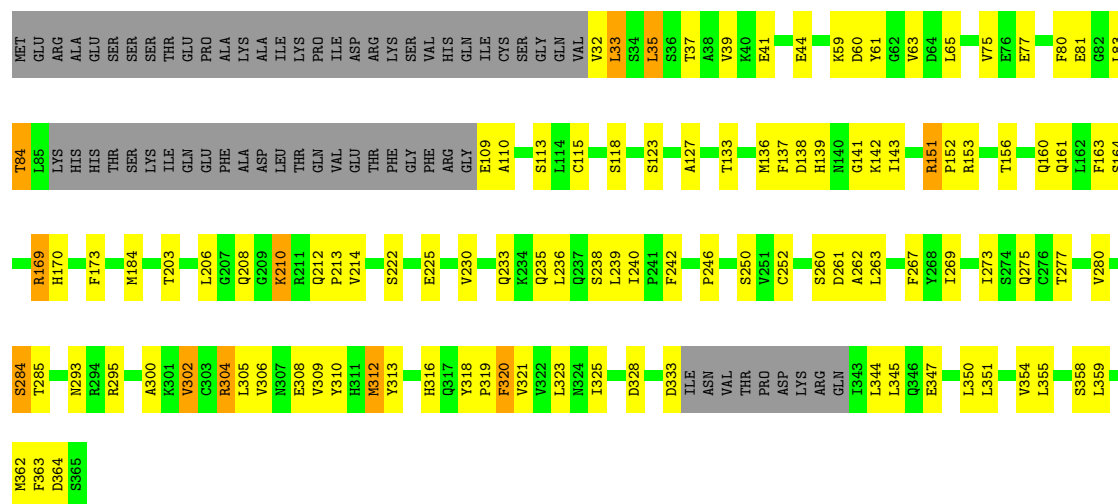
• Molecule 1: MISMATCH REPAIR ENDONUCLEASE PMS2

Chain A: 



• Molecule 1: MISMATCH REPAIR ENDONUCLEASE PMS2

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.36Å 73.87Å 136.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.45 – 2.70 24.45 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (24.45-2.70) 94.0 (24.45-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.71Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.237 , 0.270 0.230 , 0.258	Depositor DCC
R_{free} test set	1384 reflections (6.83%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.105 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4808	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: AGS, 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	A	0.57	2/2418 (0.1%)	1.07	16/3269 (0.5%)
1	B	0.59	2/2373 (0.1%)	1.16	16/3209 (0.5%)
All	All	0.58	4/4791 (0.1%)	1.12	32/6478 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	ASP	C-N	-5.82	1.25	1.33
1	B	364	ASP	C-N	-5.51	1.25	1.33
1	A	85	LEU	CA-C	5.18	1.59	1.52
1	B	344	LEU	N-CA	-5.12	1.39	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	MET	N-CA-C	-8.33	103.10	113.18
1	B	263	LEU	N-CA-C	-6.56	104.31	112.90
1	B	252	CYS	N-CA-C	-6.54	104.15	111.28
1	B	328	ASP	N-CA-C	6.46	118.89	110.43
1	A	346	GLN	N-CA-C	6.42	119.97	111.75
1	B	316	HIS	N-CA-C	6.41	121.25	113.17
1	A	328	ASP	N-CA-C	-6.41	100.34	109.96
1	B	262	ALA	N-CA-C	6.33	120.62	113.02
1	B	345	LEU	N-CA-C	-6.12	101.72	110.59
1	A	52	THR	N-CA-C	-6.05	105.71	114.12
1	A	86	LYS	N-CA-C	6.01	127.84	111.00
1	B	250	SER	N-CA-C	6.00	117.82	111.28
1	A	32	VAL	N-CA-C	-5.99	96.89	109.34
1	A	320	PHE	N-CA-C	-5.84	100.48	109.76
1	B	321	VAL	N-CA-C	5.81	116.65	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ALA	N-CA-C	5.75	119.93	113.02
1	A	230	VAL	N-CA-C	5.72	115.90	110.53
1	B	35	LEU	N-CA-C	-5.67	104.31	111.11
1	B	320	PHE	N-CA-C	-5.57	100.21	109.46
1	B	246	PRO	N-CA-C	-5.54	104.66	110.58
1	B	214	VAL	CB-CA-C	-5.53	107.01	111.71
1	A	237	GLN	CA-C-N	-5.38	113.15	122.14
1	A	237	GLN	C-N-CA	-5.38	113.15	122.14
1	A	149	TYR	CA-C-N	-5.36	113.64	120.23
1	A	149	TYR	C-N-CA	-5.36	113.64	120.23
1	B	127	ALA	N-CA-C	-5.31	105.40	111.14
1	B	284	SER	N-CA-C	5.20	115.92	108.74
1	B	230	VAL	N-CA-C	5.19	116.65	111.00
1	A	286	ASP	N-CA-C	-5.08	107.76	114.31
1	A	195	SER	N-CA-C	5.07	120.10	113.20
1	A	66	ILE	CB-CA-C	-5.07	105.46	111.09
1	A	267	PHE	N-CA-C	5.00	116.95	109.59

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	A	2379	0	2394	75	0
1	B	2334	0	2344	72	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	16	0	0	0	0
4	B	15	0	0	0	0
All	All	4808	0	4762	145	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 15.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PHE:CE1	1:B:323:LEU:HD13	2.05	0.92
1:A:309:VAL:HA	1:A:312:MET:HE2	1.53	0.89
1:B:359:LEU:HA	1:B:362:MET:HE2	1.59	0.83
1:B:269:ILE:HG23	1:B:323:LEU:HD11	1.63	0.80
1:B:39:VAL:HG21	1:B:184:MET:HE2	1.62	0.80
1:B:61:TYR:CE2	1:B:206:LEU:HD21	2.17	0.80
1:B:359:LEU:HD23	1:B:362:MET:CE	2.14	0.77
1:A:213:PRO:HB3	1:B:213:PRO:HD2	1.66	0.77
1:A:238:SER:HB2	1:A:280:VAL:HG13	1.68	0.76
1:A:359:LEU:HD23	1:A:362:MET:CE	2.14	0.76
1:A:335:ASN:HB3	1:A:342:GLN:HG2	1.68	0.76
1:A:39:VAL:HG21	1:A:184:MET:HE2	1.67	0.75
1:B:300:ALA:HB1	1:B:304:ARG:HH21	1.50	0.75
1:A:171:LYS:HD2	1:A:174:GLN:OE1	1.87	0.74
1:B:84:THR:HG21	1:B:137:PHE:CD2	2.23	0.73
1:B:163:PHE:O	1:B:170:HIS:HB2	1.89	0.73
1:B:269:ILE:CG2	1:B:323:LEU:HD11	2.21	0.69
1:A:311:HIS:HA	1:A:314:ASN:O	1.93	0.69
1:B:210:LYS:HD3	1:B:210:LYS:H	1.58	0.69
1:A:359:LEU:HD23	1:A:362:MET:HE3	1.75	0.67
1:A:63:VAL:CG2	1:A:177:ILE:HD13	2.25	0.67
1:A:346:GLN:HA	1:A:346:GLN:OE1	1.93	0.66
1:B:84:THR:CG2	1:B:137:PHE:CE2	2.80	0.65
1:B:242:PHE:CZ	1:B:323:LEU:HD13	2.32	0.64
1:A:348:GLU:O	1:A:352:LEU:HG	1.97	0.64
1:B:151:ARG:HD3	1:B:152:PRO:O	1.96	0.64
1:B:269:ILE:HD13	1:B:355:LEU:HD13	1.79	0.63
1:A:40:LYS:HG3	1:A:191:TYR:HE2	1.65	0.62
1:A:56:LEU:HD23	1:A:202:CYS:SG	2.40	0.61
1:A:248:SER:OG	1:A:251:VAL:HG23	2.00	0.61
1:B:313:TYR:CE2	1:B:363:PHE:HB3	2.36	0.61
1:B:210:LYS:H	1:B:210:LYS:CD	2.14	0.60
1:B:37:THR:O	1:B:41:GLU:HG2	2.02	0.60
1:A:32:VAL:HG12	1:A:32:VAL:O	2.00	0.60
1:A:302:VAL:O	1:A:306:VAL:HG23	2.02	0.60
1:A:325:ILE:HD13	1:A:351:LEU:HD21	1.83	0.59
1:B:238:SER:HB2	1:B:280:VAL:CG1	2.32	0.59
1:A:310:TYR:CD2	1:A:319:PRO:HD3	2.36	0.59
1:A:163:PHE:O	1:A:170:HIS:HB2	2.03	0.59
1:A:32:VAL:CG1	1:A:117:LEU:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:O	1:A:175:ARG:HG3	2.02	0.58
1:B:84:THR:HG22	1:B:137:PHE:CE2	2.38	0.58
1:A:61:TYR:HB2	1:A:177:ILE:HD11	1.85	0.58
1:B:84:THR:HG21	1:B:137:PHE:CE2	2.39	0.58
1:A:85:LEU:O	1:A:86:LYS:HG2	2.03	0.57
1:B:153:ARG:NH1	1:B:153:ARG:HB3	2.19	0.57
1:B:222:SER:OG	1:B:225:GLU:HG3	2.04	0.57
1:B:59:LYS:HB2	1:B:65:LEU:HB3	1.84	0.57
1:B:233:GLN:NE2	1:B:236:LEU:HD12	2.19	0.57
1:A:56:LEU:HD12	1:A:68:VAL:HG22	1.87	0.56
1:B:300:ALA:HB1	1:B:304:ARG:NH2	2.18	0.56
1:B:325:ILE:HD13	1:B:351:LEU:HD21	1.87	0.56
1:B:358:SER:O	1:B:362:MET:HG3	2.05	0.56
1:A:56:LEU:CD1	1:A:68:VAL:HG22	2.35	0.55
1:A:333:ASP:HB2	1:A:344:LEU:HB2	1.89	0.55
1:B:84:THR:O	1:B:84:THR:OG1	2.20	0.54
1:A:35:LEU:HD21	1:A:184:MET:HE3	1.89	0.53
1:A:39:VAL:O	1:A:43:VAL:HG23	2.08	0.53
1:A:40:LYS:HG3	1:A:191:TYR:CE2	2.43	0.53
1:B:302:VAL:O	1:B:306:VAL:HG23	2.09	0.53
1:B:80:PHE:HE2	1:B:133:THR:HG21	1.74	0.53
1:B:84:THR:OG1	1:B:141:GLY:HA3	2.10	0.52
1:A:115:CYS:O	1:A:139:HIS:HA	2.10	0.52
1:B:240:ILE:HG23	1:B:275:GLN:HG2	1.93	0.51
1:B:284:SER:OG	1:B:285:THR:N	2.44	0.51
1:A:75:VAL:HB	1:A:124:THR:HG21	1.93	0.51
1:A:284:SER:HA	1:A:318:TYR:CD2	2.45	0.51
1:A:32:VAL:HG12	1:A:117:LEU:CD1	2.41	0.51
1:B:359:LEU:HD23	1:B:362:MET:HE1	1.89	0.51
1:A:327:VAL:HG22	1:A:328:ASP:N	2.25	0.50
1:A:238:SER:HB2	1:A:280:VAL:CG1	2.39	0.50
1:A:342:GLN:HE21	1:A:344:LEU:HD21	1.75	0.50
1:B:63:VAL:HA	1:B:173:PHE:CE2	2.46	0.50
1:B:238:SER:HB2	1:B:280:VAL:HG13	1.92	0.50
1:B:123:SER:OG	1:B:156:THR:HB	2.11	0.50
1:B:269:ILE:HD11	1:B:351:LEU:CD1	2.42	0.49
1:A:332:VAL:HG22	1:A:345:LEU:CD2	2.43	0.49
1:B:115:CYS:O	1:B:139:HIS:HA	2.12	0.49
1:B:350:LEU:O	1:B:354:VAL:HG23	2.13	0.49
1:B:81:GLU:HG2	1:B:143:ILE:HD11	1.95	0.48
1:B:269:ILE:HD11	1:B:351:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HA	1:B:362:MET:CE	2.36	0.48
1:B:151:ARG:NH2	1:B:156:THR:OG1	2.46	0.48
1:B:235:GLN:O	1:B:239:LEU:HG	2.13	0.48
1:A:240:ILE:HG23	1:A:275:GLN:HG2	1.94	0.48
1:A:316:HIS:O	1:A:317:GLN:HG3	2.13	0.48
1:B:138:ASP:OD2	1:B:142:LYS:HB2	2.13	0.48
1:A:73:CYS:HA	1:A:153:ARG:HE	1.79	0.48
1:A:300:ALA:O	1:A:304:ARG:HG3	2.13	0.48
1:B:35:LEU:CG	1:B:184:MET:HE3	2.44	0.48
1:A:32:VAL:HG11	1:A:117:LEU:HD12	1.95	0.47
1:A:309:VAL:HG13	1:A:312:MET:CE	2.44	0.47
1:A:33:LEU:CD2	1:A:37:THR:HG21	2.45	0.47
1:A:177:ILE:HG23	1:A:178:LYS:N	2.29	0.47
1:A:359:LEU:HA	1:A:362:MET:HE3	1.97	0.46
1:A:42:LEU:HD23	1:A:68:VAL:CG2	2.45	0.46
1:B:75:VAL:HG21	1:B:83:LEU:HD21	1.97	0.46
1:B:267:PHE:CE2	1:B:351:LEU:HB2	2.50	0.46
1:B:359:LEU:HD23	1:B:362:MET:HE2	1.96	0.46
1:B:59:LYS:O	1:B:60:ASP:HB2	2.16	0.46
1:A:314:ASN:OD1	1:A:317:GLN:HB2	2.15	0.46
1:A:274:SER:OG	1:A:320:PHE:HB3	2.16	0.46
1:B:118:SER:HB2	1:B:160:GLN:O	2.16	0.45
1:B:308:GLU:O	1:B:312:MET:HG3	2.16	0.45
1:A:44:GLU:OE2	1:A:191:TYR:OH	2.34	0.45
1:B:77:GLU:HA	1:B:80:PHE:CD1	2.52	0.45
1:A:33:LEU:HD23	1:A:37:THR:HG21	1.98	0.45
1:A:358:SER:O	1:A:362:MET:HG3	2.17	0.45
1:B:32:VAL:HG23	1:B:113:SER:HB3	1.99	0.45
1:A:118:SER:HB3	1:A:162:LEU:HA	1.98	0.45
1:A:268:TYR:HB2	1:A:326:SER:HB3	1.98	0.45
1:A:77:GLU:HG3	1:A:80:PHE:CE2	2.53	0.44
1:B:81:GLU:HG2	1:B:143:ILE:CD1	2.46	0.44
1:B:184:MET:O	1:B:184:MET:HG2	2.15	0.44
1:B:310:TYR:O	1:B:313:TYR:HB2	2.17	0.44
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.17	0.43
1:A:32:VAL:HG12	1:A:117:LEU:HD12	1.98	0.43
1:B:161:GLN:O	1:B:164:SER:HB3	2.19	0.43
1:A:350:LEU:O	1:A:354:VAL:HG23	2.18	0.43
1:B:35:LEU:HG	1:B:184:MET:HE3	2.00	0.43
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.86	0.43
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASP:OD2	1:A:346:GLN:NE2	2.53	0.42
1:A:138:ASP:OD1	1:A:138:ASP:C	2.63	0.42
1:B:305:LEU:HD12	1:B:309:VAL:HG23	2.01	0.42
1:A:189:HIS:O	1:A:193:ILE:HG13	2.20	0.42
1:A:160:GLN:HE21	1:A:160:GLN:HB3	1.66	0.42
1:B:273:ILE:HA	1:B:320:PHE:O	2.19	0.42
1:B:277:THR:O	1:B:280:VAL:HB	2.19	0.41
1:A:212:GLN:HA	1:A:213:PRO:HD3	1.85	0.41
1:B:77:GLU:HA	1:B:80:PHE:CE1	2.55	0.41
1:B:239:LEU:HD11	1:B:320:PHE:CE1	2.55	0.41
1:B:293:ASN:O	1:B:295:ARG:HG3	2.20	0.41
1:A:332:VAL:HG22	1:A:345:LEU:HD23	2.03	0.41
1:A:195:SER:O	1:A:196:ALA:C	2.64	0.41
1:A:216:CYS:SG	1:B:203:THR:HG21	2.61	0.41
1:A:265:ASN:C	1:A:265:ASN:HD22	2.29	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.93	0.41
1:A:359:LEU:HD23	1:A:362:MET:HE1	2.01	0.41
1:A:118:SER:HB2	1:A:160:GLN:O	2.20	0.40
1:A:140:ASN:HD22	1:A:140:ASN:HA	1.57	0.40
1:A:291:PHE:CD1	1:A:291:PHE:N	2.89	0.40
1:B:318:TYR:N	1:B:318:TYR:CD1	2.89	0.40
1:A:263:LEU:C	1:A:265:ASN:H	2.29	0.40
1:B:33:LEU:O	1:B:169:ARG:NH1	2.55	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	302/365 (83%)	288 (95%)	14 (5%)	0	100	100
1	B	296/365 (81%)	282 (95%)	13 (4%)	1 (0%)	36	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	598/730 (82%)	570 (95%)	27 (4%)	1 (0%)	43 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	ALA

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	273/325 (84%)	260 (95%)	13 (5%)	23 50
1	B	268/325 (82%)	251 (94%)	17 (6%)	16 39
All	All	541/650 (83%)	511 (94%)	30 (6%)	19 45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	33	LEU
1	A	42	LEU
1	A	76	GLU
1	A	78	GLU
1	A	111	LEU
1	A	130	LYS
1	A	136	MET
1	A	140	ASN
1	A	160	GLN
1	A	171	LYS
1	A	250	SER
1	A	346	GLN
1	B	33	LEU
1	B	44	GLU
1	B	84	THR
1	B	109	GLU

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Mol	Chain	Res	Type
1	B	136	MET
1	B	151	ARG
1	B	169	ARG
1	B	208	GLN
1	B	210	LYS
1	B	212	GLN
1	B	260	SER
1	B	261	ASP
1	B	302	VAL
1	B	304	ARG
1	B	319	PRO
1	B	333	ASP
1	B	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	160	GLN
1	A	205	GLN
1	A	208	GLN
1	A	233	GLN
1	A	265	ASN
1	A	288	GLN
1	A	307	ASN
1	A	342	GLN
1	B	140	ASN
1	B	174	GLN
1	B	189	HIS
1	B	208	GLN
1	B	233	GLN
1	B	237	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
3	AGS	A	1366	2	32,33,33	3.46	12 (37%)	45,52,52	4.36	12 (26%)
3	AGS	B	1366	2	32,33,33	2.29	12 (37%)	45,52,52	3.45	11 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	A	1366	2	-	3/21/38/38	0/3/3/3
3	AGS	B	1366	2	-	5/21/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1366	AGS	PB-O3B	-13.53	1.44	1.59
3	A	1366	AGS	PG-O2G	-6.07	1.35	1.54
3	A	1366	AGS	PA-O5'	-5.20	1.39	1.59
3	B	1366	AGS	PB-O3A	4.92	1.64	1.59
3	A	1366	AGS	C4-N3	4.58	1.43	1.34
3	B	1366	AGS	C4-N3	4.39	1.42	1.34
3	A	1366	AGS	PA-O3A	-4.30	1.54	1.59
3	B	1366	AGS	O5'-C5'	-4.25	1.28	1.44
3	B	1366	AGS	PG-S1G	-4.13	1.81	1.90
3	A	1366	AGS	O5'-C5'	-4.08	1.29	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1366	AGS	PA-O1A	-4.07	1.36	1.50
3	B	1366	AGS	PB-O3B	-3.91	1.55	1.59
3	A	1366	AGS	O4'-C1'	3.56	1.50	1.42
3	B	1366	AGS	PA-O3A	-3.55	1.55	1.59
3	B	1366	AGS	PA-O5'	-3.38	1.46	1.59
3	A	1366	AGS	C3'-C4'	-2.96	1.45	1.53
3	A	1366	AGS	PB-O1B	-2.90	1.40	1.50
3	A	1366	AGS	PB-O3A	2.78	1.62	1.59
3	B	1366	AGS	O4'-C1'	2.66	1.48	1.42
3	B	1366	AGS	PB-O1B	-2.47	1.42	1.50
3	B	1366	AGS	PB-O2B	-2.30	1.44	1.55
3	A	1366	AGS	C8-N9	2.09	1.41	1.37
3	B	1366	AGS	PA-O1A	-2.05	1.43	1.50
3	B	1366	AGS	PA-O2A	-2.04	1.45	1.55

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1366	AGS	O5'-C5'-C4'	17.90	169.94	108.99
3	B	1366	AGS	O5'-C5'-C4'	15.35	161.25	108.99
3	A	1366	AGS	O3A-PB-O1B	-12.74	72.38	110.70
3	A	1366	AGS	O2A-PA-O3A	10.98	136.96	107.27
3	B	1366	AGS	O3A-PB-O1B	-8.88	84.00	110.70
3	A	1366	AGS	O2B-PB-O3B	8.81	131.10	107.27
3	A	1366	AGS	C5'-C4'-C3'	-6.76	90.86	115.21
3	A	1366	AGS	PA-O5'-C5'	6.28	157.31	121.35
3	B	1366	AGS	C5'-C4'-C3'	-6.21	92.86	115.21
3	B	1366	AGS	O5'-PA-O1A	-6.20	84.35	108.94
3	B	1366	AGS	O2B-PB-O3B	4.92	120.57	107.27
3	B	1366	AGS	PA-O5'-C5'	4.60	147.70	121.35
3	A	1366	AGS	O4'-C4'-C3'	4.34	113.78	105.15
3	B	1366	AGS	O4'-C4'-C3'	4.19	113.46	105.15
3	B	1366	AGS	O2A-PA-O3A	4.11	118.39	107.27
3	B	1366	AGS	O3A-PA-O1A	3.71	121.86	110.70
3	A	1366	AGS	O2A-PA-O5'	-3.44	91.97	107.57
3	A	1366	AGS	O3G-PG-O3B	-3.27	93.71	104.64
3	A	1366	AGS	O3'-C3'-C4'	2.79	119.10	111.08
3	B	1366	AGS	C3'-C2'-C1'	2.73	106.63	101.46
3	A	1366	AGS	O2G-PG-O3B	2.71	113.67	104.64
3	B	1366	AGS	O2B-PB-O3A	-2.49	100.54	107.27
3	A	1366	AGS	C3'-C2'-C1'	2.29	105.80	101.46

There are no chirality outliers.

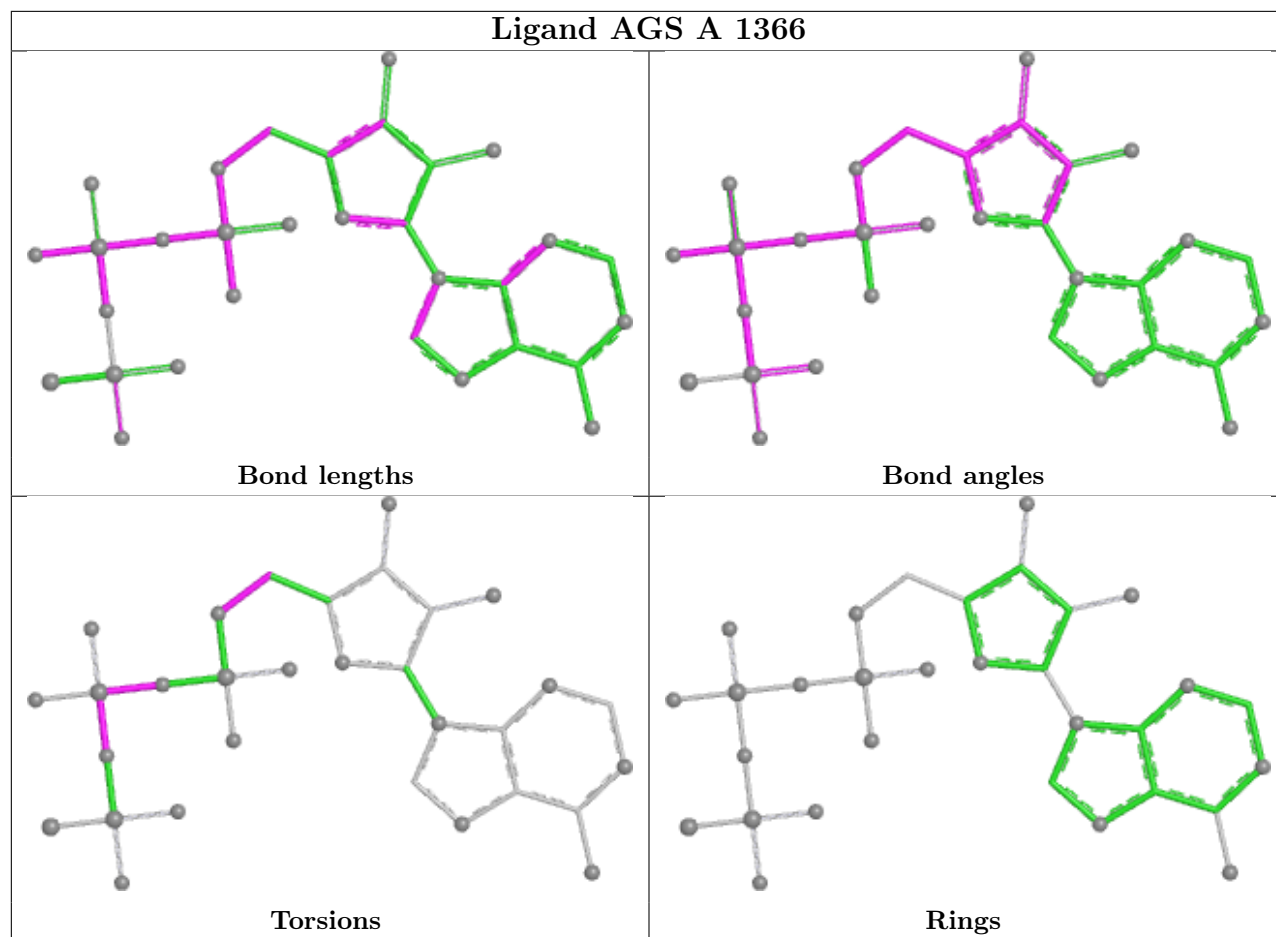
All (8) torsion outliers are listed below:

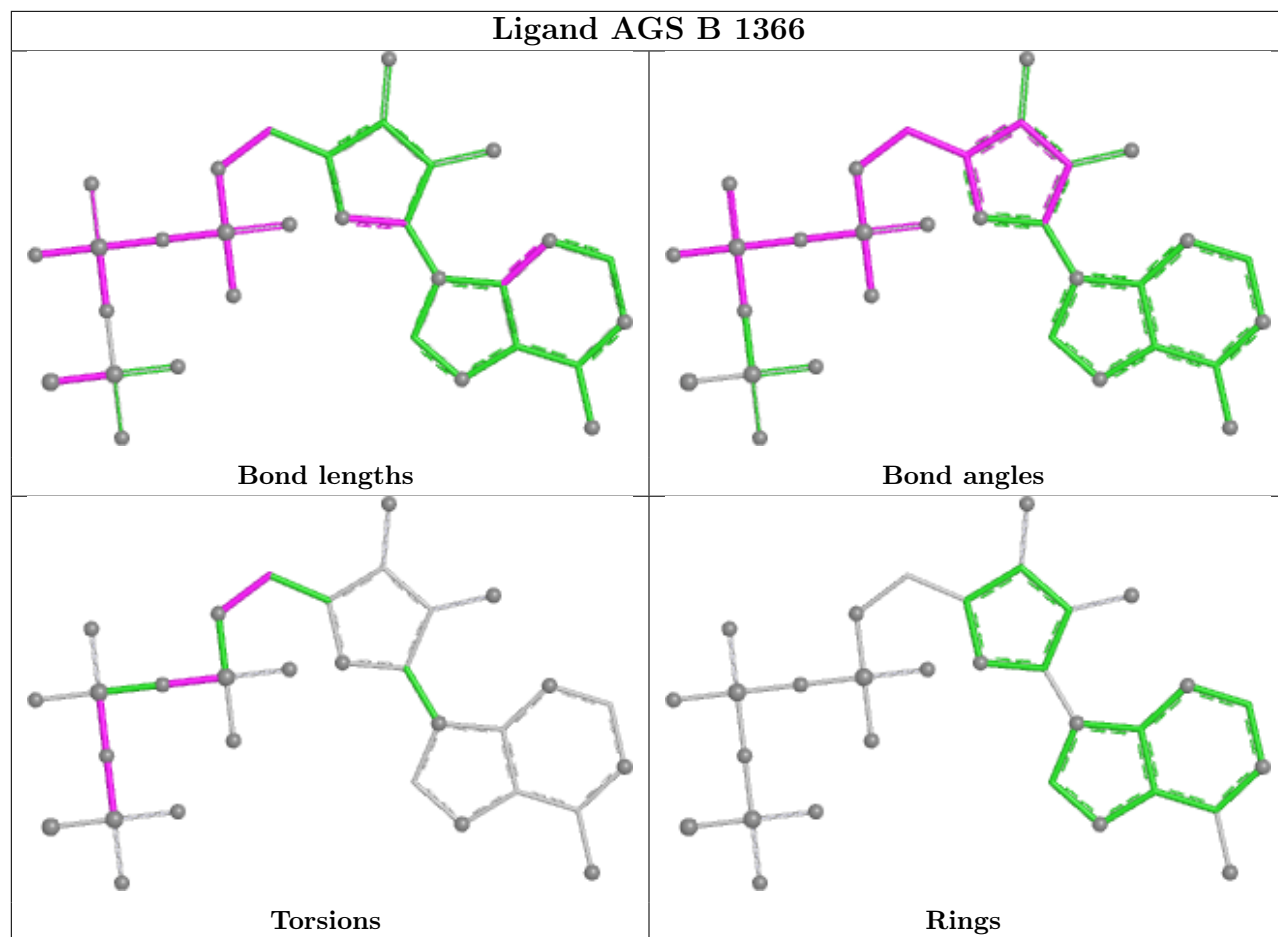
Mol	Chain	Res	Type	Atoms
3	A	1366	AGS	C4'-C5'-O5'-PA
3	B	1366	AGS	PB-O3B-PG-O2G
3	B	1366	AGS	PB-O3B-PG-O3G
3	A	1366	AGS	PA-O3A-PB-O1B
3	B	1366	AGS	C4'-C5'-O5'-PA
3	A	1366	AGS	PG-O3B-PB-O2B
3	B	1366	AGS	PG-O3B-PB-O2B
3	B	1366	AGS	PB-O3A-PA-O1A

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.





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	308/365 (84%)	-1.47	0 100 100	27, 48, 80, 100	0
1	B	302/365 (82%)	-1.43	0 100 100	31, 56, 92, 100	0
All	All	610/730 (83%)	-1.45	0 100 100	27, 51, 87, 100	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

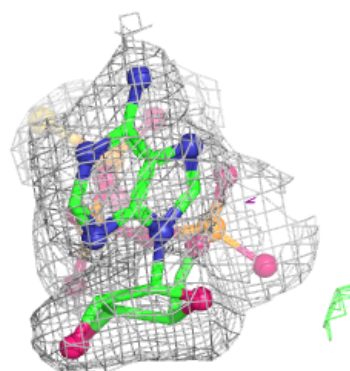
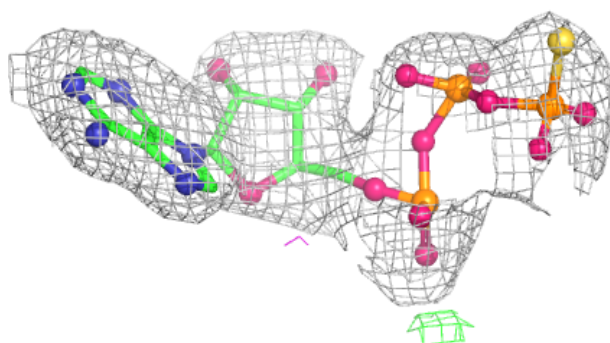
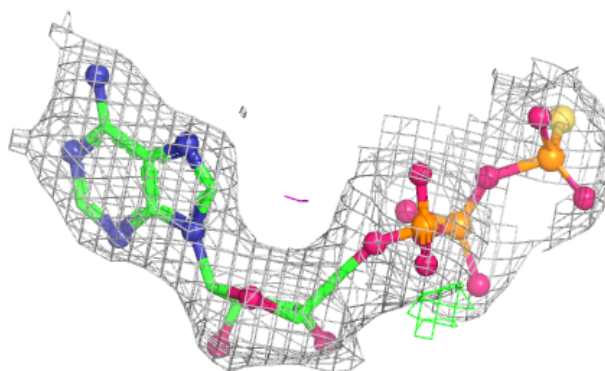
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	1365	1/1	0.99	0.04	45,45,45,45	0
2	MG	B	1365	1/1	0.99	0.02	45,45,45,45	0
3	AGS	A	1366	31/31	0.99	0.03	37,50,89,93	0
3	AGS	B	1366	31/31	0.99	0.04	62,67,99,100	0

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.

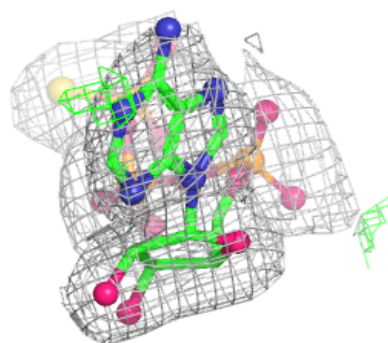
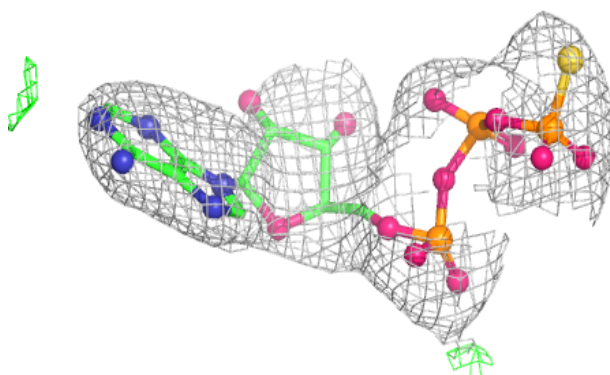
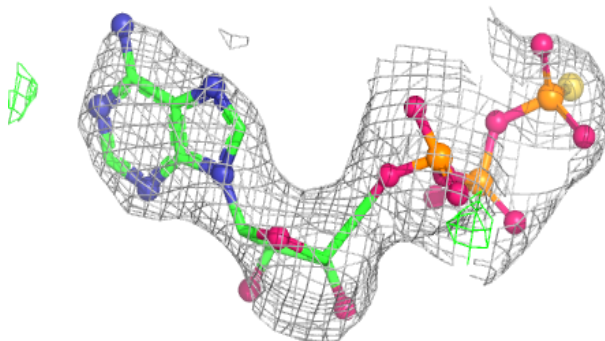
Electron density around AGS A 1366:

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



Electron density around AGS B 1366:

$2mF_o-DF_c$ (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.