



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:02 AM UTC

PDB ID : 1KJI / pdb_00001kji
Title : Crystal structure of glycineamide ribonucleotide transformylase in complex with Mg-AMPPCP
Authors : Thoden, J.B.; Firestone, S.M.; Benkovic, S.J.; Holden, H.M.
Deposited on : 2001-12-04
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

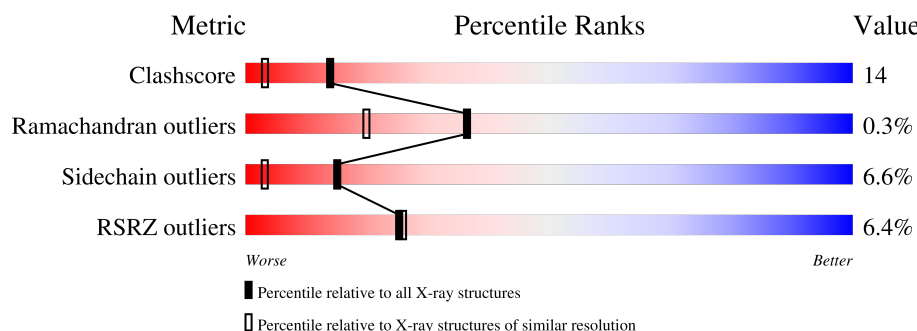
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	391	3% 76% 21% ...
1	B	391	9% 68% 25% 6% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6963 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 phosphoribosylglycinamide formyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			2967	1868	528	557	14			
1	B	389	Total	C	N	O	S	0	0	0
			2965	1867	528	557	13			

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

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

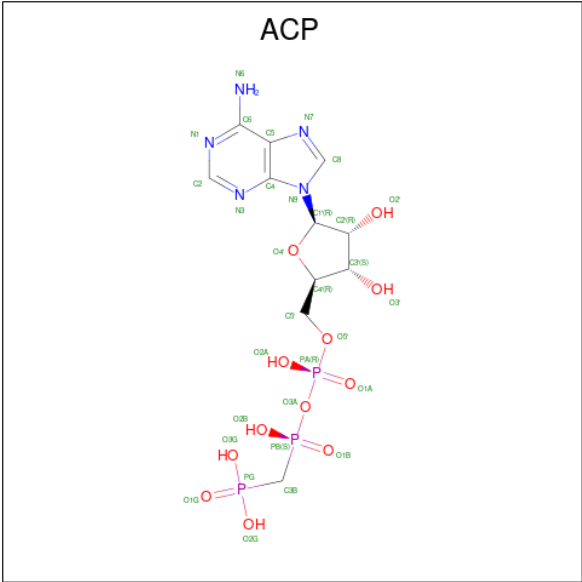
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

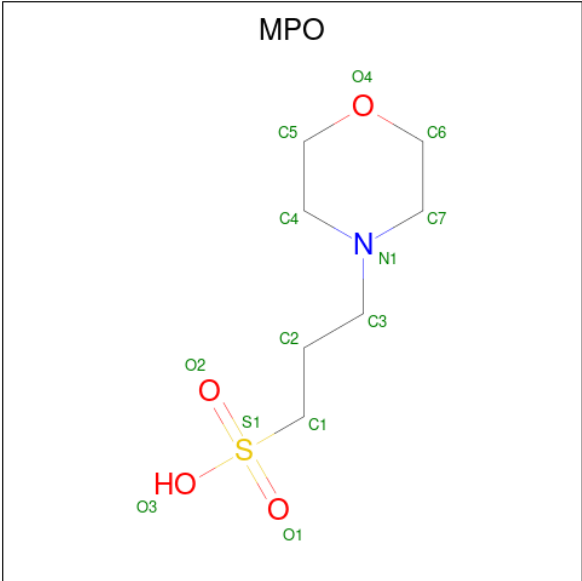
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

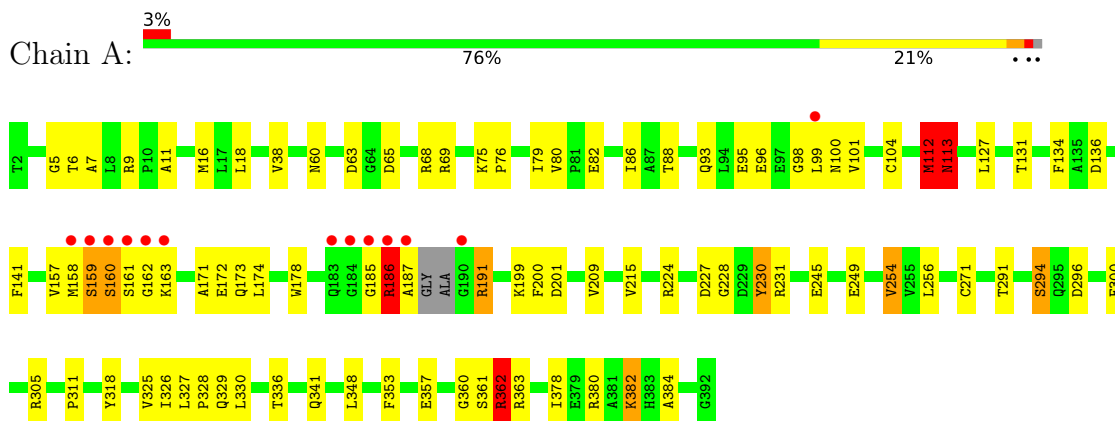
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	504	Total	O	0	0
			504	504		
8	B	440	Total	O	0	0
			440	440		

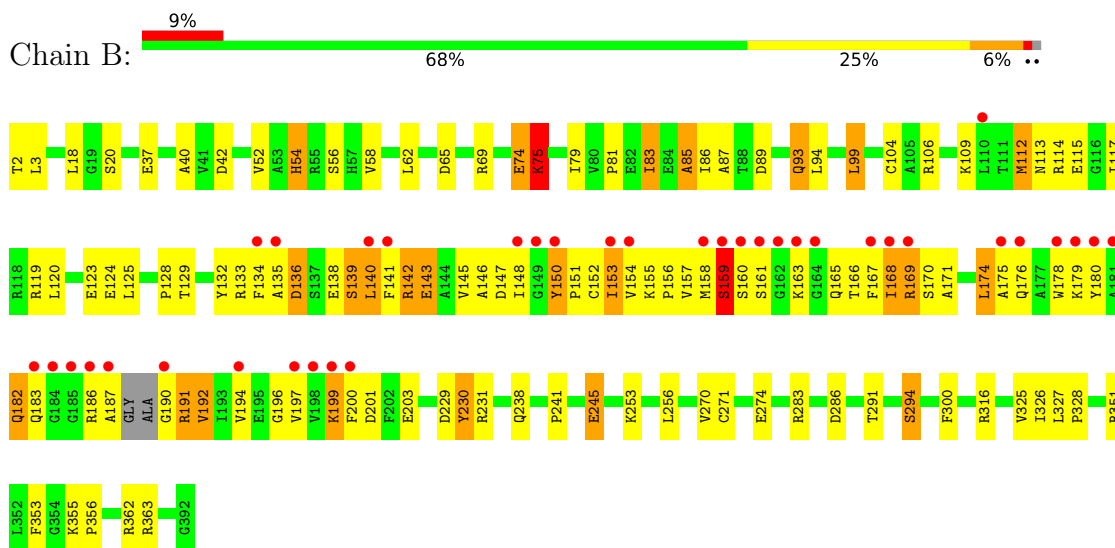
3 Residue-property plots

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: phosphoribosylglycinamide formyltransferase 2



- Molecule 1: phosphoribosylglycinamide formyltransferase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.20Å 179.20Å 76.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.60) 93.3 (30.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 1.55Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.183 , 0.229 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 120.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: CL, EDO, MG, MPO, NA, ACP

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	0.96	1/3020 (0.0%)	1.53	26/4091 (0.6%)
1	B	0.97	0/3014	1.57	25/4083 (0.6%)
All	All	0.97	1/6034 (0.0%)	1.55	51/8174 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	ARG	NE-CZ	6.67	1.40	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	PHE	N-CA-C	11.63	125.08	111.71
1	A	353	PHE	N-CA-C	9.11	123.65	112.54
1	B	128	PRO	N-CA-CB	8.37	108.84	103.23
1	A	362	ARG	CG-CD-NE	7.95	129.50	112.00
1	A	294	SER	N-CA-C	7.76	122.75	113.28
1	A	362	ARG	CD-NE-CZ	7.64	135.09	124.40
1	B	168	ILE	N-CA-C	7.02	118.00	107.75
1	B	170	SER	N-CA-C	6.98	120.90	109.24
1	B	203	GLU	CB-CA-C	-6.60	96.33	109.33
1	A	362	ARG	NE-CZ-NH2	6.56	125.10	119.20
1	B	300	PHE	CA-CB-CG	-6.34	107.45	113.80
1	A	80	VAL	N-CA-C	6.28	114.37	108.15
1	B	326	ILE	N-CA-C	-6.17	98.09	106.85
1	A	134	PHE	CA-CB-CG	-6.06	107.74	113.80
1	A	131	THR	N-CA-C	-5.97	102.49	110.55
1	B	153	ILE	CA-C-N	-5.94	115.36	123.14
1	B	153	ILE	C-N-CA	-5.94	115.36	123.14
1	A	104	CYS	N-CA-CB	5.91	120.55	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	NH1-CZ-NH2	-5.85	111.69	119.30
1	A	113	ASN	CA-CB-CG	5.83	118.43	112.60
1	B	104	CYS	N-CA-CB	5.79	120.44	111.24
1	A	112	MET	CA-C-O	5.77	126.50	119.11
1	A	318	TYR	N-CA-C	5.77	120.18	113.20
1	A	173	GLN	N-CA-C	5.77	119.93	113.01
1	A	362	ARG	CB-CG-CD	5.76	124.55	111.30
1	A	300	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	296	ASP	N-CA-C	-5.75	105.09	111.36
1	B	192	VAL	N-CA-C	5.73	116.95	108.65
1	B	117	ILE	N-CA-C	5.70	116.43	110.62
1	A	76	PRO	CB-CA-C	-5.57	103.66	110.95
1	A	159	SER	N-CA-C	5.56	116.71	108.60
1	A	326	ILE	N-CA-C	-5.54	98.98	106.85
1	A	38	VAL	N-CA-C	5.54	115.86	108.11
1	A	224	ARG	CA-CB-CG	-5.51	103.08	114.10
1	B	120	LEU	CA-C-O	5.50	126.60	120.82
1	B	74	GLU	CA-C-N	-5.50	116.89	122.83
1	B	74	GLU	C-N-CA	-5.50	116.89	122.83
1	B	196	GLY	N-CA-C	-5.49	104.11	112.51
1	B	294	SER	N-CA-C	5.43	119.91	113.28
1	A	325	VAL	N-CA-C	5.40	116.31	110.21
1	B	230	TYR	N-CA-C	-5.40	102.89	110.50
1	B	75	LYS	CA-C-O	5.38	124.62	120.48
1	B	20	SER	N-CA-C	5.22	118.77	111.30
1	B	159	SER	N-CA-C	5.16	117.65	109.50
1	B	274	GLU	N-CA-C	5.11	117.94	109.46
1	A	230	TYR	N-CA-C	-5.09	102.74	110.28
1	B	325	VAL	N-CA-C	5.09	116.57	109.80
1	A	201	ASP	N-CA-C	-5.07	105.45	111.69
1	B	54	HIS	CA-CB-CG	-5.05	108.75	113.80
1	B	150	TYR	O-C-N	5.05	126.47	121.57
1	A	113	ASN	CB-CA-C	5.03	119.63	109.68

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	2967	0	2989	64	0
1	B	2965	0	2988	110	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	31	0	14	2	0
5	B	31	0	14	4	0
6	A	13	0	15	0	0
7	A	4	0	6	0	0
8	A	504	0	0	8	0
8	B	440	0	0	14	0
All	All	6963	0	6026	173	1

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 14.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HG	1:A:79:ILE:HD11	1.29	1.13
1:B:161:SER:N	5:B:396:ACP:H3B1	1.85	0.91
1:B:161:SER:H	5:B:396:ACP:H3B1	1.34	0.90
1:B:79:ILE:HD11	1:B:99:LEU:HD22	1.53	0.89
1:B:153:ILE:HD12	1:B:197:VAL:HG22	1.60	0.83
1:B:94:LEU:HB3	1:B:99:LEU:HD13	1.62	0.82
1:B:65:ASP:O	1:B:69:ARG:HG3	1.83	0.79
1:B:132:TYR:O	1:B:133:ARG:HD2	1.84	0.78
1:B:191:ARG:HG3	1:B:192:VAL:N	1.98	0.77
1:B:153:ILE:CD1	1:B:197:VAL:HG22	2.14	0.76
1:B:183:GLN:O	1:B:187:ALA:HB2	1.87	0.74
1:B:156:PRO:HG2	1:B:159:SER:HB2	1.68	0.73
1:B:115:GLU:HG3	1:B:134:PHE:CE2	2.26	0.70
1:B:351:ARG:NH2	8:B:815:HOH:O	2.25	0.70
1:B:89:ASP:HB2	8:B:768:HOH:O	1.94	0.68
1:B:171:ALA:O	1:B:174:LEU:HG	1.94	0.67
1:B:138:GLU:OE2	1:B:142:ARG:NH1	2.28	0.67
1:B:180:TYR:O	1:B:183:GLN:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:ND2	8:A:637:HOH:O	2.28	0.67
1:B:141:PHE:CE1	1:B:145:VAL:HG21	2.30	0.66
1:B:169:ARG:HH11	1:B:169:ARG:HG3	1.60	0.65
1:B:175:ALA:HB3	8:B:836:HOH:O	1.96	0.65
1:A:185:GLY:O	1:A:187:ALA:N	2.30	0.64
1:A:249:GLU:HG2	8:A:885:HOH:O	1.96	0.64
1:A:18:LEU:CG	1:A:79:ILE:HD11	2.19	0.64
1:B:114:ARG:NH2	1:B:159:SER:O	2.31	0.64
1:B:115:GLU:HG3	1:B:134:PHE:CD2	2.32	0.64
1:B:231:ARG:NH2	8:B:631:HOH:O	2.28	0.64
1:B:115:GLU:HA	1:B:134:PHE:CZ	2.33	0.63
1:B:174:LEU:HD23	1:B:174:LEU:N	2.12	0.63
1:A:79:ILE:HB	1:A:99:LEU:HD21	1.80	0.63
1:B:156:PRO:HG2	1:B:159:SER:CB	2.28	0.62
1:B:186:ARG:NH1	1:B:190:GLY:N	2.48	0.62
1:A:200:PHE:HA	1:A:271[A]:CYS:SG	2.40	0.62
1:B:355:LYS:HD3	1:B:362:ARG:HE	1.66	0.61
1:B:316:ARG:HD2	8:B:727:HOH:O	1.99	0.60
1:B:125:LEU:O	8:B:694:HOH:O	2.15	0.60
1:B:150:TYR:HB3	1:B:151:PRO:HA	1.83	0.60
1:B:200:PHE:HA	1:B:271:CYS:SG	2.41	0.60
1:B:160:SER:H	1:B:163:LYS:HG2	1.65	0.60
1:A:16:MET:O	1:A:79:ILE:HD12	2.00	0.59
1:A:136:ASP:HB3	1:A:191:ARG:HD3	1.82	0.59
1:B:151:PRO:HB2	1:B:167:PHE:CE1	2.38	0.59
1:A:100:ASN:C	1:A:100:ASN:HD22	2.10	0.59
1:A:82:GLU:HB2	8:A:439:HOH:O	2.01	0.58
1:B:143:GLU:O	1:B:146:ALA:HB3	2.04	0.58
1:A:348:LEU:HD11	1:A:384:ALA:CB	2.34	0.57
1:B:153:ILE:HD12	1:B:197:VAL:CG2	2.32	0.57
1:A:380:ARG:HB2	8:A:859:HOH:O	2.04	0.56
1:B:81:PRO:HB3	1:B:86:ILE:HD13	1.87	0.56
1:A:185:GLY:C	1:A:187:ALA:H	2.14	0.56
1:A:60:ASN:ND2	1:A:63:ASP:HB2	2.21	0.56
1:A:136:ASP:HB3	1:A:191:ARG:CD	2.36	0.55
1:A:96:GLU:C	1:A:98:GLY:H	2.13	0.55
1:A:68:ARG:HD3	8:A:667:HOH:O	2.07	0.55
1:B:136:ASP:OD2	1:B:136:ASP:N	2.30	0.55
1:A:245:GLU:O	1:A:249:GLU:HG3	2.07	0.55
1:B:115:GLU:O	1:B:119:ARG:HG3	2.07	0.54
1:A:88:THR:HG23	1:A:112:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:NH2	8:A:783:HOH:O	2.35	0.54
1:B:150:TYR:HE2	1:B:168:ILE:HG22	1.73	0.54
1:B:283:ARG:NH2	8:B:516:HOH:O	2.41	0.53
1:B:186:ARG:HG3	1:B:187:ALA:H	1.72	0.53
1:B:79:ILE:CD1	1:B:99:LEU:HD22	2.34	0.53
1:B:186:ARG:HG3	1:B:187:ALA:N	2.23	0.53
1:A:65:ASP:O	1:A:69:ARG:HG3	2.09	0.53
1:B:159:SER:HB2	1:B:163:LYS:O	2.09	0.52
1:A:96:GLU:HG3	8:A:741:HOH:O	2.09	0.52
1:B:150:TYR:CB	1:B:151:PRO:HA	2.38	0.52
1:B:141:PHE:CD2	1:B:178:TRP:HB2	2.46	0.51
1:A:161:SER:N	5:A:1:ACP:H3B1	2.26	0.51
1:B:183:GLN:HA	8:B:809:HOH:O	2.11	0.51
1:B:138:GLU:HA	1:B:141:PHE:HB3	1.92	0.51
1:A:93:GLN:OE1	1:A:93:GLN:HA	2.10	0.51
5:B:396:ACP:H8	5:B:396:ACP:O5'	2.10	0.51
1:B:141:PHE:CE1	1:B:145:VAL:CG2	2.94	0.50
1:A:327:LEU:HD12	1:A:363:ARG:HA	1.94	0.50
1:A:16:MET:HB3	1:A:79:ILE:HD13	1.93	0.50
1:B:113:ASN:ND2	1:B:158:MET:HE2	2.26	0.50
1:B:150:TYR:CE2	1:B:168:ILE:HG22	2.47	0.50
1:B:201:ASP:N	1:B:270:VAL:O	2.45	0.50
1:B:166:THR:HG22	1:B:168:ILE:CG1	2.42	0.49
1:B:83:ILE:O	1:B:86:ILE:HD12	2.12	0.49
1:A:327:LEU:HD12	1:A:363:ARG:CA	2.42	0.49
1:A:330:LEU:HD23	1:A:330:LEU:N	2.27	0.49
1:B:119:ARG:O	1:B:123:GLU:HB2	2.12	0.49
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.24	0.49
1:A:127:LEU:HD11	1:A:254:VAL:HG23	1.95	0.48
1:A:82:GLU:HG2	1:A:82:GLU:O	2.14	0.48
1:A:357:GLU:H	1:A:362:ARG:HH21	1.60	0.48
1:B:79:ILE:HD11	1:B:99:LEU:CD2	2.36	0.48
1:B:166:THR:HG22	1:B:168:ILE:HG13	1.95	0.48
1:A:171:ALA:HA	1:A:174:LEU:HG	1.96	0.48
1:B:154:VAL:O	1:B:165:GLN:HA	2.14	0.48
1:B:253:LYS:HG3	8:B:518:HOH:O	2.14	0.48
1:B:40:ALA:O	1:B:56:SER:HB2	2.14	0.47
1:A:99:LEU:HG	1:A:100:ASN:N	2.29	0.47
1:B:52:VAL:HA	8:B:745:HOH:O	2.13	0.47
1:A:291:THR:HA	1:A:294:SER:OG	2.15	0.47
1:B:160:SER:O	1:B:163:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ILE:HG13	1:B:194:VAL:HG12	1.97	0.47
1:B:132:TYR:HA	1:B:194:VAL:O	2.14	0.47
1:A:159:SER:HA	8:A:868:HOH:O	2.14	0.47
1:A:88:THR:CG2	1:A:112:MET:HE3	2.45	0.46
1:A:160:SER:O	1:A:163:LYS:HG2	2.15	0.46
1:B:160:SER:HA	5:B:396:ACP:O1B	2.16	0.46
1:B:178:TRP:O	1:B:182:GLN:NE2	2.49	0.46
1:A:378:ILE:O	1:A:382:LYS:HG3	2.16	0.45
1:A:95:GLU:HA	1:A:99:LEU:O	2.16	0.45
1:B:238:GLN:HA	8:B:773:HOH:O	2.16	0.45
1:B:152:CYS:N	1:B:168:ILE:O	2.46	0.45
1:B:291:THR:HA	1:B:294:SER:OG	2.17	0.45
1:B:157:VAL:C	1:B:158:MET:HG2	2.43	0.44
1:B:141:PHE:CD1	1:B:141:PHE:C	2.96	0.44
1:A:113:ASN:HB2	1:A:158:MET:HG2	1.99	0.44
1:B:135:ALA:O	1:B:191:ARG:HD3	2.18	0.44
1:B:150:TYR:HA	1:B:151:PRO:C	2.41	0.44
1:A:113:ASN:HB2	1:A:158:MET:CG	2.48	0.44
1:A:209:VAL:O	1:A:215:VAL:HA	2.18	0.44
1:B:153:ILE:HD11	1:B:197:VAL:HG22	1.98	0.44
1:B:182:GLN:O	1:B:187:ALA:HA	2.18	0.44
1:B:283:ARG:NH1	8:B:602:HOH:O	2.33	0.44
1:B:327:LEU:HD12	1:B:362:ARG:C	2.42	0.44
1:B:86:ILE:HG22	1:B:87:ALA:N	2.32	0.44
1:B:109:LYS:O	1:B:112:MET:HG3	2.18	0.44
1:B:151:PRO:CB	1:B:167:PHE:CE1	3.01	0.44
1:A:79:ILE:CB	1:A:99:LEU:HD21	2.47	0.44
1:A:186:ARG:HG3	1:A:187:ALA:N	2.32	0.44
1:B:186:ARG:CG	1:B:187:ALA:H	2.31	0.44
1:B:115:GLU:HA	1:B:134:PHE:CE2	2.53	0.43
1:B:186:ARG:O	1:B:187:ALA:HB3	2.18	0.43
1:B:199:LYS:HD2	1:B:199:LYS:HA	1.76	0.43
1:A:329:GLN:HA	1:A:360:GLY:O	2.18	0.43
1:A:336:THR:HB	1:B:3:LEU:HD11	2.01	0.43
1:B:69:ARG:HD3	8:B:683:HOH:O	2.17	0.43
1:B:160:SER:H	1:B:163:LYS:CG	2.31	0.43
1:B:286:ASP:OD2	1:B:363:ARG:NH2	2.50	0.43
1:A:157:VAL:HG23	1:A:158:MET:HG3	2.01	0.43
1:A:162:GLY:HA3	1:A:228:GLY:HA2	2.00	0.43
1:B:93:GLN:NE2	1:B:93:GLN:HA	2.30	0.43
1:A:185:GLY:C	1:A:187:ALA:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1:ACP:H8	5:A:1:ACP:O5'	2.18	0.43
1:B:140:LEU:HD12	8:B:782:HOH:O	2.19	0.42
1:B:176:GLN:HE21	1:B:176:GLN:HA	1.84	0.42
1:B:180:TYR:C	1:B:183:GLN:HB3	2.45	0.42
1:A:16:MET:CG	1:A:79:ILE:HD13	2.50	0.42
1:A:348:LEU:HD11	1:A:384:ALA:HB2	2.01	0.42
1:A:79:ILE:HG22	1:A:101:VAL:HA	2.01	0.42
1:B:42:ASP:O	1:B:58:VAL:HA	2.19	0.42
1:A:382:LYS:HB3	1:A:382:LYS:HE3	1.75	0.42
1:B:141:PHE:HE1	1:B:145:VAL:HG21	1.78	0.42
1:B:156:PRO:C	1:B:158:MET:H	2.28	0.42
1:A:5:GLY:HA3	1:A:11:ALA:O	2.19	0.42
1:B:74:GLU:O	1:B:75:LYS:C	2.61	0.42
1:B:241:PRO:O	1:B:245:GLU:HB2	2.20	0.42
1:A:141:PHE:CE2	1:A:178:TRP:HB2	2.54	0.42
1:B:328:PRO:HD2	1:B:362:ARG:O	2.19	0.42
1:B:83:ILE:HG12	1:B:86:ILE:HD11	2.02	0.41
1:B:139:SER:O	1:B:143:GLU:HB2	2.19	0.41
1:A:341:GLN:OE1	1:B:2:THR:N	2.54	0.41
1:B:186:ARG:CG	1:B:187:ALA:N	2.83	0.41
1:A:6:THR:O	1:A:7:ALA:C	2.63	0.41
1:A:9:ARG:HD3	1:B:356:PRO:HA	2.02	0.41
1:B:18:LEU:HB2	1:B:81:PRO:HA	2.03	0.41
1:B:37:GLU:HA	1:B:54:HIS:CE1	2.54	0.41
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.92	0.41
1:A:305:ARG:HD3	1:A:311:PRO:O	2.21	0.41
1:A:127:LEU:CD1	1:A:254:VAL:HG23	2.51	0.40
1:A:96:GLU:C	1:A:98:GLY:N	2.78	0.40
1:B:85:ALA:C	1:B:86:ILE:HG13	2.47	0.40
1:A:328:PRO:HD2	1:A:362:ARG:O	2.21	0.40
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.87	0.40
1:B:154:VAL:HG12	1:B:166:THR:HB	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH2	1:B:191:ARG:NH2[2_555]	2.01	0.19

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	386/391 (99%)	372 (96%)	13 (3%)	1 (0%)	36	20
1	B	385/391 (98%)	367 (95%)	17 (4%)	1 (0%)	36	20
All	All	771/782 (99%)	739 (96%)	30 (4%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ARG
1	B	85	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	312/311 (100%)	297 (95%)	15 (5%)	23	6
1	B	311/311 (100%)	285 (92%)	26 (8%)	10	1
All	All	623/622 (100%)	582 (93%)	41 (7%)	15	3

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	86	ILE
1	A	112	MET
1	A	113	ASN

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Mol	Chain	Res	Type
1	A	160	SER
1	A	172	GLU
1	A	186	ARG
1	A	191	ARG
1	A	199	LYS
1	A	227	ASP
1	A	230	TYR
1	A	254	VAL
1	A	361	SER
1	A	362	ARG
1	A	382	LYS
1	B	75	LYS
1	B	83	ILE
1	B	93	GLN
1	B	99	LEU
1	B	106	ARG
1	B	112	MET
1	B	124	GLU
1	B	129	THR
1	B	136	ASP
1	B	139	SER
1	B	140	LEU
1	B	142	ARG
1	B	143	GLU
1	B	147	ASP
1	B	155	LYS
1	B	159	SER
1	B	169	ARG
1	B	174	LEU
1	B	179	LYS
1	B	182	GLN
1	B	191	ARG
1	B	199	LYS
1	B	229	ASP
1	B	230	TYR
1	B	245	GLU
1	B	256	LEU

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

Mol	Chain	Res	Type
1	A	100	ASN

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Mol	Chain	Res	Type
1	A	183	GLN
1	A	223	HIS
1	A	329	GLN
1	A	342	ASN
1	A	383	HIS
1	B	126	GLN
1	B	165	GLN
1	B	176	GLN
1	B	248	GLN
1	B	333	GLN
1	B	342	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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
5	ACP	A	1	2	31,33,33	1.50	4 (12%)	47,52,52	1.56	6 (12%)
6	MPO	A	398	-	13,13,13	2.01	2 (15%)	17,17,17	1.57	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	399	-	3,3,3	0.38	0	2,2,2	0.46	0
5	ACP	B	396	2	31,33,33	1.27	6 (19%)	47,52,52	1.31	6 (12%)

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
5	ACP	A	1	2	-	6/19/38/38	0/3/3/3
6	MPO	A	398	-	-	1/7/15/15	0/1/1/1
7	EDO	A	399	-	-	1/1/1/1	-
5	ACP	B	396	2	-	3/19/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	398	MPO	C3-N1	5.09	1.59	1.47
5	A	1	ACP	PB-O3A	4.54	1.63	1.58
6	A	398	MPO	C1-S1	4.19	1.83	1.77
5	A	1	ACP	C6-N6	-2.91	1.26	1.34
5	A	1	ACP	C2-N1	2.90	1.39	1.33
5	B	396	ACP	PB-O3A	2.85	1.61	1.58
5	A	1	ACP	PG-O3G	2.85	1.61	1.55
5	B	396	ACP	C6-N6	-2.72	1.27	1.34
5	B	396	ACP	C2-N1	2.41	1.38	1.33
5	B	396	ACP	PG-O3G	2.16	1.59	1.55
5	B	396	ACP	PB-O2B	-2.15	1.51	1.56
5	B	396	ACP	C2-N3	-2.07	1.30	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	ACP	C2-N1-C6	5.53	127.82	118.73
5	B	396	ACP	C2-N1-C6	4.12	125.49	118.73
5	A	1	ACP	N3-C2-N1	-4.03	122.49	128.58
6	A	398	MPO	O3-S1-C1	3.41	112.67	106.00
5	A	1	ACP	O3G-PG-C3B	3.37	114.57	106.40
5	A	1	ACP	O3'-C3'-C2'	3.26	122.26	111.82
5	B	396	ACP	N3-C2-N1	-3.09	123.90	128.58
6	A	398	MPO	C2-C1-S1	-3.05	108.58	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	398	MPO	O3-S1-O1	-2.93	104.08	111.40
5	A	1	ACP	C5-C6-N1	-2.79	110.42	117.51
5	B	396	ACP	O2B-PB-C3B	2.64	117.67	106.73
5	B	396	ACP	C5-C6-N1	-2.36	111.51	117.51
5	A	1	ACP	O2B-PB-C3B	2.27	116.13	106.73
5	B	396	ACP	O2A-PA-O3A	2.16	113.12	107.27
5	B	396	ACP	C5-C6-N6	2.14	128.59	123.29
6	A	398	MPO	C7-N1-C4	2.05	113.27	108.84

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	ACP	PB-C3B-PG-O1G
5	A	1	ACP	PB-C3B-PG-O2G
5	A	1	ACP	PG-C3B-PB-O1B
5	A	1	ACP	PG-C3B-PB-O3A
5	B	396	ACP	PG-C3B-PB-O1B
5	B	396	ACP	PG-C3B-PB-O3A
7	A	399	EDO	O1-C1-C2-O2
5	A	1	ACP	PB-C3B-PG-O3G
5	A	1	ACP	PG-C3B-PB-O2B
5	B	396	ACP	PG-C3B-PB-O2B
6	A	398	MPO	C2-C3-N1-C4

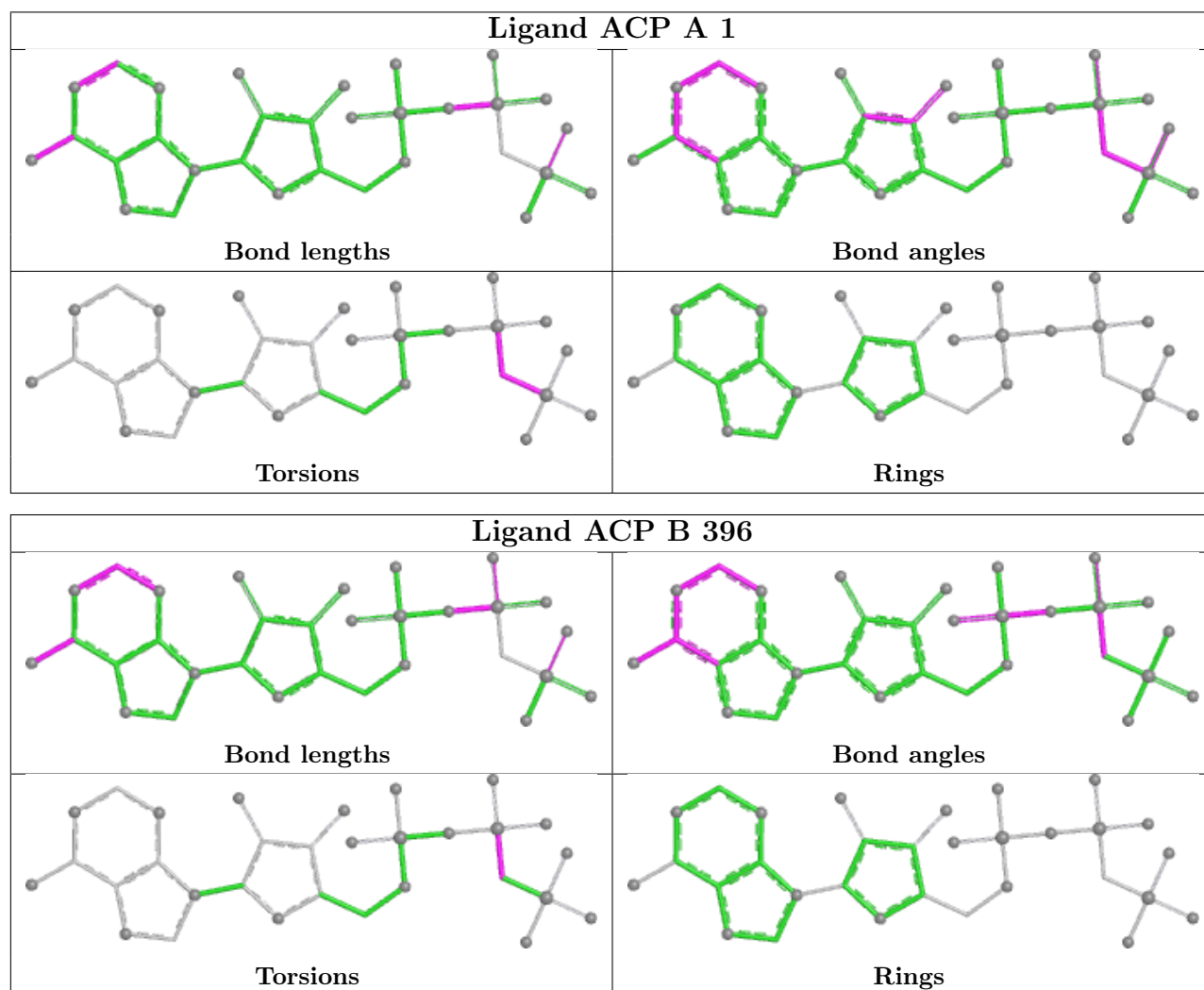
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	ACP	2	0
5	B	396	ACP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/391 (99%)	-0.17	13 (3%) 49 52	12, 19, 54, 99	1 (0%)
1	B	389/391 (99%)	0.25	37 (9%) 14 14	12, 24, 72, 96	0
All	All	778/782 (99%)	0.04	50 (6%) 25 26	12, 21, 66, 99	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	GLY	5.5
1	A	184	GLY	4.8
1	A	190	GLY	4.6
1	A	162	GLY	4.5
1	B	190	GLY	4.3
1	A	187	ALA	4.2
1	B	187	ALA	4.1
1	B	175	ALA	4.0
1	A	161	SER	4.0
1	B	159	SER	3.9
1	B	141	PHE	3.9
1	B	158	MET	3.9
1	B	185	GLY	3.7
1	B	184	GLY	3.4
1	A	183	GLN	3.4
1	B	134	PHE	3.4
1	B	160	SER	3.4
1	B	163	LYS	3.3
1	B	176	GLN	3.3
1	A	185	GLY	3.3
1	B	169	ARG	3.2
1	A	99	LEU	3.2
1	A	163	LYS	3.1
1	A	186	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	3.1
1	B	180	TYR	3.1
1	B	167	PHE	3.0
1	B	150	TYR	2.9
1	B	198	VAL	2.9
1	B	161	SER	2.9
1	B	148	ILE	2.8
1	B	154	VAL	2.7
1	B	186	ARG	2.6
1	B	168	ILE	2.6
1	B	194	VAL	2.5
1	B	181	ALA	2.5
1	B	178	TRP	2.4
1	A	158	MET	2.4
1	B	140	LEU	2.4
1	B	197	VAL	2.4
1	A	160	SER	2.4
1	B	110	LEU	2.3
1	A	159	SER	2.3
1	B	164	GLY	2.3
1	B	135	ALA	2.2
1	B	200	PHE	2.1
1	B	183	GLN	2.1
1	B	149	GLY	2.1
1	B	199	LYS	2.1
1	B	179	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

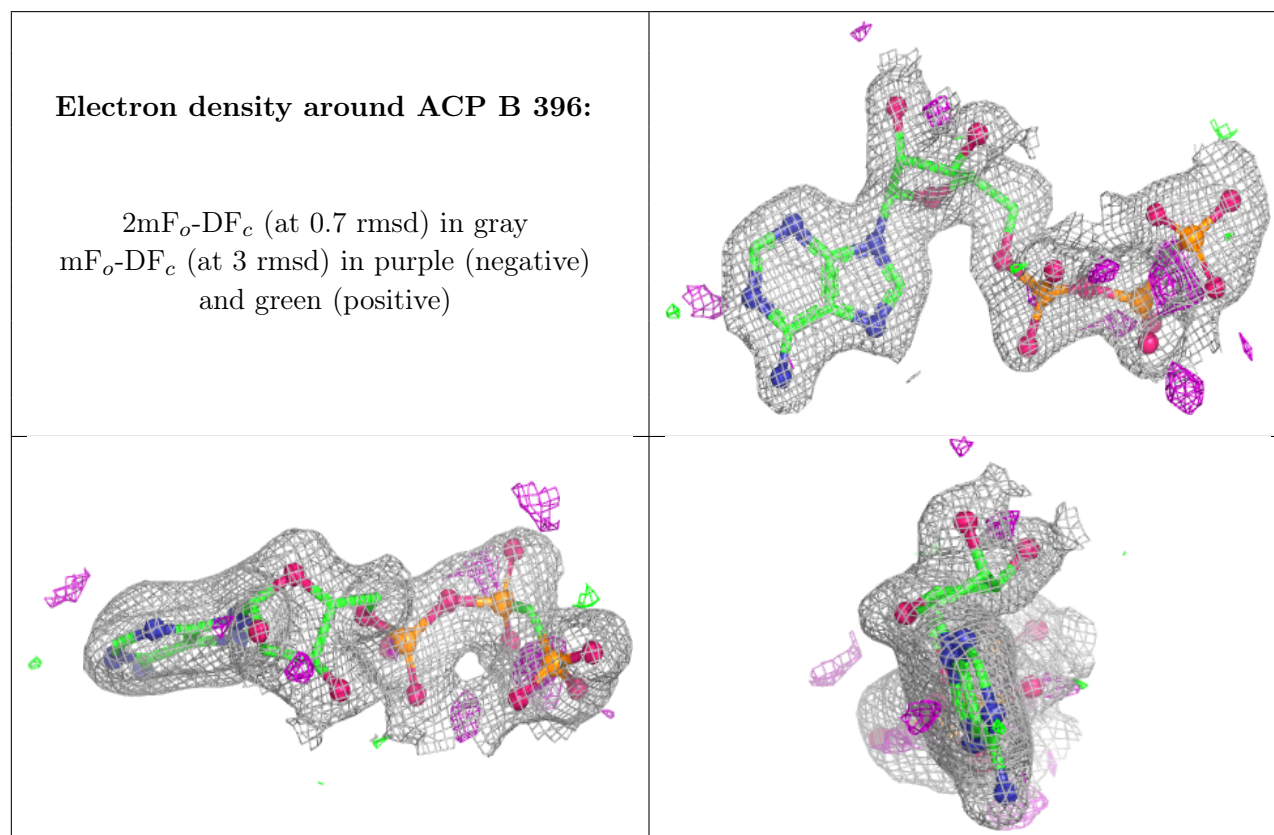
There are no oligosaccharides in this entry.

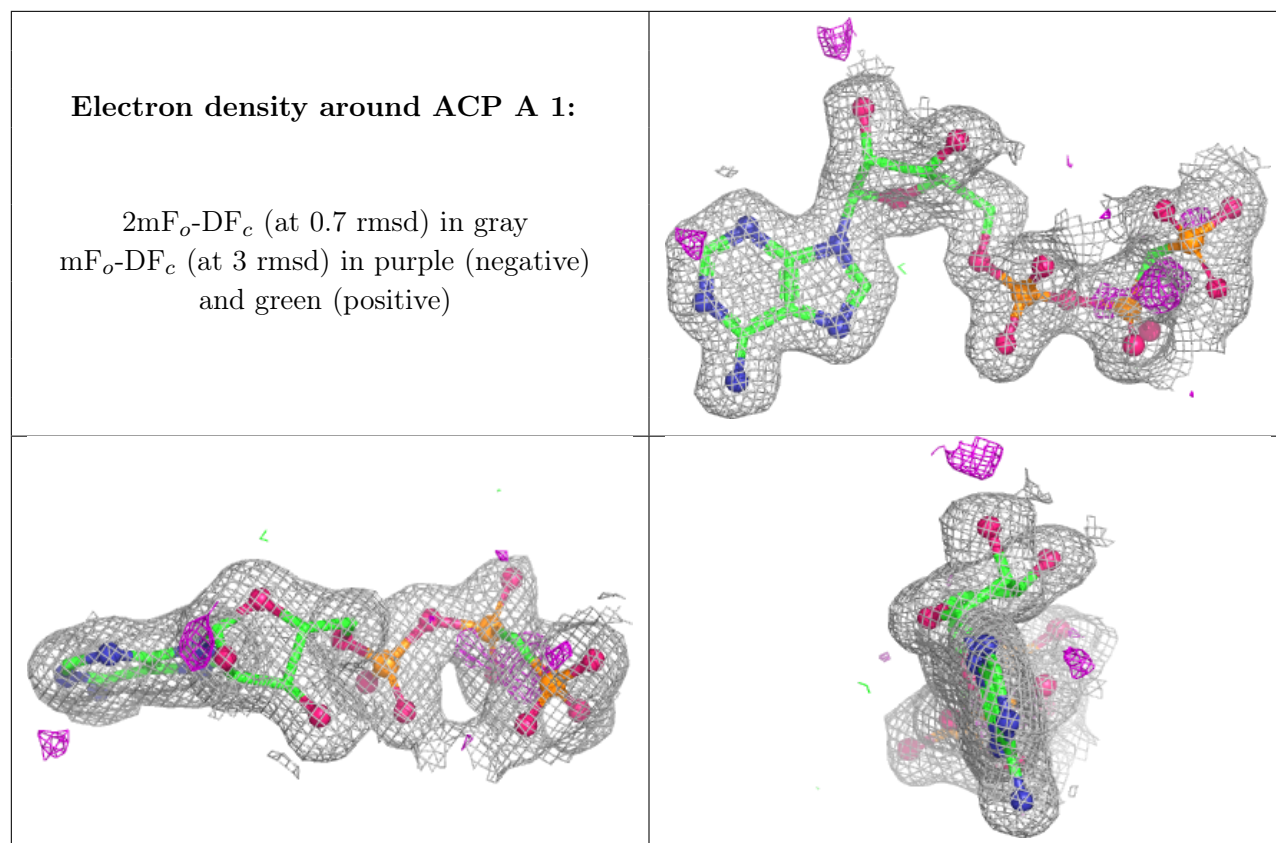
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	399	4/4	0.82	0.16	41,41,43,44	0
3	NA	A	395	1/1	0.84	0.16	47,47,47,47	0
2	MG	B	394	1/1	0.84	0.14	55,55,55,55	0
3	NA	B	395	1/1	0.88	0.12	51,51,51,51	0
5	ACP	B	396	31/31	0.93	0.09	23,35,54,98	0
2	MG	B	393	1/1	0.95	0.11	39,39,39,39	0
3	NA	A	396	1/1	0.97	0.11	30,30,30,30	0
5	ACP	A	1	31/31	0.97	0.06	17,21,38,41	0
2	MG	A	394	1/1	0.98	0.12	30,30,30,30	0
2	MG	A	393	1/1	0.98	0.07	28,28,28,28	0
6	MPO	A	398	13/13	0.98	0.06	16,20,23,25	0
4	CL	A	397	1/1	0.98	0.06	25,25,25,25	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.