Full wwPDB X-ray Structure Validation Report (i)

Apr 3, 2025 – 02:11 PM EDT

PDB ID	:	9E70 / pdb_00009e70
Title	:	Human XRN1 with Adenosine-3',5'-Bisphosphate (pAp) Bound
Authors	:	Lockbaum, G.J.; Lynes, M.M.; Sickmier, E.A.; Grigoriu, S.; Boriack-Sjodin, P.A.
Deposited on	:	2024-10-31
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

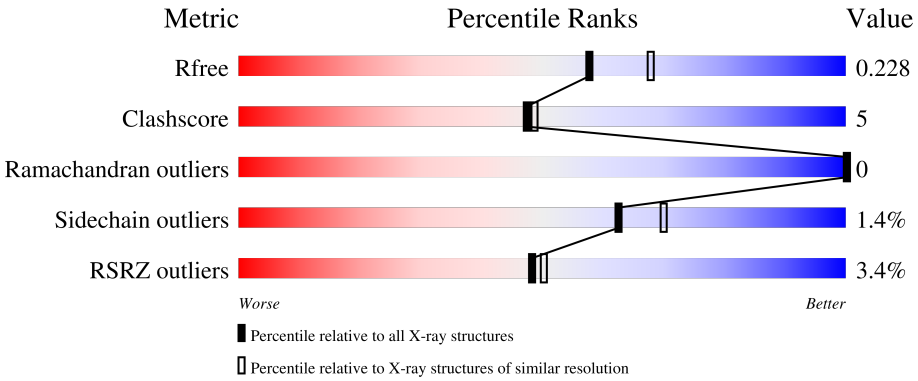
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	A	661	2% 74% 9% • 16%
1	B	661	4% 74% 8% • 17%

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
4	EDO	A	714	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10178 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.

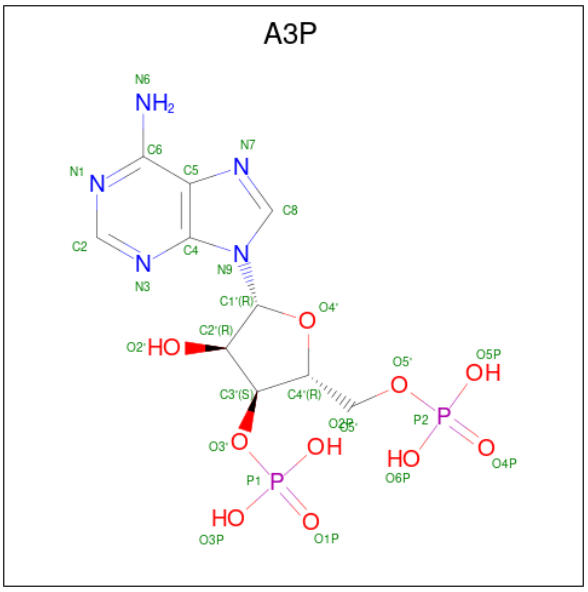
- Molecule 1 is a protein called 5'-3' exoribonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	11	0
			4709	3057	780	844	28			
1	B	547	Total	C	N	O	S	0	4	0
			4618	3000	770	824	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	654	ASP	-	expression tag	UNP Q8IZH2
A	655	TYR	-	expression tag	UNP Q8IZH2
A	656	LYS	-	expression tag	UNP Q8IZH2
A	657	ASP	-	expression tag	UNP Q8IZH2
A	658	ASP	-	expression tag	UNP Q8IZH2
A	659	ASP	-	expression tag	UNP Q8IZH2
A	660	ASP	-	expression tag	UNP Q8IZH2
A	661	LYS	-	expression tag	UNP Q8IZH2
B	654	ASP	-	expression tag	UNP Q8IZH2
B	655	TYR	-	expression tag	UNP Q8IZH2
B	656	LYS	-	expression tag	UNP Q8IZH2
B	657	ASP	-	expression tag	UNP Q8IZH2
B	658	ASP	-	expression tag	UNP Q8IZH2
B	659	ASP	-	expression tag	UNP Q8IZH2
B	660	ASP	-	expression tag	UNP Q8IZH2
B	661	LYS	-	expression tag	UNP Q8IZH2

- Molecule 2 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

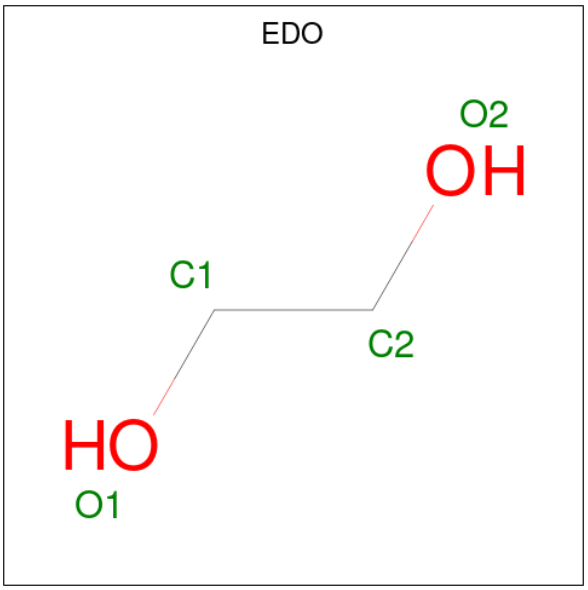


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			54	20	10	20	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

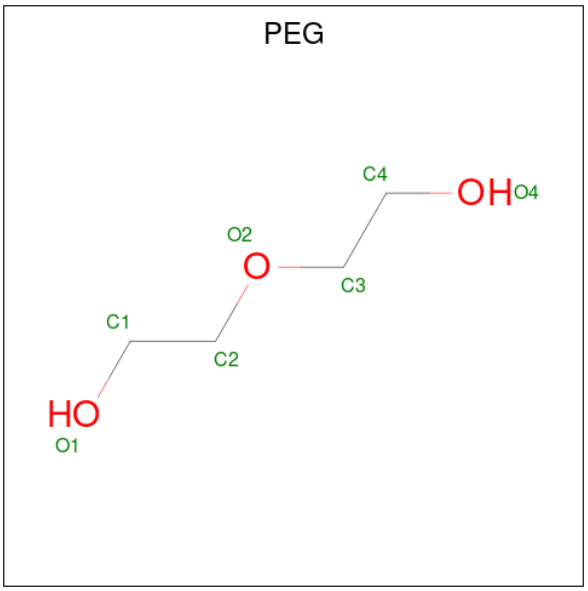


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

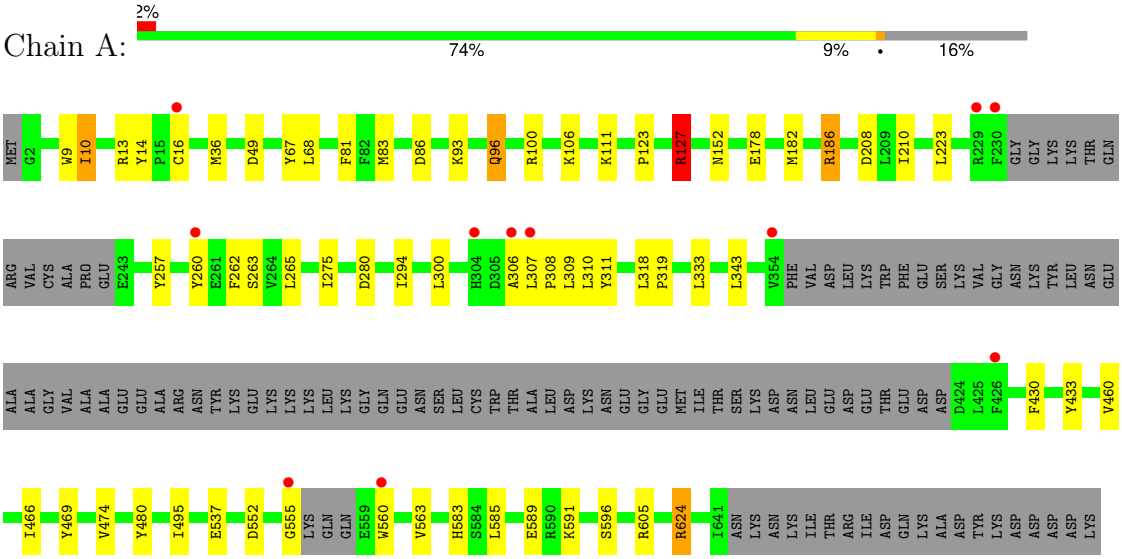
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	513	Total O 513 513	0	2
7	B	210	Total O 210 210	0	1

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.

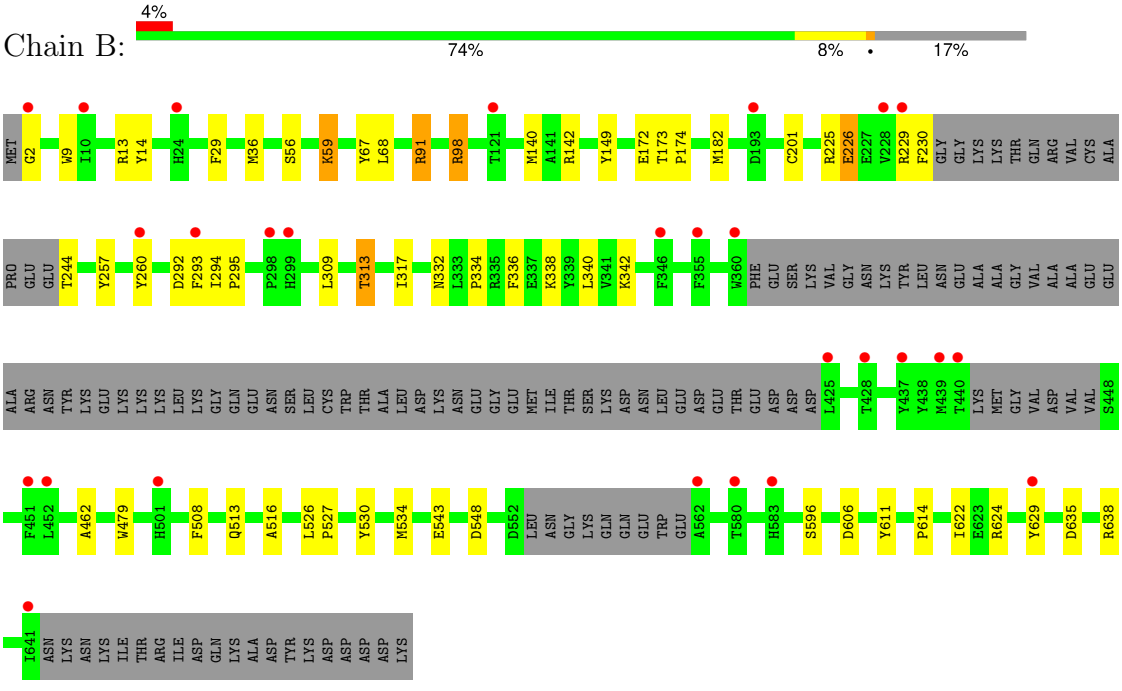
• Molecule 1: 5'-3' exoribonuclease 1

Chain A:



• Molecule 1: 5'-3' exoribonuclease 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.91Å 63.97Å 363.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.10 48.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.05-2.10) 100.0 (48.05-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.187 , 0.227 0.187 , 0.228	Depositor DCC
R_{free} test set	4332 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.031 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10178	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A3P, PEG, CL, MG, EDO

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	0.49	0/4883	0.97	7/6608 (0.1%)
1	B	0.40	0/4771	0.87	6/6459 (0.1%)
All	All	0.45	0/9654	0.92	13/13067 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	MET	CG-SD-CE	-7.18	88.72	100.20
1	A	127	ARG	CG-CD-NE	-7.04	97.02	111.80
1	A	624	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	629	TYR	CB-CA-C	-6.25	97.90	110.40
1	A	280	ASP	CB-CA-C	5.91	122.22	110.40
1	A	537	GLU	CB-CA-C	-5.82	98.76	110.40
1	A	589	GLU	CG-CD-OE2	-5.37	107.55	118.30
1	B	260	TYR	CB-CA-C	5.08	120.55	110.40
1	B	543	GLU	CG-CD-OE2	-5.05	108.19	118.30
1	B	606	ASP	CB-CA-C	5.04	120.47	110.40
1	A	182	MET	CG-SD-CE	-5.03	92.15	100.20
1	A	127	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	59	LYS	CB-CA-C	5.01	120.43	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	186	ARG	Sidechain
1	B	91	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4709	0	4595	60	0
1	B	4618	0	4484	39	0
2	A	54	0	22	4	0
3	A	2	0	0	0	0
4	A	56	0	84	13	0
4	B	8	0	12	2	0
5	A	1	0	0	0	0
6	A	7	0	10	0	0
7	A	513	0	0	8	0
7	B	210	0	0	11	0
All	All	10178	0	9207	102	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 5.

All (102) 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:583:HIS:HB2	4:A:713:EDO:H12	1.35	1.05
1:A:186:ARG:HD3	7:A:804:HOH:O	1.57	1.04
2:A:701[A]:A3P:O2'	2:A:701[A]:A3P:O1P	1.78	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ARG:HD2	4:A:714:EDO:H11	1.54	0.90
1:A:36[B]:MET:SD	1:A:83[B]:MET:SD	2.70	0.89
1:A:624:ARG:HD2	4:A:714:EDO:C1	2.10	0.82
1:A:265:LEU:HD13	1:A:318:LEU:HD23	1.66	0.78
1:A:480:TYR:H	4:A:717:EDO:H22	1.48	0.77
1:A:460:VAL:HG21	1:A:495:ILE:HD12	1.67	0.77
1:A:294:ILE:HG13	1:A:466:ILE:HD11	1.68	0.75
1:A:624:ARG:CD	4:A:714:EDO:H11	2.18	0.73
1:A:36[B]:MET:SD	1:A:83[B]:MET:CG	2.76	0.72
1:A:307:LEU:HB3	1:A:311:TYR:HE2	1.53	0.72
1:A:36[A]:MET:SD	1:A:68:LEU:HD21	2.30	0.71
2:A:701[A]:A3P:O3P	7:A:801:HOH:O	2.11	0.69
1:B:293:PHE:CD2	1:B:294:ILE:HG13	2.28	0.69
1:B:142:ARG:HD2	7:B:980:HOH:O	1.93	0.67
1:A:624:ARG:HG3	4:A:714:EDO:H11	1.77	0.66
1:A:624:ARG:CG	4:A:714:EDO:H11	2.25	0.66
1:B:624:ARG:O	7:B:801:HOH:O	2.14	0.65
1:A:591:LYS:HE2	7:A:1031:HOH:O	2.02	0.60
1:B:313:THR:O	1:B:317:ILE:HG22	2.03	0.59
1:B:292:ASP:HB3	7:B:977:HOH:O	2.03	0.58
1:A:605:ARG:HB2	7:A:1129:HOH:O	2.03	0.57
1:A:152:ASN:HD21	4:A:708:EDO:H22	1.69	0.56
1:B:508:PHE:CE1	4:B:701:EDO:H22	2.41	0.56
1:A:178:GLU:OE2	1:A:208:ASP:OD2	2.24	0.55
1:A:93:LYS:HE2	1:A:96:GLN:OE1	2.07	0.55
1:A:307:LEU:O	1:A:311:TYR:CD2	2.59	0.55
1:B:526:LEU:CD1	1:B:534:MET:SD	2.97	0.53
1:A:307:LEU:HB3	1:A:311:TYR:CE2	2.41	0.52
1:A:624:ARG:HD2	4:A:714:EDO:H12	1.89	0.52
1:A:583:HIS:CB	4:A:713:EDO:H12	2.24	0.52
1:A:469:TYR:CE1	1:A:474[B]:VAL:HG22	2.45	0.51
1:A:16:CYS:HB2	1:A:257:TYR:OH	2.10	0.51
1:A:294:ILE:CG1	1:A:466:ILE:HD11	2.40	0.51
1:B:59:LYS:NZ	7:B:803:HOH:O	2.32	0.51
1:B:336:PHE:CE2	1:B:340:LEU:HD11	2.45	0.51
1:B:309:LEU:O	1:B:313:THR:OG1	2.28	0.50
1:A:96:GLN:OE1	1:A:100:ARG:NH2	2.44	0.50
1:A:294:ILE:CD1	1:A:466:ILE:CD1	2.89	0.50
1:B:293:PHE:HD2	1:B:294:ILE:HG13	1.76	0.50
1:A:96:GLN:HE22	1:A:100:ARG:CZ	2.24	0.50
1:A:310:LEU:HD23	1:A:343:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:TYR:HB3	1:B:622:ILE:HB	1.95	0.49
1:A:10:ILE:HD11	1:A:210:ILE:HD13	1.94	0.49
1:B:149:TYR:CD2	1:B:614:PRO:HD3	2.48	0.49
1:B:225:ARG:NH2	1:B:226:GLU:O	2.46	0.48
1:B:462:ALA:HA	1:B:479:TRP:CH2	2.48	0.48
1:B:182:MET:HG2	7:B:969:HOH:O	2.14	0.48
1:B:172:GLU:CB	1:B:596:SER:HB3	2.43	0.47
1:A:307:LEU:N	1:A:308:PRO:HD2	2.29	0.47
1:A:36[B]:MET:SD	1:A:83[B]:MET:HG3	2.55	0.47
1:B:98:ARG:HD2	1:B:516:ALA:O	2.15	0.47
1:A:460:VAL:HG21	1:A:495:ILE:CD1	2.41	0.46
2:A:701[A]:A3P:O2'	2:A:701[A]:A3P:P1	2.73	0.46
1:B:635:ASP:HA	7:B:937:HOH:O	2.15	0.46
1:B:226:GLU:HG2	1:B:230:PHE:CZ	2.51	0.46
1:B:527:PRO:HD2	1:B:530:TYR:HD2	1.79	0.46
1:A:9:TRP:NE1	4:A:706:EDO:H11	2.31	0.46
1:A:49:ASP:OD1	1:A:111:LYS:HE2	2.16	0.46
1:A:81:PHE:CE2	1:A:83[B]:MET:CE	2.98	0.46
1:A:123:PRO:HB3	4:A:716:EDO:H11	1.98	0.45
1:A:96:GLN:NE2	1:A:100:ARG:NH2	2.64	0.45
1:B:225:ARG:HG2	1:B:225:ARG:HH21	1.81	0.45
1:B:332:ASN:OD1	1:B:334:PRO:HD2	2.17	0.45
1:B:2:GLY:O	1:B:225:ARG:NH1	2.51	0.44
1:B:29:PHE:CD1	1:B:201:CYS:HB2	2.53	0.44
1:B:14:TYR:CD1	1:B:257:TYR:HB3	2.52	0.44
1:B:56:SER:HA	7:B:925:HOH:O	2.17	0.44
1:A:9:TRP:CZ2	1:A:13:ARG:HD2	2.53	0.44
1:B:172:GLU:HB3	1:B:596:SER:HB3	2.00	0.44
1:A:430:PHE:O	1:A:433:TYR:HB3	2.18	0.43
1:A:474[B]:VAL:HG23	7:A:1177:HOH:O	2.18	0.43
1:A:96:GLN:CD	1:A:100:ARG:NH2	2.72	0.43
1:A:86:ASP:OD2	2:A:701[A]:A3P:H5'2	2.18	0.43
1:A:14:TYR:CD1	1:A:257:TYR:CD1	3.07	0.43
1:A:127:ARG:HB2	4:A:707:EDO:H21	2.01	0.43
1:A:552:ASP:HB3	1:A:563:VAL:HB	2.00	0.43
1:A:306:ALA:O	1:A:309:LEU:HB3	2.19	0.42
1:B:313:THR:CG2	1:B:342:LYS:HG3	2.50	0.42
1:A:14:TYR:HB3	1:A:257:TYR:CE1	2.55	0.42
1:B:91:ARG:HG2	7:B:839:HOH:O	2.19	0.42
1:B:338:LYS:HG2	7:B:1001:HOH:O	2.17	0.42
1:B:244:THR:HG23	7:B:972:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TYR:HD1	1:A:257:TYR:CD1	2.37	0.42
1:B:36:MET:SD	1:B:68:LEU:HD21	2.60	0.42
1:B:173:THR:HA	1:B:174:PRO:HD3	1.86	0.42
1:A:294:ILE:CD1	1:A:466:ILE:HD11	2.50	0.41
1:A:585:LEU:HD23	1:A:585:LEU:HA	1.90	0.41
1:B:294:ILE:HA	1:B:295:PRO:HD3	1.86	0.41
1:A:223:LEU:HD12	1:A:223:LEU:N	2.36	0.41
1:A:591:LYS:CE	7:A:1031:HOH:O	2.67	0.41
1:A:260:TYR:O	1:A:262:PHE:N	2.54	0.41
1:B:336:PHE:CZ	1:B:340:LEU:HD11	2.55	0.41
1:A:106:LYS:HE3	7:A:924[B]:HOH:O	2.20	0.41
1:A:555:GLY:HA3	1:A:560:TRP:HB2	2.02	0.41
1:A:596[B]:SER:HB3	7:A:809:HOH:O	2.21	0.40
1:B:638:ARG:CZ	7:B:869:HOH:O	2.69	0.40
1:B:9:TRP:CH2	1:B:13:ARG:HD2	2.57	0.40
1:B:91:ARG:HB2	4:B:701:EDO:O2	2.21	0.40
1:A:275:ILE:O	1:A:275:ILE:HD12	2.21	0.40

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	
1	A	559/661 (85%)	544 (97%)	15 (3%)	0	100	100
1	B	541/661 (82%)	524 (97%)	17 (3%)	0	100	100
All	All	1100/1322 (83%)	1068 (97%)	32 (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	
1	A	520/600 (87%)	512 (98%)	8 (2%)	60	67
1	B	506/600 (84%)	499 (99%)	7 (1%)	62	70
All	All	1026/1200 (86%)	1011 (98%)	15 (2%)	62	67

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	67	TYR
1	A	96	GLN
1	A	263[A]	SER
1	A	263[B]	SER
1	A	300	LEU
1	A	319	PRO
1	A	333	LEU
1	B	67	TYR
1	B	98	ARG
1	B	226	GLU
1	B	229	ARG
1	B	313	THR
1	B	513	GLN
1	B	548	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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	EDO	A	708	-	3,3,3	0.30	0	2,2,2	0.52	0
4	EDO	A	715	-	3,3,3	0.20	0	2,2,2	0.73	0
4	EDO	A	717	-	3,3,3	0.13	0	2,2,2	0.59	0
4	EDO	A	712	-	3,3,3	0.11	0	2,2,2	0.35	0
2	A3P	A	701[B]	-	25,29,29	0.74	0	31,45,45	0.97	1 (3%)
4	EDO	A	707	-	3,3,3	0.43	0	2,2,2	0.20	0
4	EDO	A	706	-	3,3,3	0.14	0	2,2,2	0.54	0
4	EDO	A	714	-	3,3,3	0.39	0	2,2,2	0.62	0
4	EDO	A	704	-	3,3,3	0.07	0	2,2,2	0.32	0
4	EDO	A	709	-	3,3,3	0.32	0	2,2,2	0.60	0
4	EDO	A	711	-	3,3,3	0.04	0	2,2,2	0.16	0
4	EDO	A	716	-	3,3,3	0.19	0	2,2,2	0.39	0
4	EDO	B	702	-	3,3,3	0.21	0	2,2,2	0.24	0
4	EDO	A	710	-	3,3,3	0.59	0	2,2,2	0.25	0
4	EDO	B	701	-	3,3,3	0.09	0	2,2,2	0.53	0
6	PEG	A	719	-	6,6,6	0.28	0	5,5,5	0.10	0
2	A3P	A	701[A]	3	25,29,29	0.79	1 (4%)	31,45,45	0.90	1 (3%)
4	EDO	A	713	-	3,3,3	0.48	0	2,2,2	0.83	0
4	EDO	A	705	-	3,3,3	0.30	0	2,2,2	0.78	0

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	EDO	A	708	-	-	1/1/1/1	-
4	EDO	A	715	-	-	0/1/1/1	-
4	EDO	A	717	-	-	0/1/1/1	-
4	EDO	A	712	-	-	0/1/1/1	-
2	A3P	A	701[B]	-	-	0/11/31/31	0/3/3/3
4	EDO	A	707	-	-	1/1/1/1	-
4	EDO	A	706	-	-	1/1/1/1	-
4	EDO	A	714	-	-	0/1/1/1	-
4	EDO	A	704	-	-	0/1/1/1	-
4	EDO	A	709	-	-	1/1/1/1	-
4	EDO	A	711	-	-	1/1/1/1	-
4	EDO	A	716	-	-	1/1/1/1	-
4	EDO	B	702	-	-	1/1/1/1	-
4	EDO	A	710	-	-	0/1/1/1	-
4	EDO	B	701	-	-	1/1/1/1	-
6	PEG	A	719	-	-	2/4/4/4	-
2	A3P	A	701[A]	3	-	3/11/31/31	0/3/3/3
4	EDO	A	713	-	-	1/1/1/1	-
4	EDO	A	705	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701[A]	A3P	P1-O3'	2.41	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701[B]	A3P	P1-O3'-C3'	-3.07	115.24	123.43
2	A	701[A]	A3P	C5-C6-N6	2.60	124.27	120.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701[A]	A3P	C5'-O5'-P2-O6P
2	A	701[A]	A3P	C4'-C3'-O3'-P1
2	A	701[A]	A3P	C2'-C3'-O3'-P1
6	A	719	PEG	O2-C3-C4-O4
4	A	713	EDO	O1-C1-C2-O2
4	A	708	EDO	O1-C1-C2-O2
4	A	711	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	716	EDO	O1-C1-C2-O2
4	B	702	EDO	O1-C1-C2-O2
4	A	707	EDO	O1-C1-C2-O2
6	A	719	PEG	C1-C2-O2-C3
4	B	701	EDO	O1-C1-C2-O2
4	A	705	EDO	O1-C1-C2-O2
4	A	706	EDO	O1-C1-C2-O2
4	A	709	EDO	O1-C1-C2-O2

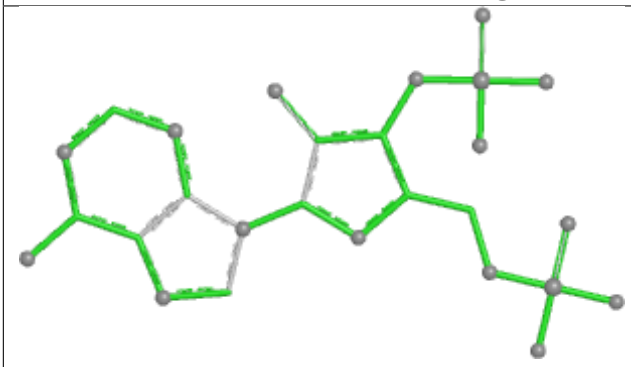
There are no ring outliers.

9 monomers are involved in 19 short contacts:

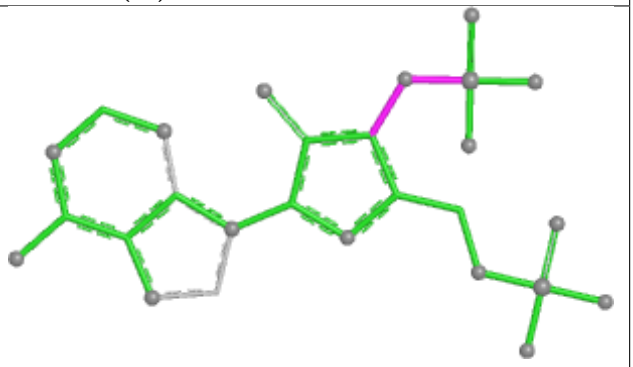
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	708	EDO	1	0
4	A	717	EDO	1	0
4	A	707	EDO	1	0
4	A	706	EDO	1	0
4	A	714	EDO	6	0
4	A	716	EDO	1	0
4	B	701	EDO	2	0
2	A	701[A]	A3P	4	0
4	A	713	EDO	2	0

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 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.

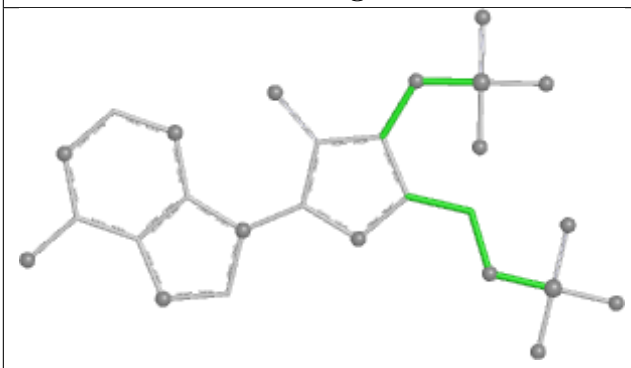
Ligand A3P A 701 (B)



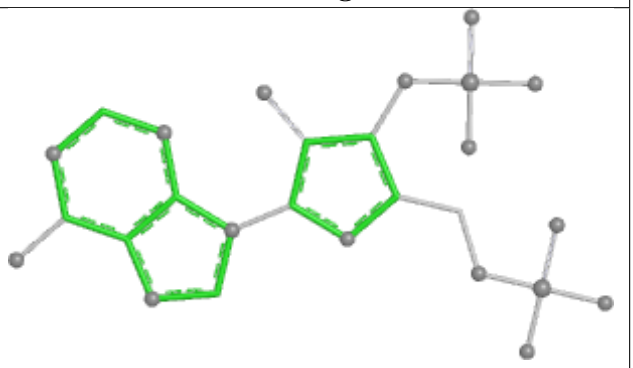
Bond lengths



Bond angles

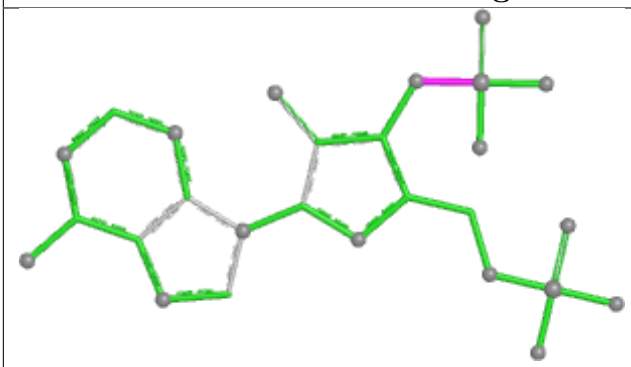


Torsions

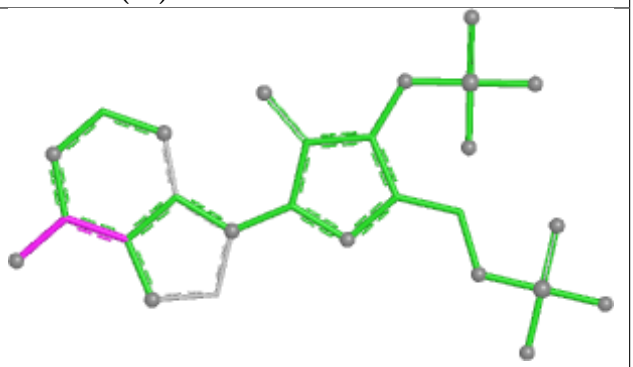


Rings

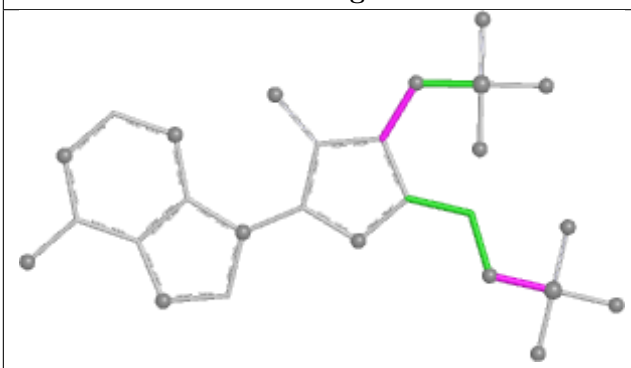
Ligand A3P A 701 (A)



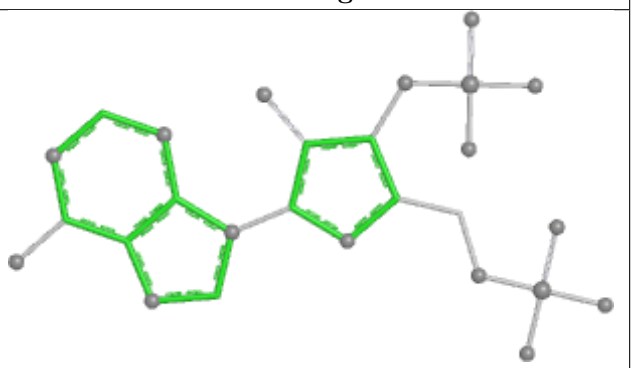
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	556/661 (84%)	-0.31	11 (1%)	64	66	11, 31, 74, 103	11 (1%)
1	B	547/661 (82%)	0.26	27 (4%)	36	38	21, 49, 89, 115	4 (0%)
All	All	1103/1322 (83%)	-0.03	38 (3%)	48	50	11, 42, 80, 115	15 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	LEU	3.9
1	B	228	VAL	3.8
1	A	426	PHE	3.4
1	A	307	LEU	3.3
1	A	354	VAL	3.3
1	A	555	GLY	3.2
1	B	641	ILE	3.2
1	B	580	THR	2.9
1	B	293	PHE	2.9
1	A	260	TYR	2.8
1	B	583	HIS	2.8
1	A	229	ARG	2.8
1	A	230	PHE	2.7
1	B	355	PHE	2.7
1	A	306	ALA	2.7
1	B	451	PHE	2.7
1	A	304	HIS	2.7
1	B	121	THR	2.7
1	B	439	MET	2.6
1	B	629	TYR	2.6
1	A	560	TRP	2.6
1	B	440	THR	2.6
1	B	24	HIS	2.5
1	B	452	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2	GLY	2.4
1	B	193[A]	ASP	2.4
1	B	346	PHE	2.3
1	B	562	ALA	2.3
1	B	260	TYR	2.2
1	B	298	PRO	2.2
1	B	10	ILE	2.2
1	A	16	CYS	2.2
1	B	299	HIS	2.2
1	B	360	TRP	2.1
1	B	437	TYR	2.0
1	B	229	ARG	2.0
1	B	428	THR	2.0
1	B	501	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
3	MG	A	703	1/1	0.79	0.20	56,56,56,56	0
4	EDO	A	716	4/4	0.79	0.17	59,67,70,75	0
4	EDO	A	711	4/4	0.80	0.11	62,71,73,76	0
4	EDO	A	704	4/4	0.80	0.19	40,59,63,68	0
4	EDO	A	705	4/4	0.81	0.20	39,60,66,69	0
6	PEG	A	719	7/7	0.82	0.15	51,56,70,70	0
4	EDO	B	701	4/4	0.84	0.16	54,61,63,67	0
4	EDO	A	714	4/4	0.85	0.18	41,46,50,52	0
4	EDO	A	706	4/4	0.85	0.16	61,63,75,82	0

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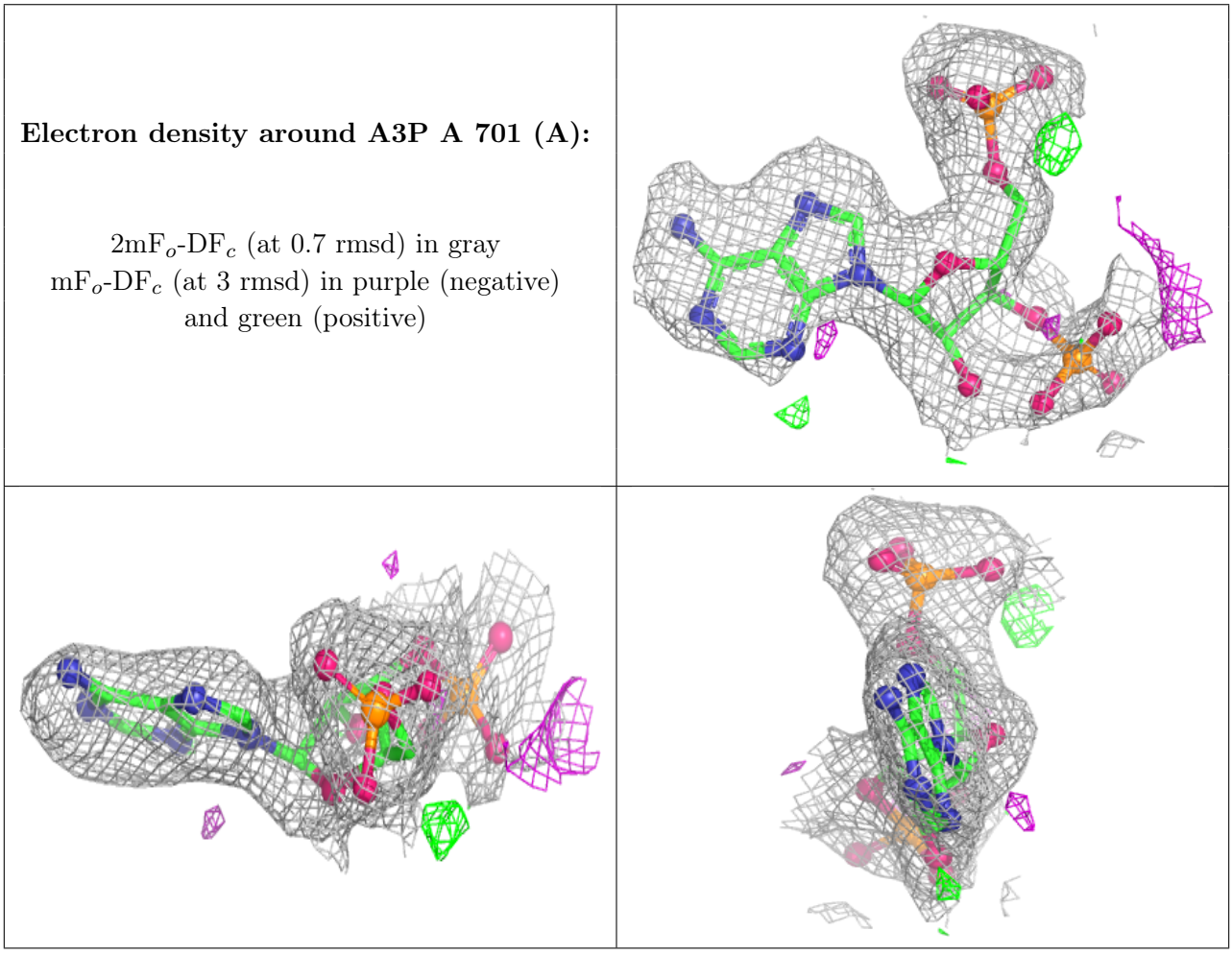
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	702	1/1	0.88	0.21	40,40,40,40	0
4	EDO	A	712	4/4	0.89	0.11	61,65,66,69	0
4	EDO	A	717	4/4	0.90	0.19	40,56,58,59	0
2	A3P	A	701[A]	27/27	0.92	0.10	29,39,45,47	27
4	EDO	A	709	4/4	0.92	0.11	38,44,44,48	0
4	EDO	B	702	4/4	0.92	0.10	45,47,51,57	0
2	A3P	A	701[B]	27/27	0.92	0.10	18,28,43,49	27
4	EDO	A	713	4/4	0.93	0.18	37,37,40,46	0
4	EDO	A	708	4/4	0.94	0.11	36,41,44,45	0
4	EDO	A	710	4/4	0.95	0.08	25,28,28,29	0
5	CL	A	718	1/1	0.95	0.10	57,57,57,57	0
4	EDO	A	707	4/4	0.95	0.09	34,35,39,39	0
4	EDO	A	715	4/4	0.96	0.06	20,29,30,36	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.

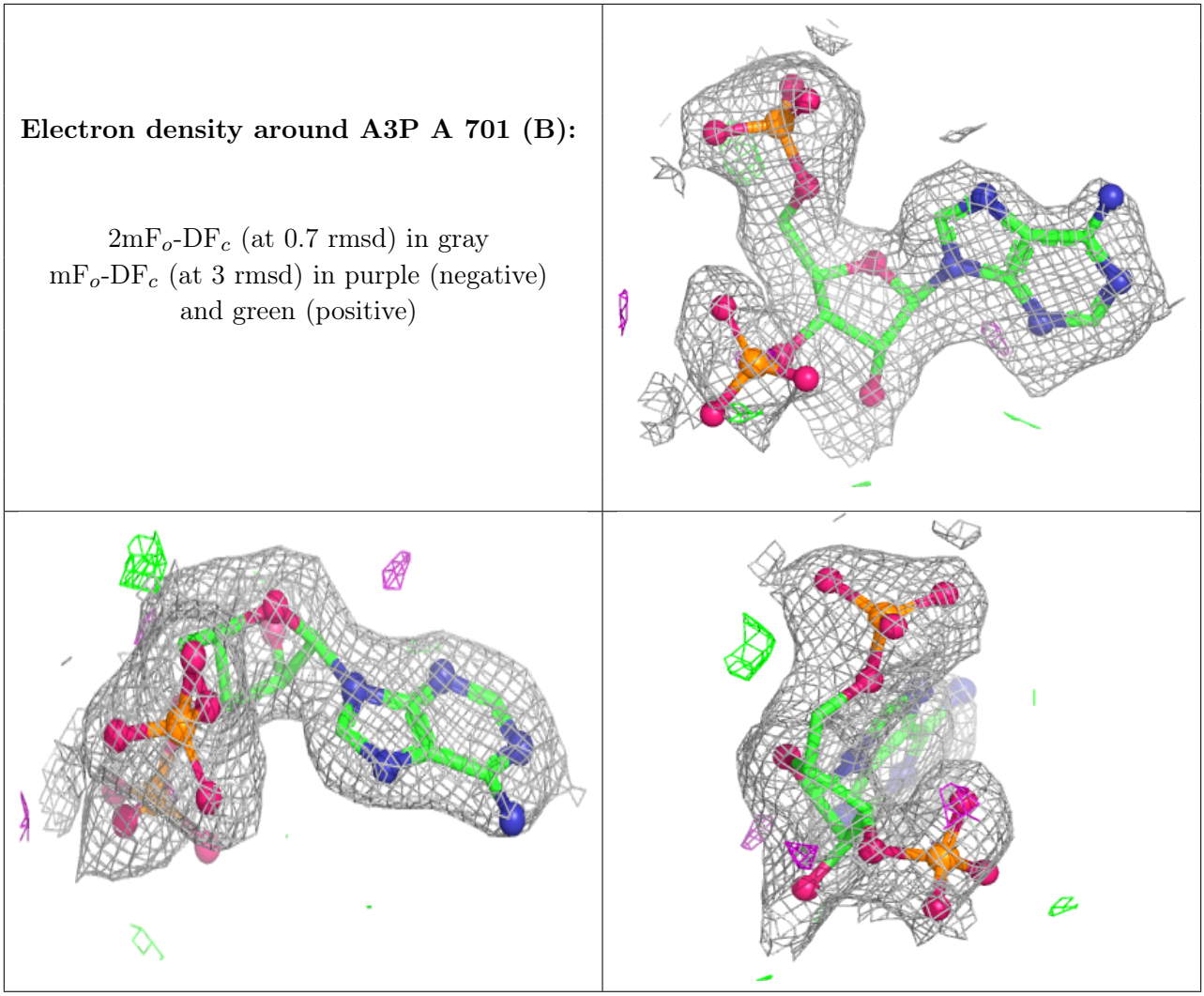
Electron density around A3P A 701 (A):

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



Electron density around A3P A 701 (B):

$2mF_o$-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

There are no such residues in this entry.