



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 06:28 pm GMT

PDB ID : 7BO7
Title : CRYSTAL STRUCTURE OF THE HUMAN PRMT5:MEP50 COMPLEX
with JNJB44355437
Authors : Brown, D.; Robinson, C.; Carr, K.H.; Pande, V.
Deposited on : 2021-01-24
Resolution : 2.83 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

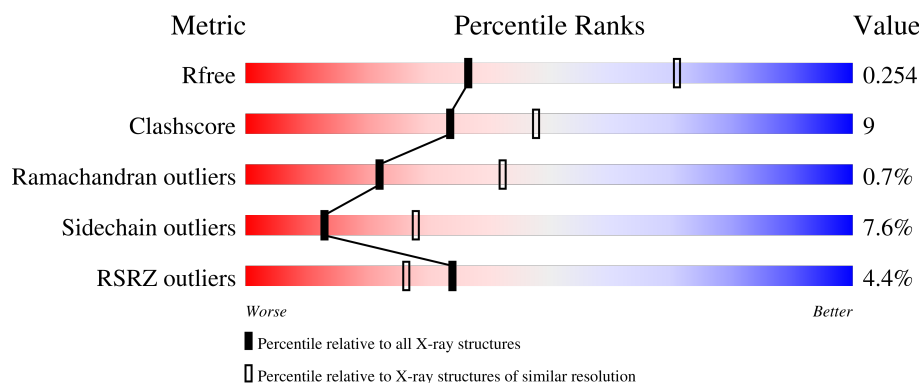
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	AAA	645	<div> <div>3%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	BBB	348	<div> <div>6%</div> <div>67%</div> <div>18%</div> <div>• 13%</div> </div>

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
3	U6K	AAA	701	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14566 atoms, of which 7155 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	625	9908	3210	4888	857	929	24	160	5	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-7	MET	-	initiating methionine	UNP O14744
AAA	-6	ASP	-	expression tag	UNP O14744
AAA	-5	TYR	-	expression tag	UNP O14744
AAA	-4	LYS	-	expression tag	UNP O14744
AAA	-3	ASP	-	expression tag	UNP O14744
AAA	-2	ASP	-	expression tag	UNP O14744
AAA	-1	ASP	-	expression tag	UNP O14744
AAA	0	ASP	-	expression tag	UNP O14744
AAA	1	LYS	-	expression tag	UNP O14744

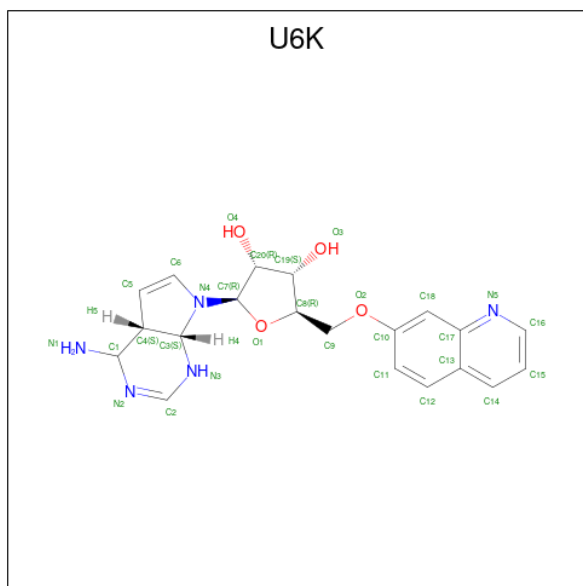
- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	BBB	303	4478	1433	2202	389	442	12	97	0	0

There are 7 discrepancies between the modelled and reference sequences:

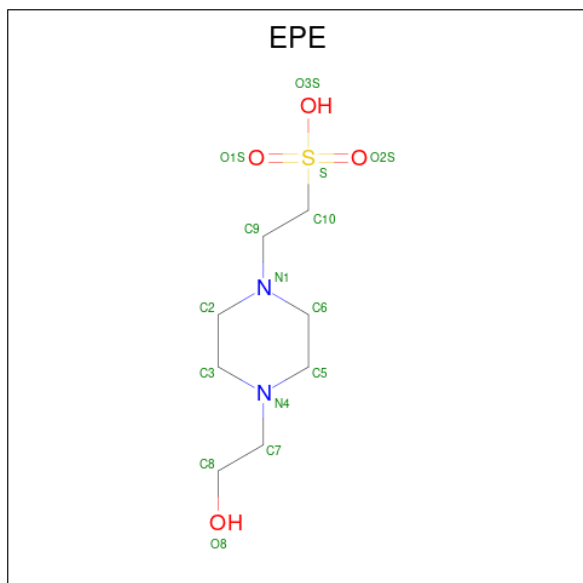
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-5	MET	-	initiating methionine	UNP Q9BQA1
BBB	-4	HIS	-	expression tag	UNP Q9BQA1
BBB	-3	HIS	-	expression tag	UNP Q9BQA1
BBB	-2	HIS	-	expression tag	UNP Q9BQA1
BBB	-1	HIS	-	expression tag	UNP Q9BQA1
BBB	0	HIS	-	expression tag	UNP Q9BQA1
BBB	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is (2 {R},3 {R},4 {S},5 {R})-2-[(4 {a} {S},7 {a} {S})-4-azanyl-1,4,4 {a} {a},7 {a}-tetrahydropyrrolo[2,3-d]pyrimidin-7-yl]-5-(quinolin-7-yloxymethyl)oxolane-3,4-diol (three-letter code: U6K) (formula: $C_{20}H_{23}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



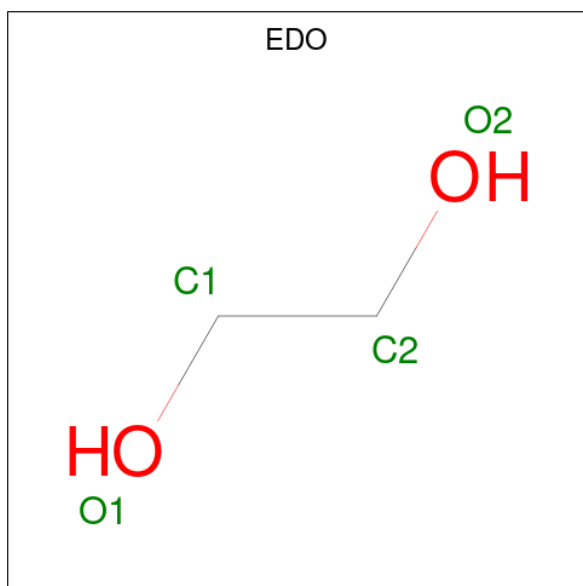
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	1	0
			48	20	19	5	4		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	H	N	O	S	
			33	8	18	2	4	1	
								2	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O		
			10	2	6	2	1	0
5	AAA	1	Total	C	H	O		
			10	2	6	2	1	0
5	AAA	1	Total	C	H	O		
			10	2	6	2	1	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			17	4	10	3		

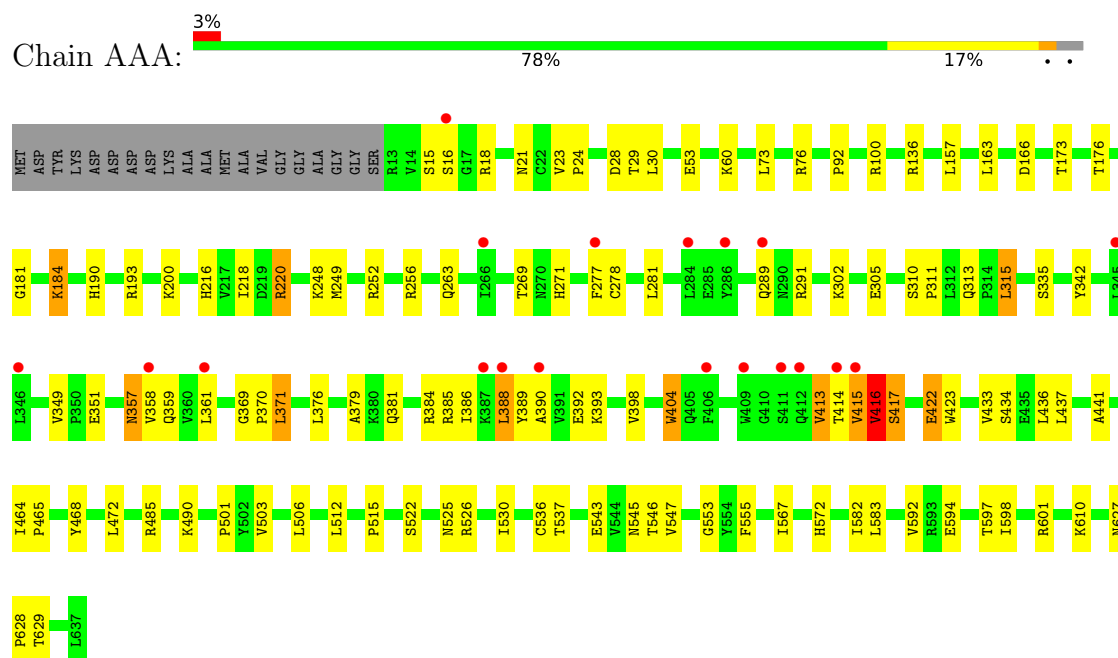
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	40	Total	O	0	0
			40	40		
7	BBB	12	Total	O	0	0
			12	12		

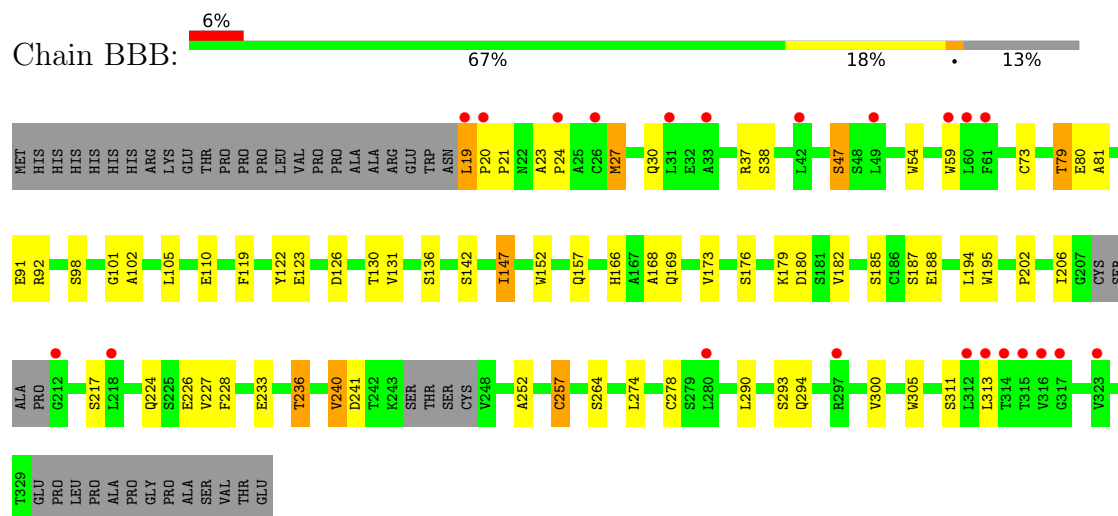
3 Residue-property plots [i](#)

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: Protein arginine N-methyltransferase 5



- Molecule 2: Methylosome protein 50



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.19Å 137.25Å 179.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.37 – 2.83 60.29 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.6 (60.37-2.83) 99.6 (60.29-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.250 0.210 , 0.254	Depositor DCC
R_{free} test set	1310 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14566	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: U6K, EDO, EPE, PEG

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	AAA	0.66	0/5161	0.87	0/7038
2	BBB	0.74	0/2330	0.86	0/3185
All	All	0.69	0/7491	0.86	0/10223

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	5020	4888	4832	77	0
2	BBB	2276	2202	2175	47	0
3	AAA	29	19	0	1	0
4	AAA	15	18	18	2	0
5	AAA	12	18	18	0	0
6	AAA	7	10	10	2	0
7	AAA	40	0	0	0	0
7	BBB	12	0	0	0	0
All	All	7411	7155	7053	123	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 9.

All (123) 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:AAA:415[B]:VAL:HG12	1:AAA:423:TRP:HE1	1.28	0.97
2:BBB:227:VAL:HG22	2:BBB:241:ASP:HB3	1.43	0.97
1:AAA:220:ARG:HG3	1:AAA:220:ARG:HH11	1.44	0.83
1:AAA:414[B]:THR:OG1	1:AAA:416[B]:VAL:HG13	1.78	0.83
2:BBB:102:ALA:HB2	2:BBB:122:TYR:CD1	2.23	0.73
1:AAA:389:TYR:CD2	1:AAA:414[B]:THR:O	2.43	0.71
1:AAA:414[A]:THR:HA	1:AAA:416[A]:VAL:HG22	1.72	0.71
2:BBB:24:PRO:HG2	2:BBB:59:TRP:CH2	2.25	0.71
1:AAA:413[B]:VAL:HG22	1:AAA:413[B]:VAL:O	1.91	0.69
1:AAA:15:SER:OG	1:AAA:263:GLN:NE2	2.25	0.69
1:AAA:415[B]:VAL:CG1	1:AAA:423:TRP:HE1	2.03	0.69
1:AAA:415[B]:VAL:HG12	1:AAA:423:TRP:NE1	2.06	0.68
1:AAA:371:LEU:HD13	1:AAA:433:VAL:HG12	1.77	0.67
1:AAA:349:VAL:HG22	1:AAA:357:ASN:HD21	1.58	0.67
1:AAA:18:ARG:CZ	1:AAA:277:PHE:CZ	2.78	0.66
1:AAA:404:TRP:CZ3	4:AAA:702:EPE:H101	2.30	0.66
1:AAA:15:SER:CB	1:AAA:263:GLN:HE21	2.11	0.64
1:AAA:379:ALA:HB2	1:AAA:386:ILE:HD13	1.79	0.64
2:BBB:37:ARG:NH1	2:BBB:91:GLU:O	2.34	0.61
2:BBB:233:GLU:HA	2:BBB:257:CYS:HB2	1.81	0.61
1:AAA:278:CYS:SG	6:AAA:706:PEG:H11	2.41	0.60
1:AAA:392:GLU:O	1:AAA:417[B]:SER:HA	2.02	0.60
1:AAA:422:GLU:OE2	1:AAA:422:GLU:HA	2.02	0.59
1:AAA:512:LEU:HD13	1:AAA:546:THR:HG21	1.84	0.59
1:AAA:53:GLU:O	1:AAA:60:LYS:HA	2.03	0.58
1:AAA:23:VAL:HG13	1:AAA:29:THR:HG21	1.86	0.58
2:BBB:147:ILE:HG23	2:BBB:168:ALA:O	2.04	0.58
2:BBB:147:ILE:HG12	2:BBB:168:ALA:C	2.24	0.57
1:AAA:358:VAL:HG22	1:AAA:385:ARG:CB	2.34	0.57
1:AAA:220:ARG:NH1	1:AAA:545:ASN:O	2.37	0.57
2:BBB:79:THR:OG1	2:BBB:81:ALA:O	2.23	0.57
2:BBB:38:SER:OG	2:BBB:91:GLU:OE2	2.23	0.56
1:AAA:220:ARG:HG3	1:AAA:220:ARG:NH1	2.15	0.56
1:AAA:592:VAL:HG21	1:AAA:598:ILE:HD11	1.88	0.56
2:BBB:147:ILE:O	2:BBB:147:ILE:HG22	2.05	0.55
2:BBB:228:PHE:CE1	2:BBB:240:VAL:HG23	2.42	0.55
1:AAA:404:TRP:HZ3	4:AAA:702:EPE:H101	1.70	0.55
2:BBB:24:PRO:HD2	2:BBB:59:TRP:CH2	2.41	0.55
1:AAA:389:TYR:HA	1:AAA:414[A]:THR:HB	1.88	0.54
2:BBB:30:GLN:HB2	2:BBB:47:SER:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:369:GLY:N	1:AAA:370:PRO:CD	2.72	0.52
2:BBB:92:ARG:NH1	2:BBB:110:GLU:HA	2.24	0.52
1:AAA:389:TYR:HD2	1:AAA:414[B]:THR:O	1.92	0.51
2:BBB:24:PRO:HG2	2:BBB:59:TRP:CZ2	2.45	0.51
1:AAA:501:PRO:HA	1:AAA:583:LEU:O	2.10	0.51
1:AAA:358:VAL:HG22	1:AAA:385:ARG:HB3	1.93	0.51
1:AAA:24:PRO:HA	2:BBB:54:TRP:O	2.10	0.51
1:AAA:15:SER:HB3	1:AAA:263:GLN:HE21	1.75	0.51
1:AAA:415[A]:VAL:HG12	1:AAA:415[A]:VAL:O	2.11	0.50
1:AAA:349:VAL:CG1	1:AAA:384:ARG:HD2	2.42	0.50
1:AAA:553:GLY:HA3	1:AAA:582:ILE:HG22	1.93	0.50
2:BBB:131:VAL:HG23	2:BBB:142:SER:HB3	1.94	0.50
2:BBB:227:VAL:CG2	2:BBB:241:ASP:HB3	2.29	0.49
1:AAA:434:SER:HB2	1:AAA:436:LEU:HD13	1.94	0.49
1:AAA:358:VAL:HG22	1:AAA:385:ARG:HB2	1.94	0.49
1:AAA:404:TRP:C	1:AAA:404:TRP:CD1	2.86	0.49
1:AAA:413[B]:VAL:O	1:AAA:413[B]:VAL:CG2	2.61	0.49
1:AAA:392:GLU:HG3	1:AAA:398:VAL:HG23	1.95	0.48
2:BBB:105:LEU:HB3	2:BBB:119:PHE:CD2	2.48	0.48
2:BBB:23:ALA:HB1	2:BBB:24:PRO:HD2	1.95	0.48
1:AAA:349:VAL:HG11	1:AAA:384:ARG:HD2	1.96	0.47
1:AAA:351:GLU:OE1	1:AAA:384:ARG:NH2	2.47	0.47
2:BBB:176:SER:HB3	2:BBB:179:LYS:O	2.14	0.47
1:AAA:278:CYS:SG	6:AAA:706:PEG:C1	3.03	0.47
2:BBB:169:GLN:HB2	2:BBB:188:GLU:HG3	1.97	0.47
2:BBB:182:VAL:HA	2:BBB:195:TRP:O	2.14	0.47
1:AAA:315:LEU:HD23	3:AAA:701:U6K:C5	2.45	0.46
2:BBB:195:TRP:HA	2:BBB:202:PRO:O	2.15	0.46
1:AAA:359:GLN:NE2	1:AAA:359:GLN:HA	2.30	0.46
1:AAA:390:ALA:HB3	1:AAA:415[A]:VAL:HA	1.96	0.46
1:AAA:543:GLU:OE2	1:AAA:543:GLU:HA	2.15	0.46
1:AAA:441:ALA:HB2	1:AAA:555:PHE:HB2	1.97	0.45
2:BBB:224:GLN:C	2:BBB:226:GLU:H	2.19	0.45
1:AAA:18:ARG:CZ	1:AAA:277:PHE:HZ	2.30	0.45
1:AAA:525:ASN:ND2	1:AAA:530:ILE:CB	2.80	0.45
1:AAA:567:ILE:HA	1:AAA:572:HIS:CD2	2.52	0.45
2:BBB:227:VAL:HG22	2:BBB:241:ASP:CB	2.31	0.45
2:BBB:264:SER:HA	2:BBB:305:TRP:CD1	2.52	0.45
1:AAA:181:GLY:O	1:AAA:184:LYS:NZ	2.50	0.45
2:BBB:23:ALA:HB1	2:BBB:24:PRO:CD	2.46	0.45
1:AAA:220:ARG:NH1	1:AAA:220:ARG:CG	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:389:TYR:CE2	1:AAA:414[A]:THR:HG21	2.53	0.44
1:AAA:413[B]:VAL:C	1:AAA:415[B]:VAL:H	2.20	0.44
2:BBB:24:PRO:CG	2:BBB:59:TRP:CH2	2.99	0.44
2:BBB:194:LEU:HB2	2:BBB:206:ILE:HD11	2.00	0.44
1:AAA:218:ILE:HG22	1:AAA:256:ARG:NH1	2.33	0.44
1:AAA:302:LYS:HA	1:AAA:305:GLU:OE2	2.19	0.43
2:BBB:101:GLY:HA2	2:BBB:126:ASP:O	2.18	0.43
2:BBB:166:HIS:CE1	2:BBB:187:SER:HB3	2.53	0.43
1:AAA:351:GLU:OE1	1:AAA:351:GLU:HA	2.18	0.43
1:AAA:92:PRO:O	1:AAA:100:ARG:HG3	2.18	0.43
2:BBB:278:CYS:HA	2:BBB:300:VAL:HG23	2.00	0.43
2:BBB:19:LEU:N	2:BBB:20:PRO:HD3	2.34	0.43
1:AAA:16:SER:OG	1:AAA:281:LEU:HD11	2.19	0.43
1:AAA:269:THR:HG23	1:AAA:271:HIS:CE1	2.54	0.43
2:BBB:166:HIS:ND1	2:BBB:187:SER:HB3	2.34	0.42
1:AAA:389:TYR:CD2	1:AAA:414[A]:THR:CG2	3.02	0.42
1:AAA:437:LEU:HD21	1:AAA:468:TYR:CD2	2.55	0.42
1:AAA:627:ASN:N	1:AAA:628:PRO:CD	2.82	0.42
2:BBB:119:PHE:CD2	2:BBB:157:GLN:HG2	2.55	0.42
2:BBB:305:TRP:CD2	2:BBB:313:LEU:HD13	2.55	0.42
1:AAA:157:LEU:HD23	1:AAA:157:LEU:HA	1.84	0.42
1:AAA:376:LEU:HD23	1:AAA:388:LEU:CD1	2.50	0.42
1:AAA:413[B]:VAL:O	1:AAA:415[B]:VAL:N	2.51	0.41
1:AAA:472:LEU:O	1:AAA:515:PRO:HA	2.21	0.41
2:BBB:38:SER:HG	2:BBB:91:GLU:CD	2.23	0.41
1:AAA:289:GLN:HE21	1:AAA:289:GLN:N	2.18	0.41
2:BBB:123:GLU:HB2	2:BBB:152:TRP:CH2	2.56	0.41
1:AAA:464:ILE:HA	1:AAA:465:PRO:HA	1.95	0.41
2:BBB:236:THR:HA	2:BBB:252:ALA:HA	2.01	0.41
1:AAA:166:ASP:CG	1:AAA:173:THR:HG23	2.41	0.41
2:BBB:105:LEU:CB	2:BBB:119:PHE:CE2	3.04	0.41
2:BBB:168:ALA:HB1	2:BBB:188:GLU:HB2	2.03	0.41
1:AAA:311:PRO:HB3	1:AAA:503:VAL:HG23	2.03	0.41
1:AAA:415[B]:VAL:HB	1:AAA:423:TRP:HZ2	1.86	0.41
2:BBB:123:GLU:HB2	2:BBB:152:TRP:HH2	1.86	0.41
2:BBB:130:THR:HG23	2:BBB:173:VAL:HG22	2.03	0.41
1:AAA:18:ARG:NH1	1:AAA:277:PHE:HZ	2.18	0.40
2:BBB:24:PRO:HD2	2:BBB:59:TRP:CZ3	2.55	0.40
2:BBB:27:MET:CB	2:BBB:59:TRP:CZ2	3.04	0.40
1:AAA:537:THR:HG23	1:AAA:601:ARG:HD3	2.03	0.40
1:AAA:190:HIS:CE1	1:AAA:547:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:166:HIS:ND1	2:BBB:187:SER:CB	2.84	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	AAA	628/645 (97%)	584 (93%)	36 (6%)	8 (1%)	12	26
2	BBB	297/348 (85%)	268 (90%)	27 (9%)	2 (1%)	22	42
All	All	925/993 (93%)	852 (92%)	63 (7%)	10 (1%)	22	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	417[A]	SER
1	AAA	417[B]	SER
2	BBB	147	ILE
2	BBB	21	PRO
1	AAA	413[A]	VAL
1	AAA	413[B]	VAL
1	AAA	415[A]	VAL
1	AAA	415[B]	VAL
1	AAA	416[A]	VAL
1	AAA	416[B]	VAL

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	AAA	544/570 (95%)	502 (92%)	42 (8%)	13	27
2	BBB	250/296 (84%)	231 (92%)	19 (8%)	13	28
All	All	794/866 (92%)	733 (92%)	61 (8%)	13	27

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	21	ASN
1	AAA	28	ASP
1	AAA	30	LEU
1	AAA	73	LEU
1	AAA	76	ARG
1	AAA	136	ARG
1	AAA	163	LEU
1	AAA	176	THR
1	AAA	184	LYS
1	AAA	193	ARG
1	AAA	200	LYS
1	AAA	216	HIS
1	AAA	220	ARG
1	AAA	248	LYS
1	AAA	249	MET
1	AAA	252	ARG
1	AAA	291	ARG
1	AAA	310	SER
1	AAA	313	GLN
1	AAA	315	LEU
1	AAA	335	SER
1	AAA	342	TYR
1	AAA	357	ASN
1	AAA	361	LEU
1	AAA	371	LEU
1	AAA	381	GLN
1	AAA	388	LEU
1	AAA	393	LYS
1	AAA	404	TRP
1	AAA	416[A]	VAL
1	AAA	416[B]	VAL
1	AAA	422	GLU
1	AAA	485	ARG

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Mol	Chain	Res	Type
1	AAA	490	LYS
1	AAA	506	LEU
1	AAA	522	SER
1	AAA	526	ARG
1	AAA	536	CYS
1	AAA	594	GLU
1	AAA	597	THR
1	AAA	610	LYS
1	AAA	629	THR
2	BBB	19	LEU
2	BBB	27	MET
2	BBB	47	SER
2	BBB	73	CYS
2	BBB	79	THR
2	BBB	80	GLU
2	BBB	98	SER
2	BBB	136	SER
2	BBB	180	ASP
2	BBB	185	SER
2	BBB	217	SER
2	BBB	236	THR
2	BBB	240	VAL
2	BBB	257	CYS
2	BBB	274	LEU
2	BBB	290	LEU
2	BBB	293	SER
2	BBB	294	GLN
2	BBB	311	SER

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands 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$
5	EDO	AAA	704	-	3,3,3	0.12	0	2,2,2	0.33	0
5	EDO	AAA	703	-	3,3,3	0.07	0	2,2,2	0.30	0
5	EDO	AAA	705	-	3,3,3	0.09	0	2,2,2	0.09	0
3	U6K	AAA	701	-	27,33,33	2.77	4 (14%)	34,48,48	1.62	1 (2%)
6	PEG	AAA	706	-	6,6,6	0.24	0	5,5,5	0.22	0
4	EPE	AAA	702	-	15,15,15	0.74	1 (6%)	18,20,20	0.70	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
5	EDO	AAA	704	-	-	0/1/1/1	-
5	EDO	AAA	703	-	-	0/1/1/1	-
5	EDO	AAA	705	-	-	1/1/1/1	-
3	U6K	AAA	701	-	3/3/11/12	2/9/48/48	0/5/5/5
6	PEG	AAA	706	-	-	1/4/4/4	-
4	EPE	AAA	702	-	-	4/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	701	U6K	C3-N3	-8.83	1.35	1.46
3	AAA	701	U6K	C4-C3	-8.75	1.41	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	701	U6K	C3-N4	-4.96	1.38	1.47
3	AAA	701	U6K	C4-C5	-4.71	1.43	1.51
4	AAA	702	EPE	O3S-S	2.63	1.56	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	701	U6K	C4-C3-N3	8.33	125.19	113.04

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AAA	701	U6K	C1
3	AAA	701	U6K	C3
3	AAA	701	U6K	C4

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	701	U6K	O1-C8-C9-O2
3	AAA	701	U6K	C19-C8-C9-O2
4	AAA	702	EPE	C8-C7-N4-C5
6	AAA	706	PEG	O2-C3-C4-O4
5	AAA	705	EDO	O1-C1-C2-O2
4	AAA	702	EPE	C10-C9-N1-C2
4	AAA	702	EPE	C10-C9-N1-C6
4	AAA	702	EPE	S-C10-C9-N1

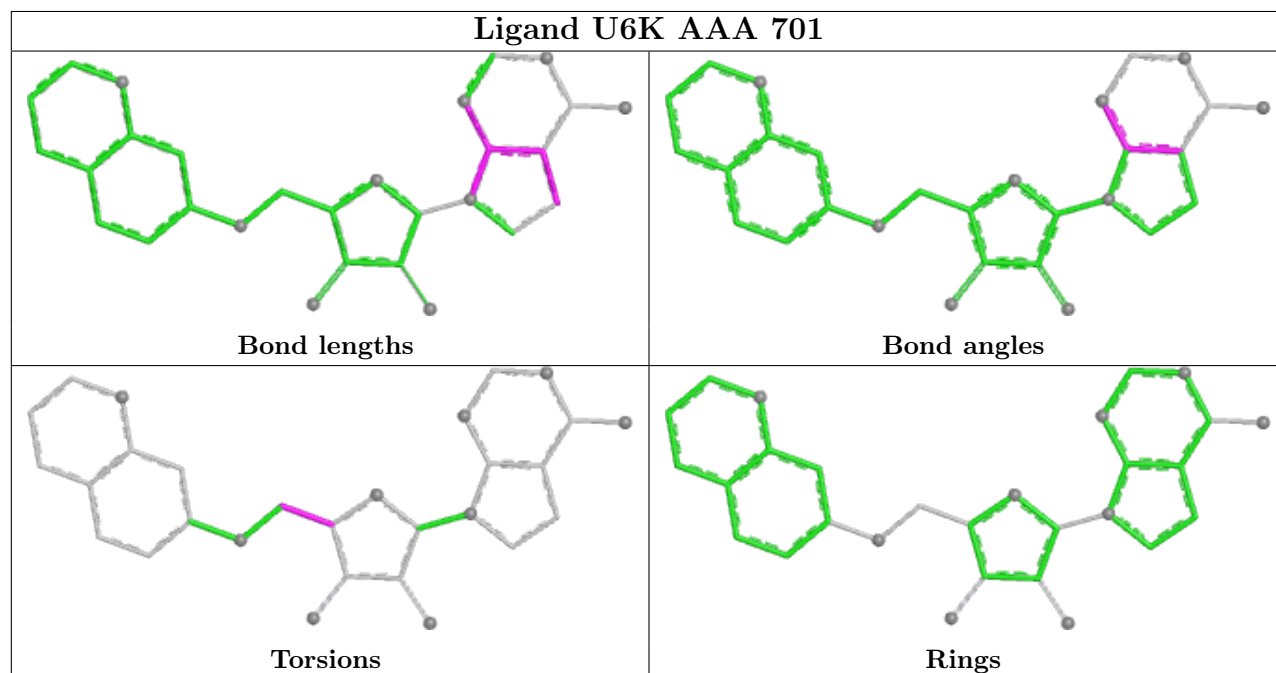
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	701	U6K	1	0
6	AAA	706	PEG	2	0
4	AAA	702	EPE	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 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	AAA	625/645 (96%)	0.26	19 (3%)	50 44	39, 62, 99, 140	0
2	BBB	303/348 (87%)	0.44	22 (7%)	15 9	53, 76, 100, 143	0
All	All	928/993 (93%)	0.32	41 (4%)	34 26	39, 67, 99, 143	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	280	LEU	3.7
2	BBB	33	ALA	3.7
1	AAA	361	LEU	3.6
2	BBB	20	PRO	3.2
1	AAA	414[A]	THR	3.2
2	BBB	31	LEU	3.2
1	AAA	406	PHE	2.9
1	AAA	411	SER	2.8
1	AAA	388	LEU	2.7
2	BBB	317	GLY	2.7
1	AAA	390	ALA	2.7
2	BBB	19	LEU	2.7
2	BBB	42	LEU	2.5
1	AAA	266	ILE	2.5
2	BBB	316	VAL	2.5
2	BBB	212	GLY	2.4
2	BBB	314	THR	2.4
2	BBB	315	THR	2.3
1	AAA	284	LEU	2.3
1	AAA	415[A]	VAL	2.3
2	BBB	323	VAL	2.3
1	AAA	345	LEU	2.3
2	BBB	49	LEU	2.2
2	BBB	26	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	409	TRP	2.2
2	BBB	61	PHE	2.2
1	AAA	358	VAL	2.2
2	BBB	60	LEU	2.2
2	BBB	218	LEU	2.2
1	AAA	387	LYS	2.2
1	AAA	346	LEU	2.1
2	BBB	59	TRP	2.1
1	AAA	289	GLN	2.1
1	AAA	277	PHE	2.1
1	AAA	286	TYR	2.0
2	BBB	312	LEU	2.0
1	AAA	16	SER	2.0
2	BBB	297	ARG	2.0
1	AAA	412	GLN	2.0
2	BBB	24	PRO	2.0
2	BBB	313	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

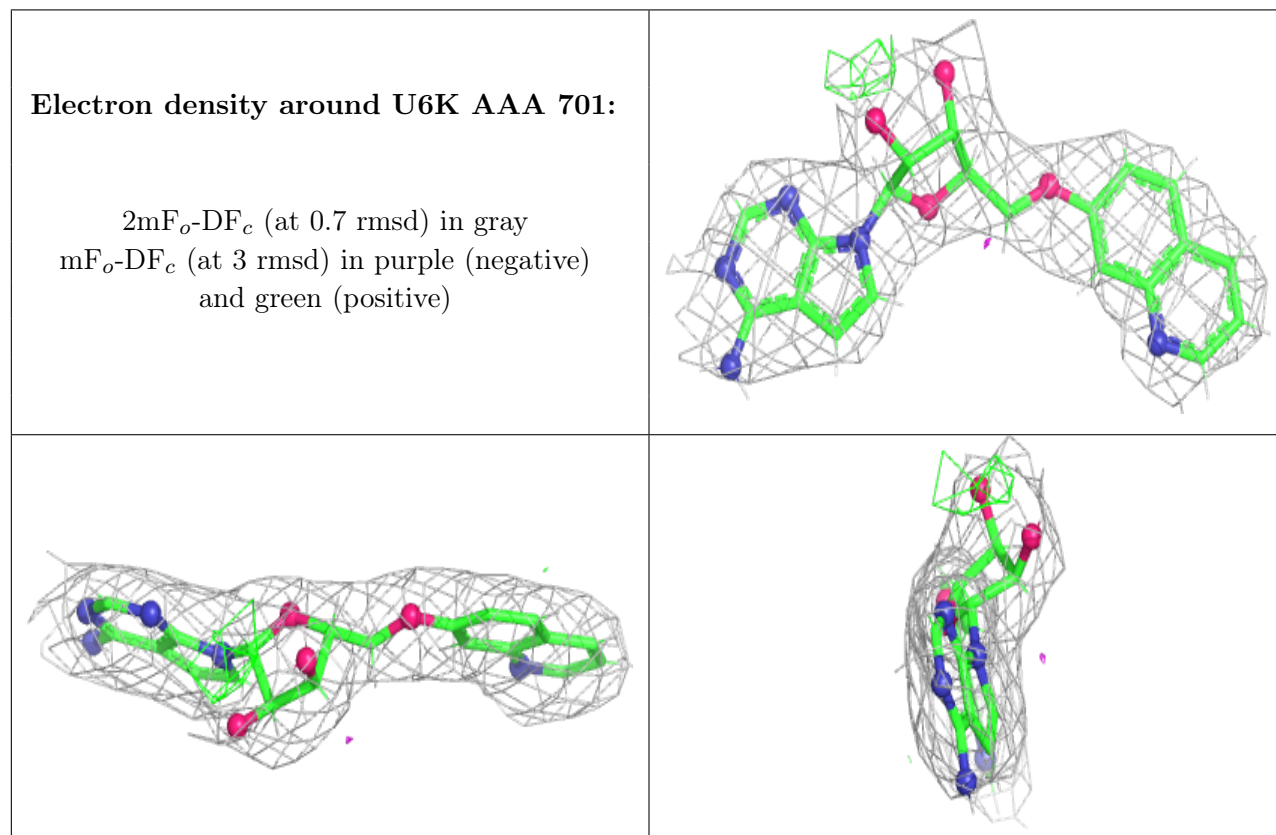
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	AAA	706	7/7	0.53	0.29	30,94,103,105	1
4	EPE	AAA	702	15/15	0.84	0.33	30,123,138,142	2
5	EDO	AAA	704	4/4	0.92	0.15	30,57,57,58	1
5	EDO	AAA	705	4/4	0.96	0.13	30,51,52,53	1
5	EDO	AAA	703	4/4	0.97	0.25	30,64,66,66	1
3	U6K	AAA	701	29/29	0.98	0.20	30,51,56,61	1

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.