



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:07 PM UTC

PDB ID : 7UBY / pdb_00007uby
Title : Structure of the GTD domain of Clostridium difficile toxin A in complex with VHH AH3
Authors : Chen, B.; Rongsheng, J.; Kay, P.
Deposited on : 2022-03-15
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 ⓘ 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

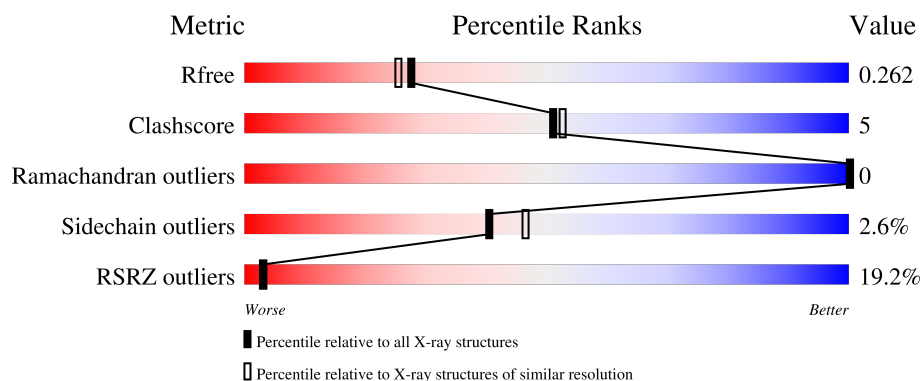
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	543	11% 88% 11%
1	B	543	23% 83% 13% ..
2	C	151	12% 73% 8% 19%
2	D	151	33% 72% 8% 21%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10704 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 Glucosyltransferase TcdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	529	Total	C	N	O	S	0	0	0
			4121	2625	678	810	8			
1	A	542	Total	C	N	O	S	0	0	0
			4368	2782	725	853	8			

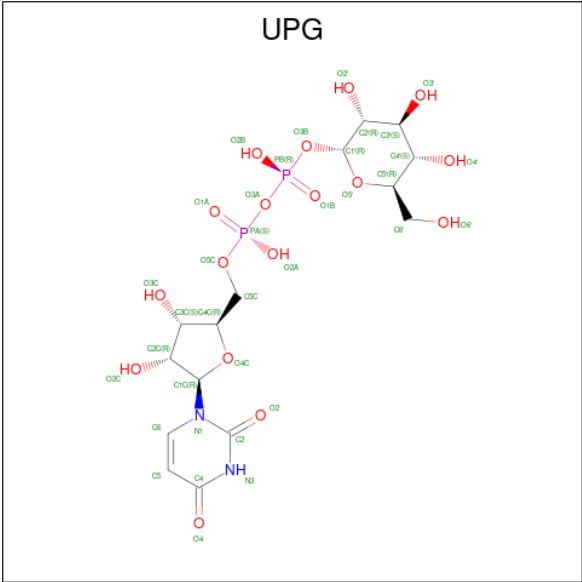
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P16154
B	190	ALA	LYS	engineered mutation	UNP P16154
A	0	SER	-	expression tag	UNP P16154
A	190	ALA	LYS	engineered mutation	UNP P16154

- Molecule 2 is a protein called Nanobody VHH AH3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	120	Total	C	N	O	S	3	0	0
			849	528	145	170	6			
2	C	123	Total	C	N	O	S	0	0	0
			893	557	152	178	6			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	2	0
			36	15	2	17	2		
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

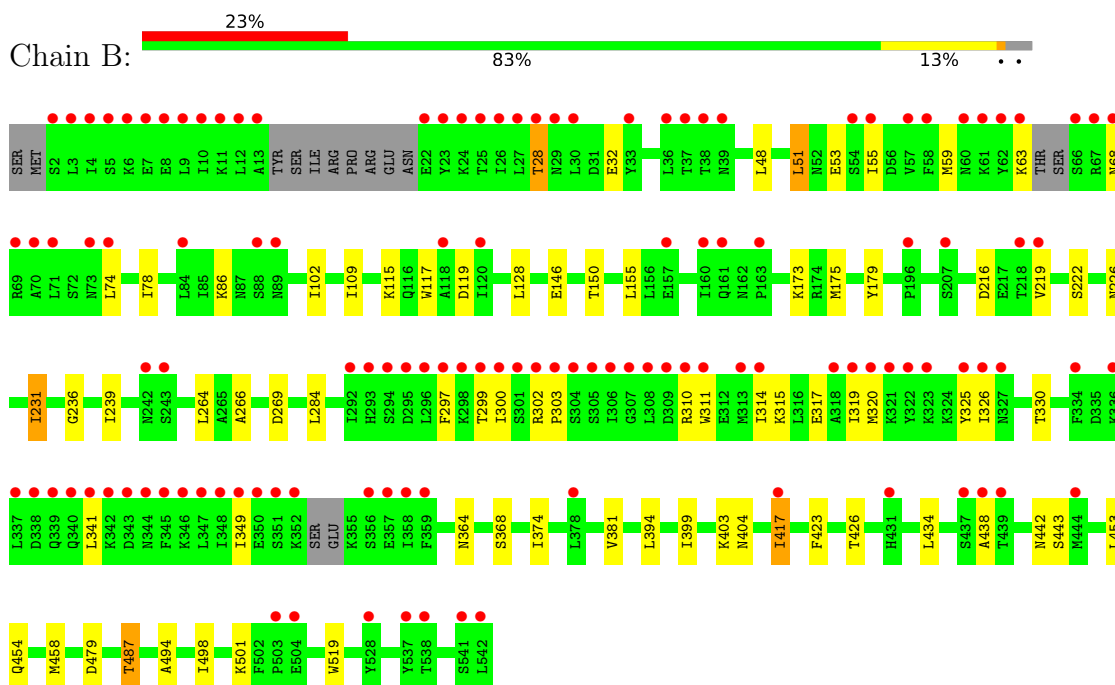
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	124	Total O 124 124	0	0
7	D	17	Total O 17 17	0	0
7	A	167	Total O 167 167	0	0
7	C	33	Total O 33 33	0	0

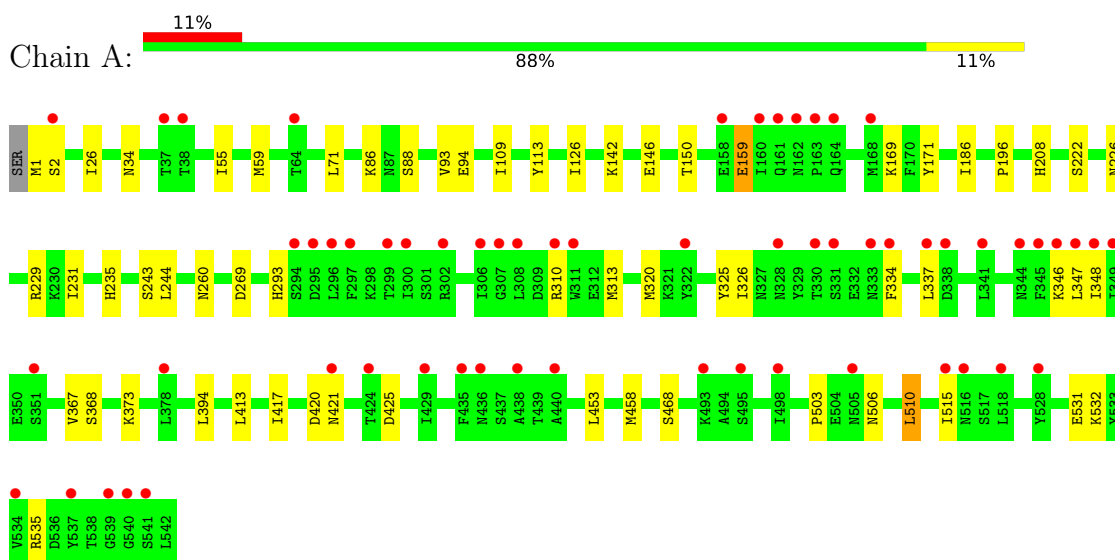
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

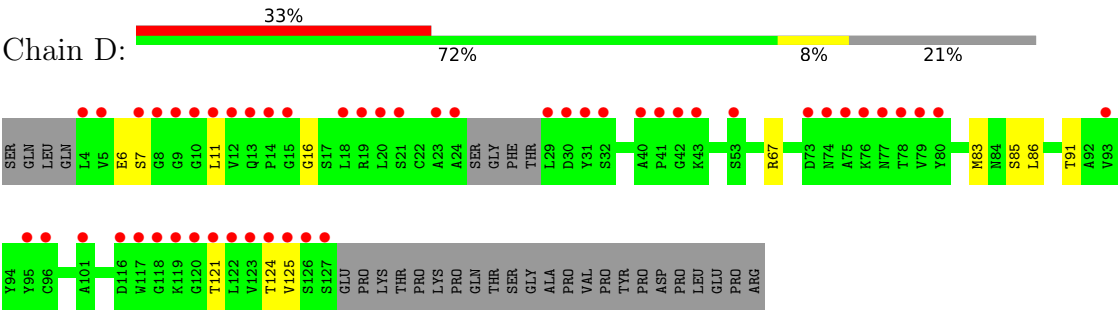
• Molecule 1: Glucosyltransferase TcdA



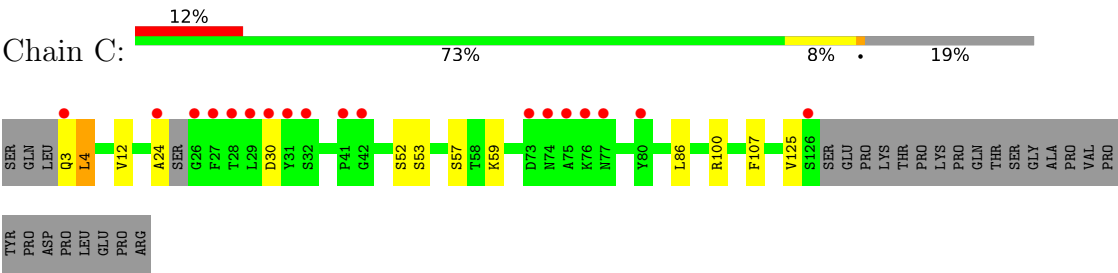
• Molecule 1: Glucosyltransferase TcdA



● Molecule 2: Nanobody VHH AH3



● Molecule 2: Nanobody VHH AH3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.12Å 131.64Å 83.80Å 90.00° 110.02° 90.00°	Depositor
Resolution (Å)	67.57 – 2.10 67.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (67.57-2.10) 99.3 (67.57-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.218 , 0.261 0.218 , 0.262	Depositor DCC
R_{free} test set	1988 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10704	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: MN, EDO, PEG, UPG

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	0.42	1/4446 (0.0%)	0.53	0/6011
1	B	0.41	0/4191	0.54	0/5683
2	C	0.37	0/910	0.53	0/1231
2	D	0.50	0/865	0.61	0/1172
All	All	0.42	1/10412 (0.0%)	0.54	0/14097

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	LYS	C-O	-5.23	1.18	1.24

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	A	4368	0	4308	37	0
1	B	4121	0	3912	51	0
2	C	893	0	841	8	0
2	D	849	0	780	8	0
3	A	36	0	22	1	0
3	B	36	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	14	0	20	4	0
6	A	28	0	42	2	0
6	B	16	0	24	1	0
7	A	167	0	0	3	0
7	B	124	0	0	1	0
7	C	33	0	0	0	0
7	D	17	0	0	0	0
All	All	10704	0	9971	106	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 (106) 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:442:ASN:HD22	5:B:604:PEG:H11	1.37	0.89
1:B:320:MET:HE1	1:B:325:TYR:HB2	1.58	0.85
1:B:364:ASN:HD22	6:B:608:EDO:H12	1.42	0.83
1:B:297:PHE:HD2	1:B:315:LYS:HD3	1.49	0.78
1:B:310:ARG:O	1:B:314:ILE:HD12	1.87	0.75
1:A:226:ASN:OD1	1:A:229:ARG:NH2	2.21	0.72
1:A:503:PRO:HB2	1:A:506:ASN:HD22	1.57	0.69
1:B:454:GLN:HG2	1:B:458:MET:HE3	1.76	0.67
1:B:109:ILE:H	1:B:109:ILE:HD12	1.59	0.67
2:D:91:THR:HG23	2:D:124:THR:HA	1.75	0.67
1:A:196:PRO:HG3	2:C:3:GLN:HG2	1.77	0.66
1:B:297:PHE:CD2	1:B:315:LYS:HD3	2.30	0.66
1:B:417:ILE:HD11	1:B:453:LEU:HD11	1.79	0.65
1:B:311:TRP:O	1:B:315:LYS:HG3	2.00	0.62
1:B:315:LYS:O	1:B:319:ILE:HD12	2.00	0.62
1:A:171:TYR:HB3	1:A:458:MET:HG2	1.81	0.61
1:B:175:MET:HG2	1:B:458:MET:HE2	1.84	0.60
1:B:63:LYS:O	1:B:68:ASN:ND2	2.35	0.60
1:B:374:ILE:HD13	1:B:381:VAL:HB	1.83	0.59
1:A:235:HIS:ND1	6:A:605:EDO:H11	2.16	0.59
1:A:334:PHE:O	1:A:337:LEU:HD12	2.03	0.59
1:B:320:MET:CE	1:B:326:ILE:H	2.16	0.58
7:A:763:HOH:O	2:C:100:ARG:HD3	2.03	0.58
1:B:519:TRP:HE1	3:B:601:UPG:C1'	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASP:HB3	1:B:219:VAL:HG12	1.87	0.56
2:D:11:LEU:CD1	2:D:124:THR:HB	2.35	0.56
1:B:48:LEU:HG	1:B:78:ILE:HG23	1.87	0.56
1:B:319:ILE:HA	1:B:349:ILE:HD13	1.88	0.56
1:A:310:ARG:HA	1:A:313:MET:HE2	1.88	0.55
1:A:55:ILE:HG22	1:A:59:MET:HE3	1.88	0.55
1:B:55:ILE:HD11	1:B:74:LEU:HD23	1.88	0.55
2:D:83:MET:HE2	2:D:86:LEU:HD11	1.89	0.54
1:A:313:MET:HG3	1:A:510:LEU:HB3	1.89	0.54
1:B:404:ASN:ND2	5:B:603:PEG:H22	2.23	0.54
1:B:454:GLN:CG	1:B:458:MET:HE3	2.37	0.53
1:A:186:ILE:HD11	1:A:260:ASN:HA	1.91	0.52
1:A:310:ARG:HH11	1:A:310:ARG:HG3	1.74	0.52
1:B:102:ILE:O	1:B:264:LEU:HD13	2.09	0.52
1:A:310:ARG:HG3	1:A:310:ARG:NH1	2.25	0.52
1:A:55:ILE:CG2	1:A:59:MET:HE3	2.39	0.52
1:A:320:MET:HE3	1:A:326:ILE:HD12	1.93	0.51
2:D:11:LEU:HD13	2:D:124:THR:HB	1.93	0.51
1:B:115:LYS:HD3	1:B:119:ASP:OD2	2.12	0.50
2:C:30:ASP:O	2:C:53:SER:OG	2.30	0.50
2:D:6:GLU:HB3	2:D:121:THR:HG22	1.94	0.50
1:A:413:LEU:HG	1:A:417:ILE:HG12	1.93	0.50
1:B:146:GLU:O	1:B:150:THR:HG23	2.12	0.49
1:A:367:VAL:HG12	1:A:373:LYS:HE2	1.95	0.49
1:A:146:GLU:O	1:A:150:THR:HG23	2.11	0.49
1:A:2:SER:HB2	1:A:34:ASN:OD1	2.12	0.49
1:B:51:LEU:HD12	1:B:51:LEU:O	2.13	0.48
2:D:86:LEU:HD12	2:D:125:VAL:HG21	1.96	0.48
1:A:1:MET:HB2	1:A:1:MET:HE2	1.70	0.47
1:A:142:LYS:NZ	1:A:142:LYS:HB3	2.28	0.47
1:B:28:THR:O	1:B:32:GLU:HG2	2.14	0.47
1:B:498:ILE:HG22	1:B:501:LYS:HD2	1.95	0.47
1:A:421:ASN:HB3	1:A:425:ASP:HB2	1.95	0.47
1:A:1:MET:HE1	1:A:88:SER:HB2	1.96	0.47
1:A:59:MET:HE2	1:A:71:LEU:HB3	1.96	0.47
3:A:601:UPG:H6'2	3:A:601:UPG:H1'	1.45	0.47
1:B:302:ARG:HD2	1:B:303:PRO:O	2.15	0.47
2:D:16:GLY:O	2:D:86:LEU:HD23	2.15	0.47
1:A:59:MET:HE2	1:A:71:LEU:CB	2.45	0.47
1:A:109:ILE:HD11	1:A:113:TYR:HE1	1.80	0.47
1:B:216:ASP:HB3	1:B:219:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLN:CD	1:B:458:MET:HE3	2.41	0.46
2:D:67:ARG:HD2	2:D:85:SER:HB2	1.98	0.46
1:A:86:LYS:O	1:A:368:SER:HB2	2.16	0.46
2:C:52:SER:HB3	2:C:57:SER:HB2	1.99	0.45
3:B:601:UPG:O3'	3:B:601:UPG:O6'	2.33	0.45
1:B:86:LYS:O	1:B:368:SER:HB2	2.16	0.45
1:A:503:PRO:HB2	1:A:506:ASN:ND2	2.27	0.45
1:B:434:LEU:O	1:B:438:ALA:HB2	2.17	0.45
1:A:244:LEU:HD12	1:A:244:LEU:HA	1.87	0.45
1:B:404:ASN:HD21	5:B:603:PEG:H22	1.83	0.44
1:B:417:ILE:HD12	1:B:426:THR:CG2	2.48	0.44
1:A:347:LEU:C	1:A:347:LEU:HD13	2.42	0.44
1:B:128:LEU:O	1:B:236:GLY:HA2	2.17	0.44
2:C:4:LEU:HD23	2:C:24:ALA:HB2	2.00	0.43
1:B:399:ILE:O	1:B:403:LYS:HG3	2.19	0.43
1:B:231:ILE:HB	7:B:710:HOH:O	2.17	0.43
1:A:159:GLU:OE2	1:A:169:LYS:NZ	2.51	0.43
1:B:341:LEU:HD12	1:B:341:LEU:HA	1.85	0.43
2:C:12:VAL:HG21	2:C:86:LEU:HD13	2.01	0.43
1:B:442:ASN:ND2	5:B:604:PEG:H11	2.19	0.42
1:B:155:LEU:HD23	1:B:173:LYS:HG2	2.00	0.42
1:B:317:GLU:HG2	1:B:330:THR:O	2.19	0.42
1:A:26:ILE:HD11	1:A:55:ILE:HA	2.02	0.42
1:B:51:LEU:HD12	1:B:51:LEU:C	2.44	0.42
1:B:109:ILE:H	1:B:109:ILE:CD1	2.29	0.42
1:B:494:ALA:O	1:B:498:ILE:HG13	2.20	0.42
1:B:117:TRP:CE2	1:B:284:LEU:HD13	2.55	0.41
1:B:175:MET:CG	1:B:458:MET:HE2	2.49	0.41
1:A:417:ILE:HD11	1:A:453:LEU:HD21	2.02	0.41
1:B:479:ASP:OD1	1:B:487:THR:HB	2.21	0.41
1:A:320:MET:SD	1:A:325:TYR:HB2	2.60	0.41
1:A:93:VAL:HG13	1:A:94:GLU:O	2.20	0.41
1:A:269:ASP:HB3	1:A:468:SER:HB2	2.02	0.41
1:B:266:ALA:O	1:B:269:ASP:HB2	2.21	0.41
1:A:208:HIS:HE1	7:A:738:HOH:O	2.04	0.41
6:A:609:EDO:H12	7:A:856:HOH:O	2.21	0.41
2:C:12:VAL:HG23	2:C:125:VAL:HG22	2.03	0.41
2:C:59:LYS:HE2	2:C:107:PHE:HD1	1.86	0.41
1:B:179:TYR:HB3	1:B:423:PHE:HB2	2.03	0.40
1:B:302:ARG:HE	1:B:302:ARG:HB3	1.49	0.40
1:A:531:GLU:O	1:A:535:ARG:HG3	2.22	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	540/543 (99%)	530 (98%)	10 (2%)	0	100	100
1	B	521/543 (96%)	506 (97%)	15 (3%)	0	100	100
2	C	119/151 (79%)	116 (98%)	3 (2%)	0	100	100
2	D	116/151 (77%)	114 (98%)	2 (2%)	0	100	100
All	All	1296/1388 (93%)	1266 (98%)	30 (2%)	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	482/499 (97%)	470 (98%)	12 (2%)	42	48
1	B	432/499 (87%)	418 (97%)	14 (3%)	34	38
2	C	93/125 (74%)	92 (99%)	1 (1%)	65	74
2	D	85/125 (68%)	84 (99%)	1 (1%)	63	72
All	All	1092/1248 (88%)	1064 (97%)	28 (3%)	40	46

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	28	THR
1	B	51	LEU
1	B	53	GLU
1	B	59	MET
1	B	222	SER
1	B	226	ASN
1	B	231	ILE
1	B	239	ILE
1	B	299	THR
1	B	300	ILE
1	B	394	LEU
1	B	417	ILE
1	B	443	SER
1	B	487	THR
2	D	7	SER
1	A	126	ILE
1	A	159	GLU
1	A	222	SER
1	A	231	ILE
1	A	243	SER
1	A	293	HIS
1	A	348	ILE
1	A	394	LEU
1	A	420	ASP
1	A	510	LEU
1	A	515	ILE
1	A	532	LYS
2	C	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	52	ASN
1	B	68	ASN
1	B	167	ASN
1	B	235	HIS
1	B	256	GLN
1	B	293	HIS
1	B	366	ASN
1	B	384	GLN
1	B	404	ASN
1	B	407	GLN
1	B	410	ASN

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Mol	Chain	Res	Type
1	B	411	GLN
1	B	442	ASN
1	B	482	ASN
1	B	509	GLN
2	D	82	GLN
1	A	21	ASN
1	A	73	ASN
1	A	192	GLN
1	A	208	HIS
1	A	366	ASN
1	A	384	GLN
1	A	411	GLN
1	A	482	ASN
1	A	484	GLN
1	A	506	ASN
1	A	509	GLN
2	C	39	GLN

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 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
6	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.31	0
5	PEG	B	604	-	6,6,6	0.19	0	5,5,5	0.10	0
6	EDO	A	605	-	3,3,3	0.57	0	2,2,2	0.29	0
6	EDO	A	609	-	3,3,3	0.51	0	2,2,2	0.06	0
6	EDO	B	606	-	3,3,3	0.33	0	2,2,2	0.85	0
6	EDO	A	606	-	3,3,3	0.46	0	2,2,2	0.39	0
6	EDO	A	608	-	3,3,3	0.53	0	2,2,2	0.22	0
6	EDO	A	607	-	3,3,3	0.43	0	2,2,2	0.50	0
3	UPG	A	601	4	37,38,38	1.61	7 (18%)	55,58,58	1.67	12 (21%)
3	UPG	B	601	4	37,38,38	1.68	8 (21%)	55,58,58	1.84	10 (18%)
6	EDO	B	607	-	3,3,3	0.57	0	2,2,2	0.15	0
6	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.66	0
5	PEG	B	603	-	6,6,6	0.14	0	5,5,5	0.21	0
6	EDO	B	608	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.44	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
6	EDO	B	605	-	-	0/1/1/1	-
5	PEG	B	604	-	-	1/4/4/4	-
6	EDO	A	605	-	-	0/1/1/1	-
6	EDO	A	609	-	-	1/1/1/1	-
6	EDO	B	606	-	-	0/1/1/1	-
6	EDO	A	606	-	-	1/1/1/1	-
6	EDO	A	608	-	-	1/1/1/1	-
6	EDO	A	607	-	-	1/1/1/1	-
3	UPG	A	601	4	-	3/23/59/59	0/3/3/3
3	UPG	B	601	4	-	5/23/59/59	0/3/3/3
6	EDO	B	607	-	-	0/1/1/1	-
6	EDO	A	604	-	-	1/1/1/1	-
5	PEG	B	603	-	-	1/4/4/4	-
6	EDO	B	608	-	-	1/1/1/1	-
6	EDO	A	603	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	UPG	C2-N3	-4.43	1.30	1.38
3	B	601	UPG	C4-N3	-4.42	1.31	1.38
3	A	601	UPG	C4-N3	-3.80	1.32	1.38
3	B	601	UPG	C2-N3	-3.36	1.32	1.38
3	B	601	UPG	C5-C4	-3.16	1.36	1.43
3	A	601	UPG	PA-O3A	3.01	1.62	1.59
3	A	601	UPG	PB-O2B	-2.77	1.42	1.55
3	B	601	UPG	PB-O2B	-2.77	1.42	1.55
3	B	601	UPG	C6-N1	-2.77	1.31	1.38
3	B	601	UPG	PA-O1A	-2.76	1.41	1.50
3	B	601	UPG	O4C-C4C	-2.63	1.39	1.45
3	A	601	UPG	PA-O1A	-2.62	1.41	1.50
3	B	601	UPG	O4-C4	-2.23	1.20	1.24
3	A	601	UPG	C5-C4	-2.10	1.39	1.43
3	A	601	UPG	C6-N1	-2.01	1.33	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	UPG	N3-C2-N1	5.25	121.73	114.89
3	B	601	UPG	C4-N3-C2	-4.91	120.52	126.61
3	A	601	UPG	N3-C2-N1	4.40	120.61	114.89
3	A	601	UPG	C4-N3-C2	-4.11	121.51	126.61
3	A	601	UPG	C5-C4-N3	4.08	120.52	114.80
3	B	601	UPG	O3B-C1'-C2'	4.01	115.73	108.38
3	B	601	UPG	O2-C2-N1	-3.88	117.74	122.80
3	B	601	UPG	O2'-C2'-C1'	3.53	118.50	110.08
3	B	601	UPG	C5-C4-N3	3.42	119.59	114.80
3	B	601	UPG	O5'-C1'-O3B	-3.08	107.33	111.36
3	A	601	UPG	O5'-C5'-C4'	-3.01	104.28	109.70
3	B	601	UPG	O4-C4-C5	-2.91	120.14	125.16
3	A	601	UPG	O4C-C1C-N1	2.82	114.76	108.36
3	B	601	UPG	O5'-C5'-C4'	-2.70	104.84	109.70
3	A	601	UPG	O3B-C1'-C2'	2.69	113.31	108.38
3	B	601	UPG	O5C-PA-O1A	-2.67	98.36	108.94
3	A	601	UPG	O5'-C1'-O3B	-2.55	108.03	111.36
3	A	601	UPG	O2'-C2'-C1'	2.37	115.72	110.08
3	A	601	UPG	O2B-PB-O3A	-2.15	101.46	107.27
3	A	601	UPG	C1'-O5'-C5'	-2.11	109.61	113.72
3	A	601	UPG	O5C-PA-O1A	-2.10	100.60	108.94
3	A	601	UPG	O2-C2-N1	-2.04	120.14	122.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

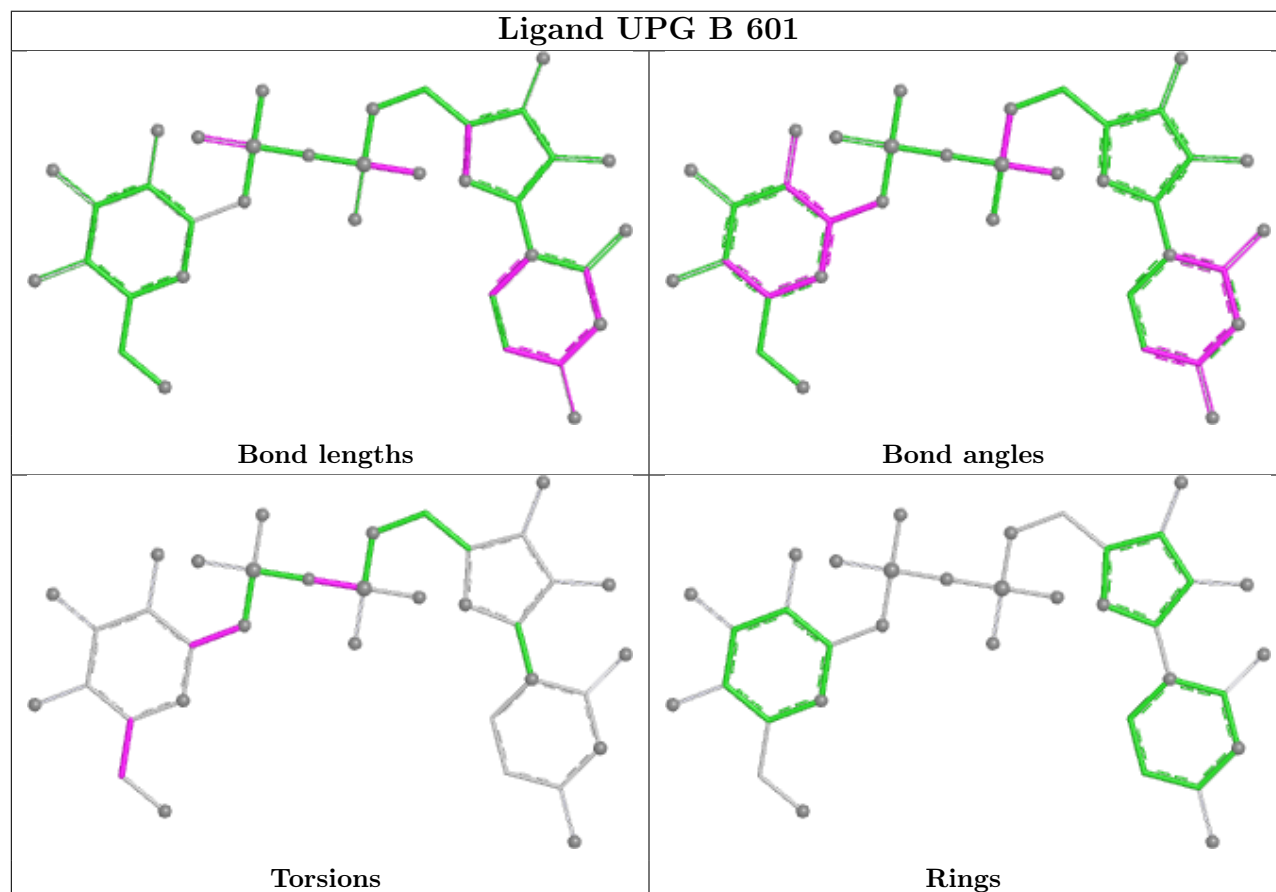
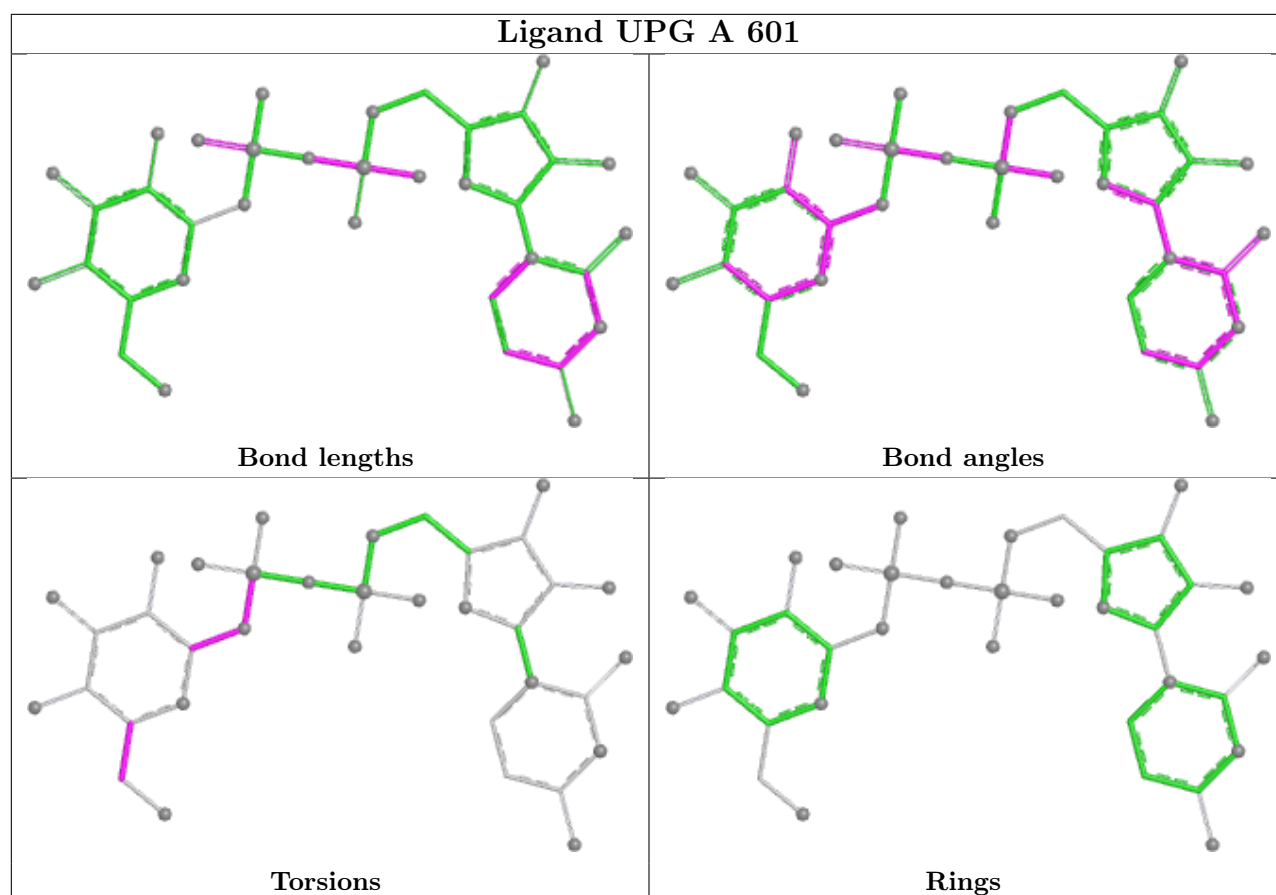
Mol	Chain	Res	Type	Atoms
3	A	601	UPG	O5'-C1'-O3B-PB
3	B	601	UPG	C4'-C5'-C6'-O6'
3	B	601	UPG	O5'-C5'-C6'-O6'
3	A	601	UPG	O5'-C5'-C6'-O6'
5	B	604	PEG	C1-C2-O2-C3
6	A	606	EDO	O1-C1-C2-O2
3	B	601	UPG	C2'-C1'-O3B-PB
5	B	603	PEG	C1-C2-O2-C3
6	B	608	EDO	O1-C1-C2-O2
6	A	607	EDO	O1-C1-C2-O2
3	A	601	UPG	C1'-O3B-PB-O1B
6	A	604	EDO	O1-C1-C2-O2
6	A	608	EDO	O1-C1-C2-O2
6	A	609	EDO	O1-C1-C2-O2
3	B	601	UPG	PB-O3A-PA-O1A
3	B	601	UPG	PB-O3A-PA-O2A

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	604	PEG	2	0
6	A	605	EDO	1	0
6	A	609	EDO	1	0
3	A	601	UPG	1	0
3	B	601	UPG	2	0
5	B	603	PEG	2	0
6	B	608	EDO	1	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	542/543 (99%)	0.56	60 (11%)	10 10	21, 34, 56, 72	0
1	B	529/543 (97%)	1.03	124 (23%)	2 2	22, 35, 90, 118	0
2	C	123/151 (81%)	0.90	18 (14%)	6 6	24, 36, 74, 92	0
2	D	120/151 (79%)	1.81	50 (41%)	0 1	28, 51, 85, 96	1 (0%)
All	All	1314/1388 (94%)	0.90	252 (19%)	3 3	21, 36, 81, 118	1 (0%)

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	ILE	7.0
1	B	341	LEU	7.0
1	B	348	ILE	6.5
2	D	75	ALA	6.4
1	B	58	PHE	6.2
1	B	13	ALA	6.1
2	C	26	GLY	6.1
1	B	36	LEU	6.1
1	B	347	LEU	6.0
2	D	24	ALA	5.8
2	C	27	PHE	5.8
1	B	303	PRO	5.8
1	B	349	ILE	5.7
2	D	30	ASP	5.7
1	B	296	LEU	5.6
1	B	344	ASN	5.6
2	D	29	LEU	5.5
2	C	28	THR	5.4
2	C	29	LEU	5.3
1	B	345	PHE	5.2
1	B	337	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	297	PHE	5.1
1	A	37	THR	5.0
1	B	23	TYR	5.0
1	B	306	ILE	5.0
1	B	62	TYR	4.9
1	B	27	LEU	4.9
2	D	32	SER	4.9
1	B	38	THR	4.9
1	B	4	ILE	4.7
2	D	31	TYR	4.7
1	B	10	ILE	4.7
1	B	60	ASN	4.6
1	B	351	SER	4.6
2	D	41	PRO	4.5
2	D	74	ASN	4.5
1	B	294	SER	4.5
2	D	9	GLY	4.5
2	D	11	LEU	4.5
1	B	61	LYS	4.4
1	B	307	GLY	4.4
1	B	334	PHE	4.3
1	B	319	ILE	4.2
1	B	305	SER	4.2
2	C	75	ALA	4.2
2	C	32	SER	4.2
1	B	322	TYR	4.2
2	C	24	ALA	4.2
1	B	12	LEU	4.2
1	B	308	LEU	4.2
1	B	9	LEU	4.1
2	D	12	VAL	4.1
2	D	23	ALA	4.1
1	B	299	THR	4.0
2	D	5	VAL	4.0
2	D	125	VAL	3.9
1	B	30	LEU	3.9
1	B	311	TRP	3.9
1	B	338	ASP	3.9
1	B	70	ALA	3.9
2	D	77	ASN	3.9
1	B	358	ILE	3.9
2	D	8	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	352	LYS	3.8
1	B	350	GLU	3.8
1	B	346	LYS	3.7
1	B	314	ILE	3.7
1	B	325	TYR	3.7
2	C	31	TYR	3.7
1	B	39	ASN	3.7
1	A	528	TYR	3.7
1	B	26	ILE	3.6
1	B	321	LYS	3.6
1	A	163	PRO	3.6
2	D	42	GLY	3.6
1	A	160	ILE	3.5
2	D	76	LYS	3.5
1	B	343	ASP	3.5
1	B	304	SER	3.5
1	A	440	ALA	3.4
1	B	66	SER	3.4
1	B	68	ASN	3.4
1	B	55	ILE	3.4
2	D	4	LEU	3.4
1	A	495	SER	3.4
1	A	341	LEU	3.4
1	B	295	ASP	3.3
1	B	342	LYS	3.3
1	B	88	SER	3.3
1	A	515	ILE	3.3
1	A	328	ASN	3.3
2	C	76	LYS	3.3
2	D	10	GLY	3.3
1	B	71	LEU	3.3
1	A	295	ASP	3.3
1	B	542	LEU	3.2
1	B	67	ARG	3.2
1	B	298	LYS	3.2
1	B	318	ALA	3.2
1	B	163	PRO	3.2
1	B	22	GLU	3.1
1	B	37	THR	3.1
1	B	63	LYS	3.1
1	A	436	ASN	3.1
2	C	77	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	161	GLN	3.1
1	A	308	LEU	3.1
1	B	293	HIS	3.1
1	A	38	THR	3.1
1	B	378	LEU	3.1
2	D	127	SER	3.1
1	A	505	ASN	3.1
1	B	74	LEU	3.1
1	B	313	MET	3.1
2	D	120	GLY	3.0
1	B	340	GLN	3.0
2	D	14	PRO	3.0
1	B	28	THR	3.0
1	B	11	LYS	3.0
1	B	301	SER	3.0
1	B	541	SER	3.0
1	A	294	SER	3.0
1	B	24	LYS	3.0
2	D	73	ASP	3.0
1	B	3	LEU	2.9
1	B	323	LYS	2.9
1	B	339	GLN	2.9
1	B	302	ARG	2.9
1	A	307	GLY	2.9
1	B	161	GLN	2.9
1	B	292	ILE	2.8
2	C	41	PRO	2.8
2	D	121	THR	2.8
1	B	57	VAL	2.8
1	B	6	LYS	2.8
1	B	25	THR	2.8
1	B	73	ASN	2.7
1	A	347	LEU	2.7
1	B	528	TYR	2.7
1	A	322	TYR	2.7
1	A	162	ASN	2.7
2	D	126	SER	2.7
1	A	2	SER	2.7
1	A	429	ILE	2.7
2	D	21	SER	2.6
2	C	42	GLY	2.6
2	C	3	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	84	LEU	2.6
1	B	537	TYR	2.6
1	A	345	PHE	2.6
1	A	498	ILE	2.6
1	B	336	LYS	2.6
2	D	78	THR	2.6
1	B	417	ILE	2.5
1	A	168	MET	2.5
2	D	80	TYR	2.5
2	C	126	SER	2.5
1	A	518	LEU	2.5
2	D	122	LEU	2.5
1	B	320	MET	2.5
1	A	534	VAL	2.4
1	B	357	GLU	2.4
1	B	2	SER	2.4
1	A	541	SER	2.4
1	A	164	GLN	2.4
1	A	537	TYR	2.4
2	D	95	TYR	2.4
2	C	80	TYR	2.4
2	D	119	LYS	2.4
1	A	539	GLY	2.4
2	D	15	GLY	2.4
1	A	516	ASN	2.4
2	C	74	ASN	2.4
1	A	158	GLU	2.4
1	A	334	PHE	2.4
2	C	30	ASP	2.4
1	A	348	ILE	2.4
1	B	5	SER	2.4
1	B	243	SER	2.4
1	B	356	SER	2.4
1	A	424	THR	2.4
1	B	503	PRO	2.4
1	A	378	LEU	2.4
2	D	20	LEU	2.4
2	D	13	GLN	2.4
1	A	302	ARG	2.4
1	B	54	SER	2.4
1	A	64	THR	2.4
1	B	33	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	540	GLY	2.3
2	C	73	ASP	2.3
1	B	69	ARG	2.3
2	D	7	SER	2.3
2	D	79	VAL	2.3
1	B	538	THR	2.3
1	A	435	PHE	2.3
1	A	306	ILE	2.3
2	D	118	GLY	2.3
2	D	43	LYS	2.3
1	A	300	ILE	2.3
2	D	96	CYS	2.3
1	B	309	ASP	2.3
1	B	7	GLU	2.2
1	A	297	PHE	2.2
1	A	344	ASN	2.2
1	A	438	ALA	2.2
1	B	218	THR	2.2
1	B	326	ILE	2.2
1	B	327	ASN	2.2
1	A	346	LYS	2.2
1	B	310	ARG	2.2
1	A	310	ARG	2.2
1	B	89	ASN	2.2
2	D	124	THR	2.2
1	A	493	LYS	2.2
1	A	421	ASN	2.2
1	A	299	THR	2.2
1	B	8	GLU	2.1
1	B	157	GLU	2.1
1	B	359	PHE	2.1
2	D	93	VAL	2.1
2	D	40	ALA	2.1
2	D	53	SER	2.1
1	B	439	THR	2.1
1	A	349	ILE	2.1
1	B	219	VAL	2.1
2	D	19	ARG	2.1
1	A	337	LEU	2.1
1	B	160	ILE	2.1
2	D	117	TRP	2.1
2	D	123	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	438	ALA	2.1
1	B	207	SER	2.1
1	A	296	LEU	2.1
1	A	351	SER	2.1
1	B	444	MET	2.1
1	B	29	ASN	2.1
1	B	196	PRO	2.1
1	B	120	ILE	2.1
1	A	311	TRP	2.1
1	B	118	ALA	2.1
1	B	437	SER	2.1
1	B	504	GLU	2.0
1	A	331	SER	2.1
2	D	101	ALA	2.1
1	A	333	ASN	2.0
1	A	338	ASP	2.0
2	D	116	ASP	2.0
1	B	242	ASN	2.0
2	D	18	LEU	2.0
1	B	431	HIS	2.0
1	A	330	THR	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 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.

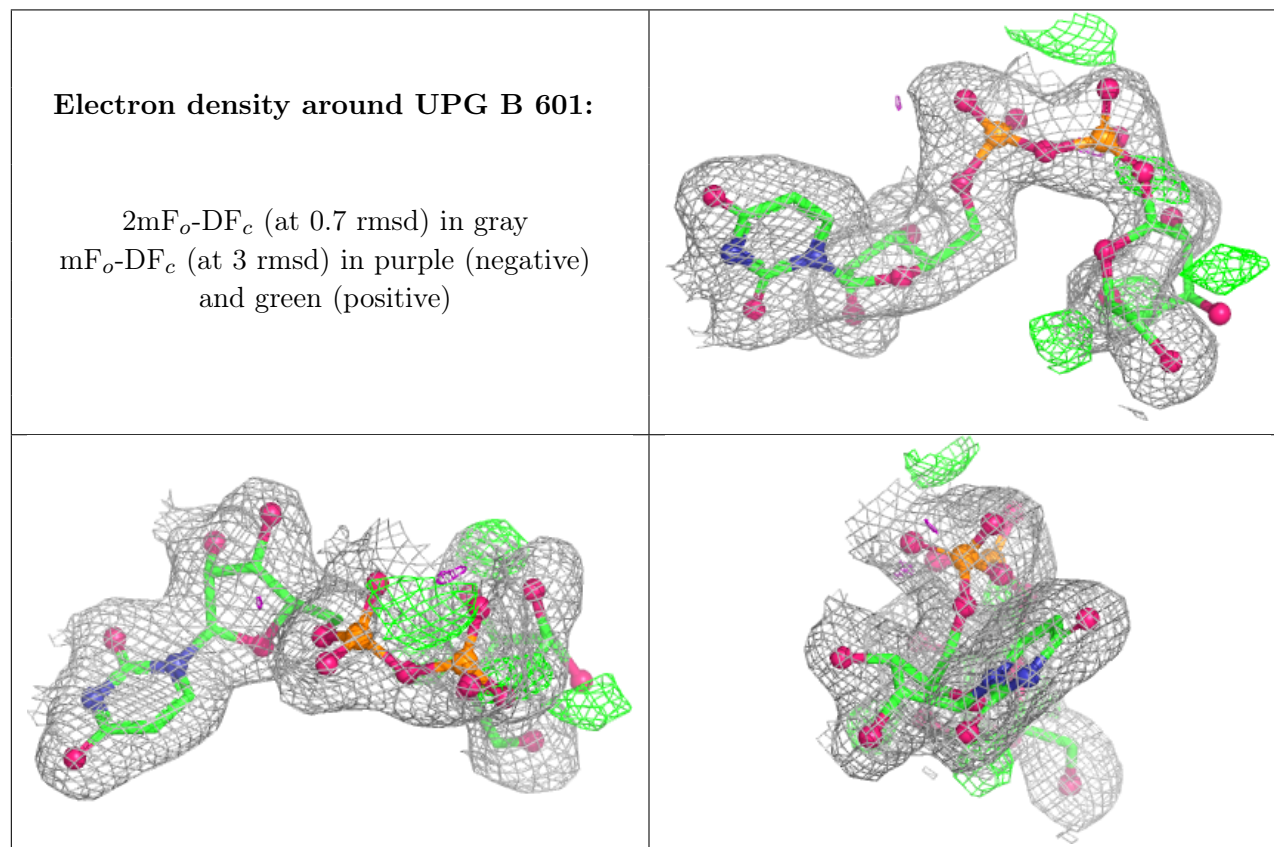
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	B	607	4/4	0.64	0.24	45,50,51,53	0
6	EDO	A	605	4/4	0.65	0.20	46,48,49,55	0

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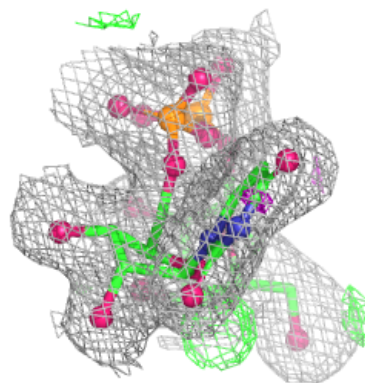
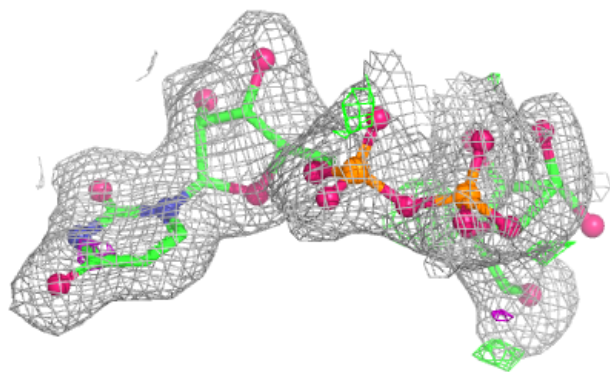
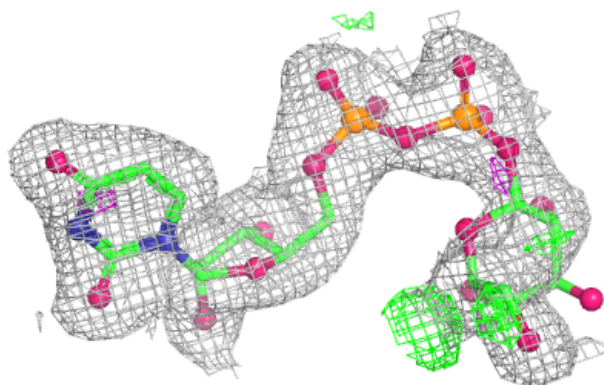
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	609	4/4	0.65	0.19	45,51,52,57	0
6	EDO	A	607	4/4	0.69	0.18	38,44,45,57	0
6	EDO	A	603	4/4	0.73	0.23	46,47,51,57	0
6	EDO	A	608	4/4	0.74	0.18	51,55,58,61	0
6	EDO	B	606	4/4	0.76	0.18	31,36,40,40	0
6	EDO	B	605	4/4	0.83	0.14	39,41,45,46	0
5	PEG	B	604	7/7	0.85	0.12	41,45,47,49	0
6	EDO	A	604	4/4	0.85	0.17	41,49,49,49	0
6	EDO	B	608	4/4	0.87	0.16	41,45,50,51	0
6	EDO	A	606	4/4	0.89	0.14	37,43,43,48	0
5	PEG	B	603	7/7	0.91	0.10	35,39,44,48	0
3	UPG	B	601	36/36	0.93	0.10	23,30,38,40	6
3	UPG	A	601	36/36	0.95	0.09	22,30,39,40	8
4	MN	B	602	1/1	0.98	0.04	37,37,37,37	0
4	MN	A	602	1/1	1.00	0.04	28,28,28,28	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 UPG A 601:

$2mF_o - DF_c$ (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.