



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:00 am BST

PDB ID : 4PQU
Title : Crystal structure of HIV-1 Reverse Transcriptase in complex with RNA/DNA and dATP
Authors : Das, K.; Bandwar, R.P.; Arnold, E.
Deposited on : 2014-03-04
Resolution : 2.51 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

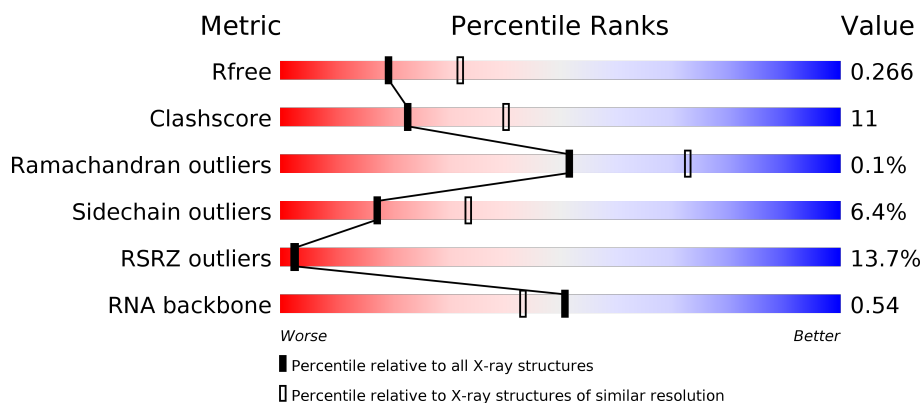
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 on 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	556	<div> <div>9%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
1	C	556	<div> <div>28%</div> <div>66%</div> <div>29%</div> <div>• •</div> </div>
2	B	428	<div> <div>4%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
2	D	428	<div> <div>11%</div> <div>71%</div> <div>22%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	27	<div><div></div><div>11%</div><div>63%</div><div>11%</div><div>•</div><div>22%</div></div>
3	T	27	<div><div></div><div>11%</div><div>48%</div><div>26%</div><div>•</div><div>22%</div></div>
4	F	21	<div><div></div><div>14%</div><div>38%</div><div>48%</div><div></div><div>14%</div></div>
4	P	21	<div><div></div><div>5%</div><div>33%</div><div>52%</div><div></div><div>14%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17849 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 HIV-1 Reverse Transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4432	2872	736	816	8			
1	C	545	Total	C	N	O	S	0	0	0
			4432	2872	736	816	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
A	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
A	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366
C	-1	MET	-	EXPRESSION TAG	UNP P03366
C	0	VAL	-	EXPRESSION TAG	UNP P03366
C	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
C	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
C	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366

- Molecule 2 is a protein called HIV-1 Reverse Transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	413	Total	C	N	O	S	0	0	0
			3406	2215	564	621	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
D	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 3 | T | 21 | Total
452 | C
202 | N
88 | O
142 | P
20 | 0 | 0 | 0 |
| 3 | E | 21 | Total
452 | C
202 | N
88 | O
142 | P
20 | 0 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 4 | P | 18 | Total
363 | C
173 | N
64 | O
109 | P
17 | 0 | 0 | 0 |
| 4 | F | 18 | Total
363 | C
173 | N
64 | O
109 | P
17 | 0 | 0 | 0 |

- # DTP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
5	C	1	Total 30	C 10	N 5	O 12	P 3	0	0

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- WORLD WIDE
PDB
PROTEIN DATA BANK

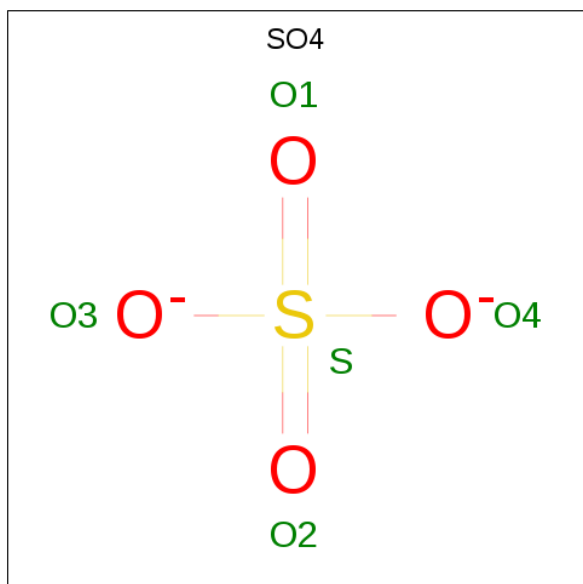
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	C	2	Total	Mg	0	0
			2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



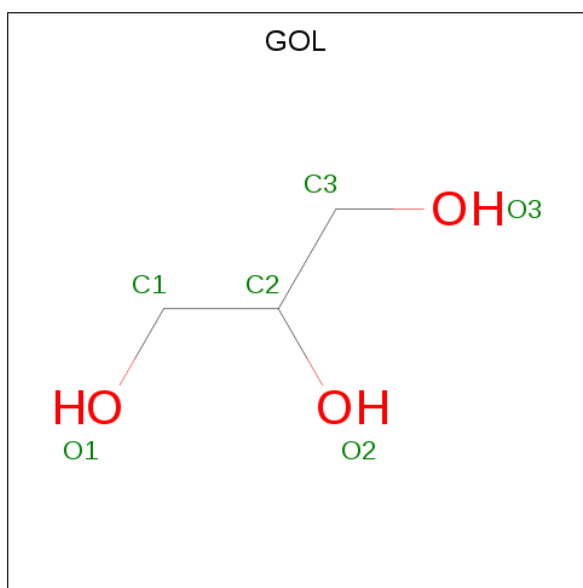
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	131	Total O 131 131	0	0

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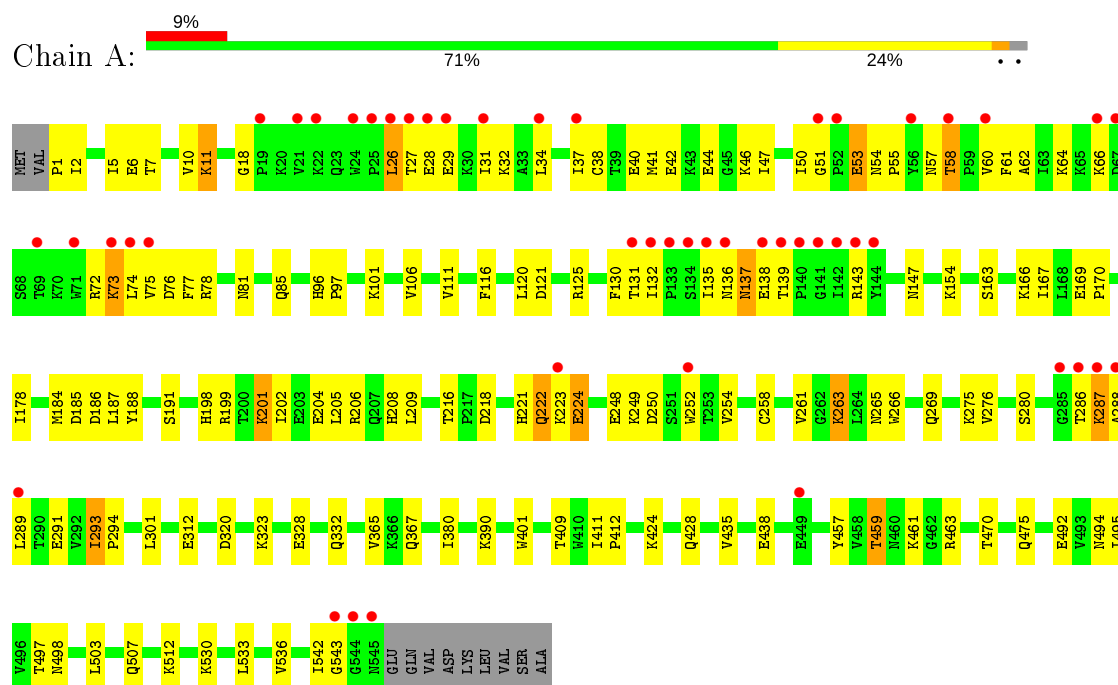
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	139	Total 139	O 139	0	0
10	C	80	Total 80	O 80	0	0
10	D	76	Total 76	O 76	0	0
10	T	3	Total 3	O 3	0	0
10	P	4	Total 4	O 4	0	0
10	E	1	Total 1	O 1	0	0
10	F	1	Total 1	O 1	0	0

3 Residue-property plots

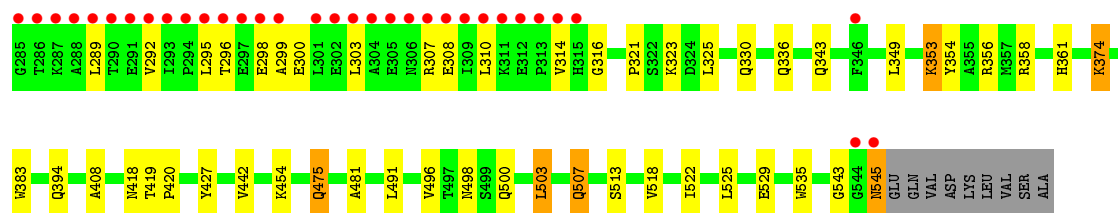
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: HIV-1 Reverse Transcriptase, p66 subunit

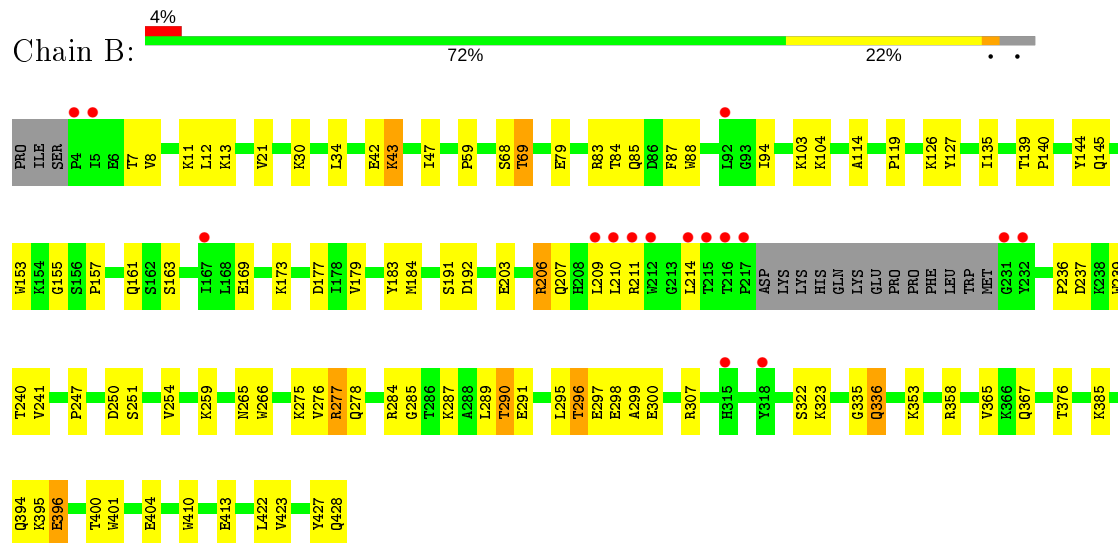


- Molecule 1: HIV-1 Reverse Transcriptase, p66 subunit

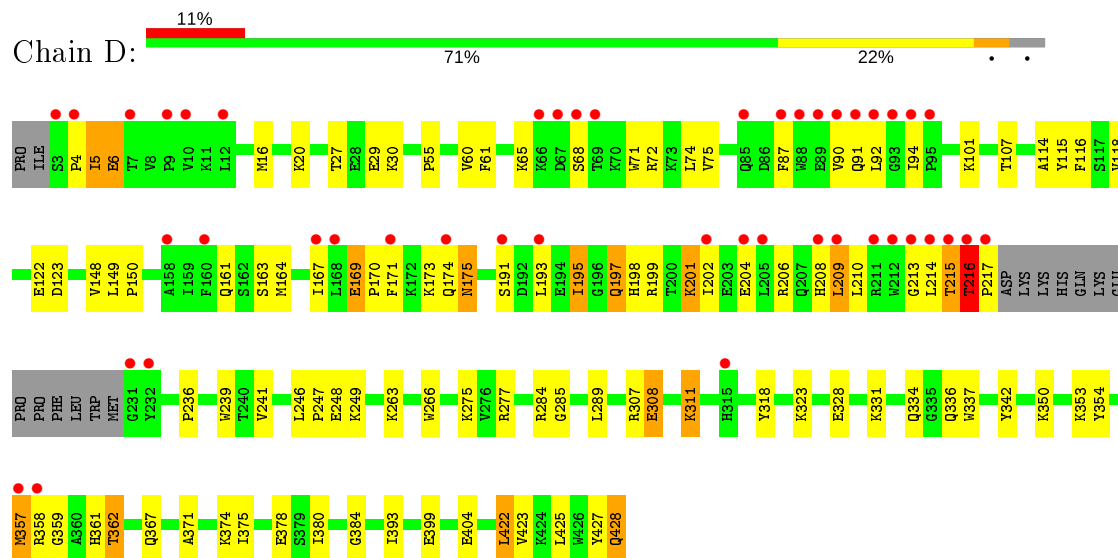




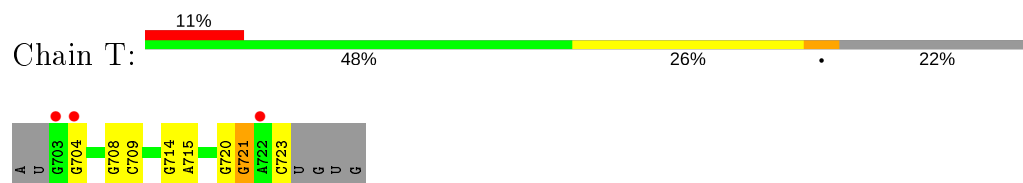
• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit



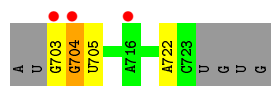
• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit



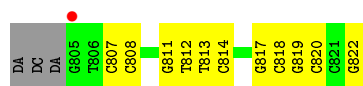
• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*A
P*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'



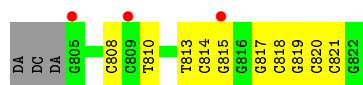
- Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'



- Molecule 4: 5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3'



- Molecule 4: 5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.44Å 128.29Å 130.68Å 90.00° 101.76° 90.00°	Depositor
Resolution (Å)	40.47 – 2.51 50.11 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (40.47-2.51) 98.1 (50.11-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202 , 0.266 0.205 , 0.266	Depositor DCC
R_{free} test set	2923 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.6	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	0.93	EDS
Total number of atoms	17849	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: GOL, MG, DTP, EDO, SO4

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	0.56	1/4550 (0.0%)	0.64	1/6183 (0.0%)
1	C	0.48	1/4550 (0.0%)	0.61	2/6183 (0.0%)
2	B	0.56	0/3497	0.64	0/4751
2	D	0.53	0/3503	0.65	3/4760 (0.1%)
3	E	0.50	0/506	0.98	0/789
3	T	0.63	0/506	1.03	0/789
4	F	0.88	0/405	1.00	0/623
4	P	1.00	0/405	1.05	0/623
All	All	0.56	2/17922 (0.0%)	0.69	6/24701 (0.0%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	GLU	CB-CG	5.29	1.62	1.52
1	C	176	PRO	N-CD	5.15	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	GLU	C-N-CD	5.80	140.58	128.40
1	A	169	GLU	C-N-CD	5.78	140.53	128.40
1	C	175	ASN	C-N-CD	5.68	140.32	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
2	D	213	GLY	N-CA-C	5.55	126.97	113.10
2	D	215	THR	N-CA-C	5.41	125.60	111.00
2	D	216	THR	C-N-CD	-5.27	109.01	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ASP	Peptide

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	4432	0	4488	97	0
1	C	4432	0	4488	133	0
2	B	3400	0	3433	69	0
2	D	3406	0	3437	81	0
3	E	452	0	232	2	0
3	T	452	0	232	4	0
4	F	363	0	202	14	0
4	P	363	0	202	12	0
5	A	30	0	12	1	0
5	C	30	0	12	2	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
7	A	4	0	6	1	0
8	A	15	0	0	2	0
8	B	10	0	0	1	0
8	C	5	0	0	0	0
8	D	10	0	0	1	0
9	B	6	0	8	2	0
10	A	131	0	0	5	0
10	B	139	0	0	7	0
10	C	80	0	0	0	0
10	D	76	0	0	3	0
10	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	1	0	0	0	0
10	P	4	0	0	1	0
10	T	3	0	0	0	0
All	All	17849	0	16752	389	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 11.

All (389) 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:C:32:LYS:HD3	1:C:33:ALA:N	1.75	1.01
1:C:168:LEU:HB3	1:C:172:LYS:HE2	1.45	0.96
1:A:459:THR:HG22	1:A:461:LYS:H	1.33	0.94
1:C:175:ASN:HB3	1:C:178:ILE:HD13	1.49	0.92
2:D:191:SER:HG	2:D:198:HIS:HD1	1.22	0.87
1:A:47:ILE:HD11	1:A:130:PHE:HZ	1.44	0.82
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.61	0.82
1:C:32:LYS:HD3	1:C:32:LYS:C	2.00	0.81
2:B:139:THR:HG22	2:B:140:PRO:O	1.81	0.80
2:D:5:ILE:CG1	2:D:5:ILE:O	2.30	0.80
1:C:3:SER:HB3	1:C:5:ILE:HG23	1.64	0.79
1:A:258:CYS:SG	10:P:903:HOH:O	2.39	0.79
1:C:491:LEU:HB3	1:C:529:GLU:HG3	1.66	0.78
1:C:125:ARG:HH11	1:C:147:ASN:HD22	1.29	0.77
1:C:498:ASN:HD21	1:C:545:ASN:HB3	1.50	0.76
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.69	0.74
1:C:31:ILE:HG23	1:C:34:LEU:HD23	1.70	0.74
1:C:475:GLN:HG3	4:F:808:DC:H5'	1.69	0.73
2:D:263:LYS:NZ	2:D:428:GLN:OE1	2.21	0.73
2:B:276:VAL:H	2:B:277:ARG:HH11	1.35	0.72
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.20	0.72
2:B:335:GLY:HA2	2:B:367:GLN:HE22	1.54	0.71
2:D:175:ASN:N	2:D:175:ASN:HD22	1.88	0.71
1:A:47:ILE:HD11	1:A:130:PHE:CZ	2.26	0.70
1:C:195:ILE:HG12	1:C:199:ARG:HH21	1.54	0.70
4:P:807:DC:H2''	4:P:808:DC:H5'	1.72	0.70
1:C:31:ILE:HA	1:C:34:LEU:HB3	1.73	0.70
2:B:307:ARG:NH1	10:B:638:HOH:O	2.21	0.70
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.74	0.69
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:ILE:HG13	2:D:5:ILE:O	1.92	0.69
4:F:814:DC:H2'	4:F:815:DG:C8	2.27	0.69
2:B:394:GLN:HE21	2:B:396:GLU:H	1.40	0.69
2:D:114:ALA:HB2	2:D:214:LEU:HD21	1.74	0.68
1:C:3:SER:HB2	1:C:119:PRO:HD3	1.75	0.68
1:C:503:LEU:CD2	1:C:535:TRP:HB2	2.22	0.68
2:B:247:PRO:O	2:B:307:ARG:NH2	2.26	0.67
1:C:107:THR:HG1	1:C:198:HIS:HE2	1.41	0.67
1:A:222:GLN:O	1:A:224:GLU:N	2.26	0.67
1:C:289:LEU:HD21	4:F:817:DG:H4'	1.77	0.67
1:A:41:MET:HB3	1:A:46:LYS:HB2	1.77	0.67
2:B:13:LYS:HD3	2:B:85:GLN:HB3	1.76	0.66
1:A:34:LEU:HD22	1:A:73:LYS:HG2	1.78	0.66
2:D:175:ASN:N	2:D:175:ASN:ND2	2.43	0.66
3:T:708:G:H2'	3:T:709:C:C6	2.30	0.66
1:C:279:LEU:HD23	1:C:299:ALA:HB1	1.78	0.66
1:C:503:LEU:HD23	1:C:535:TRP:HB2	1.76	0.65
1:C:353:LYS:HD3	1:C:353:LYS:H	1.61	0.65
1:A:27:THR:HG22	1:A:29:GLU:H	1.62	0.64
2:B:30:LYS:NZ	2:B:404:GLU:OE1	2.30	0.64
1:A:254:VAL:HG11	1:A:286:THR:HG21	1.78	0.64
2:B:276:VAL:H	2:B:277:ARG:NH1	1.95	0.63
1:A:131:THR:HG22	1:A:143:ARG:HB3	1.80	0.63
1:C:5:ILE:HG22	1:C:212:TRP:HE3	1.62	0.63
2:D:4:PRO:CD	2:D:5:ILE:H	2.10	0.63
1:C:32:LYS:CD	1:C:33:ALA:N	2.57	0.63
1:A:459:THR:CG2	1:A:461:LYS:H	2.09	0.63
2:B:336:GLN:HG2	2:B:427:TYR:CE1	2.34	0.62
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.64	0.62
1:C:233:GLU:OE2	1:C:235:HIS:NE2	2.29	0.62
1:A:503:LEU:HD23	2:B:422:LEU:HD22	1.81	0.61
1:C:32:LYS:HD3	1:C:33:ALA:CA	2.29	0.61
1:C:5:ILE:HG22	1:C:212:TRP:CE3	2.35	0.61
4:F:814:DC:H2'	4:F:815:DG:H8	1.66	0.61
1:A:459:THR:HG22	1:A:461:LYS:N	2.12	0.61
4:F:813:DT:H2'	4:F:814:DC:C6	2.36	0.60
1:A:41:MET:HG2	1:A:46:LYS:HD2	1.84	0.60
1:A:72:ARG:NH2	5:A:601:DTP:O3A	2.35	0.60
2:D:361:HIS:O	2:D:367:GLN:NE2	2.32	0.60
2:B:296:THR:HG22	2:B:299:ALA:H	1.67	0.60
1:C:253:THR:HA	1:C:292:VAL:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:819:DG:H2'	4:F:820:DC:C6	2.38	0.59
2:D:277:ARG:NE	8:D:501:SO4:O1	2.31	0.59
2:B:84:THR:HG22	2:B:87:PHE:HB3	1.84	0.59
2:D:4:PRO:HG2	2:D:5:ILE:HG23	1.83	0.59
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.68	0.59
2:D:353:LYS:NZ	10:D:622:HOH:O	2.21	0.59
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.68	0.58
1:C:217:PRO:O	1:C:219:LYS:N	2.32	0.58
2:D:167:ILE:O	2:D:208:HIS:NE2	2.35	0.58
2:D:263:LYS:HE3	2:D:425:LEU:HA	1.85	0.58
2:B:336:GLN:OE1	2:B:353:LYS:NZ	2.27	0.58
1:C:206:ARG:NH2	1:C:216:THR:O	2.30	0.58
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.38	0.58
2:D:174:GLN:HB3	2:D:175:ASN:ND2	2.19	0.58
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.85	0.57
1:A:323:LYS:NZ	10:A:819:HOH:O	2.37	0.57
1:A:163:SER:HA	1:A:166:LYS:HE3	1.86	0.57
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.85	0.57
1:C:252:TRP:HZ3	1:C:295:LEU:HB2	1.69	0.57
1:C:78:ARG:HD2	3:E:705:U:H5"	1.87	0.57
4:F:817:DG:H2'	4:F:818:DC:C6	2.40	0.57
2:D:4:PRO:HD2	2:D:5:ILE:H	1.69	0.57
1:C:10:VAL:HG11	1:C:153:TRP:HZ2	1.70	0.57
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.39	0.56
1:A:380:ILE:HD13	9:B:502:GOL:H11	1.85	0.56
1:A:293:ILE:HD12	1:A:294:PRO:HD2	1.87	0.56
1:A:6:GLU:H	1:A:6:GLU:CD	2.09	0.56
1:A:428:GLN:N	8:A:607:SO4:O1	2.34	0.56
1:C:171:PHE:CE2	1:C:205:LEU:HB2	2.40	0.56
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.35	0.56
1:A:249:LYS:HB2	1:A:252:TRP:CE2	2.41	0.56
1:A:289:LEU:HD21	4:P:817:DG:H4'	1.87	0.56
2:D:30:LYS:NZ	2:D:404:GLU:OE2	2.35	0.56
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.88	0.56
2:B:296:THR:CG2	2:B:299:ALA:H	2.19	0.56
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.40	0.56
1:C:17:ASP:OD2	1:C:56:TYR:OH	2.24	0.56
1:C:34:LEU:HD21	1:C:132:ILE:HB	1.88	0.56
2:B:358:ARG:HD2	10:B:667:HOH:O	2.06	0.55
1:C:300:GLU:OE2	1:C:307:ARG:NH2	2.39	0.55
2:B:68:SER:O	2:B:69:THR:HB	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:TYR:CE1	1:C:314:VAL:HB	2.42	0.55
2:D:92:LEU:O	2:D:161:GLN:NE2	2.39	0.55
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.06	0.55
1:A:26:LEU:HD12	1:A:31:ILE:HG13	1.89	0.55
1:A:106:VAL:HG21	8:A:605:SO4:O1	2.06	0.55
2:B:322:SER:HB3	1:C:418:ASN:HD21	1.71	0.54
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.90	0.54
1:C:139:THR:HG22	1:C:141:GLY:H	1.71	0.54
1:A:34:LEU:HA	1:A:37:ILE:HD12	1.90	0.54
2:B:84:THR:HG21	2:B:153:TRP:CZ2	2.42	0.54
2:D:247:PRO:HG2	2:D:428:GLN:HG2	1.89	0.54
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.08	0.54
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.90	0.54
1:A:135:ILE:HB	1:A:138:GLU:HB2	1.90	0.53
1:C:170:PRO:HG2	1:C:208:HIS:CE1	2.44	0.53
1:C:72:ARG:NH2	5:C:601:DTP:O2A	2.41	0.53
2:D:263:LYS:HA	2:D:423:VAL:HG11	1.90	0.53
2:B:42:GLU:OE1	2:B:43:LYS:NZ	2.41	0.53
1:A:201:LYS:HE3	1:A:204:GLU:OE2	2.09	0.53
1:C:543:GLY:HA2	2:D:285:GLY:O	2.09	0.53
1:C:289:LEU:CD2	4:F:817:DG:H4'	2.37	0.53
1:C:125:ARG:NH1	1:C:147:ASN:HD22	2.02	0.53
2:B:135:ILE:HD12	10:B:732:HOH:O	2.09	0.53
2:B:284:ARG:NH2	10:B:693:HOH:O	2.41	0.53
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.73	0.53
2:D:206:ARG:NH2	2:D:217:PRO:HB3	2.23	0.52
1:A:263:LYS:NZ	4:P:820:DC:OP1	2.43	0.52
2:D:107:THR:HG21	2:D:202:ILE:HD13	1.91	0.52
2:B:206:ARG:NH1	10:B:694:HOH:O	2.42	0.52
2:D:169:GLU:OE2	2:D:169:GLU:HA	2.02	0.52
1:C:107:THR:OG1	1:C:198:HIS:NE2	2.29	0.52
1:C:221:HIS:CD2	1:C:228:LEU:H	2.27	0.52
1:C:16:MET:HB3	1:C:83:ARG:HD3	1.92	0.52
1:C:217:PRO:C	1:C:219:LYS:H	2.13	0.52
3:T:714:G:H2'	3:T:715:A:C8	2.45	0.52
2:B:11:LYS:NZ	10:B:652:HOH:O	2.42	0.52
4:P:819:DG:H2'	4:P:820:DC:C6	2.45	0.51
1:A:287:LYS:HD2	1:A:288:ALA:H	1.76	0.51
2:B:157:PRO:HG3	2:B:184:MET:HA	1.92	0.51
1:C:229:TRP:CE2	1:C:230:MET:HG2	2.45	0.51
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:LEU:HD12	2:D:214:LEU:HD12	1.93	0.51
1:A:266:TRP:CE2	4:P:820:DC:H4'	2.46	0.51
4:P:812:DT:O2	4:P:812:DT:H2'	2.11	0.51
2:D:167:ILE:HD11	2:D:209:LEU:HA	1.93	0.51
1:A:106:VAL:H	1:A:223:LYS:HG2	1.76	0.50
1:C:296:THR:HG22	1:C:298:GLU:H	1.75	0.50
1:C:503:LEU:O	1:C:507:GLN:HB2	2.11	0.50
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.93	0.50
1:C:58:THR:HG21	1:C:77:PHE:CE1	2.46	0.50
2:D:193:LEU:HD23	2:D:198:HIS:HA	1.94	0.50
1:C:26:LEU:HD11	1:C:60:VAL:HG23	1.94	0.50
2:B:423:VAL:N	8:B:503:SO4:O3	2.34	0.49
1:C:120:LEU:HD11	1:C:124:PHE:HD2	1.77	0.49
1:C:72:ARG:HD3	1:C:74:LEU:HD21	1.93	0.49
1:A:42:GLU:HA	1:A:47:ILE:HG22	1.93	0.49
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.93	0.49
2:D:191:SER:OG	2:D:198:HIS:ND1	2.31	0.49
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.94	0.49
1:C:171:PHE:CD1	1:C:171:PHE:C	2.85	0.49
1:C:230:MET:HE3	4:F:821:DC:H4'	1.94	0.49
1:C:500:GLN:HG2	1:C:535:TRP:NE1	2.26	0.49
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.48	0.49
1:A:206:ARG:NH2	1:A:216:THR:O	2.46	0.49
1:C:29:GLU:HG3	1:C:30:LYS:HD2	1.95	0.49
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.93	0.49
1:C:84:THR:HB	1:C:154:LYS:HE2	1.94	0.48
2:D:215:THR:O	2:D:217:PRO:HD3	2.12	0.48
1:A:85:GLN:O	1:A:154:LYS:NZ	2.45	0.48
2:B:94:ILE:HG12	2:B:161:GLN:CD	2.34	0.48
1:C:10:VAL:HG21	1:C:153:TRP:HH2	1.76	0.48
1:C:113:ASP:HB3	1:C:116:PHE:HB2	1.95	0.48
1:C:408:ALA:O	2:D:393:ILE:HG13	2.13	0.48
2:D:114:ALA:CB	2:D:214:LEU:HD21	2.40	0.48
1:C:266:TRP:CE2	4:F:820:DC:H4'	2.49	0.48
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.96	0.48
1:C:168:LEU:HB3	1:C:172:LYS:CE	2.30	0.48
1:C:361:HIS:CE1	1:C:513:SER:HG	2.24	0.48
4:P:818:DC:H2''	4:P:819:DG:H5'	1.96	0.48
1:C:101:LYS:HD3	1:C:321:PRO:HG3	1.96	0.48
1:C:5:ILE:HG21	1:C:167:ILE:HD11	1.95	0.48
2:D:171:PHE:HE1	2:D:204:GLU:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:810:DT:H5"	4:F:810:DT:H6	1.78	0.48
2:D:116:PHE:O	2:D:148:VAL:HG11	2.14	0.48
1:A:275:LYS:HG3	10:A:775:HOH:O	2.13	0.48
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.96	0.48
2:D:4:PRO:CD	2:D:5:ILE:N	2.77	0.48
1:A:457:TYR:CE1	1:A:463:ARG:HG2	2.48	0.48
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.95	0.48
1:C:196:GLY:O	1:C:199:ARG:HG2	2.13	0.48
2:D:239:TRP:CZ3	2:D:378:GLU:HG3	2.49	0.47
2:D:247:PRO:CG	2:D:428:GLN:HG2	2.43	0.47
2:D:164:MET:HA	2:D:167:ILE:HG22	1.95	0.47
1:A:249:LYS:HB2	1:A:252:TRP:CD2	2.49	0.47
1:C:64:LYS:HE3	1:C:69:THR:HA	1.97	0.47
2:B:277:ARG:H	2:B:277:ARG:HD2	1.80	0.47
1:C:116:PHE:O	1:C:148:VAL:HG11	2.14	0.47
1:A:266:TRP:O	1:A:269:GLN:HG2	2.14	0.47
4:P:819:DG:H2'	4:P:820:DC:H6	1.80	0.47
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.96	0.47
1:C:84:THR:HG21	1:C:153:TRP:HE1	1.79	0.47
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.30	0.47
1:C:134:SER:OG	1:C:139:THR:HB	2.15	0.47
1:C:277:ARG:HB2	1:C:336:GLN:OE1	2.15	0.46
1:C:323:LYS:HB2	1:C:343:GLN:NE2	2.30	0.46
2:D:275:LYS:HD2	10:D:637:HOH:O	2.14	0.46
2:D:308:GLU:HA	2:D:311:LYS:HD3	1.96	0.46
2:B:203:GLU:OE2	2:B:207:GLN:NE2	2.48	0.46
2:B:84:THR:O	2:B:87:PHE:HB3	2.15	0.46
1:C:518:VAL:O	1:C:522:ILE:HG13	2.15	0.46
1:A:202:ILE:O	1:A:206:ARG:HG3	2.16	0.46
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.97	0.46
2:D:239:TRP:CH2	2:D:378:GLU:HA	2.50	0.46
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.97	0.46
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.98	0.46
1:A:7:THR:HG21	10:A:711:HOH:O	2.15	0.46
10:A:821:HOH:O	2:B:259:LYS:HG3	2.15	0.46
1:C:115:TYR:HB3	1:C:149:LEU:O	2.15	0.46
1:A:58:THR:HG21	1:A:77:PHE:CE1	2.51	0.46
2:D:29:GLU:HG3	2:D:71:TRP:CZ2	2.51	0.46
1:A:184:MET:HG2	4:P:822:DG:H2"	1.98	0.46
2:B:206:ARG:HE	2:B:206:ARG:HB3	1.40	0.46
1:C:209:LEU:HD22	1:C:214:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:TYR:HE1	1:C:314:VAL:HB	1.80	0.46
1:C:65:LYS:NZ	5:C:601:DTP:O3G	2.45	0.46
2:D:5:ILE:HG12	2:D:5:ILE:O	2.13	0.46
2:D:311:LYS:HB2	2:D:311:LYS:HE2	1.37	0.46
1:A:66:LYS:HD2	1:A:66:LYS:HA	1.77	0.45
2:B:8:VAL:HG23	10:B:682:HOH:O	2.16	0.45
1:C:10:VAL:HG11	1:C:153:TRP:CZ2	2.51	0.45
1:C:330:GLN:HG2	1:C:419:THR:HG21	1.98	0.45
1:C:60:VAL:HG12	1:C:75:VAL:HG22	1.98	0.45
1:C:38:CYS:HB3	1:C:144:TYR:HE2	1.81	0.45
3:E:703:G:C5	3:E:704:G:C8	3.05	0.45
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.98	0.45
2:D:336:GLN:NE2	2:D:353:LYS:HD2	2.31	0.45
1:C:12:LEU:HD13	1:C:124:PHE:HE1	1.82	0.45
1:C:229:TRP:CE3	1:C:234:LEU:HD21	2.51	0.45
1:C:23:GLN:NE2	1:C:26:LEU:HG	2.31	0.45
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.98	0.45
2:D:116:PHE:C	2:D:148:VAL:HG11	2.36	0.45
2:D:20:LYS:HD3	2:D:55:PRO:O	2.17	0.45
1:C:496:VAL:HG21	2:D:289:LEU:HD21	1.98	0.45
1:A:167:ILE:O	1:A:170:PRO:HD2	2.17	0.45
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.99	0.45
1:C:3:SER:OG	1:C:117:SER:O	2.30	0.45
1:C:239:TRP:CE2	1:C:316:GLY:HA3	2.52	0.45
1:C:264:LEU:O	1:C:268:SER:N	2.48	0.45
1:C:12:LEU:HD12	1:C:84:THR:HA	1.98	0.45
1:A:58:THR:HG21	1:A:77:PHE:HE1	1.81	0.45
1:C:225:PRO:HB3	1:C:236:PRO:HD3	1.97	0.45
2:B:323:LYS:O	2:B:385:LYS:NZ	2.50	0.45
1:C:223:LYS:HE2	1:C:223:LYS:HB2	1.80	0.45
2:D:65:LYS:HA	2:D:65:LYS:HD3	1.74	0.45
1:A:276:VAL:HG12	1:A:276:VAL:O	2.17	0.44
1:A:81:ASN:O	1:A:154:LYS:HE3	2.17	0.44
2:B:254:VAL:HG21	2:B:287:LYS:HB2	2.00	0.44
1:A:409:THR:OG1	7:A:604:EDO:H21	2.17	0.44
3:T:708:G:H2'	3:T:709:C:H6	1.76	0.44
1:A:61:PHE:CE1	1:A:74:LEU:HB2	2.52	0.44
2:B:287:LYS:HD3	2:B:291:GLU:OE2	2.17	0.44
2:D:115:TYR:HB3	2:D:149:LEU:HB3	1.99	0.44
2:D:87:PHE:HA	2:D:90:VAL:HG12	1.99	0.44
1:C:475:GLN:CG	4:F:808:DC:H5'	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLN:HB3	1:A:222:GLN:HE21	1.53	0.44
2:D:199:ARG:O	2:D:202:ILE:HG13	2.18	0.44
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.98	0.44
1:C:76:ASP:OD1	1:C:78:ARG:HD3	2.17	0.44
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.99	0.44
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.77	0.44
1:C:78:ARG:O	1:C:82:LYS:HG3	2.17	0.44
1:A:38:CYS:O	1:A:42:GLU:HB2	2.18	0.44
1:A:367:GLN:OE1	1:A:512:LYS:HE3	2.18	0.44
2:B:296:THR:HG22	2:B:299:ALA:CB	2.48	0.44
1:C:356:ARG:NE	1:C:358:ARG:HE	2.16	0.44
2:D:101:LYS:O	2:D:236:PRO:HB2	2.17	0.44
2:D:163:SER:O	2:D:167:ILE:HG22	2.18	0.44
1:C:58:THR:HG21	1:C:77:PHE:HE1	1.82	0.43
1:A:28:GLU:O	1:A:32:LYS:HG3	2.18	0.43
2:D:353:LYS:HE2	2:D:427:TYR:HE1	1.83	0.43
2:D:201:LYS:NZ	2:D:204:GLU:OE1	2.51	0.43
4:F:813:DT:H2'	4:F:814:DC:H6	1.82	0.43
1:A:136:ASN:ND2	1:A:137:ASN:OD1	2.51	0.43
2:B:12:LEU:HD11	2:B:127:TYR:CE1	2.53	0.43
2:B:400:THR:O	9:B:502:GOL:H12	2.18	0.43
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.54	0.43
2:D:199:ARG:HA	2:D:202:ILE:HG12	2.00	0.43
1:A:507:GLN:NE2	10:A:822:HOH:O	2.42	0.43
1:C:325:LEU:HD21	1:C:383:TRP:CD2	2.53	0.43
2:B:422:LEU:HA	2:B:422:LEU:HD23	1.66	0.43
1:C:354:TYR:HE1	1:C:374:LYS:HZ1	1.66	0.43
1:C:41:MET:HA	1:C:44:GLU:HG3	2.01	0.43
1:C:475:GLN:HG3	4:F:808:DC:C5'	2.46	0.43
1:C:503:LEU:HD21	1:C:535:TRP:HB2	1.97	0.43
1:A:34:LEU:HD22	1:A:73:LYS:CG	2.47	0.43
2:D:350:LYS:NZ	2:D:378:GLU:OE2	2.47	0.43
1:C:209:LEU:HB3	1:C:214:LEU:HB2	1.99	0.43
2:B:169:GLU:O	2:B:173:LYS:HG2	2.19	0.42
2:B:395:LYS:HE3	4:P:811:DG:O3'	2.19	0.42
1:C:47:ILE:HD11	1:C:130:PHE:HZ	1.84	0.42
1:A:186:ASP:O	1:A:187:LEU:HD23	2.19	0.42
1:A:5:ILE:HD13	1:A:163:SER:HB3	2.02	0.42
2:D:266:TRP:CD1	2:D:425:LEU:HD22	2.54	0.42
1:A:120:LEU:HD12	1:A:121:ASP:H	1.83	0.42
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:TYR:HA	10:D:666:HOH:O	2.19	0.42
2:D:357:MET:C	2:D:359:GLY:H	2.23	0.42
2:D:65:LYS:HB2	2:D:68:SER:OG	2.19	0.42
2:D:29:GLU:HG3	2:D:71:TRP:CH2	2.55	0.42
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.19	0.42
1:A:475:GLN:CD	4:P:808:DC:H5"	2.39	0.42
2:D:6:GLU:HG2	2:D:6:GLU:H	1.46	0.42
1:A:497:THR:HG21	1:A:503:LEU:HD13	2.02	0.42
2:B:69:THR:CG2	2:B:69:THR:O	2.67	0.42
1:C:215:THR:C	1:C:217:PRO:HD3	2.40	0.42
1:C:24:TRP:HB3	1:C:25:PRO:HD2	2.02	0.42
2:B:297:GLU:H	2:B:297:GLU:CD	2.23	0.42
1:C:117:SER:HB3	1:C:213:GLY:O	2.19	0.42
2:D:195:ILE:O	2:D:199:ARG:HG3	2.19	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.20	0.42
1:A:435:VAL:HG13	2:B:290:THR:HG21	2.01	0.42
1:A:40:GLU:O	1:A:44:GLU:HG3	2.19	0.42
1:C:2:ILE:HG12	1:C:3:SER:H	1.85	0.42
1:C:498:ASN:HD21	1:C:545:ASN:CB	2.28	0.42
2:D:118:VAL:HB	2:D:149:LEU:HD22	2.02	0.42
3:T:720:G:H2'	3:T:721:G:C8	2.55	0.42
1:A:47:ILE:HG21	1:A:47:ILE:HD13	1.82	0.41
1:A:543:GLY:HA2	2:B:285:GLY:O	2.20	0.41
1:C:191:SER:HB2	1:C:193:LEU:HB2	2.02	0.41
1:C:427:TYR:CE2	1:C:525:LEU:HD13	2.55	0.41
1:C:199:ARG:O	1:C:203:GLU:HG2	2.20	0.41
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.55	0.41
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.91	0.41
1:C:125:ARG:HA	1:C:128:THR:HG22	2.02	0.41
1:C:29:GLU:O	1:C:32:LYS:HB3	2.20	0.41
2:D:197:GLN:O	2:D:201:LYS:HG2	2.20	0.41
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.55	0.41
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.02	0.41
1:C:19:PRO:O	1:C:57:ASN:N	2.53	0.41
1:A:205:LEU:O	1:A:209:LEU:HG	2.20	0.41
1:A:1:PRO:HB2	1:A:2:ILE:H	1.58	0.41
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.55	0.41
1:C:500:GLN:OE1	2:D:422:LEU:HD11	2.21	0.41
1:A:76:ASP:OD1	1:A:78:ARG:NE	2.51	0.41
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.89	0.41
1:C:418:ASN:O	1:C:420:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LEU:HD21	1:C:383:TRP:CE3	2.55	0.41
2:D:328:GLU:HG3	2:D:342:TYR:HE1	1.85	0.41
2:D:60:VAL:HG12	2:D:75:VAL:HG22	2.02	0.41
1:C:13:LYS:HA	1:C:14:PRO:HD2	1.74	0.41
1:C:353:LYS:HD3	1:C:353:LYS:N	2.31	0.41
2:D:114:ALA:CA	2:D:214:LEU:HD21	2.50	0.41
4:P:813:DT:H2''	4:P:814:DC:O4'	2.21	0.41
1:A:328:GLU:OE1	1:A:390:LYS:HE2	2.21	0.41
1:C:249:LYS:HE2	1:C:249:LYS:HB2	1.84	0.41
1:A:287:LYS:HG3	1:A:287:LYS:H	1.69	0.41
2:D:334:GLN:HE21	2:D:334:GLN:HB3	1.60	0.41
2:D:354:TYR:HD2	2:D:374:LYS:HD2	1.86	0.41
1:A:10:VAL:C	1:A:11:LYS:HD2	2.41	0.40
2:B:103:LYS:HD2	2:B:191:SER:HA	2.02	0.40
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.56	0.40
2:D:174:GLN:HB3	2:D:175:ASN:HD22	1.86	0.40
1:C:50:ILE:HD11	1:C:143:ARG:HG2	2.03	0.40
2:D:380:ILE:O	2:D:384:GLY:N	2.52	0.40
2:B:275:LYS:HA	2:B:275:LYS:HD3	1.96	0.40
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.57	0.40
1:A:411:ILE:HG23	1:A:412:PRO:HD2	2.04	0.40
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.57	0.40
1:C:271:TYR:CD2	1:C:310:LEU:HD23	2.57	0.40
2:D:216:THR:HA	2:D:217:PRO:HD3	1.68	0.40
2:D:371:ALA:O	2:D:375:ILE:HG13	2.21	0.40
2:D:422:LEU:HG	2:D:422:LEU:H	1.69	0.40
1:A:136:ASN:N	1:A:136:ASN:OD1	2.53	0.40
1:A:51:GLY:HA3	1:A:53:GLU:OE2	2.21	0.40
1:C:134:SER:CB	1:C:139:THR:HB	2.51	0.40
1:C:28:GLU:HG2	1:C:28:GLU:H	1.51	0.40
1:C:300:GLU:HA	1:C:303:LEU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	543/556 (98%)	505 (93%)	37 (7%)	1 (0%)	47	68
1	C	543/556 (98%)	489 (90%)	54 (10%)	0	100	100
2	B	408/428 (95%)	386 (95%)	22 (5%)	0	100	100
2	D	409/428 (96%)	379 (93%)	29 (7%)	1 (0%)	47	68
All	All	1903/1968 (97%)	1759 (92%)	142 (8%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	362	THR
1	A	18	GLY

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	486/497 (98%)	455 (94%)	31 (6%)	17	33
1	C	486/497 (98%)	460 (95%)	26 (5%)	22	43
2	B	374/390 (96%)	353 (94%)	21 (6%)	21	40
2	D	375/390 (96%)	343 (92%)	32 (8%)	10	21
All	All	1721/1774 (97%)	1611 (94%)	110 (6%)	17	33

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	26	LEU
1	A	53	GLU
1	A	58	THR
1	A	64	LYS
1	A	73	LYS

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Mol	Chain	Res	Type
1	A	101	LYS
1	A	132	ILE
1	A	137	ASN
1	A	139	THR
1	A	178	ILE
1	A	188	TYR
1	A	191	SER
1	A	199	ARG
1	A	201	LYS
1	A	221	HIS
1	A	222	GLN
1	A	224	GLU
1	A	248	GLU
1	A	250	ASP
1	A	263	LYS
1	A	265	ASN
1	A	280	SER
1	A	287	LYS
1	A	293	ILE
1	A	301	LEU
1	A	332	GLN
1	A	424	LYS
1	A	459	THR
1	A	470	THR
1	A	498	ASN
2	B	43	LYS
2	B	69	THR
2	B	163	SER
2	B	177	ASP
2	B	206	ARG
2	B	210	LEU
2	B	211	ARG
2	B	237	ASP
2	B	240	THR
2	B	241	VAL
2	B	250	ASP
2	B	251	SER
2	B	265	ASN
2	B	266	TRP
2	B	277	ARG
2	B	290	THR
2	B	296	THR

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Mol	Chain	Res	Type
2	B	336	GLN
2	B	396	GLU
2	B	413	GLU
2	B	428	GLN
1	C	7	THR
1	C	17	ASP
1	C	21	VAL
1	C	27	THR
1	C	28	GLU
1	C	29	GLU
1	C	58	THR
1	C	67	ASP
1	C	123	ASP
1	C	172	LYS
1	C	186	ASP
1	C	199	ARG
1	C	221	HIS
1	C	240	THR
1	C	256	ASP
1	C	277	ARG
1	C	284	ARG
1	C	308	GLU
1	C	353	LYS
1	C	374	LYS
1	C	394	GLN
1	C	454	LYS
1	C	475	GLN
1	C	503	LEU
1	C	507	GLN
1	C	545	ASN
2	D	5	ILE
2	D	6	GLU
2	D	16	MET
2	D	27	THR
2	D	72	ARG
2	D	91	GLN
2	D	94	ILE
2	D	122	GLU
2	D	123	ASP
2	D	150	PRO
2	D	169	GLU
2	D	173	LYS

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Mol	Chain	Res	Type
2	D	175	ASN
2	D	195	ILE
2	D	197	GLN
2	D	201	LYS
2	D	209	LEU
2	D	210	LEU
2	D	216	THR
2	D	241	VAL
2	D	246	LEU
2	D	249	LYS
2	D	284	ARG
2	D	308	GLU
2	D	311	LYS
2	D	323	LYS
2	D	357	MET
2	D	358	ARG
2	D	362	THR
2	D	399	GLU
2	D	422	LEU
2	D	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	255	ASN
1	A	332	GLN
1	A	487	GLN
2	B	96	HIS
2	B	367	GLN
2	B	394	GLN
1	C	147	ASN
1	C	208	HIS
1	C	269	GLN
1	C	306	ASN
1	C	373	GLN
1	C	418	ASN
1	C	428	GLN
1	C	464	GLN
1	C	498	ASN
2	D	91	GLN
2	D	197	GLN

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Mol	Chain	Res	Type
2	D	334	GLN
2	D	336	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	20/27 (74%)	2 (10%)	0
3	T	20/27 (74%)	3 (15%)	0
All	All	40/54 (74%)	5 (12%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	704	G
3	T	721	G
3	T	723	C
3	E	704	G
3	E	722	A

There are no RNA pucker outliers to report.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
7	EDO	A	604	-	3,3,3	0.83	0	2,2,2	0.28	0
8	SO4	A	606	-	4,4,4	0.26	0	6,6,6	0.27	0
9	GOL	B	502	-	5,5,5	0.61	0	5,5,5	0.63	0
5	DTP	C	601	6	26,32,32	1.78	5 (19%)	30,50,50	1.54	4 (13%)
8	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.60	0
5	DTP	A	601	6	26,32,32	1.85	7 (26%)	30,50,50	1.53	3 (10%)
8	SO4	B	501	-	4,4,4	0.19	0	6,6,6	0.81	0
8	SO4	A	607	-	4,4,4	0.27	0	6,6,6	0.51	0
8	SO4	C	604	-	4,4,4	0.24	0	6,6,6	0.31	0
8	SO4	D	502	-	4,4,4	0.25	0	6,6,6	0.55	0
8	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.26	0
8	SO4	B	503	-	4,4,4	0.25	0	6,6,6	0.34	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
7	EDO	A	604	-	-	1/1/1/1	-
5	DTP	A	601	6	-	6/18/34/34	0/3/3/3
9	GOL	B	502	-	-	0/4/4/4	-
5	DTP	C	601	6	-	6/18/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	DTP	O4'-C4'	4.23	1.54	1.45
5	A	601	DTP	O4'-C4'	4.09	1.54	1.45
5	A	601	DTP	C5'-C4'	-3.99	1.39	1.51
5	C	601	DTP	C5'-C4'	-3.79	1.39	1.51
5	C	601	DTP	C6-N6	3.48	1.46	1.34
5	A	601	DTP	C6-N6	3.46	1.46	1.34
5	C	601	DTP	O3'-C3'	-2.77	1.37	1.43
5	A	601	DTP	O3'-C3'	-2.61	1.37	1.43
5	C	601	DTP	PA-O1A	2.36	1.59	1.50
5	A	601	DTP	C3'-C4'	-2.29	1.46	1.53
5	A	601	DTP	PA-O1A	2.21	1.58	1.50
5	A	601	DTP	C4-N3	-2.08	1.32	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	DTP	N3-C2-N1	-5.66	119.83	128.68
5	A	601	DTP	N3-C2-N1	-5.33	120.34	128.68
5	A	601	DTP	PB-O3B-PG	-3.35	121.32	132.83
5	C	601	DTP	PB-O3B-PG	-2.37	124.69	132.83
5	C	601	DTP	C4-C5-N7	-2.34	106.96	109.40
5	C	601	DTP	C2'-C1'-N9	-2.18	109.24	114.27
5	A	601	DTP	C4-C5-N7	-2.15	107.16	109.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	DTP	PB-O3B-PG-O2G
5	C	601	DTP	C5'-O5'-PA-O1A
5	A	601	DTP	PB-O3B-PG-O3G
5	C	601	DTP	O4'-C4'-C5'-O5'
7	A	604	EDO	O1-C1-C2-O2
5	A	601	DTP	O4'-C4'-C5'-O5'
5	C	601	DTP	PA-O3A-PB-O2B
5	A	601	DTP	PA-O3A-PB-O2B
5	C	601	DTP	C3'-C4'-C5'-O5'
5	C	601	DTP	PB-O3B-PG-O1G
5	A	601	DTP	PB-O3B-PG-O1G
5	A	601	DTP	PB-O3B-PG-O2G
5	A	601	DTP	PA-O3A-PB-O1B

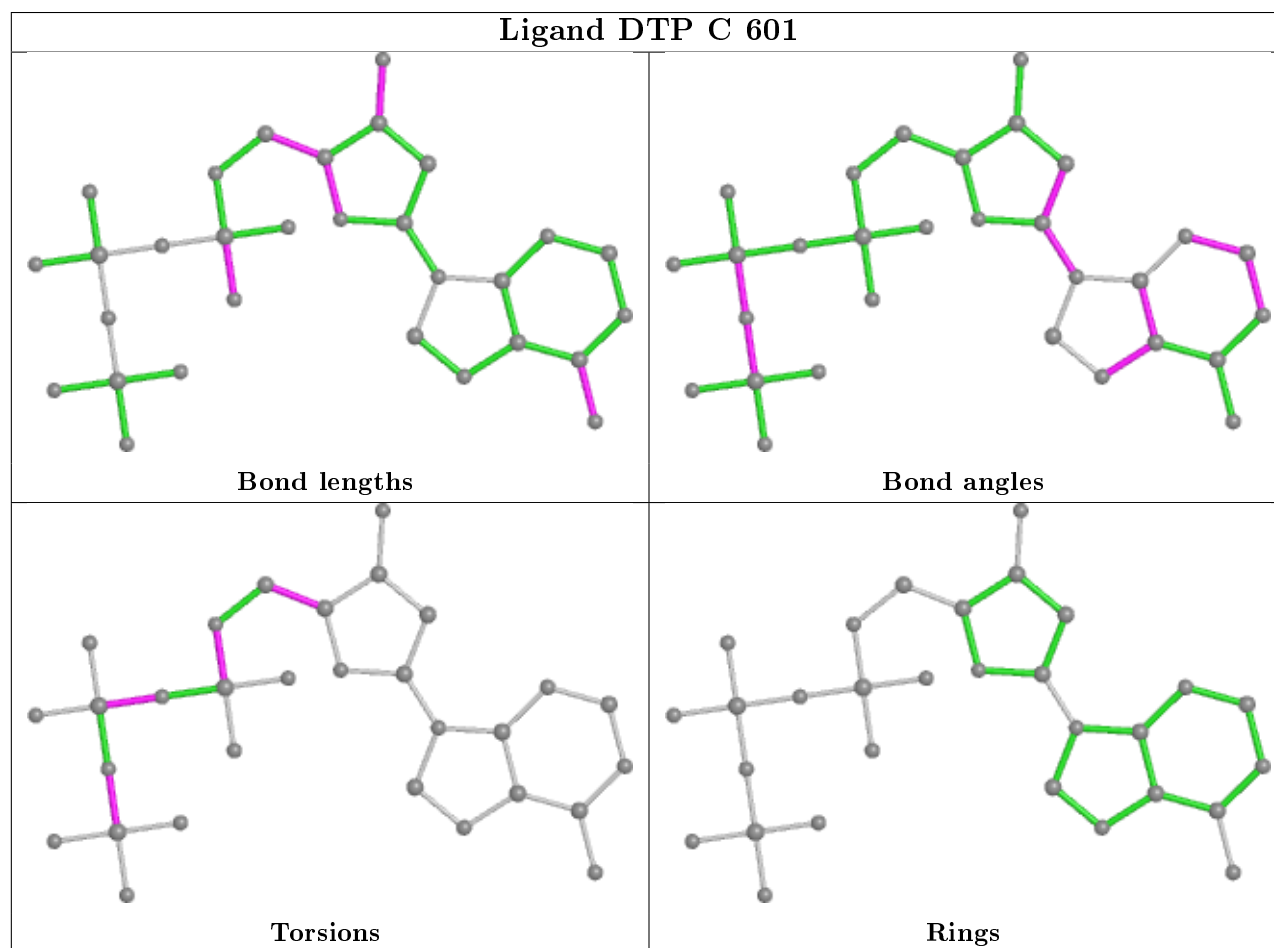
There are no ring outliers.

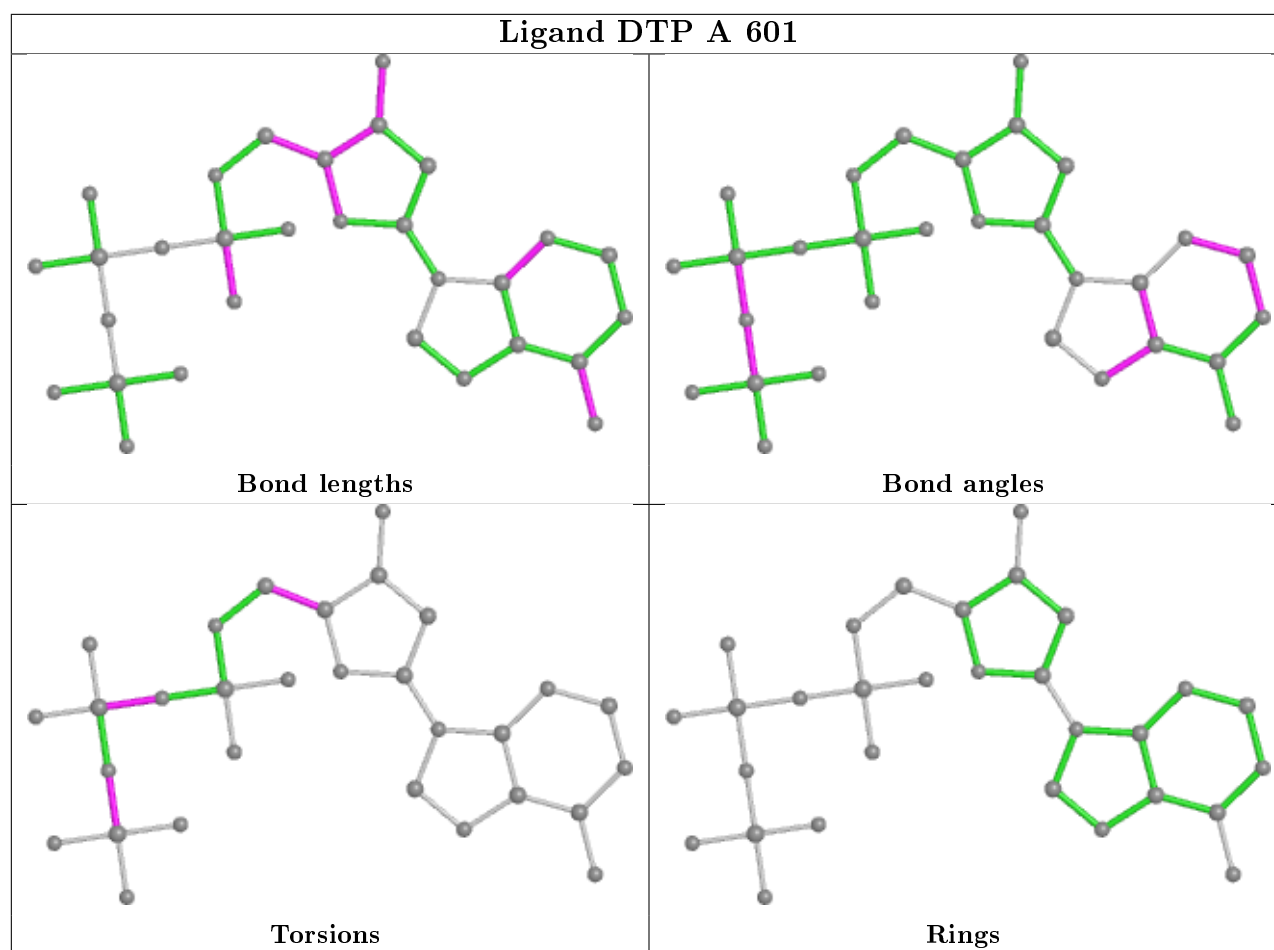
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	604	EDO	1	0
9	B	502	GOL	2	0
5	C	601	DTP	2	0
8	A	605	SO4	1	0
5	A	601	DTP	1	0
8	A	607	SO4	1	0
8	D	501	SO4	1	0
8	B	503	SO4	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	545/556 (98%)	0.55	48 (8%) 10 10	14, 40, 95, 132	0
1	C	545/556 (98%)	1.52	155 (28%) 0 0	19, 64, 140, 157	0
2	B	412/428 (96%)	0.42	16 (3%) 39 42	15, 36, 71, 84	0
2	D	413/428 (96%)	0.72	45 (10%) 5 5	18, 45, 88, 119	0
3	E	21/27 (77%)	1.43	3 (14%) 2 2	56, 92, 122, 154	0
3	T	21/27 (77%)	0.73	3 (14%) 2 2	35, 83, 95, 128	0
4	F	18/21 (85%)	1.10	3 (16%) 1 1	59, 89, 122, 124	0
4	P	18/21 (85%)	0.73	1 (5%) 24 25	34, 81, 107, 109	0
All	All	1993/2064 (96%)	0.84	274 (13%) 3 2	14, 45, 121, 157	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	PRO	11.3
1	C	247	PRO	10.7
2	D	214	LEU	10.5
1	C	252	TRP	9.9
1	C	135	ILE	9.7
1	C	142	ILE	9.4
2	D	231	GLY	9.2
1	C	293	ILE	8.8
1	C	139	THR	8.2
1	C	141	GLY	8.1
1	C	134	SER	8.1
1	C	254	VAL	7.9
1	C	136	ASN	7.7
2	D	91	GLN	7.6
3	E	703	G	7.6
1	C	297	GLU	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	22	LYS	7.4
2	D	88	TRP	7.2
1	C	131	THR	7.1
1	C	257	ILE	7.0
2	D	213	GLY	6.9
1	C	24	TRP	6.9
1	C	51	GLY	6.8
1	C	144	TYR	6.7
1	C	289	LEU	6.7
1	C	301	LEU	6.6
2	D	3	SER	6.6
1	C	292	VAL	6.6
2	D	357	MET	6.5
1	C	248	GLU	6.3
1	C	28	GLU	6.3
1	C	309	ILE	6.2
1	C	34	LEU	6.2
1	C	129	ALA	6.1
1	C	282	LEU	6.0
1	C	55	PRO	6.0
1	C	246	LEU	5.9
3	E	704	G	5.8
1	A	134	SER	5.6
1	C	137	ASN	5.6
1	C	138	GLU	5.6
2	D	4	PRO	5.5
1	C	146	TYR	5.5
1	C	66	LYS	5.5
1	C	250	ASP	5.5
1	C	294	PRO	5.3
1	C	21	VAL	5.3
2	D	90	VAL	5.3
1	C	287	LYS	5.2
1	A	545	ASN	5.2
3	T	704	G	5.2
1	A	26	LEU	5.2
3	T	703	G	5.2
1	C	244	ILE	5.1
1	C	308	GLU	5.1
2	D	212	TRP	5.1
2	D	10	VAL	5.1
1	A	141	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	20	LYS	5.0
1	C	67	ASP	5.0
1	C	256	ASP	5.0
1	C	50	ILE	4.9
1	C	260	LEU	4.9
1	C	54	ASN	4.9
1	C	47	ILE	4.8
2	B	214	LEU	4.7
1	C	264	LEU	4.7
1	A	544	GLY	4.7
1	C	33	ALA	4.6
2	D	87	PHE	4.6
1	C	283	LEU	4.6
1	A	37	ILE	4.6
1	A	135	ILE	4.6
1	A	67	ASP	4.6
1	C	30	LYS	4.6
1	C	280	SER	4.6
1	C	37	ILE	4.6
2	D	209	LEU	4.5
1	C	313	PRO	4.5
2	B	217	PRO	4.5
1	C	53	GLU	4.5
2	D	168	LEU	4.5
2	B	215	THR	4.5
1	C	58	THR	4.5
2	B	231	GLY	4.4
1	C	35	VAL	4.4
1	C	310	LEU	4.3
1	A	131	THR	4.3
1	A	28	GLU	4.3
1	C	296	THR	4.3
1	A	133	PRO	4.2
1	C	285	GLY	4.2
1	C	307	ARG	4.2
1	C	305	GLU	4.2
1	C	222	GLN	4.1
1	C	25	PRO	4.1
1	C	73	LYS	4.1
1	C	286	THR	4.1
1	A	75	VAL	4.1
1	C	271	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	48	SER	4.1
1	C	251	SER	4.1
1	C	304	ALA	4.1
1	A	34	LEU	4.0
1	A	140	PRO	4.0
1	A	142	ILE	4.0
1	C	302	GLU	4.0
1	C	278	GLN	4.0
1	C	255	ASN	4.0
1	C	49	LYS	3.9
1	C	249	LYS	3.9
2	D	216	THR	3.9
1	C	288	ALA	3.9
1	C	71	TRP	3.9
1	C	62	ALA	3.9
1	C	132	ILE	3.8
1	C	74	LEU	3.8
1	C	61	PHE	3.8
1	C	15	GLY	3.8
1	C	223	LYS	3.8
1	A	24	TRP	3.7
2	D	94	ILE	3.7
1	C	133	PRO	3.7
1	C	245	VAL	3.7
1	C	195	ILE	3.7
2	D	217	PRO	3.7
1	A	136	ASN	3.7
2	D	92	LEU	3.7
2	D	89	GLU	3.7
1	C	127	TYR	3.7
2	D	171	PHE	3.6
1	C	277	ARG	3.6
2	D	211	ARG	3.6
1	C	284	ARG	3.6
1	C	59	PRO	3.6
1	C	26	LEU	3.6
2	B	211	ARG	3.5
1	C	52	PRO	3.5
1	A	27	THR	3.5
1	C	545	ASN	3.5
1	C	39	THR	3.5
1	A	19	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	281	LYS	3.5
1	C	43	LYS	3.4
1	A	285	GLY	3.4
1	A	144	TYR	3.4
2	D	202	ILE	3.4
1	C	306	ASN	3.4
1	C	57	ASN	3.3
1	A	21	VAL	3.3
1	C	19	PRO	3.3
1	C	56	TYR	3.3
1	C	126	LYS	3.3
2	B	92	LEU	3.3
1	C	2	ILE	3.2
2	D	7	THR	3.2
1	C	261	VAL	3.2
1	C	295	LEU	3.2
1	C	311	LYS	3.2
2	D	93	GLY	3.2
4	P	805	DG	3.2
2	D	208	HIS	3.2
1	C	299	ALA	3.2
1	A	132	ILE	3.2
1	C	124	PHE	3.1
1	C	290	THR	3.1
1	C	298	GLU	3.1
2	D	232	TYR	3.1
1	C	274	ILE	3.1
1	C	145	GLN	3.1
1	C	69	THR	3.1
1	C	76	ASP	3.1
1	C	226	PRO	3.1
1	C	42	GLU	3.0
1	C	346	PHE	3.0
2	B	212	TRP	3.0
2	D	215	THR	3.0
1	A	22	LYS	3.0
1	C	41	MET	3.0
1	A	143	ARG	3.0
2	B	232	TYR	3.0
1	C	544	GLY	3.0
1	C	17	ASP	2.9
1	C	46	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	139	THR	2.9
1	A	138	GLU	2.9
1	C	79	GLU	2.8
1	C	83	ARG	2.8
1	C	14	PRO	2.8
1	C	23	GLN	2.8
2	D	174	GLN	2.8
2	D	193	LEU	2.8
1	C	219	LYS	2.8
2	D	191	SER	2.8
1	A	73	LYS	2.8
4	F	805	DG	2.8
1	C	143	ARG	2.8
1	A	51	GLY	2.8
1	C	303	LEU	2.8
2	D	95	PRO	2.8
1	C	228	LEU	2.7
1	A	449	GLU	2.7
1	C	275	LYS	2.7
1	A	60	VAL	2.7
2	D	68	SER	2.7
1	A	56	TYR	2.7
2	D	9	PRO	2.7
2	B	216	THR	2.7
1	C	263	LYS	2.7
1	C	75	VAL	2.7
1	C	130	PHE	2.7
1	C	70	LYS	2.7
4	F	815	DG	2.6
2	B	4	PRO	2.6
2	B	315	HIS	2.6
1	C	16	MET	2.6
1	A	52	PRO	2.6
1	A	223	LYS	2.6
1	A	29	GLU	2.6
2	D	66	LYS	2.5
1	C	258	CYS	2.5
1	A	58	THR	2.5
2	B	318	TYR	2.4
1	A	69	THR	2.4
1	C	40	GLU	2.4
1	A	287	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	199	ARG	2.4
2	D	69	THR	2.4
1	C	12	LEU	2.4
2	B	210	LEU	2.4
1	C	314	VAL	2.4
3	T	722	A	2.4
2	B	167	ILE	2.4
1	C	224	GLU	2.4
1	C	65	LYS	2.3
1	A	25	PRO	2.3
1	C	279	LEU	2.3
1	A	31	ILE	2.3
2	D	160	PHE	2.3
2	D	358	ARG	2.3
2	D	67	ASP	2.3
1	C	276	VAL	2.3
1	C	31	ILE	2.3
1	C	68	SER	2.3
1	A	289	LEU	2.3
1	A	252	TRP	2.3
1	A	66	LYS	2.3
1	A	288	ALA	2.3
1	C	266	TRP	2.3
2	B	5	ILE	2.3
1	C	102	LYS	2.2
2	D	205	LEU	2.2
1	C	217	PRO	2.2
1	C	196	GLY	2.2
1	A	543	GLY	2.2
4	F	809	DC	2.2
2	D	85	GLN	2.2
1	A	286	THR	2.2
1	A	71	TRP	2.2
1	C	45	GLY	2.1
1	C	312	GLU	2.1
2	D	12	LEU	2.1
1	C	315	HIS	2.1
2	D	167	ILE	2.1
2	D	158	ALA	2.1
2	B	209	LEU	2.1
3	E	716	A	2.0
1	C	200	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	315	HIS	2.0
1	C	291	GLU	2.0
1	C	18	GLY	2.0
1	A	74	LEU	2.0
1	C	202	ILE	2.0
2	D	204	GLU	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](#)

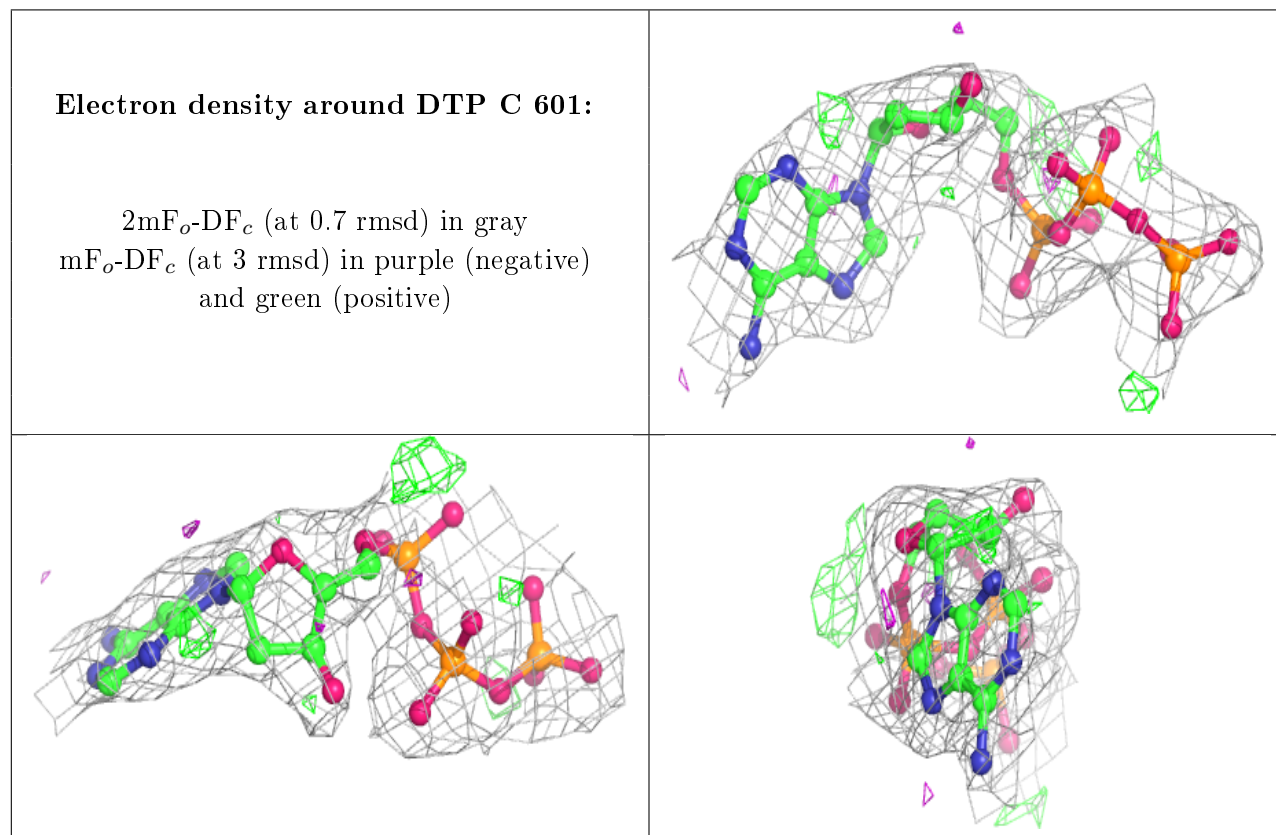
There are no carbohydrates in this entry.

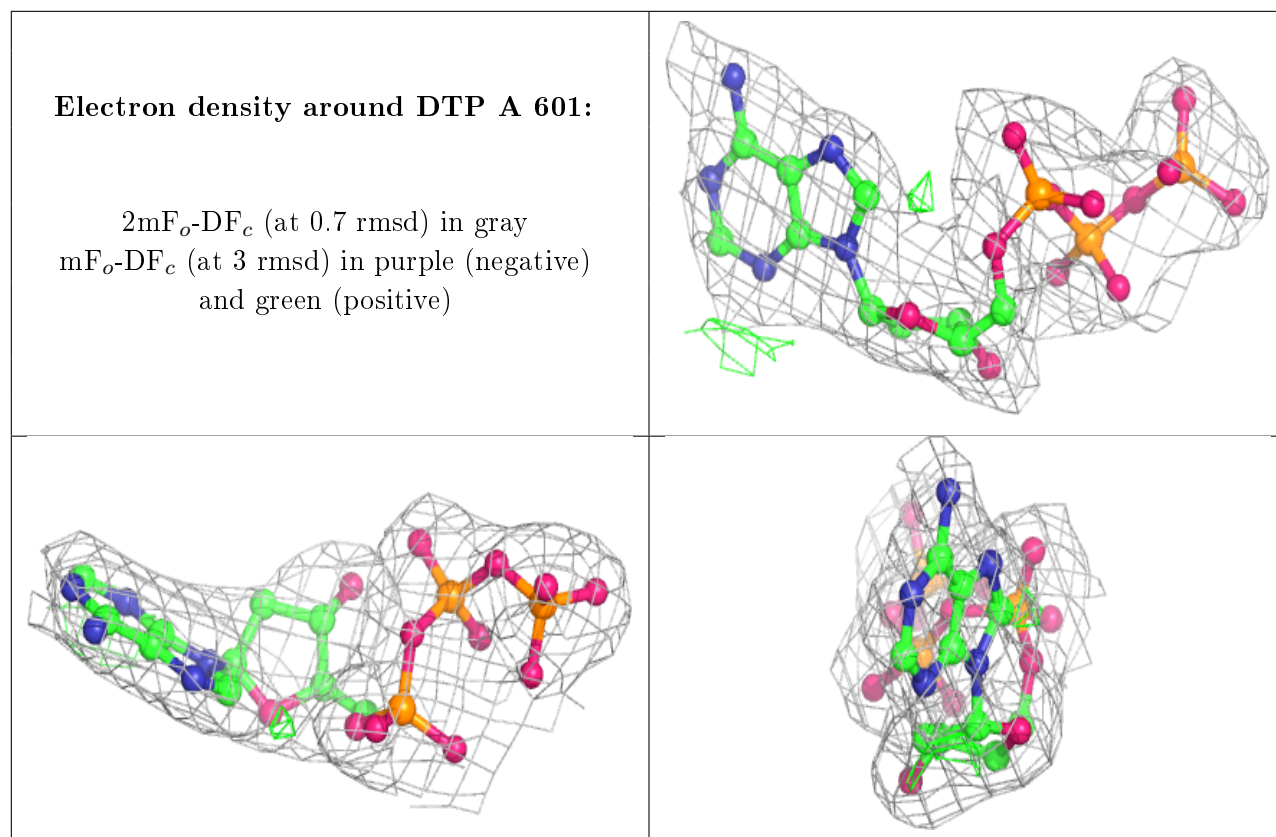
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	C	603	1/1	0.51	0.14	63,63,63,63	0
9	GOL	B	502	6/6	0.77	0.29	36,36,43,47	0
5	DTP	C	601	30/30	0.89	0.17	63,71,85,88	0
8	SO4	D	502	5/5	0.89	0.28	58,67,72,86	0
8	SO4	A	607	5/5	0.90	0.29	45,46,60,70	0
8	SO4	C	604	5/5	0.92	0.21	51,63,69,83	0
8	SO4	A	606	5/5	0.93	0.14	53,58,66,77	0
6	MG	A	602	1/1	0.94	0.12	30,30,30,30	0
6	MG	C	602	1/1	0.95	0.13	59,59,59,59	0
6	MG	A	603	1/1	0.95	0.12	35,35,35,35	0
5	DTP	A	601	30/30	0.95	0.14	33,43,53,55	0
8	SO4	B	501	5/5	0.96	0.14	32,37,46,54	0
8	SO4	D	501	5/5	0.96	0.09	49,57,63,68	0
8	SO4	B	503	5/5	0.96	0.14	54,54,65,77	0
8	SO4	A	605	5/5	0.97	0.18	37,39,51,57	0
7	EDO	A	604	4/4	0.97	0.25	21,22,23,24	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.