



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2022 – 09:24 am BST

PDB ID : 7PZB
Title : Structure of the Clr-cAMP-DNA complex
Authors : Werel, L.; Essen, L.-O.
Deposited on : 2021-10-11
Resolution : 3.12 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

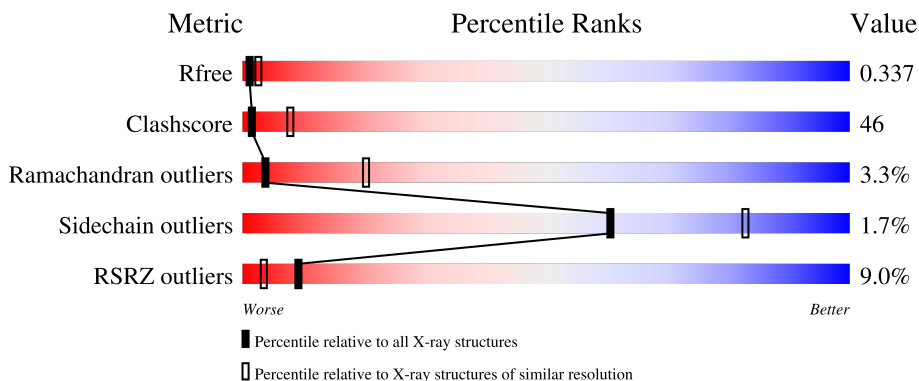
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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.



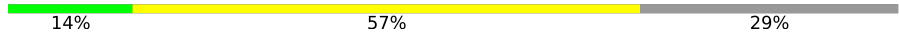
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	244	 2% 37% 52% 7%
1	B	244	 16% 40% 48% 7%
2	C	19	 11% 89%
2	E	19	 16% 58% 26%
3	D	14	 7% 93%

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Mol	Chain	Length	Quality of chain
3	F	14	 14% 57% 29%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4698 atoms, of which 22 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 Putative cAMP-binding protein-catabolite gene activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1739	1098	310	323	8	0	0	0
1	B	226	1727	1091	306	322	8	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	LEU	-	expression tag	UNP Q92SD2
A	236	GLU	-	expression tag	UNP Q92SD2
A	237	HIS	-	expression tag	UNP Q92SD2
A	238	HIS	-	expression tag	UNP Q92SD2
A	239	HIS	-	expression tag	UNP Q92SD2
A	240	HIS	-	expression tag	UNP Q92SD2
A	241	HIS	-	expression tag	UNP Q92SD2
A	242	HIS	-	expression tag	UNP Q92SD2
A	243	HIS	-	expression tag	UNP Q92SD2
A	244	HIS	-	expression tag	UNP Q92SD2
B	235	LEU	-	expression tag	UNP Q92SD2
B	236	GLU	-	expression tag	UNP Q92SD2
B	237	HIS	-	expression tag	UNP Q92SD2
B	238	HIS	-	expression tag	UNP Q92SD2
B	239	HIS	-	expression tag	UNP Q92SD2
B	240	HIS	-	expression tag	UNP Q92SD2
B	241	HIS	-	expression tag	UNP Q92SD2
B	242	HIS	-	expression tag	UNP Q92SD2
B	243	HIS	-	expression tag	UNP Q92SD2
B	244	HIS	-	expression tag	UNP Q92SD2

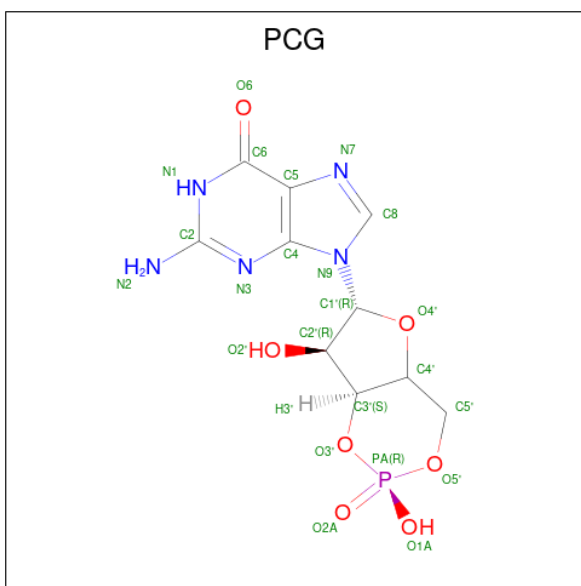
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*AP*GP*GP*TP*AP*AP*CP*AP*TP*TP*AP*CP*TP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	19	Total 385	C 185	N 70	O 112	P 18	0	0	0
2	E	14	Total 283	C 137	N 52	O 81	P 13	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*AP*GP*TP*AP*AP*TP*GP*TP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	Total 287	C 138	N 54	O 82	P 13	0	0	0
3	F	10	Total 206	C 99	N 36	O 61	P 10	0	0	0

- Molecule 4 is CYCLIC GUANOSINE MONOPHOSPHATE (three-letter code: PCG) (formula: $C_{10}H_{12}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
4	A	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0
4	B	1	Total 34	C 10	H 11	N 5	O 7	P 1	0	0

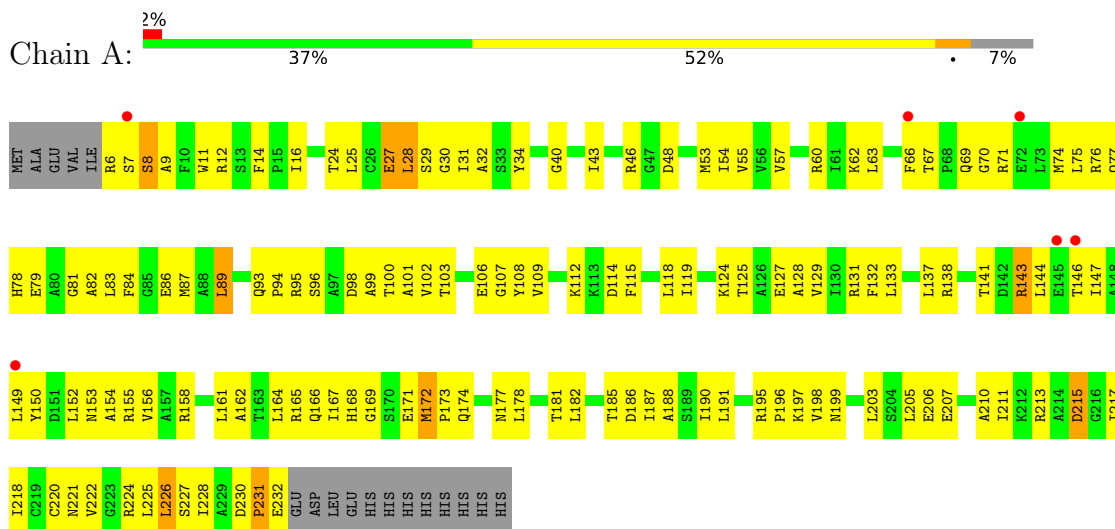
- Molecule 5 is water.

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

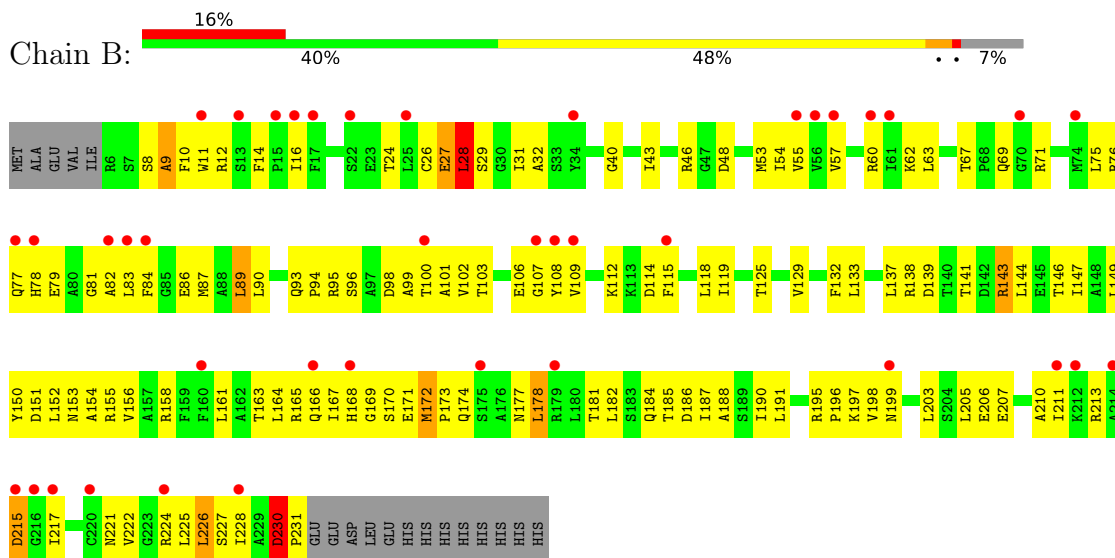
3 Residue-property plots [i](#)

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.

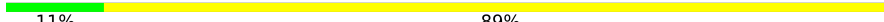
- Molecule 1: Putative cAMP-binding protein-catabolite gene activator



- Molecule 1: Putative cAMP-binding protein-catabolite gene activator

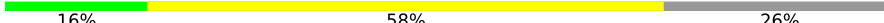


- Molecule 2: DNA (5'-D(*CP*TP*AP*GP*GP*TP*AP*AP*CP*AP*TP*TP*AP*CP*TP*CP*GP*CP*G)-3')

Chain C:  11% 89%

C1	T2	A3	G4	G5	T6	C9	A10	T11	T12	A13	C14	T15	C16	G17	C18	G19
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- Molecule 2: DNA (5'-D(*CP*TP*AP*GP*GP*TP*AP*AP*CP*AP*TP*TP*AP*CP*TP*CP*GP*CP*G)-3')

Chain E:  16% 58% 26%

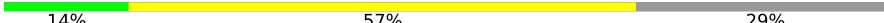
C1	T2	A3	G4	G5	T6	A7	A10	T11	T12	A13	C14	DT	DC	DG	DC	DG
----	----	----	----	----	----	----	-----	-----	-----	-----	-----	----	----	----	----	----

- Molecule 3: DNA (5'-D(*GP*CP*GP*AP*GP*TP*AP*AP*TP*GP*TP*TP*AP*C)-3')

Chain D:  7% 93%

G1	C2	G3	A4	G5	T6	A7	A8	T9	G10	T11	T12	A13	C14
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- Molecule 3: DNA (5'-D(*GP*CP*GP*AP*GP*TP*AP*AP*TP*GP*TP*TP*AP*C)-3')

Chain F:  14% 57% 29%

DG	DC	DG	DA	G5	T6	A7	A8	T9	G10	T11	T12	A13	C14
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.71Å 72.90Å 199.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.12 49.20 – 3.12	Depositor EDS
% Data completeness (in resolution range)	69.9 (49.20-3.12) 70.0 (49.20-3.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.289 , 0.333 0.289 , 0.337	Depositor DCC
R_{free} test set	469 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	100.3	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4698	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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: PCG

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	0.32	0/1766	0.62	1/2386 (0.0%)
1	B	0.34	0/1754	0.69	3/2371 (0.1%)
2	C	0.59	0/431	0.88	0/663
2	E	0.60	0/316	0.90	0/483
3	D	0.67	0/322	0.95	0/496
3	F	0.64	0/230	1.00	0/353
All	All	0.43	0/4819	0.74	4/6752 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ASP	C-N-CD	-10.78	96.88	120.60
1	B	178	LEU	CA-CB-CG	-6.16	101.13	115.30
1	A	28	LEU	CA-CB-CG	-5.39	102.91	115.30
1	B	28	LEU	CB-CG-CD1	5.02	119.53	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	169	GLY	Peptide
1	B	170	SER	Peptide
1	B	230	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	1739	0	1758	188	1
1	B	1727	0	1743	167	0
2	C	385	0	216	33	0
2	E	283	0	161	17	0
3	D	287	0	160	22	0
3	F	206	0	115	22	0
4	A	23	11	9	5	0
4	B	23	11	9	6	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
All	All	4676	22	4171	406	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (406) 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)
4:B:301:PCG:C4'	4:B:301:PCG:C3'	1.81	1.46
4:A:301:PCG:C3'	4:A:301:PCG:C4'	1.81	1.42
1:A:138:ARG:HH12	1:B:93:GLN:HB2	0.99	1.15
1:A:93:GLN:HB2	1:B:138:ARG:HH12	0.95	1.11
1:A:28:LEU:HD13	1:A:118:LEU:HD11	1.40	1.04
1:A:93:GLN:CB	1:B:138:ARG:HH12	1.74	1.01
1:A:138:ARG:NH1	1:B:93:GLN:HB2	1.76	0.99
1:A:93:GLN:HB2	1:B:138:ARG:NH1	1.78	0.97
1:B:167:ILE:HD12	1:B:178:LEU:HD11	1.46	0.96
1:B:28:LEU:O	1:B:31:ILE:HG12	1.64	0.96
1:A:231:PRO:HG3	1:B:69:GLN:HG3	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ARG:NH1	4:B:301:PCG:O1A	2.03	0.92
1:A:95:ARG:NH1	4:A:301:PCG:O2A	2.03	0.92
1:A:199:ASN:HD21	3:D:10:DG:H5''	1.33	0.92
1:B:197:LYS:NZ	2:E:5:DG:N7	2.20	0.90
1:A:199:ASN:ND2	3:D:10:DG:OP2	2.05	0.89
1:A:186:ASP:O	1:A:190:ILE:HG13	1.73	0.88
1:A:93:GLN:HB3	1:A:94:PRO:HD2	1.54	0.88
2:C:14:DC:H1'	2:C:15:DT:H5'	1.55	0.88
1:A:138:ARG:HH12	1:B:93:GLN:CB	1.84	0.88
1:B:186:ASP:O	1:B:190:ILE:HG13	1.73	0.88
1:A:75:LEU:O	1:A:143:ARG:NH2	2.08	0.87
1:B:93:GLN:HB3	1:B:94:PRO:HD2	1.54	0.86
1:B:75:LEU:O	1:B:143:ARG:NH2	2.08	0.86
1:B:167:ILE:CD1	1:B:178:LEU:HD11	2.05	0.86
1:A:231:PRO:HD3	1:B:69:GLN:HE21	1.42	0.84
1:A:57:VAL:HG22	1:A:107:GLY:HA2	1.60	0.83
1:B:57:VAL:HG22	1:B:107:GLY:HA2	1.60	0.83
1:B:167:ILE:HD12	1:B:178:LEU:CD1	2.10	0.82
2:C:18:DC:H2''	2:C:19:DG:H3'	1.61	0.81
2:C:14:DC:H6	2:C:14:DC:H5'	1.45	0.80
1:B:8:SER:C	1:B:10:PHE:H	1.85	0.80
1:B:26:CYS:SG	1:B:27:GLU:N	2.51	0.80
1:A:62:LYS:HE2	1:A:100:THR:HG21	1.63	0.80
2:C:14:DC:H5'	2:C:14:DC:C6	2.18	0.79
1:A:11:TRP:CE2	1:A:29:SER:HB3	2.19	0.78
1:A:221:ASN:ND2	1:A:224:ARG:HG3	1.99	0.78
1:B:62:LYS:HE2	1:B:100:THR:HG21	1.64	0.78
1:B:221:ASN:ND2	1:B:224:ARG:HG3	1.99	0.78
1:A:60:ARG:HD2	1:A:103:THR:HG23	1.66	0.77
1:B:60:ARG:HD2	1:B:103:THR:HG23	1.66	0.77
1:B:77:GLN:N	1:B:77:GLN:OE1	2.17	0.77
1:A:213:ARG:NH2	3:D:10:DG:OP1	2.18	0.77
1:B:11:TRP:CE2	1:B:29:SER:HB3	2.19	0.77
1:B:171:GLU:O	1:B:172:MET:HB2	1.85	0.76
1:A:171:GLU:O	1:A:172:MET:HB2	1.84	0.76
1:A:177:ASN:HB3	1:A:217:ILE:HD11	1.67	0.76
1:B:164:LEU:HD22	1:B:168:HIS:HE1	1.52	0.75
1:B:177:ASN:HB3	1:B:217:ILE:HD11	1.67	0.74
1:A:11:TRP:CZ2	1:A:29:SER:HB3	2.23	0.74
1:B:11:TRP:CZ2	1:B:29:SER:HB3	2.23	0.74
3:D:2:DC:H2'	3:D:3:DG:C8	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:DT:H2''	2:C:3:DA:C8	2.23	0.73
1:A:162:ALA:O	1:A:166:GLN:HG2	1.88	0.73
1:A:165:ARG:HG2	1:A:172:MET:SD	2.29	0.73
1:A:231:PRO:HD3	1:B:69:GLN:NE2	2.02	0.73
1:A:164:LEU:HD22	1:A:168:HIS:HE1	1.52	0.72
4:B:301:PCG:C3'	4:B:301:PCG:C5'	2.66	0.72
4:A:301:PCG:C3'	4:A:301:PCG:C5'	2.66	0.72
1:B:8:SER:O	1:B:10:PHE:N	2.23	0.71
1:A:137:LEU:HD12	1:B:137:LEU:HD12	1.71	0.71
1:A:60:ARG:HH22	1:A:181:THR:HG21	1.56	0.71
1:B:60:ARG:HH22	1:B:181:THR:HG21	1.55	0.70
2:C:13:DA:H1'	2:C:14:DC:H5''	1.73	0.70
1:B:60:ARG:HH22	1:B:181:THR:CG2	2.05	0.70
1:A:171:GLU:HG3	1:A:172:MET:N	2.08	0.69
2:E:10:DA:H2'	2:E:11:DT:C7	2.22	0.69
2:E:10:DA:H2'	2:E:11:DT:H72	1.74	0.68
1:A:60:ARG:HH22	1:A:181:THR:CG2	2.05	0.68
1:A:181:THR:O	1:A:182:LEU:HD22	1.94	0.68
2:E:6:DT:H2''	2:E:7:DA:H5'	1.76	0.67
1:B:181:THR:O	1:B:182:LEU:HD22	1.94	0.67
1:A:60:ARG:HD2	1:A:103:THR:CG2	2.25	0.67
1:A:168:HIS:CD2	1:A:172:MET:HG2	2.30	0.67
1:B:151:ASP:HA	2:E:4:DG:OP1	1.94	0.67
1:A:62:LYS:HG2	1:A:100:THR:CG2	2.25	0.66
1:B:62:LYS:HG2	1:B:100:THR:CG2	2.25	0.66
1:B:168:HIS:CD2	1:B:172:MET:HG2	2.30	0.66
1:B:86:GLU:N	1:B:86:GLU:OE1	2.28	0.66
1:A:63:LEU:O	1:A:75:LEU:HB2	1.95	0.66
1:A:224:ARG:HA	1:A:227:SER:OG	1.96	0.66
1:A:62:LYS:HE2	1:A:100:THR:CG2	2.26	0.66
1:B:55:VAL:CG2	1:B:108:TYR:HB2	2.26	0.66
1:B:60:ARG:HD2	1:B:103:THR:CG2	2.25	0.65
1:A:55:VAL:CG2	1:A:108:TYR:HB2	2.26	0.65
1:B:224:ARG:HA	1:B:227:SER:OG	1.95	0.65
1:A:43:ILE:HD12	1:A:43:ILE:H	1.60	0.65
1:B:89:LEU:HD11	1:B:112:LYS:HA	1.79	0.65
1:A:89:LEU:HD11	1:A:112:LYS:HA	1.79	0.65
1:B:62:LYS:HE2	1:B:100:THR:CG2	2.26	0.65
1:B:63:LEU:O	1:B:75:LEU:HB2	1.96	0.65
1:B:93:GLN:HB3	1:B:94:PRO:CD	2.26	0.65
1:B:205:LEU:HD23	1:B:228:ILE:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HE	1:A:77:GLN:H	1.45	0.64
1:B:43:ILE:HD12	1:B:43:ILE:H	1.60	0.64
1:B:184:GLN:NE2	3:F:9:DT:H5''	2.12	0.64
2:C:11:DT:H2'	2:C:12:DT:C7	2.28	0.64
2:E:14:DC:H4'	2:E:14:DC:OP1	1.96	0.63
1:A:27:GLU:O	1:A:29:SER:N	2.31	0.63
1:A:46:ARG:N	1:A:98:ASP:OD1	2.32	0.63
1:A:205:LEU:HD23	1:A:228:ILE:HD13	1.79	0.63
1:B:8:SER:C	1:B:10:PHE:N	2.51	0.63
2:C:18:DC:H2''	2:C:19:DG:C5'	2.29	0.63
3:F:12:DT:H2'	3:F:13:DA:C8	2.33	0.63
1:B:46:ARG:N	1:B:98:ASP:OD1	2.32	0.63
1:A:182:LEU:HD12	1:A:186:ASP:HB3	1.81	0.63
3:F:11:DT:H2'	3:F:12:DT:H71	1.81	0.63
1:A:86:GLU:N	1:A:86:GLU:OE1	2.28	0.62
1:B:27:GLU:O	1:B:29:SER:N	2.31	0.62
1:B:28:LEU:HD13	1:B:118:LEU:CD2	2.29	0.62
1:A:7:SER:O	1:A:8:SER:HB2	1.98	0.62
1:B:155:ARG:HB3	1:B:191:LEU:HD13	1.80	0.62
1:A:155:ARG:HB3	1:A:191:LEU:HD13	1.81	0.62
1:A:115:PHE:O	1:A:119:ILE:HG13	2.01	0.61
1:A:27:GLU:CB	1:A:28:LEU:HD23	2.31	0.61
1:A:28:LEU:HB3	1:A:118:LEU:HD21	1.83	0.61
1:A:127:GLU:HG3	1:A:131:ARG:HE	1.65	0.61
1:B:182:LEU:HD12	1:B:186:ASP:HB3	1.81	0.61
1:A:76:ARG:NE	1:A:77:GLN:H	1.97	0.61
1:B:28:LEU:HD23	1:B:29:SER:OG	2.01	0.61
1:A:147:ILE:HD11	1:B:147:ILE:HD11	1.81	0.61
1:A:178:LEU:HD21	1:A:218:ILE:HB	1.82	0.61
1:B:115:PHE:O	1:B:119:ILE:HG13	2.01	0.61
3:F:12:DT:H2'	3:F:13:DA:H8	1.65	0.60
1:A:178:LEU:CD2	1:A:218:ILE:HB	2.31	0.60
1:B:141:THR:O	1:B:144:LEU:HB3	2.02	0.60
1:A:28:LEU:HD13	1:A:118:LEU:CD1	2.26	0.60
1:A:141:THR:O	1:A:144:LEU:HB3	2.01	0.60
1:A:231:PRO:O	1:A:232:GLU:HG2	2.02	0.59
1:A:222:VAL:O	1:A:226:LEU:HD12	2.03	0.59
1:A:28:LEU:HD23	1:A:28:LEU:N	2.17	0.59
1:B:156:VAL:CG2	1:B:205:LEU:HD11	2.33	0.59
1:A:75:LEU:C	1:A:143:ARG:HH22	2.03	0.59
1:A:203:LEU:HD11	3:D:10:DG:C5'	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:C	1:B:143:ARG:HH22	2.03	0.59
1:B:96:SER:H	4:B:301:PCG:H5'1	1.68	0.59
2:E:2:DT:H2''	2:E:3:DA:N7	2.18	0.59
1:A:156:VAL:CG2	1:A:205:LEU:HD11	2.33	0.58
1:B:222:VAL:O	1:B:226:LEU:HD12	2.03	0.58
1:A:127:GLU:HG3	1:A:131:ARG:NE	2.18	0.58
1:A:93:GLN:HB3	1:A:94:PRO:CD	2.26	0.58
1:A:96:SER:H	4:A:301:PCG:H5'1	1.68	0.58
1:A:55:VAL:HG22	1:A:108:TYR:HB2	1.85	0.58
1:B:28:LEU:HD13	1:B:118:LEU:HD23	1.86	0.58
3:D:5:DG:H2''	3:D:6:DT:O5'	2.03	0.58
1:A:71:ARG:NH1	1:B:149:LEU:O	2.37	0.58
1:A:60:ARG:HH11	1:A:77:GLN:NE2	2.02	0.57
1:A:149:LEU:O	1:B:71:ARG:NH1	2.37	0.57
1:A:93:GLN:CB	1:B:138:ARG:NH1	2.53	0.57
1:A:28:LEU:HB3	1:A:118:LEU:CD2	2.34	0.57
1:A:67:THR:HG23	1:B:149:LEU:HD13	1.86	0.57
1:B:55:VAL:HG22	1:B:108:TYR:HB2	1.85	0.57
1:B:9:ALA:HB1	1:B:12:ARG:CZ	2.34	0.57
2:C:9:DC:H2''	2:C:10:DA:H8	1.70	0.57
1:A:185:THR:HG23	1:A:195:ARG:CD	2.35	0.56
1:A:203:LEU:HD11	3:D:10:DG:H5''	1.87	0.56
1:B:185:THR:HG23	1:B:195:ARG:CD	2.35	0.56
1:A:231:PRO:CG	1:B:69:GLN:HG3	2.27	0.56
1:A:152:LEU:HA	1:A:155:ARG:HD2	1.87	0.55
1:B:163:THR:O	1:B:166:GLN:HB3	2.07	0.55
1:B:152:LEU:HA	1:B:155:ARG:HD2	1.87	0.55
1:A:74:MET:HE1	1:A:77:GLN:OE1	2.07	0.55
1:A:221:ASN:C	1:A:225:LEU:HD12	2.27	0.55
1:A:137:LEU:HD23	1:B:87:MET:SD	2.47	0.55
3:F:10:DG:H2''	3:F:11:DT:H5'	1.88	0.55
1:B:199:ASN:ND2	3:F:10:DG:OP2	2.40	0.54
1:B:60:ARG:HG3	1:B:102:VAL:HG23	1.90	0.54
1:B:168:HIS:HD2	1:B:172:MET:HA	1.72	0.54
1:A:168:HIS:HD2	1:A:172:MET:HA	1.72	0.54
1:A:24:THR:CG2	1:A:28:LEU:HD12	2.37	0.54
1:A:171:GLU:HG3	1:A:172:MET:H	1.72	0.54
1:B:221:ASN:C	1:B:225:LEU:HD12	2.27	0.54
1:A:24:THR:HG23	1:A:28:LEU:HD12	1.89	0.54
1:A:185:THR:CG2	1:A:195:ARG:HD3	2.37	0.54
1:B:185:THR:CG2	1:B:195:ARG:HD3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:O	1:A:169:GLY:HA2	2.08	0.53
1:B:40:GLY:N	1:B:101:ALA:O	2.40	0.53
1:B:230:ASP:O	1:B:231:PRO:O	2.25	0.53
2:C:11:DT:H2'	2:C:12:DT:H72	1.89	0.53
1:A:74:MET:HE2	1:A:77:GLN:HB2	1.90	0.53
1:A:161:LEU:O	1:A:165:ARG:HG3	2.08	0.53
1:A:60:ARG:HG3	1:A:102:VAL:HG23	1.90	0.53
2:E:5:DG:C8	2:E:6:DT:H72	2.44	0.53
3:D:6:DT:H2'	3:D:7:DA:C8	2.42	0.53
3:D:6:DT:H4'	3:D:6:DT:OP1	2.09	0.53
1:A:62:LYS:HG2	1:A:100:THR:HG23	1.91	0.53
1:A:138:ARG:NH1	1:B:93:GLN:CB	2.56	0.53
1:A:171:GLU:CG	1:A:172:MET:H	2.22	0.53
1:B:62:LYS:HG2	1:B:100:THR:HG23	1.91	0.53
2:C:5:DG:C8	2:C:6:DT:H72	2.44	0.53
1:B:76:ARG:HH22	1:B:139:ASP:HB3	1.74	0.53
1:B:221:ASN:HD22	1:B:224:ARG:HG3	1.72	0.53
2:C:13:DA:H1'	2:C:14:DC:C5'	2.39	0.53
1:A:83:LEU:HD23	1:A:84:PHE:N	2.24	0.52
1:B:83:LEU:HD23	1:B:84:PHE:N	2.25	0.52
1:B:96:SER:H	4:B:301:PCG:C5'	2.23	0.52
2:C:1:DC:C5'	3:F:14:DC:H1'	2.39	0.52
3:F:8:DA:H2'	3:F:9:DT:H71	1.90	0.52
1:B:156:VAL:HG21	1:B:205:LEU:HD11	1.92	0.52
1:A:127:GLU:O	1:A:131:ARG:HG2	2.09	0.52
2:C:16:DC:H4'	2:C:16:DC:OP1	2.10	0.52
1:A:87:MET:SD	1:B:137:LEU:HD23	2.51	0.51
3:D:8:DA:H2''	3:D:9:DT:H5'	1.92	0.51
2:E:3:DA:H8	2:E:3:DA:H5''	1.75	0.51
2:C:1:DC:O5'	3:F:14:DC:H1'	2.09	0.51
1:B:27:GLU:O	1:B:28:LEU:C	2.48	0.51
1:A:96:SER:H	4:A:301:PCG:C5'	2.23	0.51
2:C:9:DC:H2''	2:C:10:DA:C8	2.45	0.51
2:C:18:DC:H2''	2:C:19:DG:C3'	2.35	0.51
1:B:62:LYS:HG2	1:B:100:THR:HG22	1.93	0.51
1:B:168:HIS:HD2	1:B:172:MET:HG2	1.76	0.51
1:A:60:ARG:NH1	1:A:77:GLN:NE2	2.59	0.50
1:A:181:THR:O	1:A:181:THR:HG22	2.11	0.50
2:C:14:DC:C1'	2:C:15:DT:H5'	2.35	0.50
3:D:13:DA:H2''	3:D:14:DC:O5'	2.11	0.50
3:F:10:DG:H2''	3:F:11:DT:C5'	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:NH2	3:F:10:DG:OP1	2.44	0.50
1:A:60:ARG:CD	1:A:103:THR:HG23	2.40	0.50
1:A:221:ASN:HD22	1:A:224:ARG:HG3	1.72	0.50
1:A:156:VAL:HG21	1:A:205:LEU:HD11	1.92	0.50
2:C:1:DC:H5''	3:F:14:DC:H1'	1.92	0.50
1:A:46:ARG:O	1:A:95:ARG:HB2	2.12	0.50
1:A:60:ARG:HG3	1:A:102:VAL:CG2	2.42	0.50
2:E:5:DG:C2'	2:E:6:DT:H72	2.42	0.50
1:A:188:ALA:HA	1:A:198:VAL:HG21	1.94	0.50
1:B:60:ARG:HG3	1:B:102:VAL:CG2	2.42	0.50
1:B:174:GLN:HA	1:B:222:VAL:CG1	2.42	0.50
1:A:206:GLU:HA	1:A:211:ILE:O	2.12	0.49
1:B:46:ARG:O	1:B:95:ARG:HB2	2.12	0.49
1:B:181:THR:O	1:B:181:THR:HG22	2.11	0.49
1:B:16:ILE:HD11	1:B:132:PHE:CD2	2.48	0.49
1:B:188:ALA:HA	1:B:198:VAL:HG21	1.94	0.49
1:B:205:LEU:HD21	1:B:228:ILE:HG21	1.94	0.49
1:A:40:GLY:N	1:A:101:ALA:O	2.40	0.49
1:A:62:LYS:HG2	1:A:100:THR:HG22	1.93	0.49
1:A:203:LEU:HD21	1:A:213:ARG:HH22	1.77	0.49
1:B:24:THR:O	1:B:28:LEU:HB2	2.11	0.49
2:C:18:DC:C2'	2:C:19:DG:H3'	2.36	0.49
3:F:12:DT:H2''	3:F:13:DA:H5'	1.95	0.49
1:A:171:GLU:CG	1:A:172:MET:N	2.73	0.49
1:B:28:LEU:HG	1:B:29:SER:N	2.19	0.49
1:B:203:LEU:HD21	1:B:213:ARG:HH22	1.77	0.49
2:C:3:DA:H2''	2:C:4:DG:C5'	2.42	0.49
2:C:18:DC:H2''	2:C:19:DG:H5'	1.94	0.49
3:D:8:DA:H2''	3:D:9:DT:C5'	2.42	0.49
1:B:167:ILE:CD1	1:B:178:LEU:HD21	2.42	0.49
1:B:206:GLU:HA	1:B:211:ILE:O	2.12	0.49
1:B:60:ARG:CD	1:B:103:THR:HG23	2.40	0.49
1:A:60:ARG:NH1	1:A:77:GLN:HE21	2.11	0.49
1:A:129:VAL:O	1:A:133:LEU:HG	2.13	0.49
1:A:205:LEU:CD2	1:A:228:ILE:HG21	2.43	0.49
2:C:3:DA:H2''	2:C:4:DG:H5''	1.95	0.49
1:B:205:LEU:CD2	1:B:228:ILE:HG21	2.43	0.49
1:A:16:ILE:HD11	1:A:132:PHE:CD2	2.48	0.48
1:A:205:LEU:HD21	1:A:228:ILE:HG21	1.94	0.48
1:A:24:THR:O	1:A:28:LEU:HD12	2.13	0.48
1:A:182:LEU:CD1	1:A:186:ASP:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:O	1:B:133:LEU:HG	2.13	0.48
1:A:67:THR:HG23	1:B:149:LEU:CD1	2.44	0.48
1:A:174:GLN:HA	1:A:222:VAL:CG1	2.42	0.48
1:A:230:ASP:HB3	1:A:231:PRO:HD2	1.96	0.48
1:A:31:ILE:HD12	1:A:114:ASP:HB3	1.96	0.47
1:B:203:LEU:HD21	3:F:10:DG:P	2.54	0.47
3:D:5:DG:H2''	3:D:6:DT:O4'	2.14	0.47
1:B:31:ILE:HD12	1:B:114:ASP:HB3	1.97	0.47
1:A:196:PRO:HB3	3:D:11:DT:C7	2.45	0.47
1:B:182:LEU:CD1	1:B:186:ASP:HB3	2.43	0.47
1:A:168:HIS:CD2	1:A:172:MET:HA	2.50	0.47
1:A:168:HIS:HD2	1:A:172:MET:HG2	1.75	0.47
1:A:178:LEU:HD22	1:A:220:CYS:SG	2.55	0.47
1:A:203:LEU:CD2	1:A:213:ARG:HH22	2.28	0.47
1:A:14:PHE:CE1	1:A:81:GLY:HA2	2.50	0.47
3:D:1:DG:H1'	3:D:2:DC:C6	2.50	0.46
1:B:57:VAL:HG22	1:B:107:GLY:CA	2.38	0.46
1:A:156:VAL:HG21	1:A:205:LEU:CD1	2.45	0.46
3:D:6:DT:H2'	3:D:7:DA:H8	1.79	0.46
1:B:178:LEU:HD12	1:B:178:LEU:HA	1.64	0.46
1:B:203:LEU:CD2	1:B:213:ARG:HH22	2.28	0.46
1:A:27:GLU:C	1:A:29:SER:H	2.18	0.46
1:A:197:LYS:HD2	2:C:4:DG:H2'	1.96	0.46
1:B:77:GLN:HG3	1:B:182:LEU:HD21	1.97	0.46
1:B:203:LEU:O	1:B:207:GLU:HG3	2.16	0.46
1:B:14:PHE:CE1	1:B:81:GLY:HA2	2.50	0.46
1:B:164:LEU:HD22	1:B:168:HIS:CE1	2.42	0.46
3:F:8:DA:C2'	3:F:9:DT:H71	2.46	0.46
1:A:195:ARG:HB3	1:A:196:PRO:HD3	1.97	0.46
1:B:76:ARG:CB	1:B:78:HIS:CE1	2.99	0.46
1:B:156:VAL:HG21	1:B:205:LEU:CD1	2.45	0.46
3:D:14:DC:H2'	2:E:1:DC:O4'	2.16	0.46
1:A:67:THR:HB	1:A:69:GLN:OE1	2.16	0.45
2:E:6:DT:H2''	2:E:7:DA:C5'	2.44	0.45
1:A:89:LEU:HD11	1:A:112:LYS:CA	2.45	0.45
1:B:77:GLN:O	1:B:77:GLN:HG2	2.16	0.45
1:B:89:LEU:HD11	1:B:112:LYS:CA	2.45	0.45
2:C:17:DG:H4'	2:C:17:DG:OP1	2.16	0.45
1:B:60:ARG:HA	1:B:79:GLU:HG2	1.99	0.45
1:B:168:HIS:CD2	1:B:172:MET:HA	2.50	0.45
1:A:75:LEU:HA	1:A:143:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:O	1:A:207:GLU:HG3	2.16	0.45
2:C:4:DG:H8	2:C:4:DG:H5'	1.82	0.45
3:F:12:DT:H2''	3:F:13:DA:C5'	2.47	0.45
1:A:60:ARG:HA	1:A:79:GLU:HG2	1.99	0.45
1:A:137:LEU:CD1	1:B:137:LEU:HA	2.47	0.45
1:B:195:ARG:HB3	1:B:196:PRO:HD3	1.98	0.45
1:A:57:VAL:HG22	1:A:107:GLY:CA	2.39	0.44
1:B:75:LEU:HA	1:B:143:ARG:NH2	2.32	0.44
2:C:3:DA:C2'	2:C:4:DG:H5''	2.46	0.44
1:B:12:ARG:HE	1:B:12:ARG:HB2	1.60	0.44
1:A:131:ARG:NH1	1:B:90:LEU:HB3	2.33	0.44
1:A:188:ALA:HB2	1:A:198:VAL:HG21	2.00	0.44
1:B:67:THR:HB	1:B:69:GLN:OE1	2.16	0.44
1:B:53:MET:HG2	1:B:54:ILE:N	2.32	0.44
2:E:10:DA:C8	2:E:11:DT:H72	2.52	0.44
1:B:167:ILE:HD11	1:B:178:LEU:HD21	2.00	0.44
1:B:174:GLN:HA	1:B:222:VAL:HG12	2.00	0.44
1:A:124:LYS:O	1:A:127:GLU:HB3	2.17	0.44
1:B:48:ASP:O	1:B:95:ARG:HG2	2.18	0.44
1:B:221:ASN:HD21	1:B:224:ARG:HG3	1.80	0.44
1:A:24:THR:HA	1:A:28:LEU:CD1	2.48	0.44
1:A:174:GLN:HA	1:A:222:VAL:HG12	2.00	0.44
2:C:14:DC:H2'	2:C:15:DT:H71	2.00	0.44
1:A:164:LEU:HD22	1:A:168:HIS:CE1	2.42	0.43
3:D:11:DT:H2''	3:D:12:DT:O5'	2.18	0.43
3:F:8:DA:H2''	3:F:9:DT:H6	1.83	0.43
1:A:53:MET:HG2	1:A:54:ILE:N	2.32	0.43
1:A:146:THR:HG23	1:A:158:ARG:HD3	2.00	0.43
1:B:146:THR:HG23	1:B:158:ARG:HD3	2.00	0.43
2:E:10:DA:H2''	2:E:11:DT:C6	2.54	0.43
1:A:9:ALA:CB	1:A:12:ARG:HH11	2.32	0.43
1:A:48:ASP:O	1:A:95:ARG:HG2	2.18	0.43
1:A:124:LYS:HE3	1:A:124:LYS:HA	2.00	0.43
1:A:231:PRO:O	1:A:232:GLU:CG	2.65	0.43
1:B:165:ARG:C	1:B:167:ILE:H	2.22	0.43
1:A:11:TRP:CE2	1:A:29:SER:CB	2.98	0.43
1:B:89:LEU:HB3	1:B:90:LEU:H	1.74	0.43
1:B:210:ALA:O	1:B:221:ASN:HB3	2.18	0.43
2:C:4:DG:H2''	2:C:5:DG:H8	1.83	0.43
2:C:11:DT:H2''	2:C:12:DT:C6	2.54	0.43
1:A:12:ARG:HG3	1:A:25:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:CD1	1:B:147:ILE:HD11	2.48	0.43
1:A:210:ALA:O	1:A:221:ASN:HB3	2.18	0.43
2:C:14:DC:H2''	2:C:15:DT:O5'	2.18	0.43
2:C:18:DC:H2''	2:C:19:DG:O5'	2.19	0.43
3:D:2:DC:O5'	3:D:2:DC:H6	2.01	0.43
1:A:87:MET:CE	1:B:137:LEU:HD23	2.48	0.43
1:A:230:ASP:HB3	1:A:231:PRO:CD	2.48	0.43
1:B:164:LEU:CD2	1:B:168:HIS:HE1	2.29	0.43
1:A:156:VAL:CG2	1:A:205:LEU:CD1	2.97	0.42
1:B:188:ALA:HB2	1:B:198:VAL:HG21	2.00	0.42
1:A:125:THR:O	1:A:129:VAL:HG23	2.19	0.42
1:A:178:LEU:HD23	1:A:218:ILE:O	2.20	0.42
1:A:187:ILE:HA	1:A:190:ILE:HD12	1.99	0.42
1:B:125:THR:O	1:B:129:VAL:HG23	2.19	0.42
1:B:203:LEU:HD21	3:F:10:DG:OP1	2.19	0.42
1:B:83:LEU:HD23	1:B:83:LEU:C	2.40	0.42
1:B:187:ILE:HA	1:B:190:ILE:HD12	2.00	0.42
1:A:28:LEU:CB	1:A:118:LEU:HD21	2.48	0.42
1:A:83:LEU:HD23	1:A:83:LEU:C	2.39	0.42
2:E:4:DG:H2''	2:E:5:DG:OP2	2.19	0.42
2:E:13:DA:H2'	2:E:14:DC:P	2.59	0.42
1:A:141:THR:HG21	4:B:301:PCG:N2	2.34	0.42
1:A:188:ALA:CA	1:A:198:VAL:HG21	2.49	0.42
1:B:230:ASP:HB3	1:B:231:PRO:CD	2.50	0.42
1:A:32:ALA:HA	1:A:109:VAL:O	2.20	0.42
1:A:34:TYR:OH	1:A:106:GLU:OE1	2.26	0.42
1:B:188:ALA:CA	1:B:198:VAL:HG21	2.49	0.42
2:E:13:DA:N6	3:F:6:DT:O4	2.53	0.42
1:A:43:ILE:HD12	1:A:43:ILE:N	2.32	0.41
1:A:78:HIS:HD2	1:A:82:ALA:HB1	1.85	0.41
1:A:158:ARG:HA	1:A:161:LEU:HD12	2.02	0.41
1:B:78:HIS:HD2	1:B:82:ALA:HB1	1.86	0.41
1:B:11:TRP:CE2	1:B:29:SER:CB	2.98	0.41
1:A:137:LEU:HA	1:B:137:LEU:CD1	2.50	0.41
1:A:147:ILE:HD11	1:B:147:ILE:CD1	2.50	0.41
1:A:178:LEU:HD23	1:A:218:ILE:HB	2.02	0.41
2:C:15:DT:H2''	2:C:16:DC:C6	2.55	0.41
1:A:6:ARG:HD2	1:A:6:ARG:N	2.36	0.41
1:A:185:THR:CG2	1:A:195:ARG:CD	2.97	0.41
1:A:203:LEU:HD11	3:D:10:DG:H5'	2.01	0.41
1:B:32:ALA:HA	1:B:109:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HD13	1:B:99:ALA:HA	2.02	0.41
1:B:8:SER:OG	1:B:10:PHE:HB3	2.21	0.41
1:B:150:TYR:HB3	1:B:154:ALA:HB3	2.03	0.41
1:A:153:ASN:O	1:A:156:VAL:HG22	2.21	0.41
1:A:185:THR:HG23	1:A:195:ARG:HD3	2.01	0.41
1:A:188:ALA:CB	1:A:198:VAL:HG21	2.51	0.41
1:A:211:ILE:O	1:A:211:ILE:HG13	2.21	0.41
1:B:156:VAL:CG2	1:B:205:LEU:CD1	2.97	0.41
1:B:184:GLN:CD	3:F:9:DT:H5''	2.40	0.41
1:A:27:GLU:CB	1:A:28:LEU:CD2	2.99	0.41
1:A:221:ASN:HD21	1:A:224:ARG:HG3	1.80	0.41
1:B:43:ILE:HD12	1:B:43:ILE:N	2.32	0.41
3:F:11:DT:H2'	3:F:12:DT:C6	2.55	0.41
1:A:66:PHE:CZ	1:A:70:GLY:HA2	2.56	0.40
1:B:153:ASN:O	1:B:156:VAL:HG22	2.21	0.40
1:A:63:LEU:HD13	1:A:99:ALA:HA	2.02	0.40
1:A:127:GLU:HG2	1:A:128:ALA:N	2.33	0.40
1:A:150:TYR:HB3	1:A:154:ALA:HB3	2.03	0.40
1:B:57:VAL:HG22	1:B:106:GLU:O	2.22	0.40
3:D:2:DC:H6	3:D:2:DC:C5'	2.34	0.40
3:D:11:DT:H2''	3:D:12:DT:C5'	2.51	0.40
1:B:32:ALA:HB1	1:B:108:TYR:HB3	2.04	0.40
1:B:118:LEU:HD12	1:B:118:LEU:HA	1.87	0.40
1:B:158:ARG:HA	1:B:161:LEU:HD12	2.02	0.40
1:A:57:VAL:HG22	1:A:106:GLU:O	2.22	0.40
3:F:12:DT:C2'	3:F:13:DA:C8	3.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLY:O	1:A:177:ASN:ND2[4_555]	1.88	0.32

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	225/244 (92%)	198 (88%)	19 (8%)	8 (4%)	3	19
1	B	224/244 (92%)	198 (88%)	19 (8%)	7 (3%)	4	22
All	All	449/488 (92%)	396 (88%)	38 (8%)	15 (3%)	4	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	172	MET
1	B	9	ALA
1	B	28	LEU
1	B	172	MET
1	A	215	ASP
1	B	27	GLU
1	B	215	ASP
1	A	89	LEU
1	B	89	LEU
1	A	27	GLU
1	A	231	PRO
1	A	173	PRO
1	B	173	PRO
1	A	167	ILE

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	181/201 (90%)	178 (98%)	3 (2%)	60	83
1	B	180/201 (90%)	177 (98%)	3 (2%)	60	83
All	All	361/402 (90%)	355 (98%)	6 (2%)	60	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ARG
1	A	215	ASP
1	A	226	LEU
1	B	143	ARG
1	B	215	ASP
1	B	226	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	168	HIS
1	A	199	ASN
1	A	221	ASN
1	B	78	HIS
1	B	168	HIS
1	B	199	ASN
1	B	221	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
4	PCG	B	301	1	22,26,26	7.29	17 (77%)	25,41,41	3.28	14 (56%)
4	PCG	A	301	1	22,26,26	7.33	18 (81%)	25,41,41	3.34	16 (64%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCG	B	301	1	-	0/0/31/31	0/4/4/4
4	PCG	A	301	1	-	0/0/31/31	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	PCG	PA-O5'	15.50	1.75	1.57
4	B	301	PCG	PA-O5'	15.50	1.75	1.57
4	A	301	PCG	C2'-C3'	-14.80	1.19	1.52
4	B	301	PCG	C2'-C3'	-14.80	1.19	1.52
4	A	301	PCG	O4'-C1'	14.70	1.61	1.41
4	B	301	PCG	O4'-C1'	14.70	1.61	1.41
4	B	301	PCG	C3'-C4'	10.61	1.81	1.52
4	A	301	PCG	C3'-C4'	10.61	1.81	1.52
4	A	301	PCG	C2'-C1'	9.14	1.67	1.53
4	B	301	PCG	C2'-C1'	9.14	1.67	1.53
4	B	301	PCG	PA-O3'	8.53	1.71	1.57
4	A	301	PCG	PA-O3'	8.52	1.71	1.57
4	B	301	PCG	O5'-C5'	7.19	1.56	1.46
4	A	301	PCG	O5'-C5'	7.19	1.56	1.46
4	A	301	PCG	O4'-C4'	-6.75	1.29	1.45
4	B	301	PCG	O4'-C4'	-6.75	1.29	1.45
4	A	301	PCG	C2-N3	5.46	1.46	1.33
4	B	301	PCG	C2-N3	5.46	1.46	1.33
4	B	301	PCG	C4-N3	4.71	1.48	1.37
4	A	301	PCG	C4-N3	4.71	1.48	1.37
4	B	301	PCG	C2-N2	4.49	1.44	1.34
4	A	301	PCG	C2-N2	4.49	1.44	1.34
4	A	301	PCG	PA-O2A	3.89	1.64	1.50
4	A	301	PCG	C6-N1	3.69	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	PCG	C6-N1	3.68	1.43	1.37
4	B	301	PCG	C5-C6	3.03	1.53	1.47
4	A	301	PCG	C5-C6	3.03	1.53	1.47
4	A	301	PCG	C2-N1	2.79	1.44	1.37
4	B	301	PCG	C2-N1	2.79	1.44	1.37
4	B	301	PCG	O2'-C2'	2.59	1.49	1.43
4	A	301	PCG	O2'-C2'	2.59	1.49	1.43
4	A	301	PCG	C5-C4	-2.48	1.36	1.43
4	B	301	PCG	C5-C4	-2.48	1.36	1.43
4	A	301	PCG	C5'-C4'	2.28	1.55	1.51
4	B	301	PCG	C5'-C4'	2.28	1.55	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	PCG	O3'-C3'-C2'	7.74	123.19	115.61
4	A	301	PCG	O3'-C3'-C2'	7.73	123.19	115.61
4	A	301	PCG	O5'-C5'-C4'	6.87	121.74	105.71
4	B	301	PCG	O5'-C5'-C4'	6.87	121.74	105.71
4	A	301	PCG	O5'-PA-O3'	6.30	114.36	105.68
4	B	301	PCG	O5'-PA-O3'	6.30	114.36	105.68
4	A	301	PCG	O3'-C3'-C4'	4.68	114.24	110.71
4	B	301	PCG	O3'-C3'-C4'	4.68	114.24	110.71
4	A	301	PCG	C5'-C4'-C3'	-3.82	104.75	112.49
4	B	301	PCG	C5'-C4'-C3'	-3.82	104.75	112.49
4	A	301	PCG	C2-N1-C6	-3.46	118.73	125.10
4	B	301	PCG	C2-N1-C6	-3.46	118.73	125.10
4	A	301	PCG	O1A-PA-O2A	-3.32	98.33	108.73
4	B	301	PCG	O1A-PA-O2A	-3.32	98.33	108.73
4	B	301	PCG	C5-C6-N1	3.22	119.63	113.95
4	A	301	PCG	C5-C6-N1	3.22	119.63	113.95
4	A	301	PCG	O4'-C4'-C5'	3.11	121.66	112.37
4	B	301	PCG	O4'-C4'-C5'	3.11	121.66	112.37
4	B	301	PCG	C2'-C3'-C4'	2.79	108.17	103.22
4	A	301	PCG	C2'-C3'-C4'	2.79	108.17	103.22
4	A	301	PCG	O4'-C1'-C2'	-2.71	102.96	106.93
4	B	301	PCG	O4'-C1'-C2'	-2.71	102.96	106.93
4	A	301	PCG	C3'-C2'-C1'	2.64	105.74	99.89
4	B	301	PCG	C3'-C2'-C1'	2.64	105.74	99.89
4	A	301	PCG	O1A-PA-O5'	2.48	113.20	107.16
4	A	301	PCG	O1A-PA-O3'	2.46	112.76	107.04
4	A	301	PCG	C8-N7-C5	2.38	107.53	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	PCG	C8-N7-C5	2.38	107.52	102.99
4	B	301	PCG	O6-C6-C5	-2.37	119.73	124.37
4	A	301	PCG	O6-C6-C5	-2.37	119.74	124.37

There are no chirality outliers.

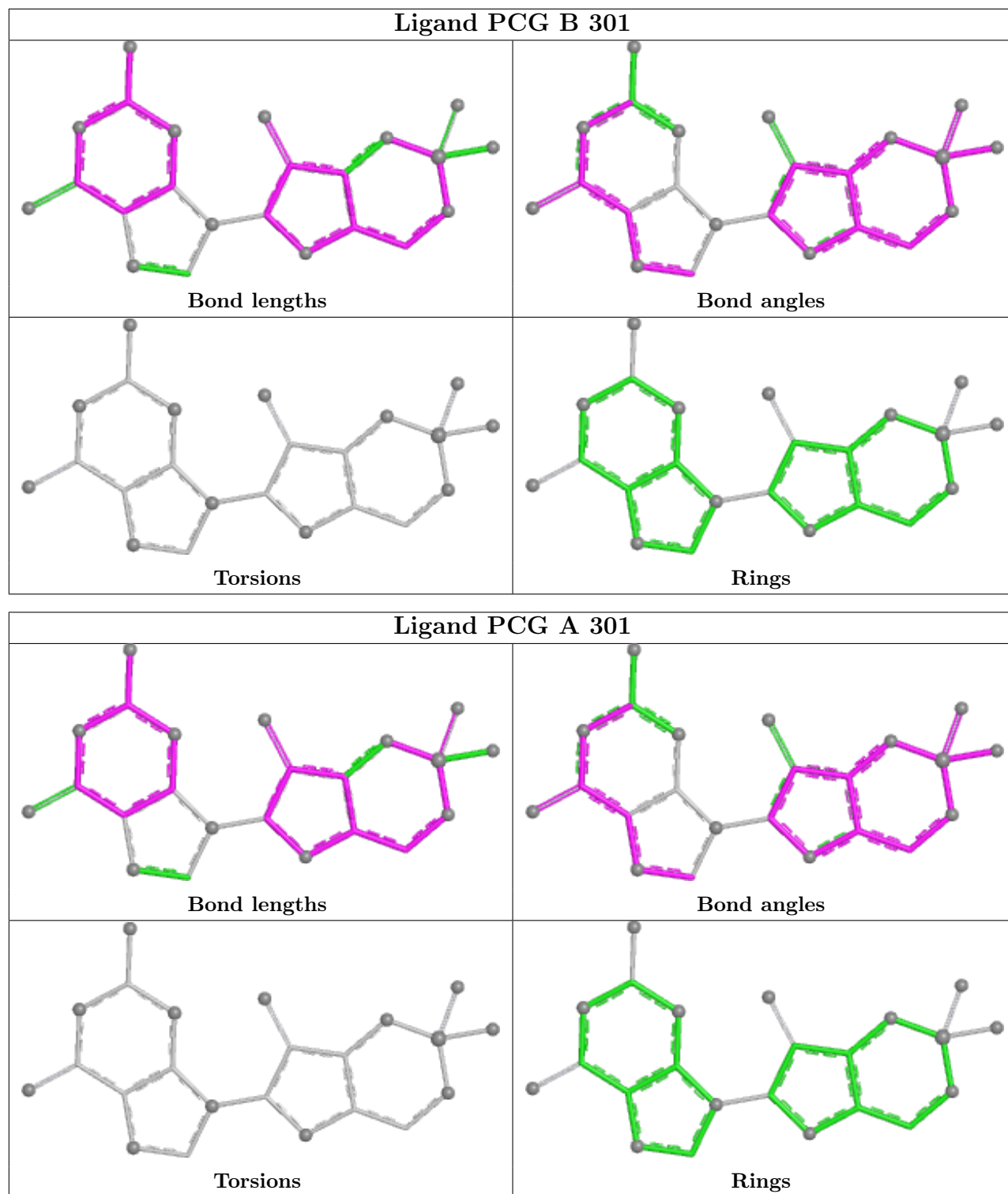
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	PCG	6	0
4	A	301	PCG	5	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	13:DA	O3'	14:DC	P	4.56

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	227/244 (93%)	0.19	6 (2%) 56 33	66, 93, 128, 154	0
1	B	226/244 (92%)	1.03	40 (17%) 1 0	89, 138, 169, 194	0
2	C	19/19 (100%)	-0.40	0 100 100	102, 131, 178, 182	0
2	E	14/19 (73%)	-0.39	0 100 100	124, 144, 170, 176	0
3	D	14/14 (100%)	-0.50	0 100 100	90, 123, 167, 173	0
3	F	10/14 (71%)	-0.30	0 100 100	118, 140, 186, 193	0
All	All	510/554 (92%)	0.49	46 (9%) 9 3	66, 117, 167, 194	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	ASP	16.7
1	B	216	GLY	9.0
1	B	83	LEU	7.0
1	B	77	GLN	5.9
1	B	56	VAL	4.7
1	B	224	ARG	4.4
1	B	78	HIS	4.0
1	B	217	ILE	3.9
1	B	179	ARG	3.7
1	A	149	LEU	3.6
1	B	60	ARG	3.6
1	B	220	CYS	3.5
1	B	107	GLY	3.4
1	B	11	TRP	3.4
1	B	17	PHE	3.3
1	B	61	ILE	3.3
1	B	16	ILE	3.3
1	B	199	ASN	3.2
1	B	84	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	22	SER	3.2
1	A	7	SER	3.1
1	B	214	ALA	3.1
1	B	34	TYR	3.1
1	B	25	LEU	3.0
1	B	13	SER	3.0
1	B	55	VAL	2.8
1	B	15	PRO	2.8
1	B	211	ILE	2.7
1	B	228	ILE	2.6
1	B	212	LYS	2.6
1	B	100	THR	2.6
1	B	70	GLY	2.5
1	B	160	PHE	2.5
1	B	166	GLN	2.4
1	B	175	SER	2.3
1	B	74	MET	2.3
1	A	146	THR	2.3
1	B	108	TYR	2.3
1	B	57	VAL	2.3
1	A	66	PHE	2.3
1	A	72	GLU	2.2
1	B	82	ALA	2.2
1	A	145	GLU	2.1
1	B	168	HIS	2.1
1	B	109	VAL	2.1
1	B	115	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

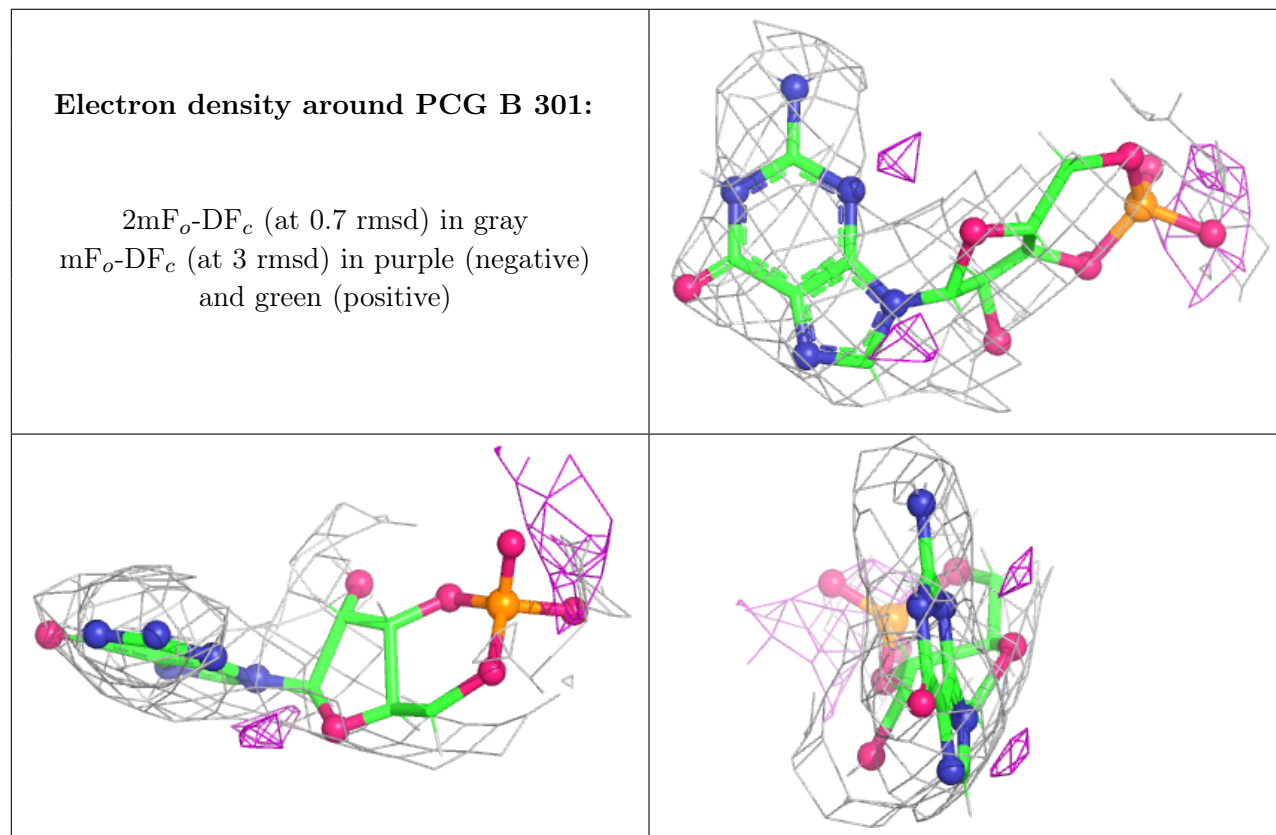
6.4 Ligands [i](#)

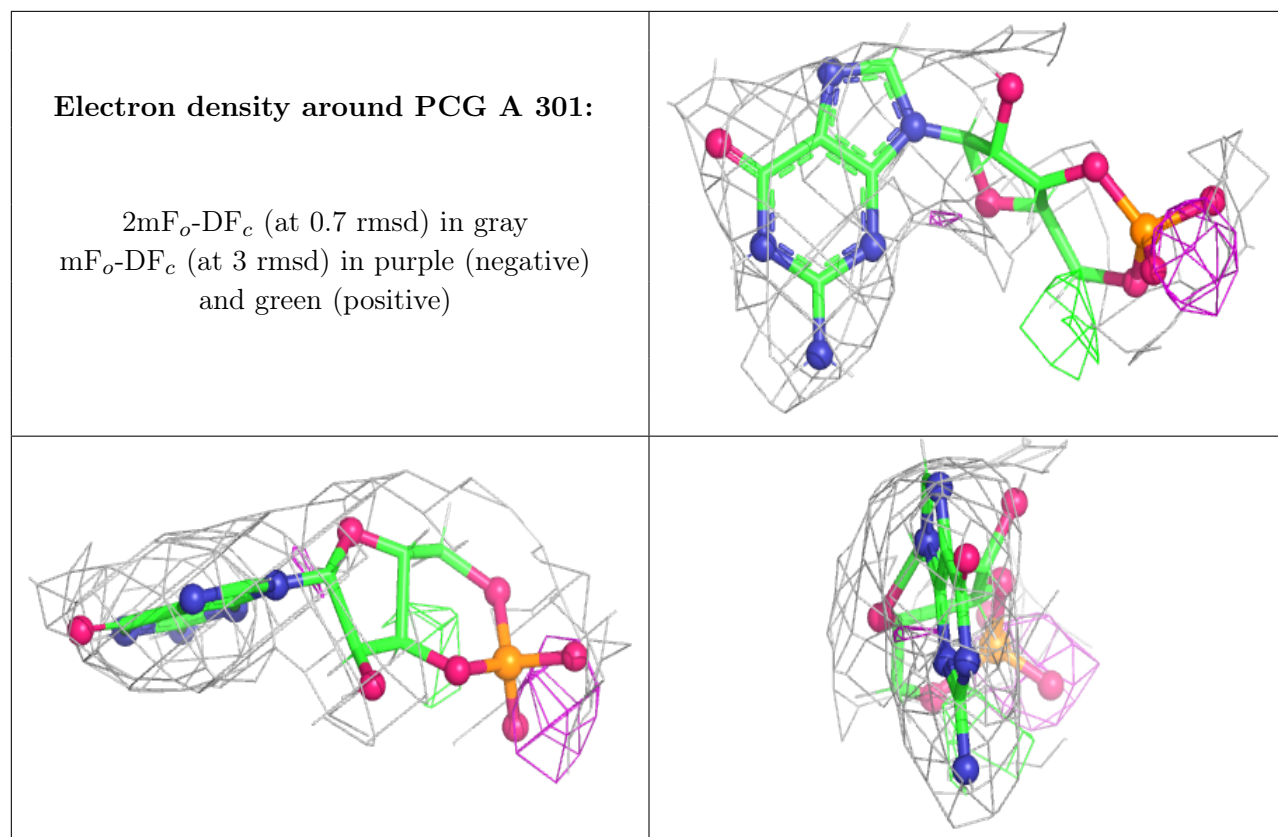
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
4	PCG	B	301	23/23	0.87	0.24	34,96,131,141	0
4	PCG	A	301	23/23	0.88	0.24	32,77,102,116	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.