



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:20 PM UTC

PDB ID : 1O3T / pdb_00001o3t
Title : PROTEIN-DNA RECOGNITION AND DNA DEFORMATION REVEALED
IN CRYSTAL STRUCTURES OF CAP-DNA COMPLEXES
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Deposited on : 2003-03-18
Resolution : 2.80 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

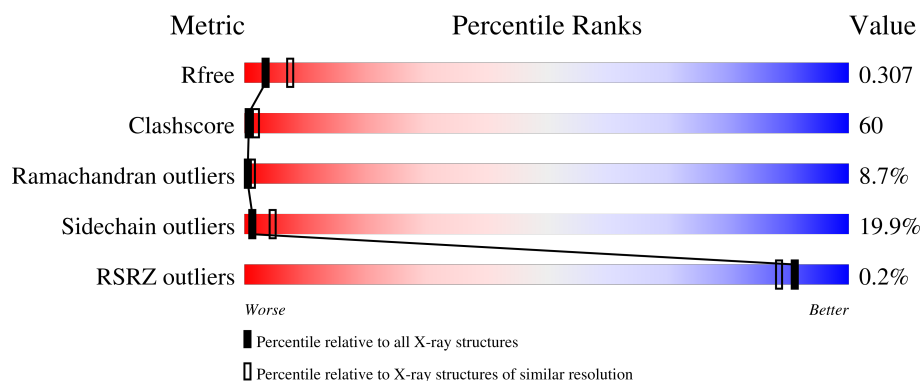
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	C	14	100%
1	F	14	14% 86%
2	D	17	12% 82% 6%
2	E	17	18% 76% 6%
3	A	200	26% 45% 28%

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Mol	Chain	Length	Quality of chain
3	B	200	 A horizontal bar chart showing the quality of chain 3. The bar is divided into three segments: green (19%), yellow (54%), and orange (22%). The segments are labeled with their respective percentages. The bar ends with a small red segment and two dots.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CMP	B	761	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4491 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 DNA chain called 5'-D(*GP*CP*GP*AP*AP*AP*AP*AP*TP*GP*CP*GP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	14	Total	C	N	O	P	0	0	0
			289	138	60	78	13			
1	F	14	Total	C	N	O	P	0	0	0
			289	138	60	78	13			

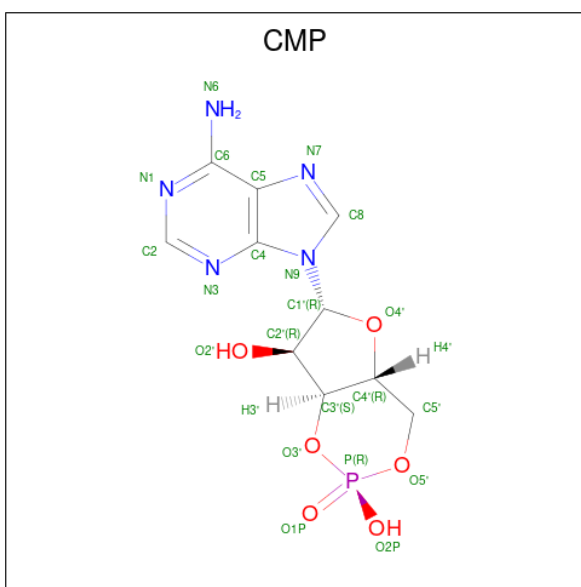
- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*GP*AP*TP*CP*GP*CP*AP*TP*TP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	P	0	0	0
			342	166	56	104	16			
2	E	17	Total	C	N	O	P	0	0	0
			342	166	56	104	16			

- Molecule 3 is a protein called CATABOLITE GENE ACTIVATOR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	199	Total	C	N	O	S	0	0	0
			1573	997	275	292	9			
3	B	197	Total	C	N	O	S	0	0	0
			1556	986	273	288	9			

- Molecule 4 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: C₁₀H₁₂N₅O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

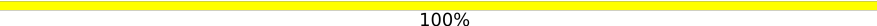
- Molecule 5 is water.

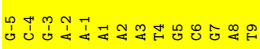
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total	O	0	0
			4	4		
5	D	7	Total	O	0	0
			7	7		
5	E	5	Total	O	0	0
			5	5		
5	F	2	Total	O	0	0
			2	2		
5	A	19	Total	O	0	0
			19	19		
5	B	19	Total	O	0	0
			19	19		

3 Residue-property plots

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

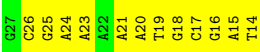
- Molecule 1: 5'-D(*GP*CP*GP*AP*AP*AP*AP*AP*TP*GP*CP*GP*AP*T)-3'

Chain C:  100%


G-5 C-4 G-3 A-2 A-1 A1 A2 A3 T4 T5 G6 G7 G8 T9

- Molecule 1: 5'-D(*GP*CP*GP*AP*AP*AP*AP*AP*TP*GP*CP*GP*AP*T)-3'

Chain F:  14% 86%


G27 C26 G25 A24 A23 A22 A21 A20 T19 T18 G18 C17 G16 A15 T14

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

Chain D:  12% 82% 6%

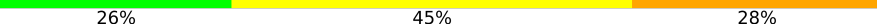

G13 T12 A11 G10 A9 T8 C7 G6 C5 A4 T3 T2 T1 T-1 T-2 C-3 G-4

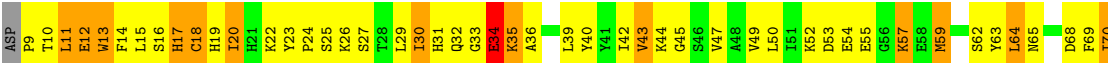
- Molecule 2: 5'-D(*CP*TP*AP*GP*AP*TP*CP*GP*CP*AP*TP*TP*TP*TP*TP*CP*G)-3',

Chain E:  18% 76% 6%

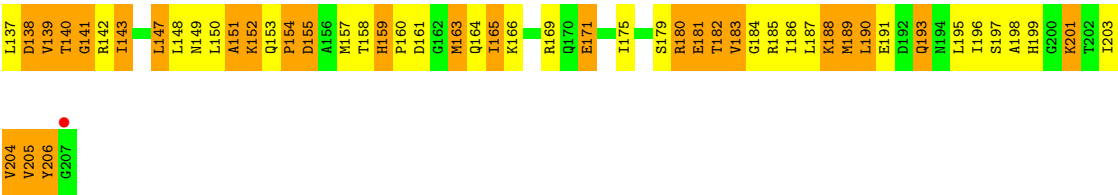

G10 T11 A12 G13 A14 T15 C16 G17 C18 A19 T20 T21 T22 C25 G26

- Molecule 3: CATABOLITE GENE ACTIVATOR PROTEIN

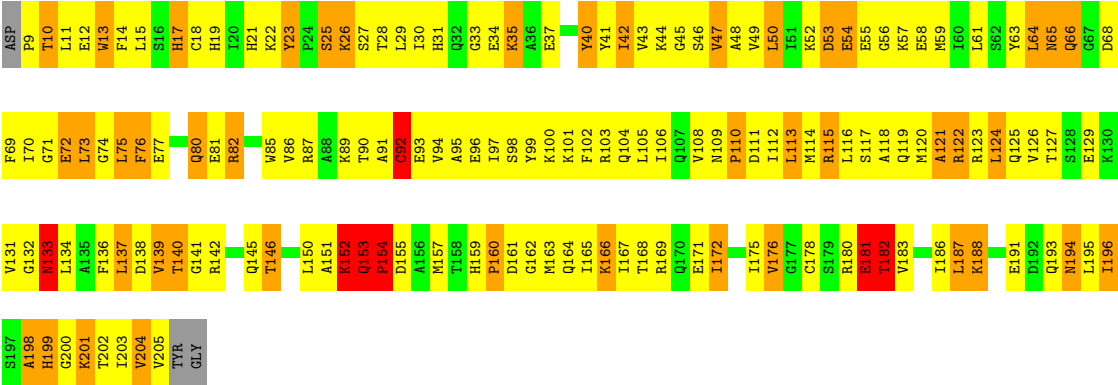
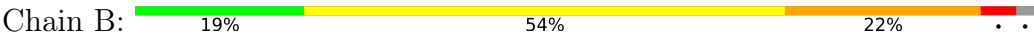
Chain A:  26% 45% 28%


ASP P9 T10 L73 L11 E12 M13 F14 L15 S16 H17 Q80 E81 R82 S83 A84 W85 A88 E83 V94 I97 S98 Y99 K100 K101 F102 R103 A36 I106 Q107 Y108 M109 P110 D111 I112 L113 M114 R115 L116 S117 A118 Q119 K120 D121 R122 E123 L124 Q125 V126 E127 S128 E129 K130 Y131 V132 G133 N133 L134 A135 F136


G71 E72 G74 L75 F76 E77 E78 G79 Q80 E81 R82 S83 A84 W85 A88 E83 V94 I97 S98 Y99 K100 K101 F102 R103 A36 I106 Q107 Y108 M109 P110 D111 I112 L113 M114 R115 L116 S117 A118 Q119 K120 D121 R122 E123 L124 Q125 V126 E127 S128 E129 K130 Y131 V132 G133 N133 L134 A135 F136



● Molecule 3: CATABOLITE GENE ACTIVATOR PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	136.99Å 152.80Å 76.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	72.2 (20.00-2.80) 72.0 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 2.48Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.230 , 0.303 0.228 , 0.307	Depositor DCC
R_{free} test set	919 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 96.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4491	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CMP

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	C	0.32	0/326	0.68	0/502
1	F	0.36	0/326	0.77	0/502
2	D	0.35	0/381	0.88	2/586 (0.3%)
2	E	0.37	0/381	0.91	1/586 (0.2%)
3	A	0.70	0/1598	1.24	23/2150 (1.1%)
3	B	0.74	0/1580	1.26	23/2127 (1.1%)
All	All	0.63	0/4592	1.13	49/6453 (0.8%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	153	GLN	CA-C-N	9.02	131.12	119.84
3	B	153	GLN	C-N-CA	9.02	131.12	119.84
3	A	143	ILE	N-CA-C	-8.94	104.12	111.81
3	B	50	LEU	N-CA-C	8.90	123.03	109.23
3	B	133	ASN	N-CA-C	7.75	119.80	111.36
3	A	12	GLU	N-CA-C	-7.25	103.38	111.71
3	A	93	GLU	N-CA-C	-7.14	96.76	108.41
3	A	13	TRP	N-CA-C	-6.95	103.63	111.14
3	A	159	HIS	N-CA-C	-6.94	101.37	110.39
3	B	182	THR	N-CA-C	-6.93	96.03	110.80
3	B	131	VAL	N-CA-C	-6.93	103.72	110.72
3	B	151	ALA	N-CA-C	-6.92	104.81	113.18
3	B	113	LEU	N-CA-C	-6.79	103.67	112.23
3	B	198	ALA	N-CA-C	6.77	119.73	109.23
3	A	179	SER	N-CA-C	6.75	120.52	110.52
3	B	132	GLY	N-CA-C	-6.65	104.75	112.73
3	B	172	ILE	N-CA-C	-6.47	104.21	110.42
3	A	126	VAL	N-CA-C	6.41	116.45	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	109	ASN	CA-C-N	6.31	127.73	119.84
3	A	109	ASN	C-N-CA	6.31	127.73	119.84
3	A	23	TYR	CA-C-N	6.27	126.76	119.99
3	A	23	TYR	C-N-CA	6.27	126.76	119.99
3	A	120	MET	N-CA-C	-6.20	103.83	111.33
3	B	65	ASN	N-CA-C	6.18	116.59	108.07
3	A	164	GLN	N-CA-C	6.16	119.52	107.57
3	A	30	ILE	N-CA-C	6.16	117.56	108.45
3	A	83	SER	N-CA-C	6.13	120.62	113.20
3	B	10	THR	N-CA-C	-5.99	104.09	111.40
3	B	92	CYS	N-CA-C	5.94	119.08	109.40
3	B	23	TYR	CA-C-N	5.86	127.25	120.98
3	B	23	TYR	C-N-CA	5.86	127.25	120.98
3	A	118	ALA	N-CA-C	-5.72	106.30	113.28
3	B	17	HIS	N-CA-C	-5.56	106.39	114.12
3	A	171	GLU	N-CA-C	-5.55	105.13	111.07
2	D	5	DC	N1-C1'-C2'	5.51	121.77	113.50
3	A	193	GLN	N-CA-C	-5.48	105.85	112.54
3	A	180	ARG	N-CA-C	-5.44	104.59	111.11
3	A	69	PHE	N-CA-C	-5.42	101.74	110.14
3	B	109	ASN	CA-C-N	5.40	126.59	119.84
3	B	109	ASN	C-N-CA	5.40	126.59	119.84
2	D	-3	DC	N1-C1'-C2'	5.33	121.50	113.50
3	A	130	LYS	N-CA-C	-5.25	105.45	111.07
3	B	76	PHE	N-CA-C	5.24	119.95	113.50
3	B	122	ARG	N-CA-C	-5.24	105.63	112.23
3	B	181	GLU	N-CA-C	5.24	117.47	109.62
3	B	94	VAL	N-CA-C	5.07	115.27	108.17
3	A	190	LEU	N-CA-C	-5.06	105.27	111.75
2	E	18	DC	N1-C1'-C2'	5.05	121.08	113.50
3	A	54	GLU	N-CA-C	5.02	121.49	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	C	289	0	158	34	0
1	F	289	0	158	24	0
2	D	342	0	196	31	0
2	E	342	0	196	28	0
3	A	1573	0	1612	183	0
3	B	1556	0	1600	226	0
4	A	22	0	11	3	0
4	B	22	0	11	7	0
5	A	19	0	0	2	0
5	B	19	0	0	4	0
5	C	4	0	0	1	0
5	D	7	0	0	1	0
5	E	5	0	0	0	0
5	F	2	0	0	0	0
All	All	4491	0	3942	504	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 60.

All (504) 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:A:762:CMP:C2	4:A:762:CMP:H2	0.97	1.49
4:B:761:CMP:C2	4:B:761:CMP:H2	0.97	1.48
1:F:26:DC:H2''	1:F:25:DG:H5''	1.24	1.17
3:B:196:ILE:HG22	3:B:204:VAL:HA	1.25	1.15
3:B:115:ARG:HB2	3:B:115:ARG:HH11	1.04	1.06
3:A:36:ALA:HB2	3:A:82:ARG:HD3	1.43	1.00
3:B:106:ILE:HD13	3:B:113:LEU:HD13	1.44	0.99
3:B:115:ARG:HB2	3:B:115:ARG:NH1	1.80	0.96
3:A:153:GLN:HG2	3:A:154:PRO:HD2	1.46	0.95
3:B:50:LEU:HD12	3:B:85:TRP:HB2	1.47	0.95
3:A:75:LEU:O	3:A:75:LEU:HD22	1.67	0.95
1:C:9:DT:C2'	2:E:10:DC:H5''	1.99	0.91
2:D:11:DA:H2''	2:D:10:DG:H5''	1.50	0.90
1:F:26:DC:H2''	1:F:25:DG:C5'	2.02	0.89
1:C:9:DT:H2''	2:E:10:DC:H5''	1.56	0.87
1:C:5:DG:H2''	1:C:6:DC:H5''	1.56	0.87
1:F:26:DC:C2'	1:F:25:DG:H5''	2.05	0.86
3:B:122:ARG:HH22	3:B:125:GLN:NE2	1.73	0.85
3:A:106:ILE:CG2	3:A:113:LEU:HD12	2.06	0.84
3:B:116:LEU:HD23	3:B:117:SER:H	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:DC:O5'	1:F:14:DT:H2''	1.76	0.84
3:A:36:ALA:CB	3:A:82:ARG:HD3	2.08	0.84
1:C:1:DA:H1'	1:C:2:DA:H5''	1.60	0.83
3:B:182:THR:O	3:B:186:ILE:HG12	1.78	0.83
2:E:20:DT:H2''	2:E:21:DT:H5'	1.62	0.81
3:B:30:ILE:HD11	4:B:761:CMP:H5'2	1.62	0.81
3:B:69:PHE:H	3:B:119:GLN:HE22	1.29	0.81
3:A:11:LEU:HD23	3:A:115:ARG:HH12	1.46	0.80
3:B:42:ILE:HD11	3:B:70:ILE:HD11	1.62	0.80
3:A:125:GLN:HG2	3:B:73:LEU:HD13	1.62	0.80
3:A:188:LYS:O	3:A:191:GLU:HB3	1.81	0.80
3:B:19:HIS:O	3:B:95:ALA:HA	1.81	0.78
3:A:204:VAL:HG22	3:A:205:VAL:HG23	1.65	0.78
2:E:13:DG:H2''	2:E:14:DA:OP2	1.84	0.78
3:A:43:VAL:HG22	3:A:93:GLU:HB3	1.65	0.78
3:A:191:GLU:HG3	3:A:197:SER:HA	1.64	0.77
1:C:-1:DA:H2''	1:C:1:DA:OP2	1.85	0.77
3:B:41:TYR:HB3	3:B:95:ALA:HB3	1.67	0.77
3:B:46:SER:N	3:B:92:CYS:SG	2.57	0.77
1:F:15:DA:H2''	1:F:14:DT:H5''	1.65	0.77
1:C:5:DG:H2''	1:C:6:DC:C5'	2.14	0.76
3:B:146:THR:O	3:B:150:LEU:HG	1.85	0.76
3:A:13:TRP:O	3:A:16:SER:HB3	1.85	0.76
3:B:165:ILE:HG22	3:B:166:LYS:N	2.01	0.76
3:B:204:VAL:HG12	3:B:204:VAL:O	1.83	0.76
3:B:9:PRO:O	3:B:12:GLU:HB2	1.84	0.76
3:B:13:TRP:CZ2	3:B:105:LEU:HB3	2.21	0.76
3:B:199:HIS:C	3:B:201:LYS:H	1.93	0.76
3:B:69:PHE:HB2	3:B:119:GLN:HE22	1.52	0.75
3:A:149:ASN:HA	3:A:152:LYS:HZ1	1.52	0.75
3:B:136:PHE:O	3:B:137:LEU:HD13	1.87	0.74
3:B:110:PRO:HG2	3:B:111:ASP:H	1.53	0.74
3:A:11:LEU:HD23	3:A:115:ARG:NH1	2.03	0.74
3:B:69:PHE:HB2	3:B:119:GLN:NE2	2.02	0.74
3:B:45:GLY:HA3	3:B:92:CYS:SG	2.28	0.73
3:B:90:THR:HG22	3:B:91:ALA:H	1.52	0.73
3:A:153:GLN:HG2	3:A:154:PRO:CD	2.18	0.73
3:A:39:LEU:HD11	3:A:72:GLU:HB3	1.70	0.73
3:A:106:ILE:HG21	3:A:113:LEU:HD12	1.68	0.73
2:E:25:DC:H2''	2:E:26:DG:OP2	1.88	0.73
3:B:12:GLU:HA	3:B:15:LEU:HD12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:120:MET:O	3:B:120:MET:HG3	1.89	0.72
3:B:11:LEU:HD13	3:B:15:LEU:HD11	1.70	0.72
3:B:193:GLN:O	3:B:194:ASN:HB2	1.89	0.72
3:A:196:ILE:HG22	3:A:204:VAL:HA	1.70	0.72
1:F:20:DA:H1'	1:F:19:DT:H5''	1.69	0.72
1:F:15:DA:C2'	1:F:14:DT:H5''	2.19	0.71
3:A:64:LEU:HD23	3:A:70:ILE:HG23	1.72	0.71
1:C:5:DG:C2'	1:C:6:DC:H5''	2.20	0.71
2:E:18:DC:H1'	2:E:19:DA:N7	2.06	0.71
3:A:65:ASN:N	3:A:68:ASP:OD2	2.24	0.71
2:D:5:DC:H1'	2:D:4:DA:N7	2.06	0.70
1:C:6:DC:H2''	1:C:7:DG:H5''	1.73	0.70
3:A:73:LEU:HD23	3:B:125:GLN:HG3	1.72	0.70
3:B:102:PHE:O	3:B:105:LEU:HB2	1.91	0.70
2:D:5:DC:H1'	2:D:4:DA:C8	2.27	0.70
3:B:35:LYS:H	3:B:81:GLU:HB2	1.56	0.70
3:B:122:ARG:NH2	3:B:125:GLN:CD	2.49	0.70
2:D:9:DA:H2''	2:D:8:DT:H5'	1.73	0.69
2:E:20:DT:H2'	2:E:21:DT:H71	1.75	0.69
3:A:151:ALA:O	3:A:163:MET:HE2	1.92	0.69
3:B:31:HIS:O	3:B:82:ARG:HG3	1.93	0.69
2:D:3:DT:H2''	2:D:2:DT:C6	2.28	0.69
3:B:42:ILE:CD1	3:B:70:ILE:HD11	2.22	0.69
3:A:154:PRO:O	3:A:155:ASP:HB3	1.90	0.68
3:A:97:ILE:HD12	3:A:97:ILE:H	1.58	0.68
3:A:97:ILE:HD12	3:A:97:ILE:N	2.09	0.68
3:B:102:PHE:HA	3:B:105:LEU:HD12	1.75	0.68
3:B:115:ARG:HH11	3:B:115:ARG:CB	1.94	0.68
2:E:19:DA:H2''	2:E:20:DT:H5''	1.75	0.67
3:B:68:ASP:HA	3:B:119:GLN:OE1	1.95	0.67
3:B:69:PHE:CB	3:B:119:GLN:HE22	2.08	0.67
3:B:40:TYR:CD1	3:B:40:TYR:N	2.62	0.66
3:B:201:LYS:O	3:B:201:LYS:HG2	1.94	0.66
1:C:4:DT:H2''	1:C:5:DG:H5'	1.77	0.66
2:D:1:DT:H2''	2:D:-1:DT:OP2	1.94	0.66
1:F:16:DG:H2''	1:F:15:DA:N7	2.11	0.66
2:D:13:DC:H5'	1:F:14:DT:O3'	1.95	0.66
2:D:11:DA:C2'	2:D:10:DG:H5''	2.23	0.66
3:A:47:VAL:HG12	3:A:88:ALA:HA	1.77	0.66
3:B:69:PHE:HD2	3:B:119:GLN:NE2	1.94	0.66
3:A:50:LEU:HB2	3:A:59:MET:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:26:LYS:HE2	3:B:87:ARG:HH11	1.61	0.65
3:B:50:LEU:HD21	3:B:87:ARG:HH21	1.60	0.65
3:B:75:LEU:HD12	3:B:75:LEU:O	1.95	0.65
1:C:2:DA:H2''	1:C:3:DA:H8	1.62	0.65
3:A:98:SER:OG	3:A:101:LYS:HB2	1.97	0.65
3:B:165:ILE:HG22	3:B:166:LYS:H	1.61	0.65
2:D:3:DT:H2'	2:D:2:DT:H71	1.79	0.65
3:B:199:HIS:HD2	3:B:201:LYS:HZ2	1.42	0.65
3:A:106:ILE:HG23	3:A:113:LEU:HD12	1.77	0.65
2:D:10:DG:H3'	3:A:182:THR:HG21	1.79	0.65
3:B:168:THR:O	3:B:171:GLU:HB3	1.97	0.65
2:E:15:DT:H72	3:B:181:GLU:HG3	1.78	0.64
3:A:117:SER:HA	3:A:120:MET:HE3	1.80	0.64
3:B:172:ILE:O	3:B:176:VAL:HG23	1.97	0.64
3:A:149:ASN:HA	3:A:152:LYS:NZ	2.12	0.64
3:A:57:LYS:HE2	3:A:57:LYS:HA	1.79	0.64
3:A:78:GLU:HA	3:A:78:GLU:OE1	1.98	0.64
3:B:35:LYS:N	3:B:81:GLU:HB2	2.12	0.64
3:A:42:ILE:HD11	3:A:70:ILE:CD1	2.28	0.64
1:F:15:DA:H1'	1:F:14:DT:H5''	1.79	0.63
3:B:199:HIS:HD2	3:B:201:LYS:NZ	1.96	0.63
3:A:62:SER:OG	3:A:63:TYR:N	2.30	0.63
3:A:42:ILE:HD11	3:A:70:ILE:HD13	1.79	0.63
3:A:116:LEU:CD2	3:A:120:MET:HE2	2.28	0.63
3:A:169:ARG:HG2	3:A:183:VAL:HG12	1.79	0.63
3:B:10:THR:C	3:B:12:GLU:H	2.06	0.63
3:B:122:ARG:NH2	3:B:125:GLN:NE2	2.44	0.63
3:B:159:HIS:CG	3:B:160:PRO:HD2	2.33	0.63
3:B:69:PHE:H	3:B:119:GLN:NE2	1.95	0.63
3:B:159:HIS:CD2	3:B:160:PRO:HD2	2.34	0.63
3:B:198:ALA:O	3:B:199:HIS:HB2	1.99	0.63
2:E:19:DA:H2''	2:E:20:DT:C5'	2.28	0.62
1:F:25:DG:H2''	1:F:24:DA:C8	2.34	0.62
3:A:124:LEU:HD22	3:B:73:LEU:HD11	1.81	0.62
1:C:9:DT:H2''	2:E:10:DC:C5'	2.29	0.62
3:B:21:HIS:CD2	3:B:96:GLU:HG3	2.34	0.62
3:A:109:ASN:C	3:A:109:ASN:HD22	2.07	0.62
3:B:162:GLY:C	3:B:163:MET:HE2	2.25	0.62
3:A:33:GLY:O	3:A:81:GLU:HB3	2.00	0.62
3:A:116:LEU:O	3:A:119:GLN:HB2	1.99	0.62
2:E:21:DT:H2'	2:E:22:DT:H71	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:DT:C6	2:D:-1:DT:H72	2.34	0.61
3:B:33:GLY:N	3:B:82:ARG:HB2	2.14	0.61
3:A:181:GLU:O	3:A:183:VAL:N	2.33	0.61
3:A:181:GLU:HB3	3:A:185:ARG:HD3	1.82	0.61
3:B:44:LYS:HZ1	3:B:91:ALA:HB3	1.64	0.61
3:B:162:GLY:O	3:B:163:MET:HE2	2.00	0.61
1:F:19:DT:OP1	3:B:169:ARG:N	2.34	0.61
3:B:13:TRP:HZ2	3:B:105:LEU:HB3	1.64	0.61
2:E:19:DA:C2'	2:E:20:DT:H5''	2.30	0.61
3:A:124:LEU:C	3:A:124:LEU:HD23	2.25	0.61
3:B:164:GLN:HG3	3:B:203:ILE:CD1	2.31	0.61
3:A:77:GLU:HB2	3:A:80:GLN:HE22	1.66	0.61
3:A:122:ARG:CZ	3:A:122:ARG:HB2	2.29	0.61
2:D:4:DA:H1'	2:D:3:DT:H5''	1.83	0.60
2:D:9:DA:OP2	3:A:182:THR:OG1	2.08	0.60
3:A:57:LYS:HA	3:A:57:LYS:CE	2.31	0.60
3:B:26:LYS:HE2	3:B:87:ARG:NH1	2.17	0.60
3:B:199:HIS:O	3:B:201:LYS:HD3	2.02	0.60
3:B:152:LYS:O	3:B:153:GLN:C	2.45	0.60
3:A:20:ILE:HD12	3:A:20:ILE:C	2.27	0.59
3:B:102:PHE:HA	3:B:105:LEU:CD1	2.31	0.59
2:E:20:DT:H2''	2:E:21:DT:C5'	2.30	0.59
3:A:120:MET:O	3:A:121:ALA:C	2.43	0.59
2:E:21:DT:H1'	2:E:22:DT:H5''	1.85	0.59
3:B:199:HIS:O	3:B:201:LYS:N	2.36	0.59
3:A:132:GLY:O	3:A:136:PHE:HB2	2.03	0.59
3:B:72:GLU:O	3:B:74:GLY:N	2.36	0.58
1:C:-2:DA:H1'	1:C:-1:DA:H5'	1.85	0.58
3:A:159:HIS:CE1	3:A:160:PRO:HG2	2.39	0.57
3:A:199:HIS:O	3:A:201:LYS:HD3	2.04	0.57
3:B:13:TRP:CH2	3:B:105:LEU:HD22	2.39	0.57
3:A:122:ARG:HH11	3:A:122:ARG:HA	1.69	0.57
1:F:20:DA:H2''	1:F:19:DT:OP2	2.03	0.57
3:B:119:GLN:O	3:B:123:ARG:HG3	2.05	0.57
3:B:169:ARG:NH2	3:B:198:ALA:HB1	2.18	0.57
3:B:37:GLU:HA	3:B:99:TYR:CD2	2.39	0.57
3:A:101:LYS:HD3	3:A:101:LYS:C	2.29	0.57
3:A:143:ILE:HD12	3:A:186:ILE:HG21	1.86	0.57
3:B:152:LYS:O	3:B:153:GLN:O	2.23	0.57
3:A:29:LEU:C	3:A:30:ILE:HG13	2.29	0.57
3:A:101:LYS:HD3	3:A:101:LYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:ILE:CG2	3:A:204:VAL:HA	2.34	0.57
3:B:42:ILE:HD11	3:B:47:VAL:HG13	1.87	0.57
3:A:85:TRP:HZ3	5:A:767:HOH:O	1.86	0.56
3:B:17:HIS:CE1	3:B:105:LEU:HD21	2.40	0.56
3:B:199:HIS:C	3:B:201:LYS:N	2.63	0.56
3:A:18:CYS:O	3:A:19:HIS:C	2.48	0.56
3:B:34:GLU:O	3:B:35:LYS:O	2.23	0.56
2:E:18:DC:H1'	2:E:19:DA:C8	2.40	0.56
3:B:136:PHE:O	3:B:137:LEU:CD1	2.54	0.56
3:A:118:ALA:O	3:A:121:ALA:HB3	2.06	0.56
3:B:69:PHE:CD2	3:B:119:GLN:NE2	2.74	0.56
3:A:122:ARG:HB2	3:A:122:ARG:NH1	2.21	0.56
3:B:44:LYS:NZ	3:B:91:ALA:HB3	2.21	0.56
1:C:-3:DG:H5'	1:C:-3:DG:H8	1.71	0.56
1:C:9:DT:C3'	2:E:10:DC:H5''	2.35	0.56
3:A:121:ALA:HA	3:B:120:MET:HE1	1.86	0.56
3:B:116:LEU:CD2	3:B:117:SER:H	2.17	0.56
3:A:182:THR:O	3:A:186:ILE:HB	2.06	0.56
3:B:14:PHE:CZ	3:B:18:CYS:SG	2.99	0.56
3:B:26:LYS:CE	3:B:87:ARG:HD3	2.36	0.56
3:B:40:TYR:N	3:B:40:TYR:HD1	2.03	0.56
3:A:39:LEU:HB3	3:A:97:ILE:CD1	2.35	0.56
3:B:165:ILE:CG2	3:B:166:LYS:N	2.69	0.56
3:A:124:LEU:O	3:A:128:SER:HB2	2.06	0.55
3:B:49:VAL:CG2	3:B:64:LEU:HD22	2.36	0.55
3:A:122:ARG:O	3:A:126:VAL:HG23	2.07	0.55
1:C:3:DA:H1'	1:C:4:DT:H5''	1.89	0.55
3:A:9:PRO:C	3:A:11:LEU:H	2.14	0.55
3:B:139:VAL:HG21	3:B:178:CYS:HB3	1.89	0.55
3:A:18:CYS:O	3:A:20:ILE:HG22	2.06	0.55
3:B:25:SER:O	3:B:26:LYS:CB	2.54	0.55
3:B:157:MET:O	3:B:164:GLN:HB3	2.05	0.55
2:E:21:DT:H2''	2:E:22:DT:H5'	1.87	0.55
1:C:7:DG:H2''	1:C:8:DA:N7	2.22	0.55
3:A:20:ILE:HD11	3:A:22:LYS:HE3	1.88	0.55
3:B:28:THR:HG21	3:B:31:HIS:CD2	2.42	0.55
3:B:133:ASN:HD21	3:B:145:GLN:HG3	1.71	0.55
3:B:52:LYS:HE2	3:B:58:GLU:OE2	2.06	0.55
3:B:69:PHE:N	3:B:119:GLN:HE22	2.00	0.54
3:A:97:ILE:O	3:A:98:SER:CB	2.54	0.54
3:B:110:PRO:HG2	3:B:111:ASP:N	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:45:GLY:CA	3:B:92:CYS:SG	2.96	0.54
3:A:39:LEU:HB3	3:A:97:ILE:HD13	1.88	0.54
3:B:30:ILE:HD12	3:B:82:ARG:HD2	1.90	0.54
1:F:18:DG:O6	3:B:180:ARG:NH2	2.38	0.54
3:B:10:THR:C	3:B:12:GLU:N	2.63	0.54
3:B:26:LYS:HE2	3:B:87:ARG:HD3	1.89	0.54
3:B:42:ILE:CD1	3:B:47:VAL:HG13	2.37	0.54
3:B:57:LYS:HG3	3:B:58:GLU:N	2.23	0.54
3:B:45:GLY:C	3:B:92:CYS:SG	2.90	0.54
3:B:116:LEU:HD23	3:B:117:SER:N	2.19	0.54
3:B:205:VAL:HG11	5:B:768:HOH:O	2.07	0.54
2:D:5:DC:H5	5:D:123:HOH:O	1.90	0.54
2:E:21:DT:C2'	2:E:22:DT:H71	2.37	0.54
3:B:28:THR:HG21	3:B:31:HIS:NE2	2.23	0.53
3:A:109:ASN:C	3:A:109:ASN:ND2	2.64	0.53
2:E:12:DA:H2''	2:E:13:DG:H5'	1.90	0.53
2:E:21:DT:H2''	2:E:22:DT:OP2	2.08	0.53
3:A:11:LEU:HA	3:A:14:PHE:HB3	1.91	0.53
3:A:44:LYS:HB3	3:A:93:GLU:HB2	1.91	0.53
3:B:13:TRP:CD1	3:B:14:PHE:N	2.76	0.53
1:C:-5:DG:H2''	1:C:-4:DC:OP2	2.09	0.53
3:B:22:LYS:NZ	3:B:93:GLU:OE1	2.41	0.53
1:C:-4:DC:H2''	1:C:-3:DG:H5''	1.89	0.53
3:B:182:THR:O	3:B:183:VAL:C	2.52	0.53
3:A:140:THR:O	3:A:141:GLY:C	2.50	0.53
3:A:72:GLU:OE1	3:A:73:LEU:HD13	2.09	0.53
3:A:18:CYS:SG	3:A:97:ILE:HG13	2.49	0.52
3:A:143:ILE:HD12	3:A:186:ILE:CG2	2.39	0.52
3:B:169:ARG:HG2	3:B:187:LEU:CD2	2.39	0.52
1:F:17:DC:H2''	1:F:16:DG:C8	2.44	0.52
1:C:7:DG:H2''	1:C:8:DA:C8	2.45	0.52
3:B:25:SER:O	3:B:26:LYS:HB2	2.10	0.52
3:B:103:ARG:C	3:B:105:LEU:N	2.67	0.52
3:B:159:HIS:CE1	3:B:161:ASP:H	2.28	0.52
3:A:113:LEU:HD23	3:A:113:LEU:O	2.10	0.52
3:A:195:LEU:O	3:A:206:TYR:N	2.29	0.52
3:A:150:LEU:O	3:A:152:LYS:N	2.43	0.52
3:B:72:GLU:C	3:B:74:GLY:H	2.18	0.52
3:A:159:HIS:O	3:A:160:PRO:C	2.51	0.51
3:A:180:ARG:NE	3:A:181:GLU:OE2	2.43	0.51
3:B:167:ILE:HG13	3:B:171:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:116:LEU:C	3:A:116:LEU:HD23	2.36	0.51
3:B:199:HIS:CD2	3:B:201:LYS:NZ	2.78	0.51
1:C:-5:DG:C2	1:C:-4:DC:N4	2.78	0.51
2:D:11:DA:H2''	2:D:10:DG:C8	2.44	0.51
3:B:35:LYS:HA	3:B:80:GLN:O	2.10	0.51
3:B:165:ILE:CG2	3:B:166:LYS:H	2.23	0.51
3:A:157:MET:HE2	3:A:157:MET:H	1.76	0.51
3:B:169:ARG:HG2	3:B:187:LEU:HD23	1.90	0.51
3:B:116:LEU:O	3:B:119:GLN:N	2.44	0.51
3:A:74:GLY:C	3:A:99:TYR:HE2	2.19	0.51
3:A:180:ARG:HG3	3:A:181:GLU:OE2	2.11	0.51
3:B:204:VAL:O	3:B:205:VAL:C	2.54	0.51
3:A:9:PRO:HD2	3:A:11:LEU:HD11	1.92	0.51
3:A:198:ALA:O	3:A:199:HIS:HB3	2.11	0.51
3:B:188:LYS:O	3:B:191:GLU:HB3	2.11	0.51
2:D:3:DT:H2'	2:D:2:DT:C7	2.41	0.50
3:A:11:LEU:HD12	3:A:12:GLU:N	2.26	0.50
2:D:11:DA:H2''	2:D:10:DG:H8	1.76	0.50
3:A:117:SER:HA	3:A:120:MET:CE	2.41	0.50
3:B:23:TYR:HB3	3:B:27:SER:OG	2.11	0.50
3:B:50:LEU:CD1	3:B:85:TRP:HB2	2.31	0.50
3:B:13:TRP:CH2	3:B:105:LEU:HB3	2.46	0.50
3:B:52:LYS:HE2	3:B:58:GLU:HG2	1.93	0.50
3:A:114:MET:O	3:A:115:ARG:C	2.53	0.50
3:B:43:VAL:O	3:B:66:GLN:HG3	2.12	0.50
3:B:71:GLY:HA2	4:B:761:CMP:P	2.51	0.50
3:B:167:ILE:CG1	3:B:171:GLU:HG2	2.42	0.50
1:C:-2:DA:H2''	1:C:-1:DA:OP2	2.11	0.50
1:F:15:DA:C1'	1:F:14:DT:H5''	2.40	0.50
3:B:116:LEU:O	3:B:119:GLN:HB2	2.11	0.50
2:E:21:DT:H1'	2:E:22:DT:C5'	2.42	0.50
2:D:13:DC:C5'	1:F:14:DT:H2''	2.42	0.49
2:D:10:DG:H2''	2:D:9:DA:OP2	2.11	0.49
3:A:32:GLN:HB2	3:A:84:ALA:HA	1.94	0.49
3:A:97:ILE:O	3:A:98:SER:HB3	2.10	0.49
1:C:9:DT:H4'	1:C:9:DT:OP1	2.12	0.49
2:E:20:DT:C2'	2:E:21:DT:H71	2.39	0.49
3:A:20:ILE:O	3:A:20:ILE:HG13	2.12	0.49
3:A:150:LEU:C	3:A:152:LYS:H	2.21	0.49
3:A:183:VAL:HG12	3:A:184:GLY:N	2.27	0.49
3:A:169:ARG:HG2	3:A:183:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:116:LEU:HD23	3:B:116:LEU:N	2.26	0.49
3:B:30:ILE:HD11	4:B:761:CMP:C5'	2.37	0.49
3:B:103:ARG:C	3:B:105:LEU:H	2.20	0.49
1:C:8:DA:H2''	1:C:9:DT:O5'	2.13	0.49
1:F:24:DA:H2''	1:F:23:DA:H5'	1.94	0.49
3:A:184:GLY:O	3:A:187:LEU:N	2.44	0.49
2:D:9:DA:H2''	2:D:8:DT:C5'	2.40	0.49
1:F:15:DA:H2''	1:F:14:DT:C5'	2.39	0.49
3:A:75:LEU:HA	3:A:99:TYR:CE2	2.48	0.49
3:B:90:THR:HG22	3:B:91:ALA:N	2.23	0.49
2:D:2:DT:H2'	2:D:1:DT:H71	1.94	0.48
3:B:30:ILE:O	3:B:30:ILE:HG13	2.13	0.48
3:B:205:VAL:HG21	5:B:768:HOH:O	2.13	0.48
1:C:-4:DC:P	5:C:116:HOH:O	2.71	0.48
1:F:18:DG:N7	3:B:180:ARG:NH2	2.60	0.48
3:A:150:LEU:C	3:A:152:LYS:N	2.70	0.48
3:B:11:LEU:HD13	3:B:11:LEU:O	2.13	0.48
3:B:33:GLY:H	3:B:82:ARG:HB2	1.77	0.48
1:C:2:DA:H2''	1:C:3:DA:C8	2.47	0.48
3:A:139:VAL:O	3:A:143:ILE:HG13	2.13	0.48
3:B:44:LYS:O	3:B:92:CYS:HA	2.14	0.48
3:B:134:LEU:HD23	3:B:142:ARG:NH1	2.28	0.48
3:B:12:GLU:HA	3:B:12:GLU:OE2	2.13	0.48
2:D:3:DT:C2'	2:D:2:DT:H71	2.41	0.48
3:B:196:ILE:HG22	3:B:204:VAL:CA	2.18	0.48
3:A:143:ILE:O	3:A:147:LEU:HD22	2.14	0.48
3:A:189:MET:C	3:A:191:GLU:N	2.70	0.48
3:B:42:ILE:HG22	3:B:66:GLN:HA	1.95	0.48
3:B:199:HIS:CD2	3:B:201:LYS:HZ2	2.29	0.48
3:A:159:HIS:CG	3:A:160:PRO:HD2	2.49	0.48
3:A:182:THR:O	3:A:186:ILE:CG1	2.62	0.48
3:B:29:LEU:CD2	3:B:47:VAL:HG11	2.44	0.48
3:B:116:LEU:O	3:B:117:SER:C	2.57	0.48
2:D:5:DC:H4'	2:D:4:DA:OP1	2.12	0.47
2:E:17:DG:C6	2:E:18:DC:N4	2.82	0.47
1:F:21:DA:H5'	1:F:21:DA:H8	1.79	0.47
3:A:140:THR:O	3:A:142:ARG:N	2.47	0.47
3:B:53:ASP:O	3:B:56:GLY:N	2.38	0.47
3:B:63:TYR:HE2	3:B:175:ILE:HD11	1.78	0.47
3:A:153:GLN:O	3:A:155:ASP:N	2.48	0.47
3:A:191:GLU:HA	3:A:196:ILE:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:110:PRO:CG	3:B:111:ASP:H	2.22	0.47
1:F:16:DG:H2''	1:F:15:DA:C8	2.49	0.47
3:A:71:GLY:HA2	4:A:762:CMP:P	2.53	0.47
3:A:143:ILE:HG22	3:A:147:LEU:HD22	1.96	0.47
3:A:184:GLY:C	3:A:186:ILE:N	2.70	0.47
3:A:109:ASN:HD21	3:A:111:ASP:HB3	1.79	0.47
3:B:14:PHE:O	3:B:17:HIS:N	2.43	0.47
2:D:7:DC:C5	2:D:6:DG:O6	2.68	0.47
3:A:127:THR:HG22	3:B:127:THR:HG22	1.95	0.47
3:B:34:GLU:O	3:B:35:LYS:C	2.58	0.47
3:B:153:GLN:O	3:B:154:PRO:O	2.33	0.47
1:C:1:DA:C1'	1:C:2:DA:H5''	2.39	0.47
3:B:63:TYR:OH	3:B:171:GLU:OE1	2.30	0.47
3:B:118:ALA:O	3:B:121:ALA:HB3	2.15	0.47
3:B:138:ASP:O	3:B:140:THR:N	2.48	0.47
3:B:196:ILE:CG2	3:B:204:VAL:HA	2.18	0.46
3:B:53:ASP:O	3:B:54:GLU:C	2.59	0.46
3:B:146:THR:CG2	3:B:175:ILE:HG21	2.45	0.46
3:A:196:ILE:HD12	3:A:196:ILE:C	2.40	0.46
3:B:106:ILE:CD1	3:B:113:LEU:HD13	2.29	0.46
2:E:14:DA:H2''	2:E:15:DT:H5'	1.96	0.46
3:A:57:LYS:HD3	5:A:777:HOH:O	2.15	0.46
3:B:11:LEU:O	3:B:15:LEU:HG	2.16	0.46
3:B:169:ARG:O	3:B:183:VAL:HG11	2.16	0.46
3:B:35:LYS:H	3:B:81:GLU:CB	2.26	0.46
1:C:-2:DA:H1'	1:C:-1:DA:C5'	2.46	0.46
3:A:134:LEU:HA	3:A:142:ARG:HD3	1.97	0.46
3:A:205:VAL:O	3:A:206:TYR:O	2.34	0.46
3:B:71:GLY:HA2	4:B:761:CMP:O1P	2.16	0.46
3:B:124:LEU:HD12	3:B:124:LEU:O	2.16	0.46
3:B:138:ASP:O	3:B:139:VAL:C	2.59	0.46
3:A:189:MET:HE2	3:A:189:MET:HB2	1.83	0.45
3:B:100:LYS:HB2	3:B:100:LYS:HE3	1.72	0.45
3:A:25:SER:O	3:A:26:LYS:HB2	2.16	0.45
2:D:3:DT:C2	2:D:2:DT:C4	3.04	0.45
3:A:189:MET:O	3:A:193:GLN:N	2.45	0.45
3:A:199:HIS:C	3:A:201:LYS:H	2.24	0.45
3:B:75:LEU:HD12	3:B:75:LEU:C	2.42	0.45
3:B:129:GLU:O	3:B:133:ASN:HB2	2.16	0.45
3:A:124:LEU:HD23	3:A:124:LEU:O	2.16	0.45
3:A:34:GLU:HG3	3:A:35:LYS:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:159:HIS:CG	3:B:160:PRO:CD	2.98	0.45
1:C:5:DG:H2''	1:C:6:DC:H5'	1.97	0.45
3:A:130:LYS:NZ	3:A:175:ILE:HG23	2.32	0.45
3:B:40:TYR:HD1	3:B:40:TYR:H	1.65	0.45
3:B:81:GLU:O	3:B:82:ARG:O	2.34	0.45
3:B:116:LEU:HG	3:B:117:SER:N	2.31	0.45
1:C:-5:DG:H1'	1:C:-4:DC:C5	2.52	0.45
3:A:17:HIS:O	3:A:97:ILE:HG23	2.17	0.45
3:B:74:GLY:C	3:B:76:PHE:H	2.24	0.45
3:A:64:LEU:HD12	3:A:64:LEU:HA	1.60	0.44
3:A:111:ASP:C	3:A:113:LEU:H	2.25	0.44
3:A:205:VAL:O	3:A:205:VAL:HG12	2.17	0.44
3:B:29:LEU:N	3:B:29:LEU:HD12	2.31	0.44
3:B:63:TYR:HE1	3:B:89:LYS:HD3	1.83	0.44
3:B:103:ARG:O	3:B:105:LEU:N	2.50	0.44
3:A:113:LEU:HD11	3:B:114:MET:SD	2.57	0.44
3:A:77:GLU:HB2	3:A:80:GLN:NE2	2.32	0.44
3:A:106:ILE:HD13	3:A:113:LEU:CD1	2.48	0.44
3:B:61:LEU:HA	3:B:61:LEU:HD23	1.61	0.44
3:B:100:LYS:O	3:B:101:LYS:C	2.61	0.44
3:B:102:PHE:HA	3:B:105:LEU:CG	2.48	0.44
3:B:164:GLN:HG3	3:B:203:ILE:HD13	1.97	0.44
2:D:3:DT:O2	2:D:2:DT:C2	2.71	0.44
3:B:11:LEU:CD1	3:B:15:LEU:HD11	2.44	0.44
3:A:106:ILE:O	3:A:107:GLN:C	2.60	0.44
3:A:125:GLN:O	3:A:128:SER:HB3	2.17	0.43
3:B:140:THR:HG22	3:B:141:GLY:N	2.31	0.43
3:A:9:PRO:C	3:A:11:LEU:N	2.75	0.43
3:A:59:MET:HE1	3:A:134:LEU:HD11	2.00	0.43
3:A:182:THR:O	3:A:186:ILE:CB	2.66	0.43
3:B:116:LEU:CG	3:B:117:SER:N	2.80	0.43
3:B:139:VAL:CG2	3:B:178:CYS:HB3	2.47	0.43
3:B:9:PRO:HG2	3:B:10:THR:H	1.84	0.43
3:B:57:LYS:HE2	5:B:763:HOH:O	2.18	0.43
3:B:118:ALA:O	3:B:119:GLN:C	2.61	0.43
3:B:140:THR:O	3:B:142:ARG:N	2.51	0.43
1:C:-4:DC:C2'	1:C:-3:DG:H5''	2.49	0.43
3:A:111:ASP:C	3:A:113:LEU:N	2.74	0.43
3:A:157:MET:O	3:A:163:MET:HB2	2.19	0.43
3:B:42:ILE:CG1	3:B:70:ILE:HD11	2.48	0.43
3:B:110:PRO:CG	3:B:111:ASP:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:DA:C3'	2:D:10:DG:H5''	2.48	0.43
3:A:113:LEU:O	3:A:113:LEU:CD2	2.67	0.43
3:B:71:GLY:HA2	4:B:761:CMP:O3'	2.19	0.43
3:A:137:LEU:HB2	3:A:142:ARG:HG3	2.01	0.43
3:A:139:VAL:CG1	3:A:140:THR:N	2.82	0.43
3:A:186:ILE:CG2	3:A:186:ILE:O	2.67	0.43
3:B:116:LEU:HA	3:B:119:GLN:HB2	2.00	0.43
2:E:16:DC:H2''	2:E:17:DG:C8	2.54	0.43
3:B:10:THR:O	3:B:12:GLU:N	2.52	0.43
3:B:134:LEU:HD21	3:B:176:VAL:O	2.19	0.43
3:A:74:GLY:C	3:A:99:TYR:CE2	2.97	0.42
3:B:48:ALA:O	3:B:86:VAL:HA	2.19	0.42
3:B:102:PHE:HA	3:B:105:LEU:HG	2.01	0.42
3:A:122:ARG:NH1	3:A:122:ARG:CB	2.82	0.42
3:B:142:ARG:O	3:B:146:THR:OG1	2.37	0.42
3:A:43:VAL:CG2	3:A:93:GLU:HB3	2.43	0.42
3:A:44:LYS:HG2	3:A:45:GLY:N	2.34	0.42
2:D:12:DT:H2''	2:D:11:DA:OP2	2.20	0.42
3:A:11:LEU:CD2	3:A:115:ARG:HH12	2.24	0.42
3:A:198:ALA:C	3:A:201:LYS:O	2.62	0.42
3:B:46:SER:HB2	3:B:65:ASN:OD1	2.18	0.42
3:A:44:LYS:HE3	3:A:93:GLU:OE1	2.19	0.42
3:A:103:ARG:HA	3:A:106:ILE:HD12	2.01	0.42
3:A:116:LEU:HD23	3:A:120:MET:HE2	2.01	0.42
3:A:32:GLN:HG3	3:A:83:SER:C	2.44	0.42
3:A:40:TYR:HD2	3:A:94:VAL:CG1	2.32	0.42
3:B:125:GLN:O	3:B:126:VAL:C	2.62	0.42
1:C:4:DT:P	3:A:169:ARG:HB2	2.60	0.42
3:A:30:ILE:O	3:A:85:TRP:HA	2.20	0.42
3:A:40:TYR:HD2	3:A:94:VAL:HG11	1.84	0.42
3:A:127:THR:O	3:A:127:THR:CG2	2.67	0.42
3:A:138:ASP:O	3:A:139:VAL:C	2.60	0.42
2:D:11:DA:C2'	2:D:10:DG:C8	3.03	0.42
2:E:26:DG:C2	1:F:25:DG:N2	2.88	0.41
3:A:126:VAL:C	3:A:128:SER:N	2.77	0.41
3:B:26:LYS:O	3:B:26:LYS:CG	2.68	0.41
3:A:22:LYS:HD3	3:A:93:GLU:HG3	2.02	0.41
3:B:140:THR:C	3:B:142:ARG:H	2.28	0.41
3:A:121:ALA:HA	3:B:120:MET:CE	2.49	0.41
1:C:6:DC:C2'	1:C:7:DG:H5''	2.47	0.41
2:E:25:DC:C2'	2:E:26:DG:OP2	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:49:VAL:HG11	4:A:762:CMP:C4	2.54	0.41
3:B:47:VAL:HG22	3:B:64:LEU:HB2	2.03	0.41
3:B:54:GLU:C	3:B:56:GLY:H	2.28	0.41
3:A:31:HIS:ND1	3:A:85:TRP:NE1	2.66	0.41
3:A:131:VAL:HG12	3:B:59:MET:CE	2.51	0.41
3:B:116:LEU:CD2	3:B:117:SER:N	2.82	0.41
3:A:165:ILE:CG2	3:A:166:LYS:N	2.84	0.41
3:A:181:GLU:O	3:A:182:THR:C	2.64	0.41
3:A:24:PRO:O	3:A:27:SER:OG	2.37	0.41
3:A:99:TYR:O	3:A:100:LYS:C	2.63	0.41
3:A:184:GLY:O	3:A:185:ARG:C	2.62	0.41
3:A:196:ILE:HB	3:A:203:ILE:O	2.20	0.41
3:B:50:LEU:HD21	3:B:87:ARG:NH2	2.32	0.41
3:B:74:GLY:C	3:B:76:PHE:N	2.77	0.41
1:C:-3:DG:H5'	1:C:-3:DG:C8	2.53	0.41
3:B:97:ILE:HG12	3:B:98:SER:O	2.21	0.41
3:B:104:GLN:O	3:B:108:VAL:HG23	2.20	0.41
3:A:189:MET:O	3:A:190:LEU:C	2.62	0.41
3:B:11:LEU:HD23	3:B:112:ILE:HD11	2.03	0.41
3:B:123:ARG:HD3	4:B:761:CMP:C2	2.56	0.41
3:A:123:ARG:CB	3:B:124:LEU:HD21	2.50	0.41
3:A:133:ASN:HA	3:A:137:LEU:CD1	2.52	0.40
3:B:29:LEU:N	3:B:29:LEU:CD1	2.83	0.40
1:C:3:DA:N3	1:C:4:DT:C6	2.89	0.40
1:F:20:DA:H1'	1:F:19:DT:C5'	2.43	0.40
3:A:83:SER:O	3:A:84:ALA:HB2	2.22	0.40
3:A:182:THR:O	3:A:186:ILE:HG12	2.21	0.40
3:B:13:TRP:HH2	3:B:105:LEU:HA	1.86	0.40
3:A:122:ARG:HH11	3:A:122:ARG:CA	2.33	0.40
3:A:131:VAL:H	3:A:131:VAL:HG23	1.56	0.40
3:B:87:ARG:NH2	5:B:771:HOH:O	2.54	0.40
2:D:13:DC:O5'	2:D:13:DC:H6	2.04	0.40
3:A:124:LEU:C	3:A:124:LEU:CD2	2.95	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	
3	A	197/200 (98%)	152 (77%)	33 (17%)	12 (6%)	1	3
3	B	195/200 (98%)	141 (72%)	32 (16%)	22 (11%)	0	1
All	All	392/400 (98%)	293 (75%)	65 (17%)	34 (9%)	0	1

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	98	SER
3	A	155	ASP
3	A	182	THR
3	A	206	TYR
3	B	26	LYS
3	B	35	LYS
3	B	73	LEU
3	B	82	ARG
3	B	139	VAL
3	B	154	PRO
3	B	199	HIS
3	A	151	ALA
3	A	181	GLU
3	B	42	ILE
3	B	54	GLU
3	B	121	ALA
3	B	153	GLN
3	B	176	VAL
3	B	194	ASN
3	A	34	GLU
3	B	66	GLN
3	B	182	THR
3	B	200	GLY
3	A	115	ARG
3	A	140	THR

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Mol	Chain	Res	Type
3	A	141	GLY
3	A	154	PRO
3	B	55	GLU
3	B	110	PRO
3	B	152	LYS
3	B	196	ILE
3	B	140	THR
3	B	204	VAL
3	A	205	VAL

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	
3	A	171/172 (99%)	131 (77%)	40 (23%)	1	3
3	B	170/172 (99%)	142 (84%)	28 (16%)	2	8
All	All	341/344 (99%)	273 (80%)	68 (20%)	1	5

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	15	LEU
3	A	17	HIS
3	A	18	CYS
3	A	20	ILE
3	A	34	GLU
3	A	35	LYS
3	A	43	VAL
3	A	52	LYS
3	A	53	ASP
3	A	55	GLU
3	A	57	LYS
3	A	59	MET

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Mol	Chain	Res	Type
3	A	64	LEU
3	A	70	ILE
3	A	72	GLU
3	A	75	LEU
3	A	78	GLU
3	A	80	GLN
3	A	97	ILE
3	A	101	LYS
3	A	122	ARG
3	A	127	THR
3	A	134	LEU
3	A	138	ASP
3	A	139	VAL
3	A	147	LEU
3	A	148	LEU
3	A	152	LYS
3	A	158	THR
3	A	161	ASP
3	A	163	MET
3	A	165	ILE
3	A	171	GLU
3	A	183	VAL
3	A	188	LYS
3	A	189	MET
3	A	201	LYS
3	A	204	VAL
3	B	13	TRP
3	B	25	SER
3	B	40	TYR
3	B	47	VAL
3	B	53	ASP
3	B	64	LEU
3	B	72	GLU
3	B	75	LEU
3	B	77	GLU
3	B	80	GLN
3	B	92	CYS
3	B	115	ARG
3	B	124	LEU
3	B	133	ASN
3	B	137	LEU
3	B	146	THR

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Mol	Chain	Res	Type
3	B	152	LYS
3	B	153	GLN
3	B	154	PRO
3	B	155	ASP
3	B	160	PRO
3	B	166	LYS
3	B	181	GLU
3	B	187	LEU
3	B	188	LYS
3	B	195	LEU
3	B	201	LYS
3	B	202	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	65	ASN
3	A	109	ASN
3	A	125	GLN
3	A	133	ASN
3	A	145	GLN
3	A	153	GLN
3	A	170	GLN
3	B	17	HIS
3	B	119	GLN
3	B	125	GLN
3	B	133	ASN
3	B	149	ASN
3	B	164	GLN
3	B	174	GLN
3	B	194	ASN
3	B	199	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	CMP	B	761	-	25,25,25	0.95	2 (8%)	37,39,39	1.27	6 (16%)
4	CMP	A	762	-	25,25,25	1.06	2 (8%)	37,39,39	1.64	4 (10%)

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	CMP	B	761	-	-	0/4/31/31	0/4/4/4
4	CMP	A	762	-	-	0/4/31/31	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	762	CMP	O3'-C3'	-3.16	1.39	1.44
4	A	762	CMP	P-O5'	2.59	1.60	1.57
4	B	761	CMP	P-O5'	2.46	1.60	1.57
4	B	761	CMP	O3'-C3'	-2.08	1.41	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	762	CMP	O3'-C3'-C4'	-7.13	105.33	110.71
4	A	762	CMP	O2P-P-O1P	3.73	120.02	108.56
4	B	761	CMP	O2P-P-O1P	3.56	119.52	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	761	CMP	O3'-C3'-C2'	3.32	118.86	115.61
4	A	762	CMP	O3'-C3'-C2'	3.03	118.57	115.61
4	B	761	CMP	O3'-C3'-C4'	-2.95	108.49	110.71
4	A	762	CMP	O3'-P-O1P	-2.39	105.28	110.39
4	B	761	CMP	O4'-C4'-C3'	-2.26	100.16	104.92
4	B	761	CMP	C2'-C3'-C4'	-2.08	99.60	103.24
4	B	761	CMP	O5'-P-O3'	-2.02	103.00	105.70

There are no chirality outliers.

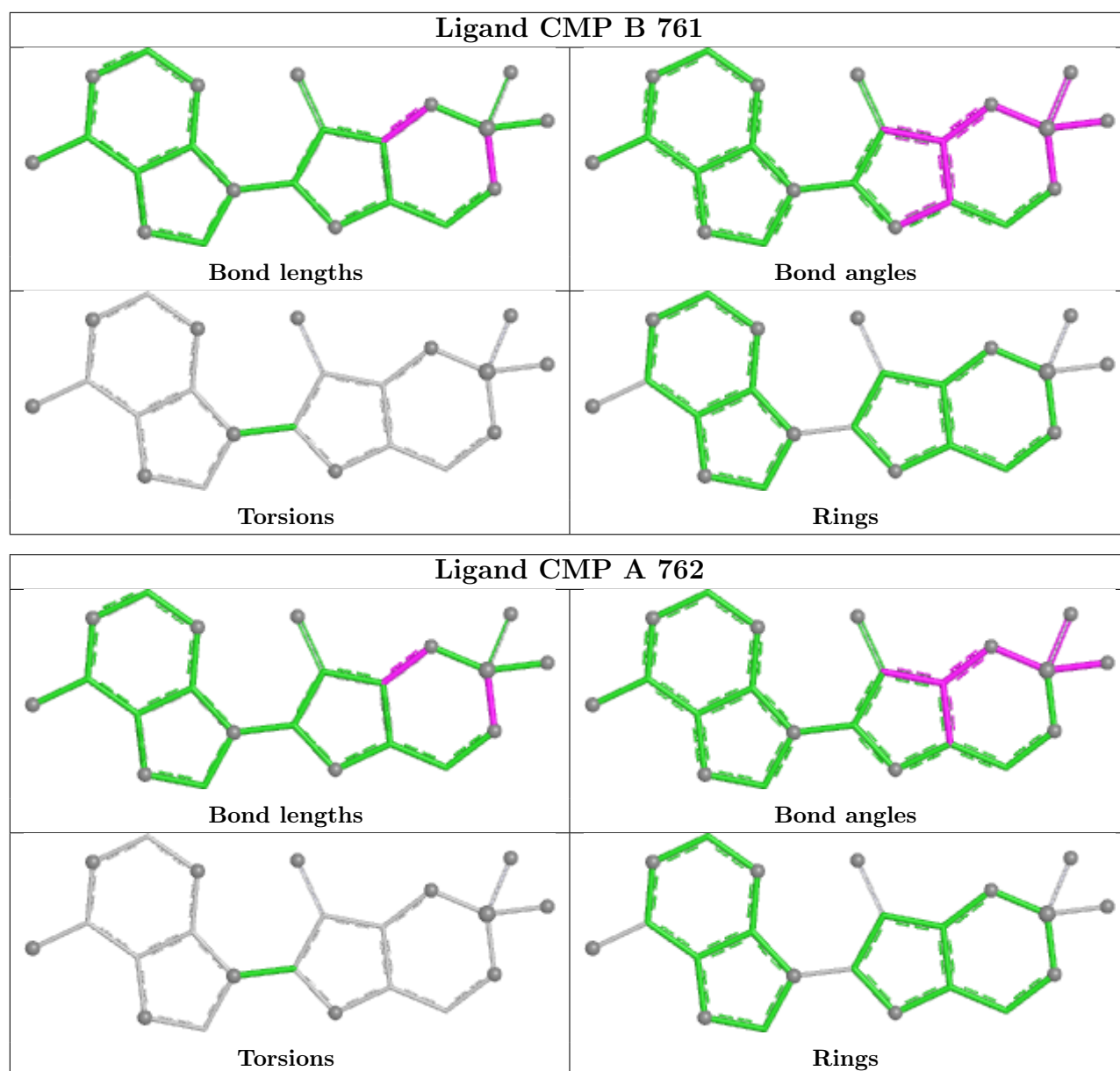
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	761	CMP	7	0
4	A	762	CMP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	C	14/14 (100%)	0.26	0	100100	32, 50, 59, 63	0
1	F	14/14 (100%)	-0.12	0	100100	26, 40, 48, 56	0
2	D	17/17 (100%)	0.02	0	100100	35, 44, 59, 63	0
2	E	17/17 (100%)	-0.17	0	100100	25, 36, 51, 53	0
3	A	199/200 (99%)	-0.39	1 (0%)	8782	4, 24, 45, 55	0
3	B	197/200 (98%)	-0.35	0	100100	2, 23, 45, 55	0
All	All	458/462 (99%)	-0.32	1 (0%)	9188	2, 26, 50, 63	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	207	GLY	4.9

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](#)

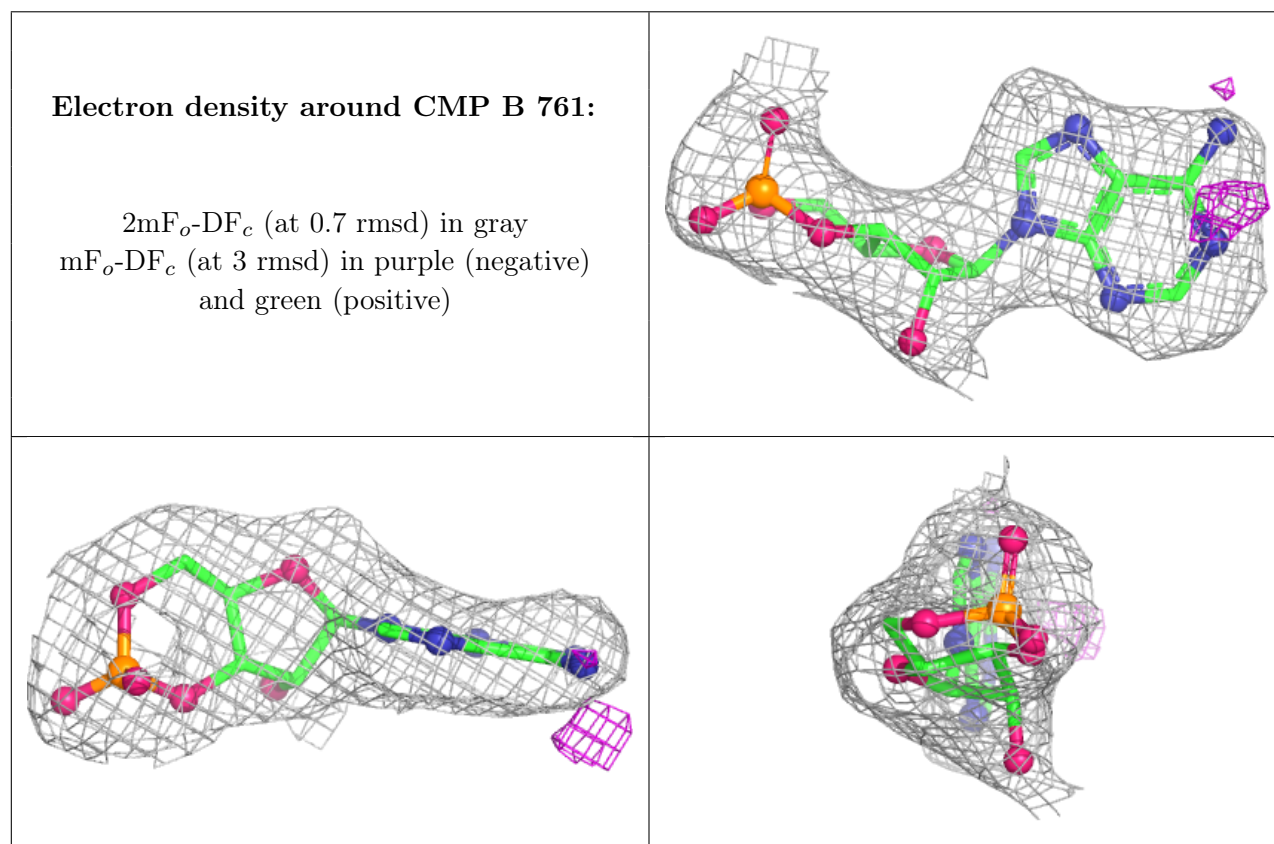
There are no oligosaccharides in this entry.

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.

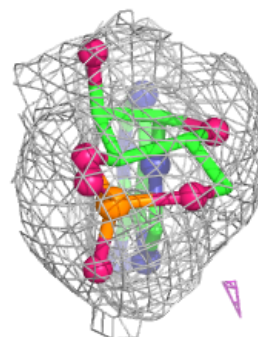
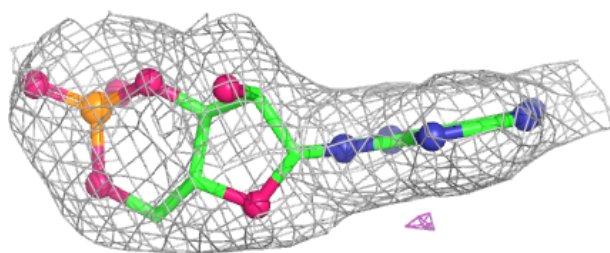
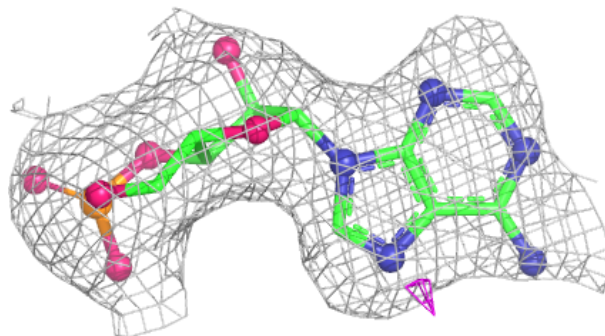
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CMP	B	761	22/22	0.97	0.06	9,14,20,21	0
4	CMP	A	762	22/22	0.98	0.05	0,7,12,15	0

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 CMP A 762:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.