



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:44 AM UTC

PDB ID : 2QBY / pdb_00002qby
Title : Crystal structure of a heterodimer of Cdc6/Orc1 initiators bound to origin DNA (from *S. solfataricus*)
Authors : Cunningham Dueber, E.L.; Corn, J.E.; Bell, S.D.; Berger, J.M.
Deposited on : 2007-06-18
Resolution : 3.35 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

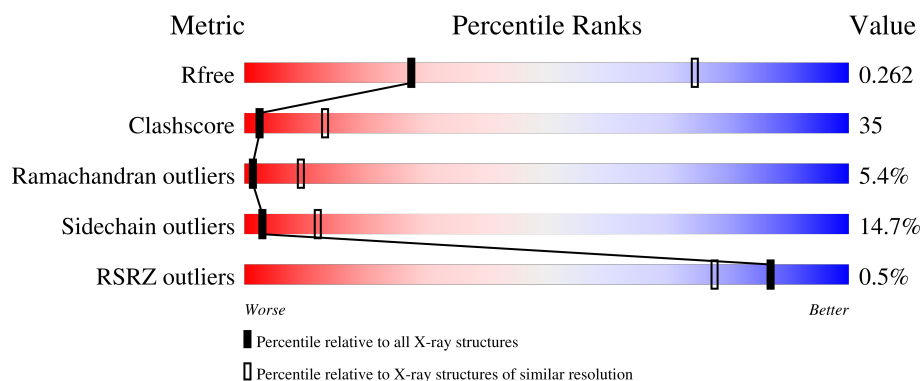
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	33	12% 85% .
2	D	33	9% 91%
3	A	386	39% 42% 13% 5%
4	B	384	% 39% 45% 10% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7309 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 DNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	P	0	0	0
			678	326	127	193	32			

- Molecule 2 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	33	Total	C	N	O	P	0	0	0
			669	324	114	199	32			

- Molecule 3 is a protein called Cell division control protein 6 homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	366	Total	C	N	O	S	0	0	0
			2937	1887	501	542	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP Q980N4
A	13	ALA	-	expression tag	UNP Q980N4
A	14	MET	-	expression tag	UNP Q980N4

- Molecule 4 is a protein called Cell division control protein 6 homolog 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	368	Total	C	N	O	S	0	0	0
			2944	1890	501	546	7			

There are 3 discrepancies between the modelled and reference sequences:

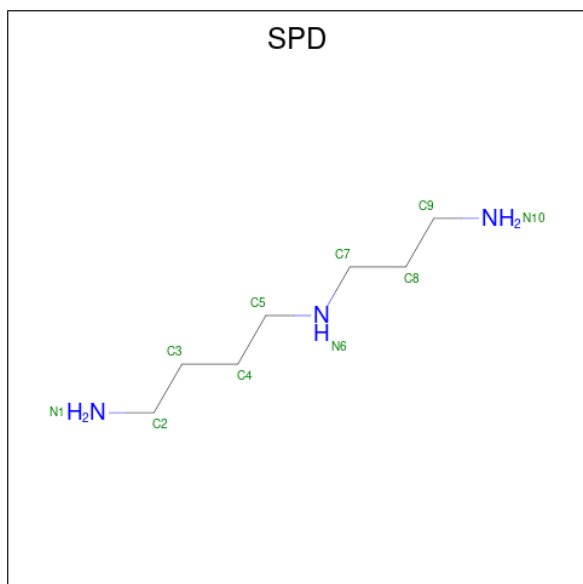
Chain	Residue	Modelled	Actual	Comment	Reference
B	11	GLY	-	expression tag	UNP Q97WM8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	-	expression tag	UNP Q97WM8
B	13	MET	-	expression tag	UNP Q97WM8

- Molecule 5 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N 10 7 3	0	0
5	C	1	Total C N 10 7 3	0	0

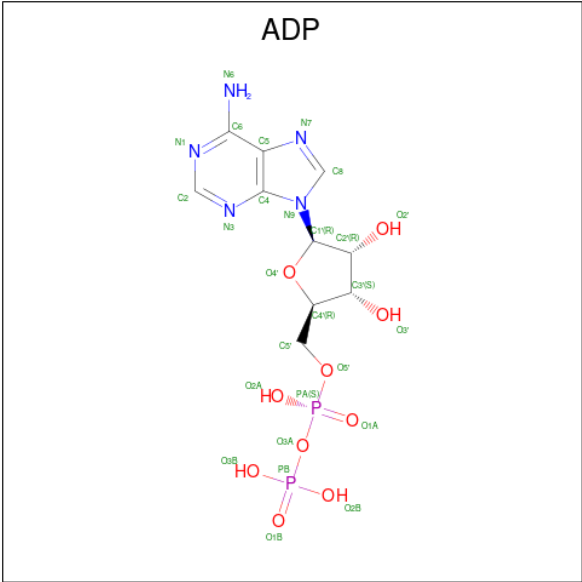
- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total K 1 1	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
8	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

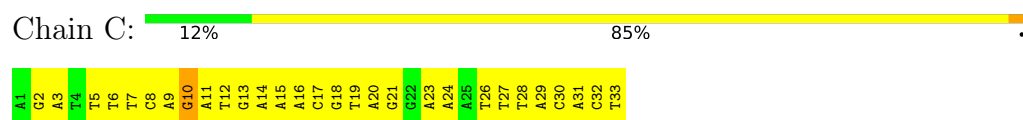
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	O	0	0
			2	2		
9	B	2	Total	O	0	0
			2	2		

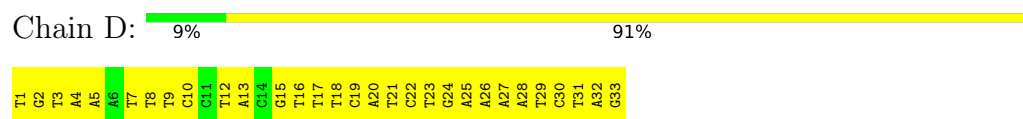
3 Residue-property plots

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.

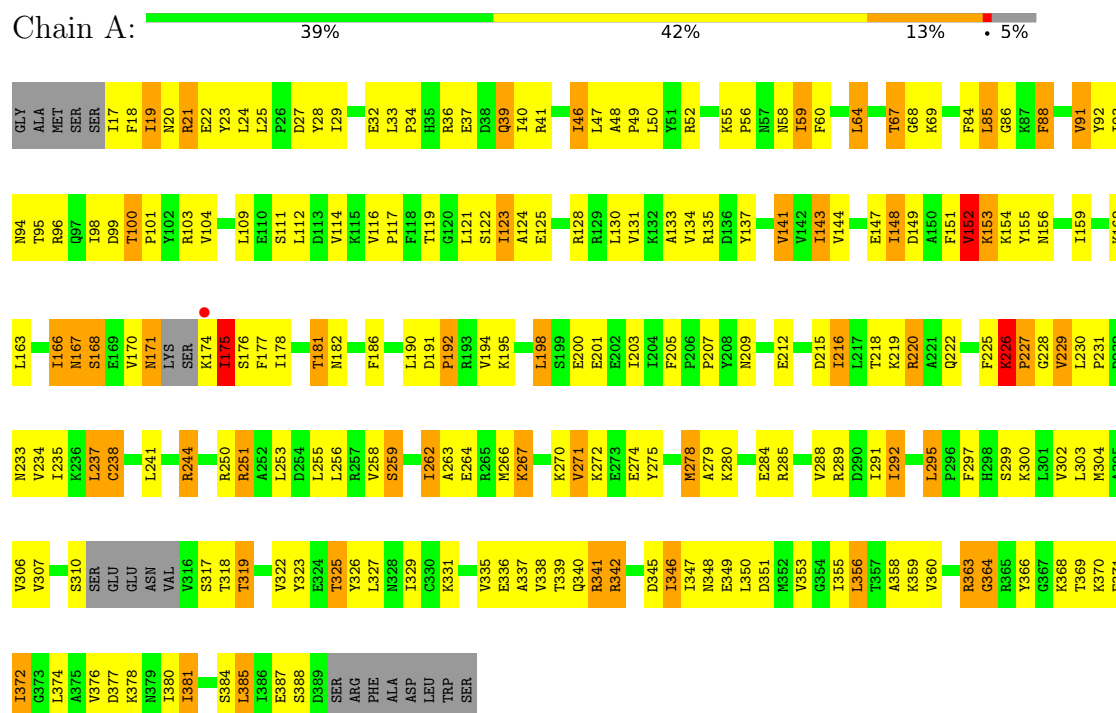
- Molecule 1: DNA (33-MER)



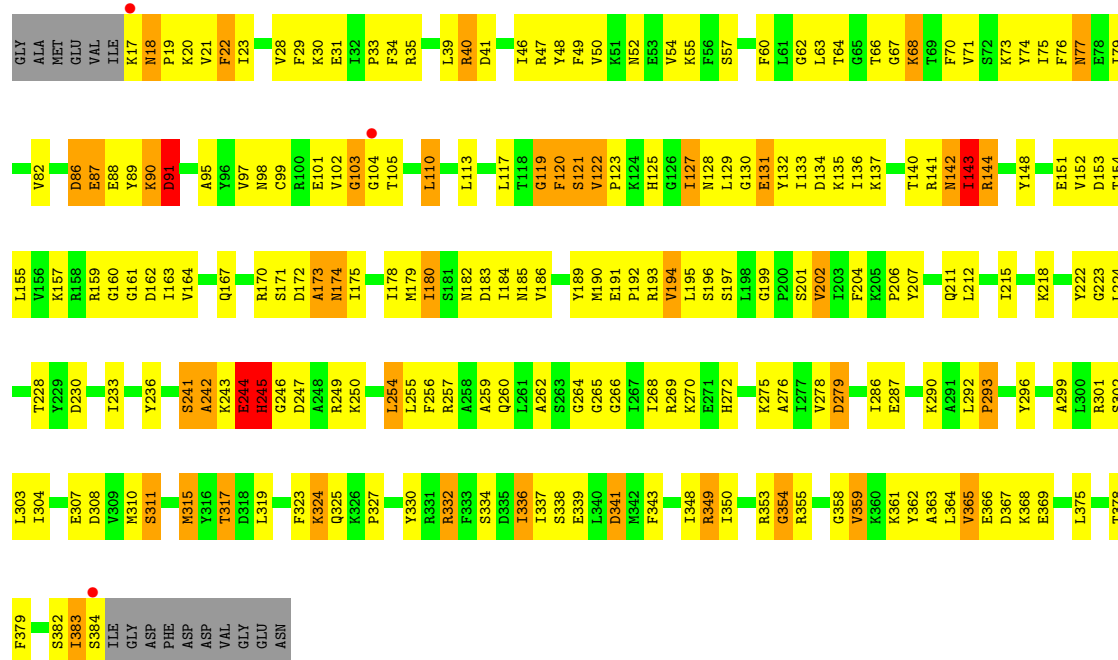
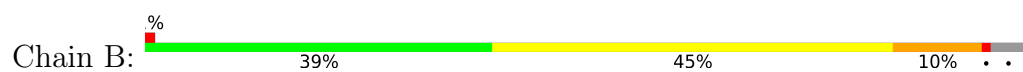
- Molecule 2: DNA (33-MER)



- Molecule 3: Cell division control protein 6 homolog 1



- Molecule 4: Cell division control protein 6 homolog 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	77.65Å 199.14Å 213.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.35 30.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-3.35) 97.9 (30.00-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.269 0.220 , 0.262	Depositor DCC
R_{free} test set	1216 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	119.2	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 93.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7309	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: ADP, K, SPD, MG

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	0.31	0/762	0.98	1/1175 (0.1%)
2	D	0.30	0/748	0.93	0/1152
3	A	0.50	0/2980	0.95	8/4022 (0.2%)
4	B	0.47	0/2993	0.95	4/4025 (0.1%)
All	All	0.45	0/7483	0.95	13/10374 (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
4	B	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	33	LEU	CA-C-N	8.51	130.48	119.84
3	A	33	LEU	C-N-CA	8.51	130.48	119.84
3	A	29	ILE	CA-C-N	7.92	128.36	120.52
3	A	29	ILE	C-N-CA	7.92	128.36	120.52
3	A	152	VAL	N-CA-C	-6.93	106.73	113.53
1	C	10	DG	C1'-O4'-C4'	-6.82	99.47	109.70
4	B	104	GLY	N-CA-C	-6.48	106.98	114.69
3	A	226	LYS	CA-C-N	-5.59	112.85	119.84
3	A	226	LYS	C-N-CA	-5.59	112.85	119.84
4	B	143	ILE	N-CA-C	-5.54	97.81	109.34
4	B	18	ASN	CA-C-N	5.21	126.35	119.84
4	B	18	ASN	C-N-CA	5.21	126.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	175	ILE	CB-CA-C	-5.19	104.08	111.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	243	LYS	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	C	678	0	375	37	0
2	D	669	0	378	51	0
3	A	2937	0	3069	229	0
4	B	2944	0	3027	198	0
5	C	20	0	38	2	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	27	0	12	2	0
8	B	27	0	12	4	0
9	A	2	0	0	0	0
9	B	2	0	0	1	0
All	All	7309	0	6911	495	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 35.

All (495) 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)
3:A:291:ILE:HG21	3:A:353:VAL:HG11	1.44	1.00
2:D:26:DA:H2'	2:D:27:DA:C8	1.99	0.98
3:A:251:ARG:HG3	3:A:251:ARG:HH11	1.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:162:ASP:HB2	4:B:194:VAL:HG21	1.47	0.96
3:A:226:LYS:HB3	3:A:227:PRO:HD3	1.49	0.95
4:B:86:ASP:O	4:B:87:GLU:HB2	1.71	0.91
4:B:34:PHE:CE1	4:B:211:GLN:HG2	2.05	0.90
3:A:119:THR:HG22	4:B:159:ARG:HH11	1.34	0.90
1:C:5:DT:H2''	1:C:6:DT:H5''	1.51	0.89
3:A:244:ARG:HG3	3:A:244:ARG:HH11	1.37	0.88
4:B:245:HIS:HE1	4:B:250:LYS:HD3	1.37	0.87
3:A:289:ARG:HG2	3:A:384:SER:HB3	1.53	0.87
2:D:15:DG:H1'	2:D:16:DT:H5''	1.53	0.87
4:B:52:ASN:HB3	4:B:54:VAL:HG23	1.55	0.85
3:A:270:LYS:HG2	3:A:271:VAL:H	1.40	0.85
3:A:17:ILE:HG21	3:A:264:GLU:HG3	1.56	0.85
1:C:27:DT:C6	1:C:28:DT:H72	2.12	0.85
4:B:97:VAL:HG21	4:B:113:LEU:HD23	1.59	0.85
3:A:84:PHE:C	3:A:86:GLY:H	1.85	0.84
3:A:152:VAL:HG11	3:A:186:PHE:HE1	1.41	0.84
3:A:369:THR:HG22	3:A:370:LYS:N	1.92	0.84
3:A:291:ILE:HG21	3:A:353:VAL:CG1	2.07	0.84
4:B:293:PRO:HB2	4:B:296:TYR:CD1	2.12	0.84
4:B:73:LYS:O	4:B:77:ASN:HB2	1.77	0.84
3:A:18:PHE:O	3:A:226:LYS:HE3	1.78	0.83
4:B:90:LYS:O	4:B:91:ASP:HB2	1.80	0.81
3:A:32:GLU:HB2	3:A:219:LYS:NZ	1.96	0.81
3:A:318:THR:HB	3:A:369:THR:HG21	1.63	0.80
3:A:225:PHE:CE1	3:A:230:LEU:HD12	2.18	0.79
3:A:135:ARG:NE	3:A:170:VAL:HG11	1.96	0.79
3:A:100:THR:HG23	3:A:103:ARG:HB2	1.64	0.78
4:B:353:ARG:H	4:B:358:GLY:HA3	1.47	0.78
1:C:20:DA:H1'	1:C:21:DG:H5'	1.66	0.77
4:B:257:ARG:HB2	4:B:276:ALA:HB1	1.67	0.77
3:A:227:PRO:HD2	3:A:229:VAL:HG23	1.67	0.76
3:A:231:PRO:HD2	3:A:271:VAL:HG12	1.68	0.76
3:A:46:ILE:O	3:A:46:ILE:HG22	1.85	0.76
4:B:375:LEU:O	4:B:378:THR:HG22	1.86	0.75
3:A:363:ARG:HD3	3:A:366:TYR:HB2	1.69	0.75
2:D:26:DA:H2''	2:D:27:DA:O5'	1.87	0.75
4:B:275:LYS:O	4:B:279:ASP:HB2	1.89	0.73
3:A:339:THR:HG22	3:A:341:ARG:H	1.54	0.73
3:A:95:THR:HB	3:A:151:PHE:CB	2.19	0.73
3:A:270:LYS:HG2	3:A:271:VAL:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:135:ARG:HD2	3:A:170:VAL:HG21	1.71	0.72
1:C:10:DG:H5"	3:A:369:THR:HG23	1.70	0.72
4:B:190:MET:HE3	4:B:195:LEU:HD13	1.71	0.72
3:A:84:PHE:C	3:A:86:GLY:N	2.46	0.72
3:A:171:ASN:ND2	3:A:171:ASN:H	1.86	0.72
3:A:17:ILE:HG23	3:A:18:PHE:H	1.55	0.72
4:B:212:LEU:HD12	4:B:242:ALA:HB2	1.72	0.71
3:A:209:ASN:HB2	3:A:212:GLU:HG3	1.69	0.71
3:A:378:LYS:O	3:A:381:ILE:HG22	1.90	0.71
4:B:57:SER:O	4:B:199:GLY:HA3	1.90	0.71
3:A:125:GLU:HA	3:A:128:ARG:HD2	1.72	0.71
3:A:342:ARG:HH21	3:A:346:ILE:CG1	2.03	0.71
4:B:304:ILE:HG23	4:B:368:LYS:HG2	1.73	0.71
4:B:46:ILE:HD13	4:B:79:ILE:HD11	1.71	0.70
3:A:95:THR:HB	3:A:151:PHE:HB2	1.73	0.70
3:A:319:THR:HG22	3:A:347:ILE:HD12	1.71	0.70
3:A:98:ILE:HG21	3:A:104:VAL:HG23	1.73	0.70
4:B:153:ASP:O	4:B:157:LYS:HG3	1.91	0.70
4:B:332:ARG:HD2	4:B:332:ARG:O	1.91	0.70
3:A:369:THR:HG22	3:A:370:LYS:H	1.57	0.69
2:D:31:DT:H2"	2:D:32:DA:OP2	1.91	0.69
4:B:142:ASN:O	4:B:143:ILE:HG13	1.92	0.69
2:D:17:DT:H2"	2:D:18:DT:H5'	1.72	0.69
4:B:62:GLY:O	4:B:68:LYS:HE3	1.93	0.69
4:B:315:MET:O	4:B:319:LEU:HD12	1.92	0.69
3:A:17:ILE:HG23	3:A:18:PHE:N	2.05	0.69
4:B:317:THR:HG22	4:B:327:PRO:CB	2.22	0.69
3:A:109:LEU:HG	3:A:130:LEU:HD13	1.75	0.69
3:A:348:ASN:HD21	3:A:370:LYS:NZ	1.91	0.68
3:A:141:VAL:HG13	3:A:175:ILE:HG22	1.72	0.68
4:B:269:ARG:H	4:B:272:HIS:HD2	1.41	0.68
3:A:226:LYS:HB3	3:A:227:PRO:CD	2.23	0.68
4:B:50:VAL:HG21	4:B:89:TYR:CE1	2.28	0.68
4:B:34:PHE:CZ	4:B:211:GLN:HG2	2.29	0.68
2:D:12:DT:H2"	2:D:13:DA:N7	2.10	0.67
3:A:39:GLN:H	3:A:39:GLN:NE2	1.92	0.67
3:A:190:LEU:HB2	3:A:195:LYS:HB2	1.75	0.67
4:B:144:ARG:HH11	4:B:144:ARG:CG	2.06	0.67
3:A:58:ASN:HB3	3:A:198:LEU:HD23	1.77	0.67
3:A:251:ARG:HG3	3:A:251:ARG:NH1	2.04	0.67
3:A:41:ARG:HG3	3:A:41:ARG:HH11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:181:THR:OG1	3:A:182:ASN:N	2.28	0.66
3:A:272:LYS:H	3:A:275:TYR:HD2	1.41	0.66
4:B:131:GLU:O	4:B:135:LYS:HG3	1.96	0.66
4:B:34:PHE:CD1	4:B:211:GLN:HG2	2.30	0.66
3:A:130:LEU:O	3:A:134:VAL:HG23	1.95	0.66
3:A:220:ARG:HH11	3:A:220:ARG:CG	2.09	0.66
3:A:251:ARG:HH11	3:A:251:ARG:CG	2.05	0.66
4:B:17:LYS:N	4:B:224:LEU:HD23	2.11	0.66
4:B:303:LEU:HD11	4:B:337:ILE:HD12	1.78	0.66
4:B:144:ARG:HH11	4:B:144:ARG:HG2	1.61	0.65
3:A:384:SER:O	3:A:387:GLU:HB2	1.96	0.65
1:C:32:DC:H2''	1:C:33:DT:OP2	1.97	0.64
3:A:234:VAL:HG21	3:A:271:VAL:HG13	1.80	0.64
3:A:348:ASN:HD21	3:A:370:LYS:HZ2	1.44	0.64
4:B:128:ASN:HD22	4:B:129:LEU:N	1.95	0.64
4:B:233:ILE:HD13	4:B:268:ILE:O	1.96	0.64
3:A:244:ARG:HH11	3:A:244:ARG:CG	2.09	0.64
4:B:257:ARG:HB2	4:B:276:ALA:CB	2.27	0.64
4:B:79:ILE:O	4:B:82:VAL:HG12	1.98	0.64
2:D:32:DA:OP2	2:D:32:DA:H2'	1.97	0.64
3:A:369:THR:CG2	3:A:370:LYS:N	2.61	0.63
4:B:167:GLN:O	4:B:171:SER:HB3	1.99	0.62
4:B:307:GLU:CD	4:B:364:LEU:HD23	2.24	0.62
2:D:26:DA:H2'	2:D:27:DA:H8	1.57	0.62
3:A:285:ARG:HA	3:A:380:ILE:HG21	1.80	0.62
3:A:119:THR:HG22	4:B:159:ARG:NH1	2.12	0.62
4:B:191:GLU:HG2	4:B:192:PRO:HD2	1.82	0.62
4:B:30:LYS:O	4:B:31:GLU:HG3	2.00	0.62
4:B:48:TYR:O	4:B:52:ASN:HB2	1.99	0.62
4:B:383:ILE:O	4:B:384:SER:HB3	2.00	0.62
2:D:4:DA:H3'	4:B:129:LEU:HD11	1.81	0.61
3:A:109:LEU:O	3:A:114:VAL:HB	2.00	0.61
4:B:22:PHE:CE1	4:B:223:GLY:HA3	2.35	0.61
4:B:382:SER:O	4:B:383:ILE:HG23	2.01	0.61
4:B:182:ASN:ND2	9:B:2:HOH:O	2.34	0.61
3:A:67:THR:HG22	3:A:207:PRO:HA	1.82	0.61
4:B:22:PHE:HD1	4:B:22:PHE:N	1.99	0.61
3:A:59:ILE:HD12	3:A:178:ILE:HG12	1.82	0.61
4:B:18:ASN:HB2	4:B:223:GLY:O	2.01	0.61
4:B:21:VAL:HG22	4:B:28:VAL:HG21	1.83	0.60
3:A:381:ILE:O	3:A:385:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:117:PRO:HD2	3:A:121:LEU:HD11	1.83	0.60
4:B:317:THR:HG22	4:B:327:PRO:HB3	1.83	0.60
2:D:7:DT:H1'	2:D:8:DT:H5'	1.84	0.59
2:D:28:DA:H2''	2:D:29:DT:OP2	2.02	0.59
3:A:318:THR:O	3:A:322:VAL:HG23	2.03	0.59
3:A:20:ASN:OD1	3:A:22:GLU:HB2	2.02	0.59
3:A:22:GLU:HG2	3:A:25:LEU:HD11	1.84	0.59
4:B:98:ASN:HB3	4:B:101:GLU:HG3	1.83	0.59
2:D:15:DG:C1'	2:D:16:DT:H5''	2.29	0.59
4:B:119:GLY:O	4:B:120:PHE:HB3	2.01	0.59
3:A:84:PHE:O	3:A:86:GLY:N	2.36	0.59
3:A:327:LEU:O	3:A:331:LYS:HG3	2.03	0.59
4:B:128:ASN:HD22	4:B:128:ASN:C	2.11	0.59
4:B:287:GLU:HA	4:B:290:LYS:HB2	1.84	0.59
3:A:95:THR:HB	3:A:151:PHE:HB3	1.85	0.58
4:B:97:VAL:HG21	4:B:113:LEU:CD2	2.32	0.58
4:B:358:GLY:O	4:B:359:VAL:HG22	2.03	0.58
3:A:285:ARG:O	3:A:289:ARG:HB2	2.03	0.58
4:B:22:PHE:N	4:B:22:PHE:CD1	2.71	0.58
4:B:95:ALA:HB2	4:B:117:LEU:HD21	1.85	0.58
1:C:28:DT:H2''	1:C:29:DA:C5'	2.32	0.58
3:A:342:ARG:HH21	3:A:346:ILE:HG13	1.67	0.58
4:B:245:HIS:CE1	4:B:250:LYS:HD3	2.29	0.58
3:A:220:ARG:HH11	3:A:220:ARG:HG2	1.68	0.58
3:A:220:ARG:HG2	3:A:220:ARG:NH1	2.18	0.58
2:D:9:DT:H1'	2:D:10:DC:H5''	1.86	0.58
3:A:226:LYS:CB	3:A:227:PRO:HD3	2.30	0.58
4:B:359:VAL:HG23	4:B:359:VAL:O	2.04	0.57
3:A:25:LEU:C	3:A:27:ASP:H	2.12	0.57
3:A:345:ASP:O	3:A:349:GLU:HG3	2.02	0.57
3:A:122:SER:O	3:A:123:ILE:C	2.48	0.57
1:C:17:DC:H5''	4:B:355:ARG:O	2.05	0.57
3:A:251:ARG:NH1	3:A:251:ARG:CG	2.65	0.57
4:B:249:ARG:HB3	4:B:249:ARG:NH2	2.19	0.57
3:A:17:ILE:HG21	3:A:264:GLU:CG	2.32	0.57
4:B:52:ASN:HB3	4:B:54:VAL:CG2	2.33	0.56
4:B:152:VAL:HG11	4:B:179:MET:HB3	1.87	0.56
3:A:39:GLN:H	3:A:39:GLN:HE21	1.52	0.56
3:A:226:LYS:CB	3:A:227:PRO:CD	2.84	0.56
3:A:255:LEU:O	3:A:259:SER:HB2	2.06	0.56
4:B:323:PHE:O	4:B:324:LYS:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:170:ARG:HE	4:B:197:SER:HB2	1.70	0.56
4:B:262:ALA:HA	4:B:272:HIS:CE1	2.40	0.56
3:A:46:ILE:O	3:A:46:ILE:CG2	2.52	0.56
4:B:249:ARG:HG3	8:B:9:ADP:H4'	1.88	0.56
2:D:4:DA:H5''	4:B:129:LEU:HG	1.87	0.56
2:D:32:DA:H2''	2:D:33:DG:OP2	2.05	0.56
3:A:18:PHE:CD2	3:A:21:ARG:HG2	2.41	0.56
3:A:376:VAL:HG22	3:A:377:ASP:N	2.21	0.56
3:A:292:ILE:HA	3:A:295:LEU:HD22	1.87	0.56
3:A:98:ILE:HG23	3:A:103:ARG:HB3	1.87	0.56
3:A:342:ARG:HH21	3:A:346:ILE:HG12	1.70	0.56
3:A:50:LEU:HD22	3:A:88:PHE:CD1	2.41	0.55
3:A:192:PRO:C	3:A:194:VAL:H	2.14	0.55
3:A:46:ILE:HG21	3:A:201:GLU:HG3	1.87	0.55
4:B:367:ASP:O	4:B:369:GLU:N	2.35	0.55
3:A:22:GLU:HA	3:A:25:LEU:HG	1.88	0.55
3:A:92:TYR:HA	3:A:144:VAL:HB	1.87	0.55
4:B:18:ASN:N	4:B:19:PRO:HD3	2.22	0.55
1:C:13:DG:C2	2:D:20:DA:C2	2.93	0.55
4:B:98:ASN:CB	4:B:101:GLU:HG3	2.36	0.55
2:D:20:DA:H2''	2:D:21:DT:OP2	2.06	0.55
3:A:230:LEU:HD21	3:A:235:ILE:HG13	1.89	0.55
2:D:25:DA:N3	3:A:364:GLY:HA2	2.22	0.55
3:A:304:MET:HE3	3:A:304:MET:HA	1.88	0.55
4:B:256:PHE:O	4:B:260:GLN:HG2	2.07	0.55
3:A:84:PHE:CD1	3:A:84:PHE:N	2.75	0.55
3:A:234:VAL:HG21	3:A:271:VAL:CG1	2.36	0.55
4:B:132:TYR:O	4:B:136:ILE:HG13	2.06	0.55
3:A:17:ILE:CG2	3:A:18:PHE:H	2.20	0.54
3:A:369:THR:CG2	3:A:370:LYS:H	2.20	0.54
2:D:17:DT:H2''	2:D:18:DT:C5'	2.36	0.54
4:B:184:ILE:C	4:B:186:VAL:H	2.16	0.54
4:B:29:PHE:CE2	8:B:9:ADP:H2	2.26	0.54
4:B:117:LEU:HD12	4:B:136:ILE:HG23	1.89	0.54
1:C:6:DT:H2''	1:C:7:DT:H5'	1.90	0.54
1:C:28:DT:H2''	1:C:29:DA:H5'	1.88	0.54
4:B:117:LEU:N	4:B:117:LEU:HD23	2.22	0.54
3:A:19:ILE:HD12	3:A:19:ILE:O	2.08	0.54
3:A:225:PHE:CZ	3:A:230:LEU:HD12	2.43	0.54
4:B:127:ILE:HG12	4:B:128:ASN:N	2.23	0.54
4:B:48:TYR:HD1	4:B:52:ASN:HD22	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:DG:H4'	3:A:368:LYS:O	2.07	0.53
3:A:348:ASN:O	3:A:351:ASP:HB3	2.07	0.53
3:A:159:ILE:O	3:A:163:LEU:HG	2.08	0.53
2:D:25:DA:H2''	2:D:26:DA:N7	2.22	0.53
3:A:319:THR:OG1	3:A:369:THR:HG23	2.07	0.53
3:A:135:ARG:CD	3:A:170:VAL:HG11	2.37	0.53
4:B:249:ARG:HB3	4:B:249:ARG:HH21	1.74	0.53
3:A:216:ILE:HD13	8:A:8:ADP:C6	2.44	0.53
3:A:141:VAL:CG1	3:A:175:ILE:HG22	2.38	0.53
4:B:17:LYS:N	4:B:224:LEU:HA	2.24	0.52
4:B:303:LEU:HD22	4:B:363:ALA:HB3	1.91	0.52
4:B:33:PRO:O	4:B:34:PHE:HB2	2.09	0.52
1:C:19:DT:H2''	1:C:20:DA:N7	2.24	0.52
2:D:4:DA:H2''	2:D:5:DA:OP2	2.08	0.52
3:A:41:ARG:HH11	3:A:41:ARG:CG	2.22	0.52
3:A:32:GLU:HB2	3:A:219:LYS:HZ2	1.73	0.52
3:A:325:THR:O	3:A:329:ILE:HG13	2.09	0.52
2:D:1:DT:HO5'	2:D:1:DT:H6	1.54	0.52
2:D:15:DG:C2'	2:D:16:DT:H5''	2.40	0.52
2:D:16:DT:H2'	2:D:17:DT:C6	2.44	0.52
3:A:50:LEU:HD22	3:A:88:PHE:HD1	1.75	0.52
4:B:151:GLU:HG3	4:B:182:ASN:ND2	2.25	0.52
4:B:244:GLU:OE2	4:B:244:GLU:HA	2.09	0.52
4:B:293:PRO:O	4:B:296:TYR:HB2	2.10	0.52
3:A:226:LYS:O	3:A:227:PRO:O	2.28	0.52
3:A:342:ARG:O	3:A:342:ARG:HD3	2.09	0.51
3:A:153:LYS:HG2	3:A:154:LYS:N	2.25	0.51
3:A:198:LEU:HD22	3:A:198:LEU:O	2.10	0.51
3:A:60:PHE:CD1	3:A:198:LEU:HD13	2.46	0.51
3:A:156:ASN:OD1	3:A:159:ILE:HD12	2.11	0.51
2:D:30:DC:H2''	2:D:31:DT:OP2	2.11	0.51
3:A:84:PHE:N	3:A:84:PHE:HD1	2.08	0.51
4:B:228:THR:O	4:B:268:ILE:HG13	2.09	0.51
4:B:250:LYS:O	4:B:254:LEU:HB2	2.10	0.51
4:B:98:ASN:CG	4:B:101:GLU:HG3	2.36	0.51
4:B:91:ASP:O	4:B:143:ILE:HG23	2.10	0.51
3:A:359:LYS:O	3:A:370:LYS:HA	2.10	0.51
3:A:131:VAL:O	3:A:135:ARG:HG3	2.10	0.51
4:B:50:VAL:HG21	4:B:89:TYR:CD1	2.46	0.51
3:A:167:ASN:C	3:A:167:ASN:ND2	2.69	0.51
3:A:263:ALA:HB2	3:A:275:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:DA:H2''	1:C:17:DC:OP2	2.10	0.50
4:B:133:ILE:O	4:B:137:LYS:HG3	2.11	0.50
3:A:297:PHE:CE2	3:A:335:VAL:HG11	2.46	0.50
2:D:17:DT:OP2	3:A:338:VAL:HG22	2.10	0.50
4:B:144:ARG:CG	4:B:144:ARG:NH1	2.68	0.50
3:A:297:PHE:HE2	3:A:335:VAL:HG11	1.77	0.50
3:A:32:GLU:HB2	3:A:219:LYS:HZ3	1.73	0.50
4:B:18:ASN:N	4:B:223:GLY:O	2.45	0.50
4:B:76:PHE:C	4:B:76:PHE:CD2	2.90	0.50
4:B:102:VAL:HG23	4:B:103:GLY:N	2.27	0.50
3:A:347:ILE:HD13	3:A:372:ILE:HD12	1.94	0.50
4:B:299:ALA:O	4:B:302:SER:HB2	2.11	0.50
3:A:220:ARG:HH11	3:A:220:ARG:HB3	1.77	0.49
4:B:97:VAL:CG2	4:B:113:LEU:HD23	2.39	0.49
4:B:301:ARG:NH1	4:B:301:ARG:HB2	2.27	0.49
1:C:28:DT:H2''	1:C:29:DA:H5''	1.94	0.49
3:A:19:ILE:HG12	3:A:226:LYS:HE2	1.94	0.49
3:A:109:LEU:HD21	3:A:130:LEU:HA	1.94	0.49
3:A:46:ILE:CG2	3:A:201:GLU:HG3	2.42	0.49
3:A:323:TYR:CE1	3:A:340:GLN:HA	2.47	0.49
4:B:46:ILE:HD13	4:B:79:ILE:CD1	2.40	0.49
3:A:17:ILE:CG2	3:A:18:PHE:N	2.73	0.49
4:B:34:PHE:O	4:B:35:ARG:HD3	2.13	0.49
4:B:230:ASP:OD1	4:B:230:ASP:C	2.55	0.49
3:A:159:ILE:HD12	3:A:159:ILE:H	1.78	0.48
4:B:183:ASP:O	4:B:186:VAL:HB	2.12	0.48
4:B:144:ARG:HH11	4:B:174:ASN:HD21	1.61	0.48
1:C:2:DG:H2''	1:C:3:DA:O5'	2.13	0.48
4:B:21:VAL:HB	4:B:22:PHE:CD1	2.47	0.48
3:A:98:ILE:O	3:A:100:THR:HG22	2.13	0.48
3:A:143:ILE:HD12	3:A:177:PHE:CE1	2.48	0.48
3:A:326:TYR:CE2	3:A:338:VAL:HG12	2.49	0.48
4:B:70:PHE:HE2	8:B:9:ADP:C2	2.31	0.48
4:B:40:ARG:CG	4:B:41:ASP:N	2.76	0.48
4:B:76:PHE:HD1	4:B:148:TYR:CE2	2.32	0.48
3:A:32:GLU:C	3:A:34:PRO:HD3	2.38	0.48
4:B:90:LYS:O	4:B:91:ASP:CB	2.59	0.48
4:B:144:ARG:HG2	4:B:174:ASN:HD21	1.77	0.48
4:B:170:ARG:NE	4:B:197:SER:HB2	2.28	0.48
3:A:112:LEU:HD23	3:A:133:ALA:HB1	1.96	0.48
3:A:192:PRO:C	3:A:194:VAL:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:160:GLY:O	4:B:164:VAL:HG23	2.14	0.48
3:A:167:ASN:HD22	3:A:168:SER:N	2.12	0.47
3:A:284:GLU:O	3:A:285:ARG:C	2.56	0.47
4:B:244:GLU:OE2	4:B:244:GLU:CA	2.62	0.47
4:B:260:GLN:HA	4:B:260:GLN:HE21	1.78	0.47
4:B:293:PRO:HB2	4:B:296:TYR:HD1	1.75	0.47
2:D:16:DT:H2'	2:D:17:DT:C5	2.48	0.47
3:A:250:ARG:HE	8:A:8:ADP:H5'1	1.79	0.47
1:C:3:DA:N6	2:D:28:DA:N6	2.63	0.47
3:A:84:PHE:O	3:A:85:LEU:HB3	2.15	0.47
1:C:30:DC:H2''	1:C:31:DA:H5'	1.96	0.47
3:A:190:LEU:CB	3:A:195:LYS:HB2	2.44	0.47
3:A:363:ARG:HD3	3:A:366:TYR:CB	2.42	0.47
2:D:17:DT:H2'	2:D:18:DT:H71	1.97	0.47
3:A:133:ALA:O	3:A:137:TYR:HB2	2.15	0.47
3:A:291:ILE:O	3:A:295:LEU:HD13	2.14	0.47
3:A:21:ARG:O	3:A:24:LEU:HB2	2.14	0.47
3:A:39:GLN:NE2	3:A:39:GLN:N	2.61	0.47
3:A:109:LEU:O	3:A:114:VAL:O	2.32	0.47
3:A:270:LYS:HE2	3:A:271:VAL:O	2.14	0.47
4:B:86:ASP:O	4:B:87:GLU:CB	2.49	0.47
4:B:324:LYS:HA	4:B:324:LYS:HD2	1.75	0.47
3:A:244:ARG:O	3:A:244:ARG:HD3	2.14	0.47
3:A:212:GLU:O	3:A:216:ILE:HG13	2.15	0.47
4:B:130:GLY:C	4:B:132:TYR:H	2.23	0.47
1:C:5:DT:C2'	1:C:6:DT:H5''	2.36	0.46
3:A:60:PHE:HD1	3:A:198:LEU:HD13	1.81	0.46
4:B:140:THR:O	4:B:141:ARG:C	2.58	0.46
4:B:192:PRO:O	4:B:193:ARG:C	2.58	0.46
1:C:12:DT:H2''	1:C:13:DG:H5'	1.98	0.46
3:A:91:VAL:HG11	3:A:111:SER:CB	2.45	0.46
3:A:231:PRO:CD	3:A:271:VAL:HG12	2.42	0.46
1:C:21:DG:H21	5:C:34:SPD:H81	1.81	0.46
2:D:26:DA:H2''	2:D:27:DA:C5'	2.46	0.46
3:A:162:LYS:O	3:A:166:ILE:HG13	2.16	0.46
3:A:190:LEU:HD22	3:A:194:VAL:CG1	2.45	0.46
2:D:8:DT:C2	2:D:9:DT:C5	3.04	0.46
4:B:66:THR:HG22	4:B:206:PRO:HA	1.96	0.46
4:B:332:ARG:HD2	4:B:332:ARG:C	2.41	0.46
3:A:55:LYS:HG3	3:A:174:LYS:HB3	1.98	0.46
3:A:91:VAL:HG11	3:A:111:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:296:TYR:CE2	4:B:336:ILE:HG23	2.51	0.46
4:B:60:PHE:HB2	4:B:180:ILE:HG23	1.98	0.46
2:D:19:DC:H2''	2:D:20:DA:OP2	2.16	0.46
1:C:26:DT:H2''	1:C:27:DT:OP2	2.15	0.46
3:A:244:ARG:CG	3:A:244:ARG:NH1	2.74	0.46
3:A:288:VAL:O	3:A:292:ILE:HG22	2.17	0.46
4:B:30:LYS:HD2	4:B:30:LYS:HA	1.80	0.46
4:B:310:MET:HA	4:B:330:TYR:CE1	2.51	0.46
3:A:148:ILE:O	3:A:149:ASP:C	2.59	0.45
3:A:244:ARG:HG3	3:A:244:ARG:NH1	2.18	0.45
3:A:225:PHE:N	3:A:225:PHE:CD2	2.84	0.45
1:C:32:DC:H1'	1:C:33:DT:H5'	1.98	0.45
2:D:16:DT:C2'	2:D:17:DT:C6	2.99	0.45
3:A:98:ILE:O	3:A:99:ASP:HB2	2.16	0.45
4:B:315:MET:O	4:B:319:LEU:CD1	2.62	0.45
1:C:3:DA:H61	2:D:28:DA:N6	2.15	0.45
3:A:68:GLY:O	3:A:69:LYS:C	2.60	0.45
4:B:186:VAL:HA	4:B:189:TYR:CD2	2.51	0.45
3:A:94:ASN:OD1	3:A:96:ARG:HB2	2.17	0.45
3:A:300:LYS:NZ	3:A:388:SER:CB	2.79	0.45
1:C:3:DA:N6	2:D:28:DA:H61	2.15	0.45
2:D:18:DT:C7	3:A:339:THR:HG21	2.46	0.45
2:D:26:DA:C2'	2:D:27:DA:O5'	2.60	0.45
3:A:225:PHE:CD1	3:A:230:LEU:HD12	2.52	0.45
3:A:285:ARG:HG2	3:A:380:ILE:HD13	1.98	0.45
4:B:310:MET:HG3	4:B:330:TYR:OH	2.16	0.45
4:B:375:LEU:O	4:B:379:PHE:CD2	2.70	0.45
3:A:266:MET:O	3:A:267:LYS:C	2.59	0.45
4:B:218:LYS:O	4:B:222:TYR:CD2	2.70	0.45
1:C:31:DA:H5''	4:B:123:PRO:HB3	1.99	0.45
4:B:22:PHE:HE1	4:B:223:GLY:HA3	1.82	0.45
3:A:220:ARG:HH11	3:A:220:ARG:CB	2.29	0.45
4:B:62:GLY:C	4:B:68:LYS:HE3	2.42	0.45
1:C:18:DG:H2''	1:C:19:DT:H72	1.99	0.44
3:A:27:ASP:O	3:A:28:TYR:C	2.60	0.44
4:B:144:ARG:HG2	4:B:174:ASN:ND2	2.32	0.44
4:B:308:ASP:HB3	4:B:311:SER:HB2	1.98	0.44
1:C:23:DA:H2''	1:C:24:DA:OP2	2.16	0.44
3:A:302:VAL:O	3:A:306:VAL:HG23	2.17	0.44
4:B:47:ARG:HG3	4:B:89:TYR:OH	2.16	0.44
4:B:341:ASP:OD2	4:B:341:ASP:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:DG:H4'	3:A:369:THR:HA	1.99	0.44
1:C:16:DA:H1'	1:C:17:DC:H5'	2.00	0.44
2:D:19:DC:H4'	4:B:355:ARG:NH1	2.33	0.44
3:A:191:ASP:HB2	3:A:192:PRO:HD3	1.99	0.44
4:B:68:LYS:HB2	8:B:9:ADP:O2B	2.18	0.44
4:B:71:VAL:HG21	4:B:204:PHE:HE2	1.83	0.44
4:B:301:ARG:HB2	4:B:301:ARG:HH11	1.83	0.44
3:A:303:LEU:HD11	3:A:381:ILE:HD11	1.99	0.44
1:C:8:DC:C4	1:C:9:DA:N6	2.85	0.44
2:D:23:DT:H2''	2:D:24:DG:C8	2.53	0.44
3:A:304:MET:O	3:A:307:VAL:HB	2.17	0.44
4:B:55:LYS:HE3	4:B:175:ILE:O	2.17	0.44
2:D:2:DG:H2''	2:D:3:DT:H5'	1.99	0.44
4:B:334:SER:O	4:B:361:LYS:NZ	2.51	0.44
3:A:190:LEU:HB3	3:A:194:VAL:HG12	1.99	0.44
3:A:233:ASN:O	3:A:237:LEU:HD23	2.17	0.44
3:A:358:ALA:HA	3:A:371:GLU:O	2.18	0.44
3:A:363:ARG:O	3:A:364:GLY:C	2.60	0.44
4:B:62:GLY:HA3	4:B:68:LYS:HD2	2.00	0.44
4:B:349:ARG:HD3	4:B:362:TYR:HB2	2.00	0.44
3:A:218:THR:O	3:A:222:GLN:HG3	2.17	0.43
4:B:292:LEU:O	4:B:293:PRO:C	2.61	0.43
3:A:101:PRO:HD3	3:A:155:TYR:CE1	2.53	0.43
4:B:131:GLU:HA	4:B:134:ASP:HB2	2.00	0.43
2:D:16:DT:O2	4:B:354:GLY:HA2	2.18	0.43
4:B:207:TYR:CE1	4:B:215:ILE:HD11	2.53	0.43
4:B:151:GLU:C	4:B:153:ASP:H	2.26	0.43
1:C:20:DA:C1'	1:C:21:DG:H5'	2.43	0.43
1:C:31:DA:H5'	4:B:125:HIS:O	2.19	0.43
4:B:40:ARG:HG2	4:B:41:ASP:N	2.33	0.43
4:B:191:GLU:CG	4:B:192:PRO:HD2	2.46	0.43
2:D:13:DA:O5'	2:D:13:DA:H2'	2.19	0.43
2:D:21:DT:H1'	2:D:22:DC:H5''	1.99	0.43
4:B:304:ILE:HG12	4:B:365:VAL:HG21	2.01	0.43
3:A:300:LYS:NZ	3:A:388:SER:HB2	2.33	0.43
2:D:15:DG:H2''	2:D:16:DT:H5''	2.01	0.43
3:A:152:VAL:HG11	3:A:186:PHE:CE1	2.34	0.43
3:A:171:ASN:ND2	3:A:171:ASN:N	2.62	0.43
3:A:350:LEU:HD13	3:A:356:LEU:HD22	2.00	0.43
4:B:39:LEU:HD21	4:B:74:TYR:HD2	1.84	0.43
2:D:7:DT:C2	2:D:8:DT:C5	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:122:SER:O	3:A:124:ALA:N	2.52	0.42
3:A:291:ILE:CG2	3:A:353:VAL:HG11	2.30	0.42
4:B:21:VAL:HB	4:B:22:PHE:HD1	1.83	0.42
4:B:211:GLN:O	4:B:215:ILE:HG13	2.19	0.42
4:B:88:GLU:O	4:B:88:GLU:HG2	2.19	0.42
4:B:121:SER:O	4:B:122:VAL:HG23	2.19	0.42
3:A:36:ARG:O	3:A:40:ILE:HG13	2.20	0.42
3:A:234:VAL:O	3:A:238:CYS:HB2	2.18	0.42
4:B:22:PHE:HD2	4:B:256:PHE:CD1	2.37	0.42
1:C:20:DA:H2	5:C:34:SPD:H41	1.84	0.42
4:B:34:PHE:CZ	4:B:211:GLN:HA	2.55	0.42
3:A:25:LEU:C	3:A:27:ASP:N	2.78	0.42
3:A:48:ALA:O	3:A:49:PRO:C	2.62	0.42
3:A:292:ILE:HD11	3:A:385:LEU:HD13	2.02	0.42
3:A:50:LEU:HG	3:A:56:PRO:HG3	2.01	0.42
3:A:342:ARG:NH2	3:A:346:ILE:HG12	2.33	0.42
4:B:378:THR:HG23	4:B:379:PHE:N	2.35	0.42
1:C:14:DA:H2''	1:C:15:DA:OP2	2.20	0.42
2:D:22:DC:H2''	2:D:23:DT:H5'	2.01	0.42
3:A:67:THR:HB	3:A:205:PHE:HB3	2.02	0.42
3:A:241:LEU:HD23	3:A:241:LEU:HA	1.84	0.42
4:B:63:LEU:HD23	4:B:184:ILE:HD11	2.01	0.42
4:B:128:ASN:C	4:B:128:ASN:ND2	2.77	0.42
1:C:11:DA:C2	1:C:12:DT:C2	3.08	0.42
4:B:170:ARG:NE	4:B:197:SER:CB	2.82	0.42
3:A:23:TYR:O	3:A:220:ARG:NH1	2.53	0.42
3:A:198:LEU:HD23	3:A:198:LEU:HA	1.58	0.42
3:A:262:ILE:C	3:A:264:GLU:H	2.28	0.42
3:A:279:ALA:O	3:A:280:LYS:C	2.61	0.42
4:B:49:PHE:CE2	4:B:144:ARG:HB3	2.55	0.42
2:D:16:DT:H2'	2:D:17:DT:H71	2.01	0.42
3:A:21:ARG:H	3:A:21:ARG:HG3	1.58	0.42
3:A:306:VAL:HG12	3:A:374:LEU:HD11	2.01	0.42
4:B:172:ASP:O	4:B:173:ALA:C	2.63	0.42
4:B:296:TYR:CD2	4:B:336:ILE:HG23	2.55	0.41
4:B:155:LEU:O	4:B:161:GLY:HA3	2.19	0.41
4:B:204:PHE:CD1	4:B:204:PHE:N	2.89	0.41
4:B:206:PRO:HB3	4:B:246:GLY:HA3	2.02	0.41
4:B:349:ARG:HD3	4:B:362:TYR:CB	2.50	0.41
2:D:27:DA:H2''	2:D:28:DA:C8	2.56	0.41
3:A:19:ILE:HD13	3:A:19:ILE:HA	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:253:LEU:HD23	3:A:253:LEU:HA	1.93	0.41
3:A:341:ARG:HA	3:A:341:ARG:HD2	1.85	0.41
4:B:67:GLY:O	4:B:68:LYS:C	2.62	0.41
4:B:110:LEU:HD12	4:B:110:LEU:HA	1.83	0.41
4:B:122:VAL:HA	4:B:123:PRO:HD3	1.86	0.41
4:B:173:ALA:O	4:B:175:ILE:N	2.53	0.41
4:B:259:ALA:O	4:B:260:GLN:C	2.63	0.41
4:B:230:ASP:CG	4:B:233:ILE:HD12	2.46	0.41
3:A:22:GLU:C	3:A:24:LEU:H	2.27	0.41
4:B:79:ILE:HA	4:B:82:VAL:HG12	2.01	0.41
3:A:227:PRO:HB2	3:A:228:GLY:H	1.55	0.41
4:B:265:GLY:N	4:B:266:GLY:CA	2.84	0.41
3:A:41:ARG:CG	3:A:41:ARG:NH1	2.83	0.41
4:B:151:GLU:HG3	4:B:182:ASN:HD22	1.85	0.41
4:B:301:ARG:HH11	4:B:301:ARG:CB	2.34	0.41
4:B:353:ARG:N	4:B:358:GLY:HA3	2.25	0.41
4:B:365:VAL:O	4:B:366:GLU:C	2.64	0.41
1:C:6:DT:C2'	1:C:7:DT:H5'	2.51	0.41
1:C:10:DG:C2'	1:C:11:DA:OP2	2.68	0.41
2:D:28:DA:H1'	2:D:29:DT:H5'	2.03	0.41
4:B:75:ILE:O	4:B:76:PHE:C	2.63	0.41
4:B:160:GLY:HA2	4:B:163:ILE:HD12	2.03	0.41
4:B:250:LYS:O	4:B:254:LEU:N	2.54	0.41
3:A:36:ARG:HA	3:A:36:ARG:HD3	1.89	0.41
3:A:262:ILE:HG22	3:A:275:TYR:CD1	2.56	0.41
4:B:310:MET:HB2	4:B:310:MET:HE3	1.83	0.41
4:B:339:GLU:O	4:B:343:PHE:HD2	2.04	0.41
4:B:52:ASN:O	4:B:54:VAL:HG23	2.21	0.41
4:B:179:MET:HB2	4:B:179:MET:HE2	1.83	0.40
2:D:12:DT:H2''	2:D:13:DA:C8	2.55	0.40
3:A:274:GLU:O	3:A:278:MET:HE3	2.20	0.40
4:B:60:PHE:HE1	4:B:202:VAL:HG21	1.86	0.40
4:B:236:TYR:OH	4:B:270:LYS:HG3	2.21	0.40
2:D:26:DA:O4'	3:A:364:GLY:HA3	2.22	0.40
3:A:50:LEU:HD13	3:A:88:PHE:CE1	2.56	0.40
3:A:258:VAL:O	3:A:259:SER:C	2.65	0.40
3:A:376:VAL:HG22	3:A:377:ASP:H	1.83	0.40
3:A:335:VAL:O	3:A:336:GLU:C	2.64	0.40
3:A:147:GLU:C	3:A:149:ASP:N	2.79	0.40
3:A:198:LEU:C	3:A:200:GLU:H	2.29	0.40
3:A:300:LYS:HZ3	3:A:388:SER:HB2	1.87	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	360/386 (93%)	295 (82%)	53 (15%)	12 (3%)	3	17
4	B	366/384 (95%)	294 (80%)	45 (12%)	27 (7%)	1	5
All	All	726/770 (94%)	589 (81%)	98 (14%)	39 (5%)	1	9

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	123	ILE
3	A	153	LYS
3	A	226	LYS
3	A	227	PRO
4	B	91	ASP
4	B	120	PHE
4	B	142	ASN
4	B	143	ILE
4	B	245	HIS
4	B	247	ASP
3	A	64	LEU
3	A	88	PHE
3	A	337	ALA
3	A	364	GLY
4	B	87	GLU
4	B	174	ASN
4	B	241	SER
4	B	242	ALA
4	B	244	GLU
4	B	264	GLY
4	B	324	LYS
4	B	354	GLY

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Mol	Chain	Res	Type
4	B	383	ILE
3	A	267	LYS
4	B	20	LYS
4	B	86	ASP
4	B	173	ALA
4	B	185	ASN
3	A	47	LEU
4	B	131	GLU
4	B	293	PRO
4	B	90	LYS
4	B	99	CYS
4	B	119	GLY
3	A	85	LEU
3	A	192	PRO
4	B	103	GLY
4	B	359	VAL
4	B	286	ILE

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	327/344 (95%)	271 (83%)	56 (17%)	2	9
4	B	319/331 (96%)	280 (88%)	39 (12%)	5	18
All	All	646/675 (96%)	551 (85%)	95 (15%)	3	12

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	19	ILE
3	A	21	ARG
3	A	37	GLU
3	A	39	GLN
3	A	46	ILE
3	A	52	ARG

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Mol	Chain	Res	Type
3	A	59	ILE
3	A	64	LEU
3	A	67	THR
3	A	91	VAL
3	A	93	ILE
3	A	100	THR
3	A	116	VAL
3	A	141	VAL
3	A	143	ILE
3	A	148	ILE
3	A	152	VAL
3	A	166	ILE
3	A	167	ASN
3	A	168	SER
3	A	171	ASN
3	A	175	ILE
3	A	176	SER
3	A	181	THR
3	A	198	LEU
3	A	203	ILE
3	A	215	ASP
3	A	216	ILE
3	A	220	ARG
3	A	229	VAL
3	A	237	LEU
3	A	238	CYS
3	A	244	ARG
3	A	251	ARG
3	A	256	LEU
3	A	259	SER
3	A	262	ILE
3	A	271	VAL
3	A	278	MET
3	A	292	ILE
3	A	295	LEU
3	A	299	SER
3	A	310	SER
3	A	317	SER
3	A	319	THR
3	A	325	THR
3	A	341	ARG
3	A	342	ARG

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Mol	Chain	Res	Type
3	A	346	ILE
3	A	355	ILE
3	A	356	LEU
3	A	360	VAL
3	A	363	ARG
3	A	372	ILE
3	A	381	ILE
3	A	385	LEU
4	B	22	PHE
4	B	23	ILE
4	B	40	ARG
4	B	64	THR
4	B	68	LYS
4	B	77	ASN
4	B	91	ASP
4	B	105	THR
4	B	110	LEU
4	B	121	SER
4	B	122	VAL
4	B	127	ILE
4	B	144	ARG
4	B	154	THR
4	B	178	ILE
4	B	180	ILE
4	B	194	VAL
4	B	196	SER
4	B	201	SER
4	B	202	VAL
4	B	241	SER
4	B	244	GLU
4	B	245	HIS
4	B	254	LEU
4	B	255	LEU
4	B	278	VAL
4	B	279	ASP
4	B	311	SER
4	B	315	MET
4	B	317	THR
4	B	325	GLN
4	B	332	ARG
4	B	336	ILE
4	B	338	SER

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Mol	Chain	Res	Type
4	B	341	ASP
4	B	348	ILE
4	B	349	ARG
4	B	350	ILE
4	B	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	35	HIS
3	A	39	GLN
3	A	81	HIS
3	A	167	ASN
3	A	171	ASN
3	A	182	ASN
3	A	233	ASN
4	B	18	ASN
4	B	94	GLN
4	B	128	ASN
4	B	167	GLN
4	B	174	ASN
4	B	245	HIS
4	B	260	GLN
4	B	272	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
8	ADP	B	9	7	28,29,29	1.46	4 (14%)	43,45,45	1.83	7 (16%)
5	SPD	C	35	-	9,9,9	0.33	0	8,8,8	0.65	0
5	SPD	C	34	-	9,9,9	0.39	0	8,8,8	0.79	0
8	ADP	A	8	-	28,29,29	1.51	4 (14%)	43,45,45	1.96	10 (23%)

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
8	ADP	B	9	7	-	7/16/32/32	0/3/3/3
5	SPD	C	35	-	-	3/7/7/7	-
5	SPD	C	34	-	-	1/7/7/7	-
8	ADP	A	8	-	-	6/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	8	ADP	C5-C4	5.07	1.48	1.39
8	B	9	ADP	C5-C4	5.04	1.48	1.39
8	A	8	ADP	C5-C6	3.09	1.49	1.41
8	B	9	ADP	C5-C6	2.86	1.49	1.41
8	A	8	ADP	C8-N7	2.57	1.36	1.31
8	B	9	ADP	C5-N7	-2.25	1.35	1.39
8	A	8	ADP	PA-O3A	2.21	1.61	1.59
8	B	9	ADP	C8-N7	2.20	1.35	1.31

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	9	ADP	C5-C4-N3	-6.14	118.26	126.72
8	A	8	ADP	C5-C4-N3	-5.42	119.26	126.72
8	B	9	ADP	N3-C4-N9	4.99	135.66	127.17
8	A	8	ADP	N3-C4-N9	4.39	134.63	127.17
8	B	9	ADP	C2-N3-C4	3.75	120.98	111.83
8	A	8	ADP	C2-N3-C4	3.59	120.60	111.83
8	A	8	ADP	C4-C5-N7	-3.44	106.65	110.58
8	B	9	ADP	C4-C5-N7	-3.36	106.74	110.58
8	A	8	ADP	O4'-C1'-N9	3.26	114.36	108.09
8	A	8	ADP	N3-C2-N1	-3.23	123.69	128.58
8	B	9	ADP	N3-C2-N1	-3.16	123.81	128.58
8	A	8	ADP	C4-N9-C8	2.89	108.78	105.74
8	A	8	ADP	C6-C5-N7	2.60	137.10	132.09
8	B	9	ADP	C5-N7-C8	2.44	107.28	103.45
8	A	8	ADP	C5-N7-C8	2.39	107.20	103.45
8	B	9	ADP	C4-N9-C8	2.28	108.14	105.74
8	A	8	ADP	O3A-PA-O1A	-2.06	104.52	110.70

There are no chirality outliers.

All (17) torsion outliers are listed below:

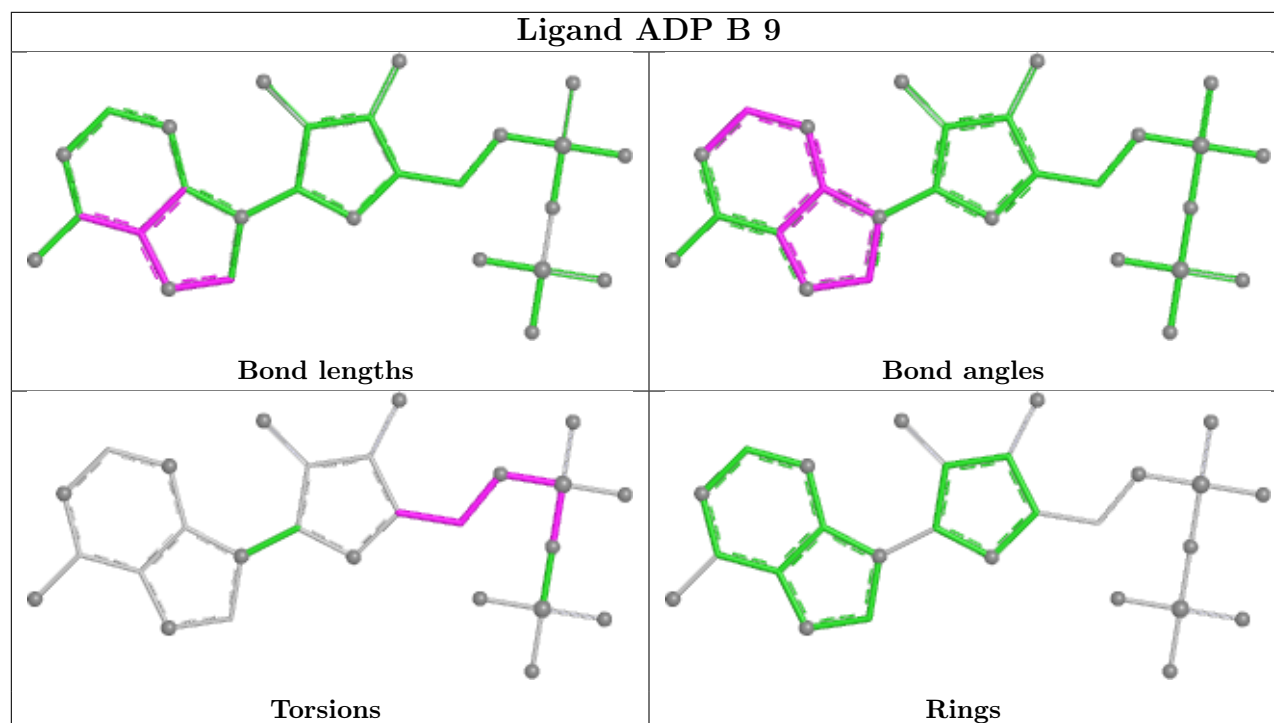
Mol	Chain	Res	Type	Atoms
8	A	8	ADP	PA-O3A-PB-O2B
8	A	8	ADP	C5'-O5'-PA-O1A
8	A	8	ADP	C5'-O5'-PA-O2A
8	A	8	ADP	C5'-O5'-PA-O3A
8	A	8	ADP	O4'-C4'-C5'-O5'
8	B	9	ADP	C5'-O5'-PA-O1A
8	B	9	ADP	C5'-O5'-PA-O2A
8	B	9	ADP	C5'-O5'-PA-O3A
5	C	35	SPD	C4-C5-N6-C7
8	A	8	ADP	C3'-C4'-C5'-O5'
8	B	9	ADP	O4'-C4'-C5'-O5'
8	B	9	ADP	C3'-C4'-C5'-O5'
5	C	35	SPD	C8-C7-N6-C5
5	C	34	SPD	C2-C3-C4-C5
8	B	9	ADP	C4'-C5'-O5'-PA
8	B	9	ADP	PB-O3A-PA-O2A
5	C	35	SPD	C7-C8-C9-N10

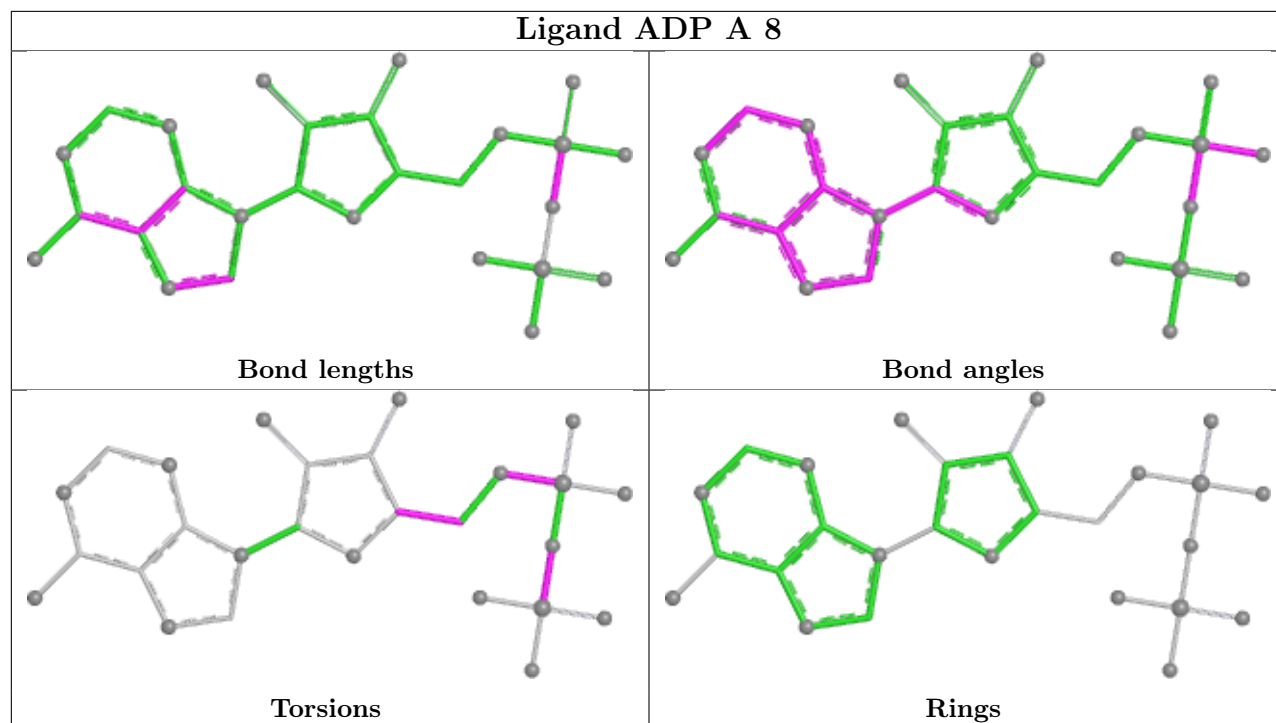
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	9	ADP	4	0
5	C	34	SPD	2	0
8	A	8	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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(Å ²)	Q<0.9
1	C	33/33 (100%)	-0.57	0	100 100	131, 168, 209, 224	0
2	D	33/33 (100%)	-0.47	0	100 100	133, 161, 210, 219	0
3	A	366/386 (94%)	-0.32	1 (0%)	90 84	115, 148, 197, 257	0
4	B	368/384 (95%)	-0.41	3 (0%)	82 71	111, 148, 200, 232	0
All	All	800/836 (95%)	-0.38	4 (0%)	87 78	111, 149, 201, 257	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	104	GLY	2.6
4	B	384	SER	2.3
3	A	174	LYS	2.2
4	B	17	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

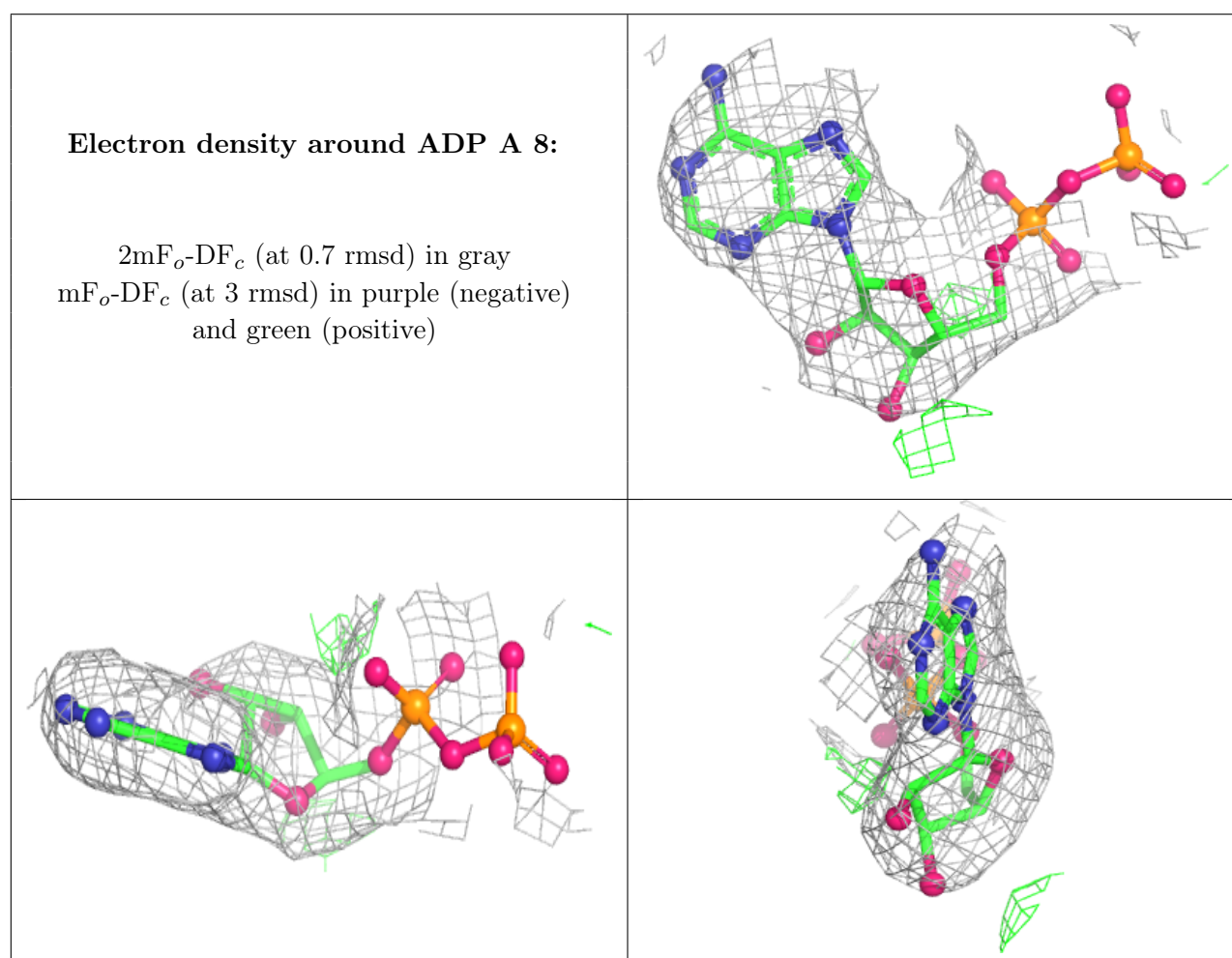
There are no oligosaccharides in this entry.

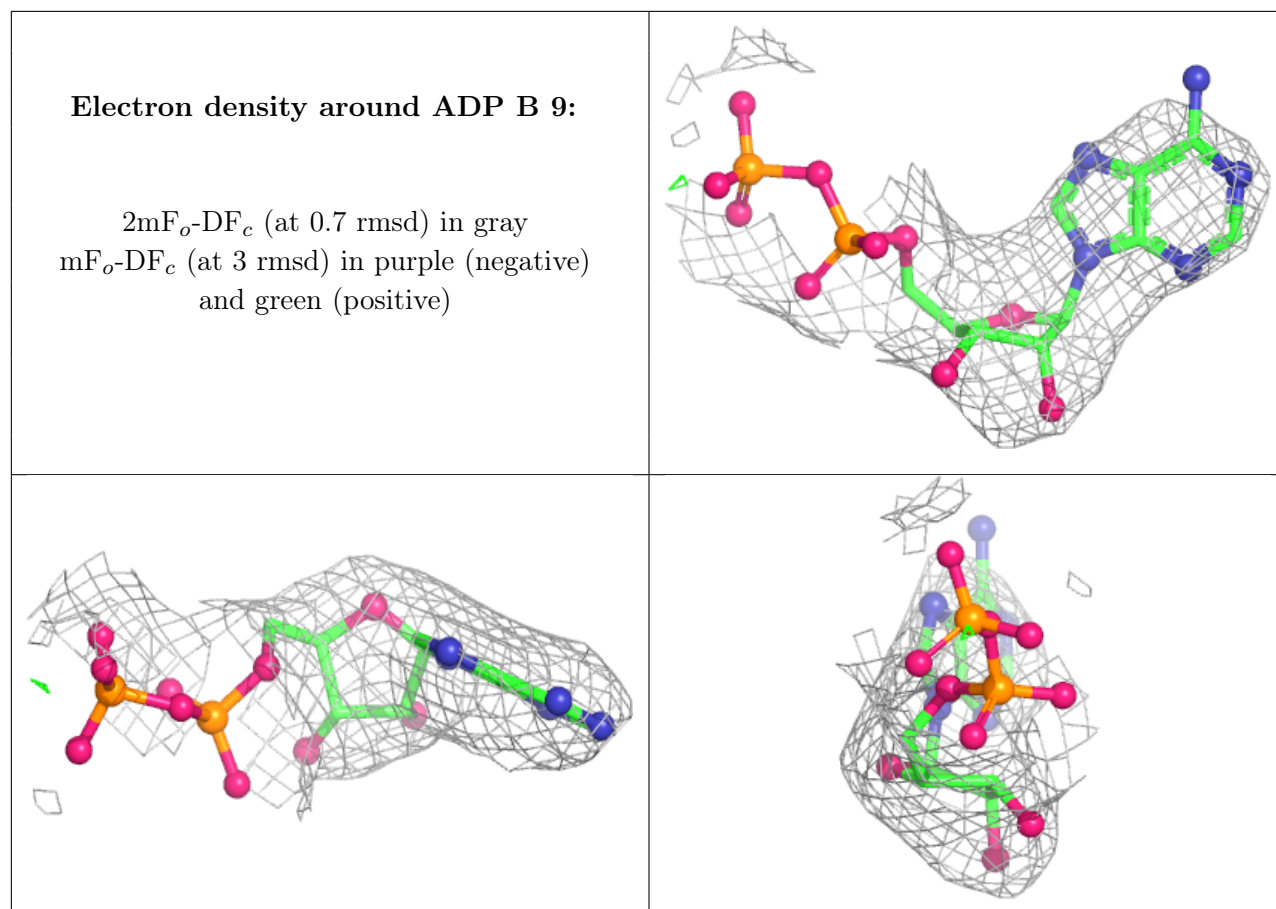
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	D	35	1/1	0.66	0.33	168,168,168,168	0
5	SPD	C	35	10/10	0.67	0.17	152,152,152,152	0
5	SPD	C	34	10/10	0.86	0.24	130,130,130,130	0
7	MG	B	7	1/1	0.95	0.06	73,73,73,73	0
8	ADP	A	8	27/27	0.96	0.08	111,111,111,111	0
7	MG	A	6	1/1	0.97	0.11	79,79,79,79	0
8	ADP	B	9	27/27	0.97	0.07	121,121,121,121	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 ⓘ

There are no such residues in this entry.