Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 04:49 AM EDT

PDB ID	:	2QBY
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:

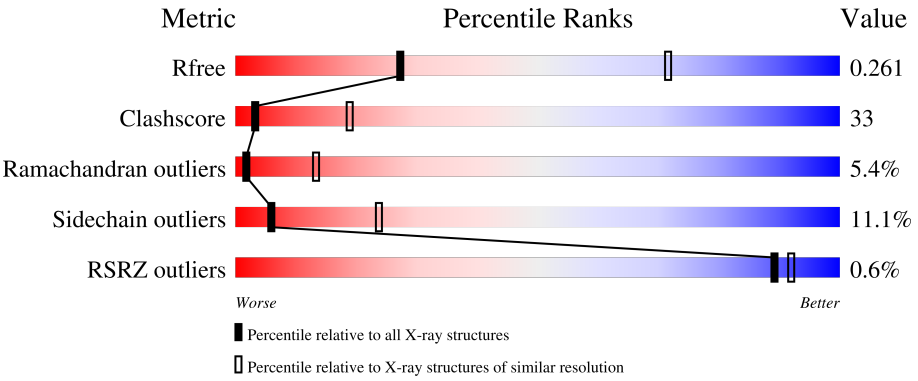
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 <=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	9% 45% 45%
2	D	33	9% 61% 30%
3	A	386	% 42% 42% 10% 5%
4	B	384	42% 44% 9%

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
5	SPD	C	34	-	-	-	X
5	SPD	C	35	-	-	-	X

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
			Total	C	N	O	P			
1	C	33	678	326	127	193	32	0	0	0

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

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

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

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

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
			Total	C	N	O	S			
4	B	368	2944	1890	501	546	7	0	0	0

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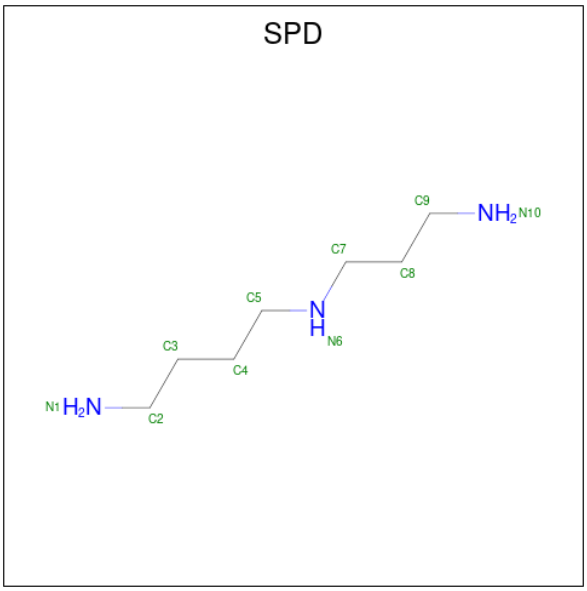
Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	-	expression tag	UNP Q97WM8
B	13	MET	-	expression tag	UNP Q97WM8

- Molecule 5 is SPERMIDINE (three-letter code: 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 (three-letter code: K) (formula: K).

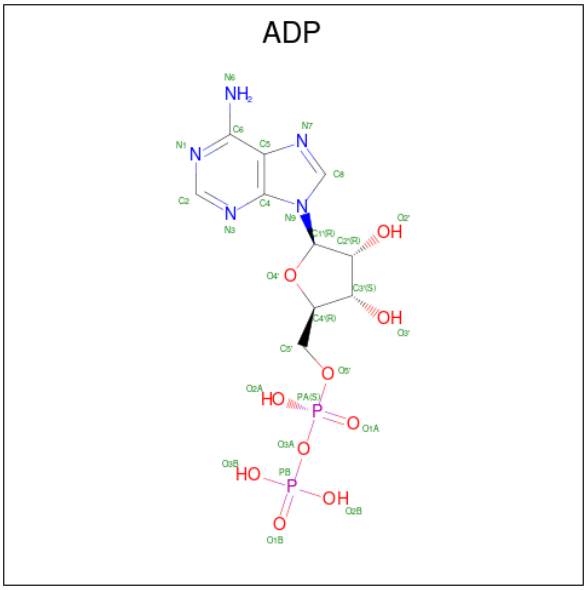
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total K 1 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: 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 (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 9 is water.

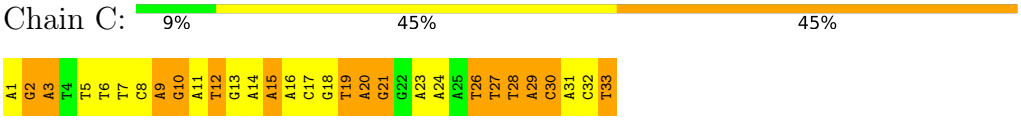
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	O	0	0
			2	2		
9	B	2	Total	O	0	0
			2	2		

3 Residue-property plots (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.

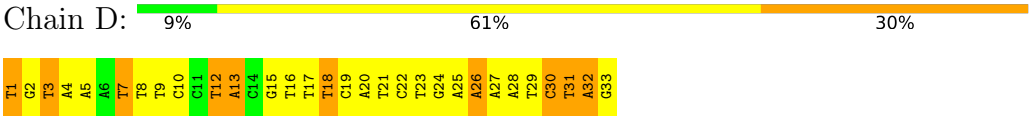
• Molecule 1: DNA (33-MER)

Chain C:



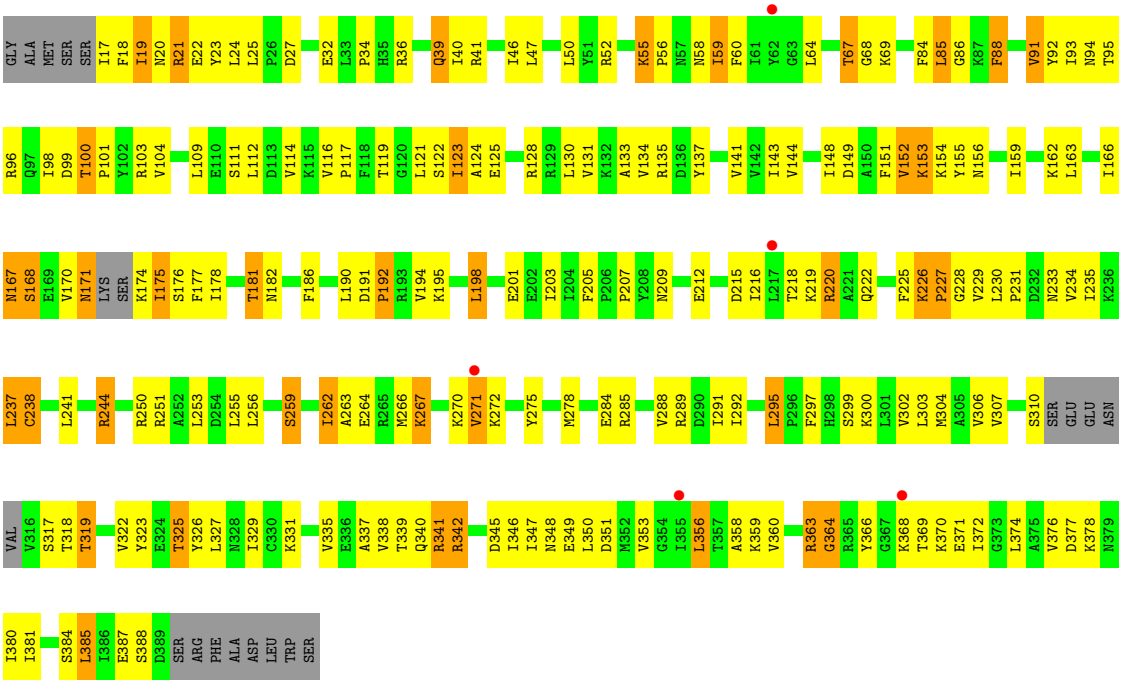
• Molecule 2: DNA (33-MER)

Chain D:



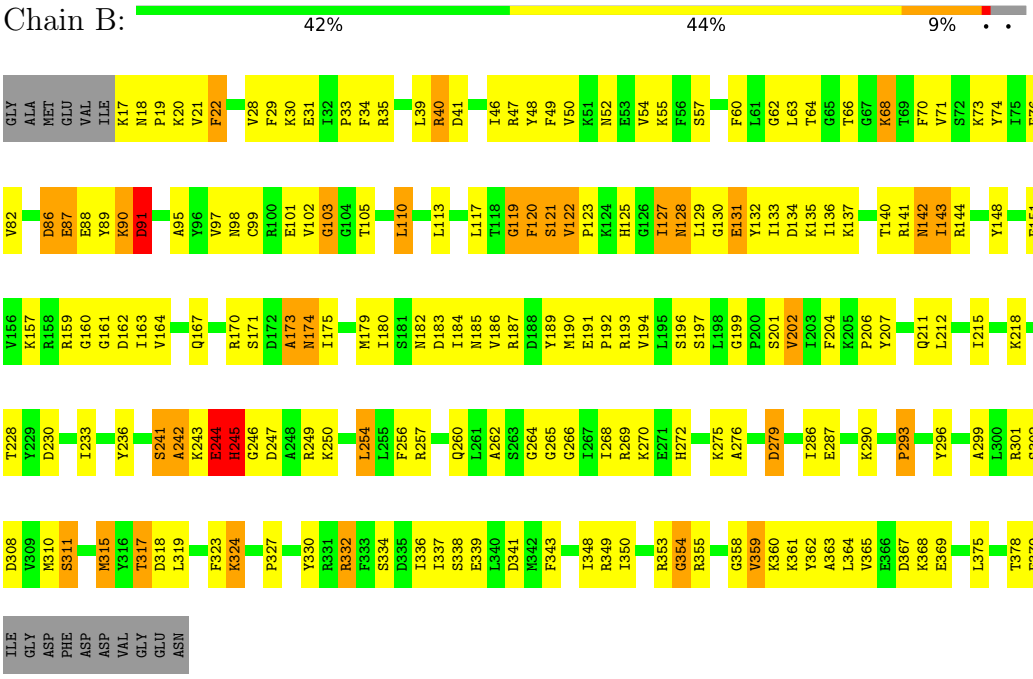
• Molecule 3: Cell division control protein 6 homolog 1

Chain A:



• Molecule 4: Cell division control protein 6 homolog 3

Chain B:


42%
44%
9%
GLY ALA MET GLU VAL ILE K17 N18 P19 K20 V21 F22 V28 F29 K30 E31 I32 P33 F34 R35 L39 R40 D41 I46 R47 Y48 F49 V50 K51 N52 E53 V54 K55 F56 S57 F60 L61 G62 L63 T64 G65 T66 G67 K68 T69 F70 V71 S72 K73 Y74 I75 F76 N77 E78 I79
V82 D86 E87 E88 Y89 K90 D91 A95 Y96 V97 N98 C99 R100 E101 V102 G103 G104 T105 L110 L113 L117 T118 G119 F120 S121 V122 P123 K124 H125 G126 I127 N128 L129 G130 E131 Y132 I133 D134 K135 I136 K137 T140 R141 N142 I143 R144 Y148 E151 V152 D153 T154 L155
V156 K157 R158 R159 G160 G161 D162 I163 V164 Q167 R170 S171 D172 A173 N174 I175 M179 I180 S181 N182 D183 I184 N185 V186 R187 D188 Y189 M190 E191 P192 R193 V194 L195 S196 S197 L198 G199 P200 S201 V202 I203 F204 K205 P206 Y207 Q211 L212 I215 K218 Y222 G223 L224
T228 Y229 D230 I233 Y236 S241 A242 K243 E244 H245 G246 D247 A248 R249 K250 L254 L255 F256 R257 Q260 L261 A262 S263 G264 G265 G266 I267 I268 R269 K270 E271 H272 K275 A276 D279 I286 E287 K290 P293 Y296 A299 L300 R301 S302 L303 I304 E307
D308 V309 M310 S311 M315 Y316 T317 D318 L319 F323 K324 P327 Y330 R331 R332 F333 S334 D335 I336 I337 S338 E339 L340 D341 M342 F343 I348 R349 I350 R353 G354 R355 G358 V359 K360 K361 Y362 A363 L364 V365 E366 D367 K368 E369 L375 T378 F379 S382 I383 S384
ILE GLY ASP PHE ASP ASP VAL GLY GLU ASN

4 Data and refinement statistics (i)

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 49.10 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-3.35) 97.9 (49.10-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.269 0.220 , 0.261	Depositor DCC
R_{free} test set	1216 reflections (5.11%)	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 , 90.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, ADP, K, SPD

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	0.69	0/762	1.55	23/1175 (2.0%)
2	D	0.65	0/748	1.51	16/1152 (1.4%)
3	A	0.39	0/2980	0.60	0/4022
4	B	0.40	0/2993	0.60	0/4025
All	All	0.46	0/7483	0.90	39/10374 (0.4%)

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 (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	10	DG	C1'-O4'-C4'	-10.63	99.47	110.10
2	D	30	DC	O4'-C1'-N1	8.74	114.12	108.00
1	C	26	DT	O4'-C1'-N1	8.50	113.95	108.00
1	C	9	DA	C4'-C3'-C2'	-7.96	95.93	103.10
1	C	33	DT	C4'-C3'-C2'	-7.72	96.15	103.10
2	D	3	DT	O4'-C1'-N1	7.47	113.23	108.00
2	D	13	DA	O4'-C4'-C3'	-7.29	101.58	104.50
2	D	32	DA	O4'-C1'-N9	6.64	112.65	108.00
2	D	32	DA	P-O3'-C3'	6.40	127.38	119.70
1	C	21	DG	O4'-C1'-N9	6.36	112.45	108.00
2	D	13	DA	C3'-C2'-C1'	-6.30	94.94	102.50
2	D	13	DA	O4'-C1'-N9	-6.26	103.62	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	9	DA	O4'-C4'-C3'	-6.16	102.03	104.50
1	C	2	DG	C1'-O4'-C4'	-6.13	103.97	110.10
1	C	15	DA	O4'-C1'-N9	6.13	112.29	108.00
1	C	19	DT	O4'-C1'-N1	6.13	112.29	108.00
1	C	1	DA	O4'-C1'-N9	-6.11	103.73	108.00
1	C	26	DT	N3-C4-O4	6.10	123.56	119.90
1	C	28	DT	N3-C4-O4	6.00	123.50	119.90
1	C	28	DT	C5-C4-O4	-6.00	120.70	124.90
1	C	20	DA	O4'-C1'-N9	-5.99	103.81	108.00
2	D	12	DT	N3-C4-O4	5.91	123.45	119.90
1	C	3	DA	O4'-C1'-N9	5.88	112.12	108.00
1	C	27	DT	N3-C4-O4	5.71	123.33	119.90
1	C	27	DT	C5-C4-O4	-5.58	121.00	124.90
1	C	26	DT	C4'-C3'-C2'	-5.52	98.13	103.10
2	D	1	DT	N3-C4-O4	5.49	123.19	119.90
1	C	30	DC	O4'-C4'-C3'	-5.42	102.33	104.50
1	C	12	DT	N3-C4-O4	5.38	123.12	119.90
2	D	18	DT	C4'-C3'-C2'	-5.35	98.29	103.10
1	C	9	DA	C3'-C2'-C1'	-5.24	96.21	102.50
2	D	31	DT	C5-C4-O4	-5.24	121.23	124.90
2	D	12	DT	C5-C4-O4	-5.20	121.26	124.90
1	C	10	DG	O4'-C4'-C3'	-5.17	102.43	104.50
2	D	26	DA	P-O3'-C3'	5.16	125.89	119.70
1	C	29	DA	P-O5'-C5'	-5.14	112.68	120.90
2	D	1	DT	P-O3'-C3'	-5.09	113.59	119.70
2	D	7	DT	P-O3'-C3'	5.06	125.77	119.70
2	D	1	DT	C5-C4-O4	-5.04	121.37	124.90

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	38	0
2	D	669	0	378	50	0
3	A	2937	0	3069	217	0
4	B	2944	0	3027	186	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	471	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 33.

All (471) 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
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
4:B:97:VAL:HG21	4:B:113:LEU:HD23	1.59	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:PHE:C	3:A:86:GLY:H	1.85	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
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
3:A:17:ILE:HG23	3:A:18:PHE:N	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:84:PHE:C	3:A:86:GLY:N	2.46	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
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
3:A:32:GLU:HB2	3:A:219:LYS:HZ2	1.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:167:GLN:O	4:B:171:SER:HB3	1.99	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
1:C:27:DT:C2'	1:C:28:DT:H71	2.31	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
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
1:C:27:DT:H2'	1:C:28:DT:H71	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:307:GLU:CD	4:B:364:LEU:HD23	2.24	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:345:ASP:O	3:A:349:GLU:HG3	2.02	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: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:348:ASN:HD21	3:A:370:LYS:HZ1	1.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:B:128:ASN:HD22	4:B:128:ASN:C	2.11	0.54
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
3:A:122:SER:O	3:A:123:ILE:C	2.48	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: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
3:A:25:LEU:C	3:A:27:ASP:H	2.12	0.52
3:A:300:LYS:HZ3	3:A:388:SER:CB	2.22	0.52
4:B:151:GLU:HG3	4:B:182:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:323:PHE:O	4:B:324:LYS:C	2.48	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:91:ASP:O	4:B:143:ILE:HG23	2.10	0.51
3:A:192:PRO:C	3:A:194:VAL:H	2.14	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:263:ALA:HB2	3:A:275:TYR:CD2	2.45	0.51
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
4:B:18:ASN:N	4:B:223:GLY:O	2.45	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:184:ILE:C	4:B:186:VAL:H	2.16	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:300:LYS:HZ3	3:A:388:SER:HB2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:34:PHE:O	4:B:35:ARG:HD3	2.13	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:DT:H2"	1:C:13:DG:H5'	1.98	0.46
4:B:98:ASN:CG	4:B:101:GLU:HG3	2.36	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
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
3:A:167:ASN:C	3:A:167:ASN:ND2	2.69	0.46
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
4:B:187:ARG:HA	4:B:190:MET:HE3	1.97	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: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
4:B:76:PHE:C	4:B:76:PHE:CD2	2.90	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
4:B:310:MET:HE1	4:B:360:LYS:HG2	1.98	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:230:ASP:OD1	4:B:230:ASP:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:18:DG:H2"	1:C:19:DT:H72	1.99	0.44
4:B:144:ARG:HG2	4:B:174:ASN:ND2	2.32	0.44
3:A:300:LYS:NZ	3:A:388:SER:CB	2.79	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
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
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
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
3:A:32:GLU:C	3:A:34:PRO:HD3	2.38	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
3:A:192:PRO:C	3:A:194:VAL:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:284:GLU:O	3:A:285:ARG:C	2.56	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
4:B:88:GLU:O	4:B:88:GLU:HG2	2.19	0.43
2:D:7:DT:C2	2:D:8:DT:C5	3.07	0.42
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: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: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
3:A:300:LYS:NZ	3:A:388:SER:HB2	2.33	0.42
4:B:63:LEU:HD23	4:B:184:ILE:HD11	2.01	0.42
4:B:130:GLY:C	4:B:132:TYR:H	2.23	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
4:B:49:PHE:CE2	4:B:144:ARG:HB3	2.55	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:140:THR:O	4:B:141:ARG:C	2.58	0.42
4:B:192:PRO:O	4:B:193:ARG:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:253:LEU:HD23	3:A:253:LEU:HA	1.93	0.41
3:A:262:ILE:HG22	3:A:263:ALA:N	2.35	0.41
3:A:341:ARG:HA	3:A:341:ARG:HD2	1.85	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: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:152:VAL:HG22	4:B:152:VAL:O	2.20	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
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: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:148:ILE:O	3:A:149:ASP:C	2.59	0.41
3:A:262:ILE:HG22	3:A:275:TYR:CD1	2.56	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
3:A:68:GLY:O	3:A:69:LYS:C	2.60	0.40
2:D:12:DT:H2"	2:D:13:DA:C8	2.55	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:376:VAL:HG22	3:A:377:ASP:H	1.83	0.40
3:A:266:MET:O	3:A:267:LYS:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	360/386 (93%)	295 (82%)	53 (15%)	12 (3%)	4 24
4	B	366/384 (95%)	294 (80%)	45 (12%)	27 (7%)	1 7
All	All	726/770 (94%)	589 (81%)	98 (14%)	39 (5%)	2 13

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
4	B	383	ILE
3	A	267	LYS
4	B	20	LYS

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Mol	Chain	Res	Type
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 (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
3	A	327/344 (95%)	285 (87%)	42 (13%)	4 18
4	B	319/331 (96%)	289 (91%)	30 (9%)	8 31
All	All	646/675 (96%)	574 (89%)	72 (11%)	6 24

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	19	ILE
3	A	21	ARG
3	A	39	GLN
3	A	52	ARG
3	A	55	LYS
3	A	59	ILE
3	A	67	THR
3	A	91	VAL
3	A	93	ILE

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Mol	Chain	Res	Type
3	A	100	THR
3	A	116	VAL
3	A	152	VAL
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	220	ARG
3	A	237	LEU
3	A	238	CYS
3	A	244	ARG
3	A	256	LEU
3	A	259	SER
3	A	262	ILE
3	A	271	VAL
3	A	278	MET
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
3	A	356	LEU
3	A	360	VAL
3	A	363	ARG
3	A	385	LEU
4	B	22	PHE
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

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Mol	Chain	Res	Type
4	B	122	VAL
4	B	127	ILE
4	B	128	ASN
4	B	154	THR
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	279	ASP
4	B	311	SER
4	B	315	MET
4	B	317	THR
4	B	318	ASP
4	B	332	ARG
4	B	338	SER
4	B	341	ASP
4	B	348	ILE
4	B	350	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	362	ASN
4	B	125	HIS
4	B	128	ASN
4	B	174	ASN
4	B	245	HIS
4	B	260	GLN
4	B	272	HIS
4	B	325	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
5	SPD	C	35	-	9,9,9	0.34	0	8,8,8	0.65	0
5	SPD	C	34	-	9,9,9	0.39	0	8,8,8	0.80	0
8	ADP	A	8	-	24,29,29	1.07	2 (8%)	29,45,45	1.54	4 (13%)
8	ADP	B	9	7	24,29,29	1.03	1 (4%)	29,45,45	1.40	4 (13%)

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
5	SPD	C	35	-	-	3/7/7/7	-
5	SPD	C	34	-	-	1/7/7/7	-
8	ADP	A	8	-	-	6/12/32/32	0/3/3/3
8	ADP	B	9	7	-	7/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	8	ADP	C5-C4	2.72	1.48	1.40
8	B	9	ADP	C5-C4	2.70	1.48	1.40
8	A	8	ADP	O4'-C1'	2.25	1.44	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	9	ADP	PA-O3A-PB	-3.52	120.76	132.83
8	A	8	ADP	N3-C2-N1	-3.19	123.69	128.68
8	A	8	ADP	PA-O3A-PB	-3.16	122.00	132.83
8	B	9	ADP	N3-C2-N1	-3.12	123.81	128.68
8	A	8	ADP	C4-C5-N7	-2.64	106.65	109.40
8	B	9	ADP	C4-C5-N7	-2.55	106.74	109.40
8	B	9	ADP	C3'-C2'-C1'	2.54	104.80	100.98
8	A	8	ADP	C1'-N9-C4	-2.05	123.04	126.64

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

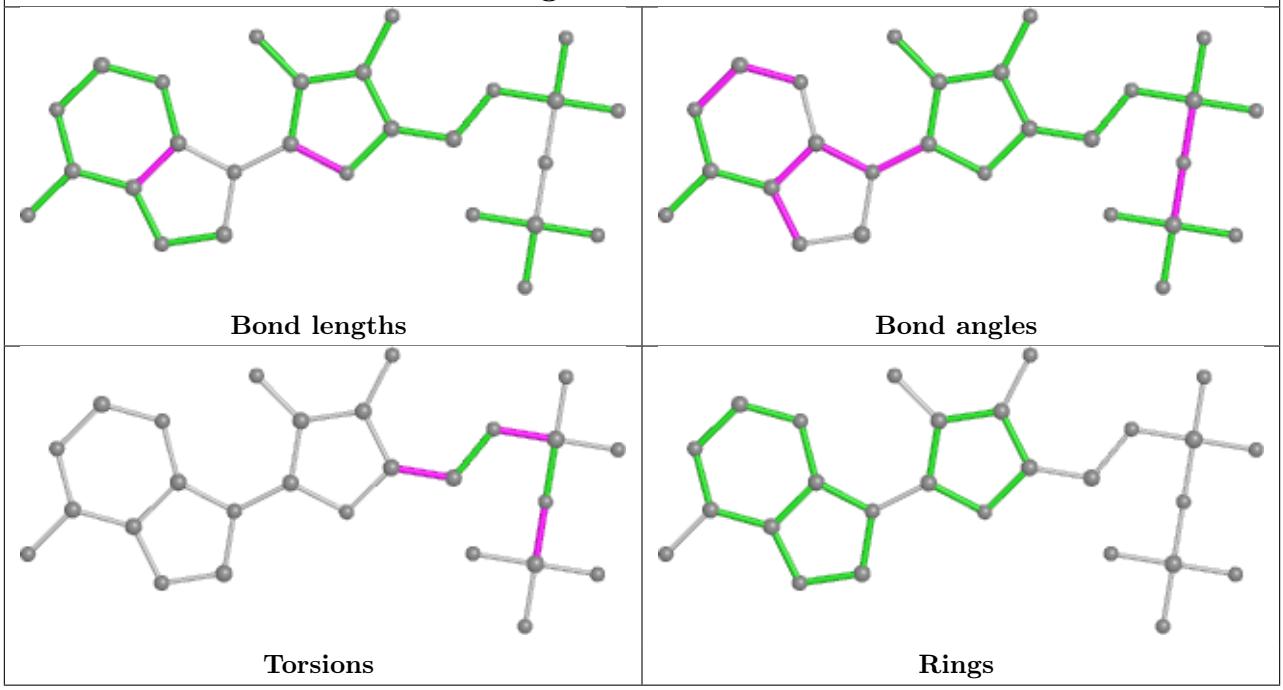
There are no ring outliers.

3 monomers are involved in 8 short contacts:

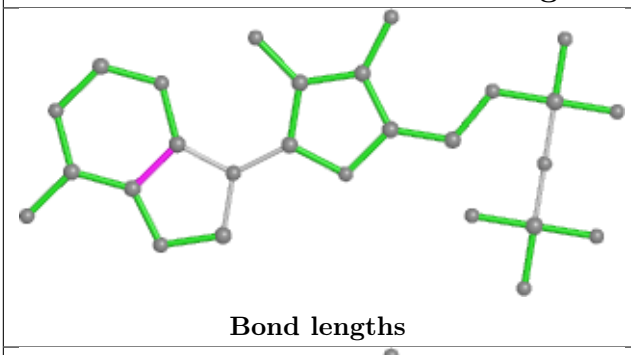
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	34	SPD	2	0
8	A	8	ADP	2	0
8	B	9	ADP	4	0

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 then 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.

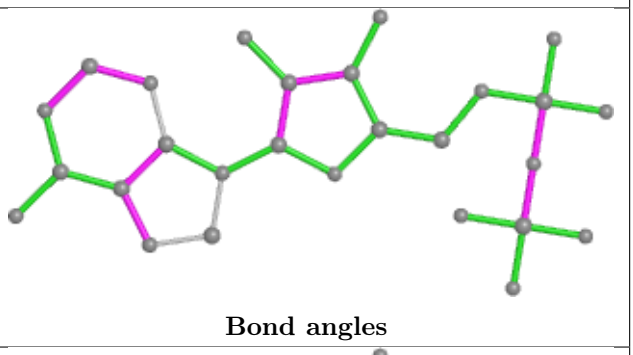
Ligand ADP A 8



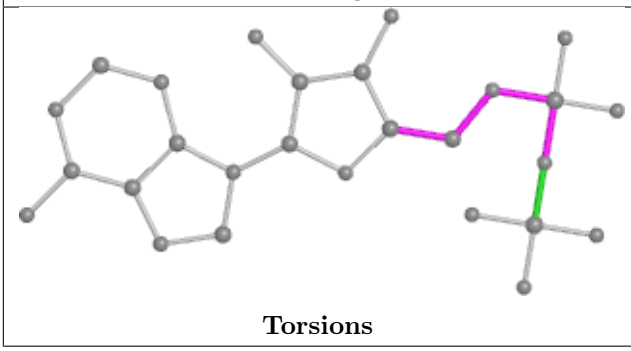
Ligand ADP B 9



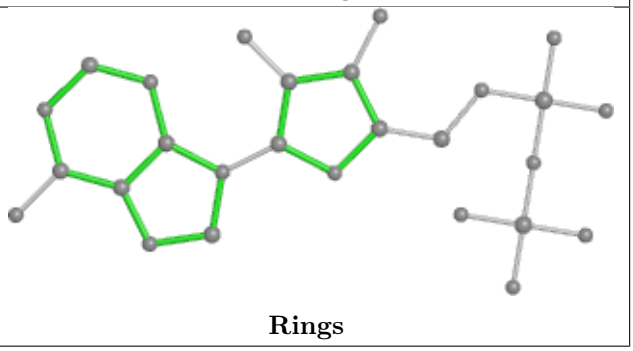
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.60	0 100 100	131, 168, 209, 224	0
2	D	33/33 (100%)	-0.65	0 100 100	133, 161, 210, 219	0
3	A	366/386 (94%)	-0.08	5 (1%) 75 78	115, 148, 197, 257	0
4	B	368/384 (95%)	-0.04	0 100 100	111, 148, 200, 232	0
All	All	800/836 (95%)	-0.10	5 (0%) 89 92	111, 149, 201, 257	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	368	LYS	2.9
3	A	217	LEU	2.4
3	A	355	ILE	2.4
3	A	271	VAL	2.4
3	A	62	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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,

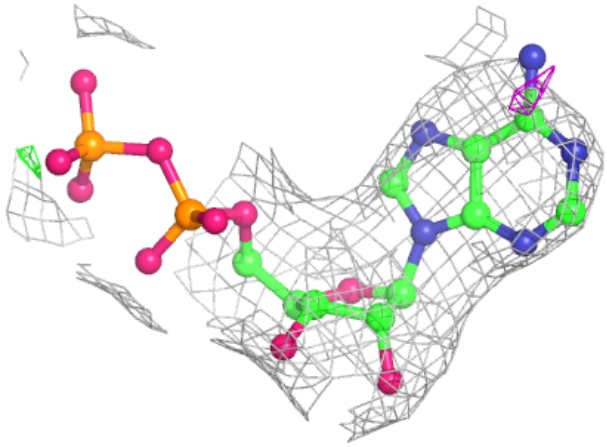
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

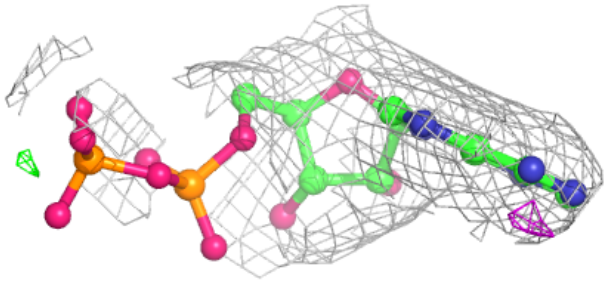
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SPD	C	35	10/10	0.24	1.01	152,152,152,152	0
5	SPD	C	34	10/10	0.77	0.59	130,130,130,130	0
8	ADP	B	9	27/27	0.91	0.25	121,121,121,121	0
6	K	D	35	1/1	0.92	1.51	168,168,168,168	0
8	ADP	A	8	27/27	0.95	0.23	111,111,111,111	0
7	MG	B	7	1/1	0.95	0.27	73,73,73,73	0
7	MG	A	6	1/1	0.99	0.27	79,79,79,79	0

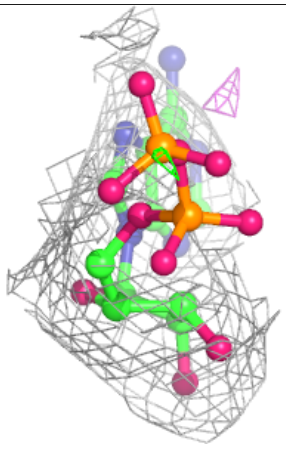
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP B 9:

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

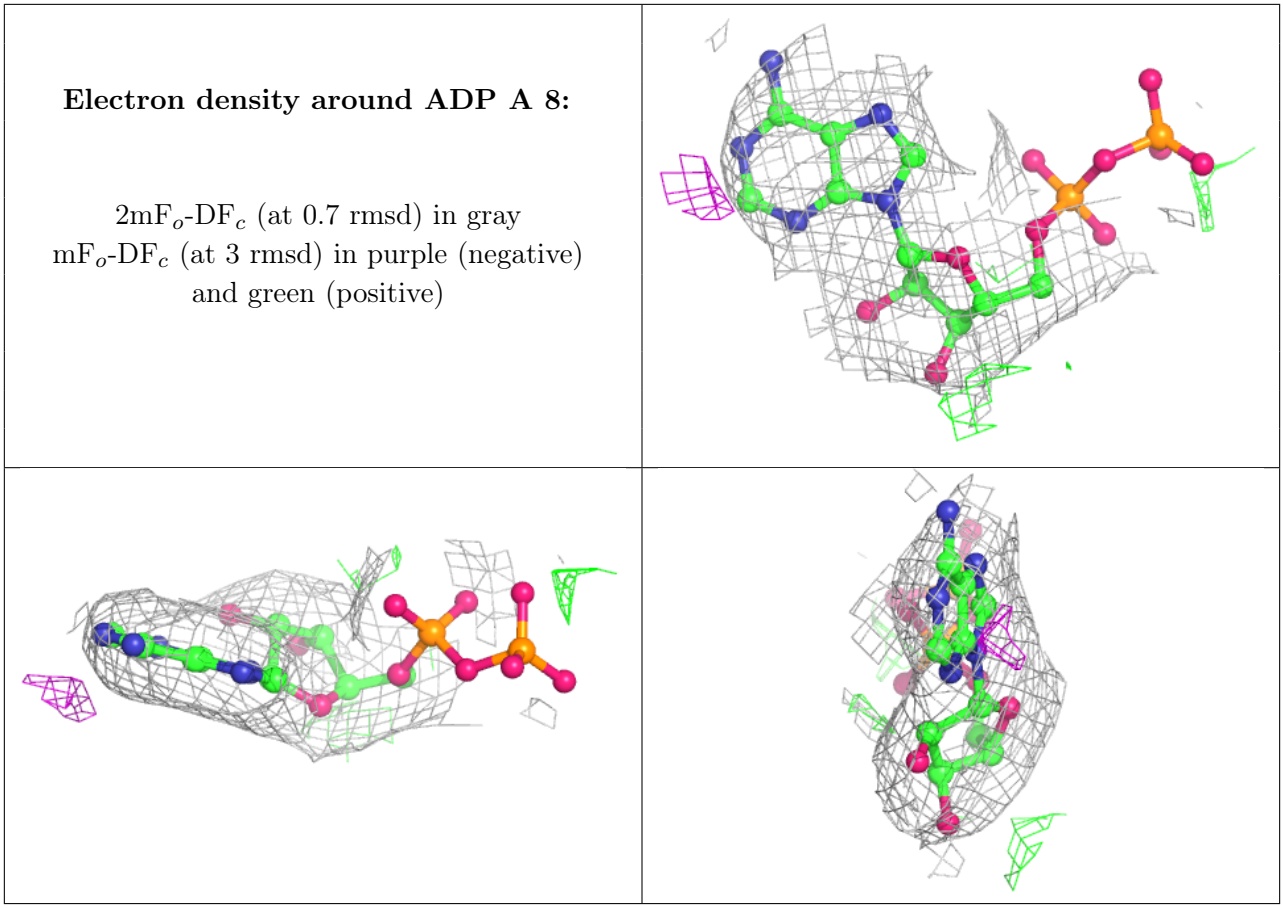






Electron density around ADP A 8:

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



6.5 Other polymers

There are no such residues in this entry.