



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:30 AM UTC

PDB ID : 1S9F / pdb_00001s9f
Title : DPO with AT matched
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Prakash, L.; Aggarwal, A.K.
Deposited on : 2004-02-04
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

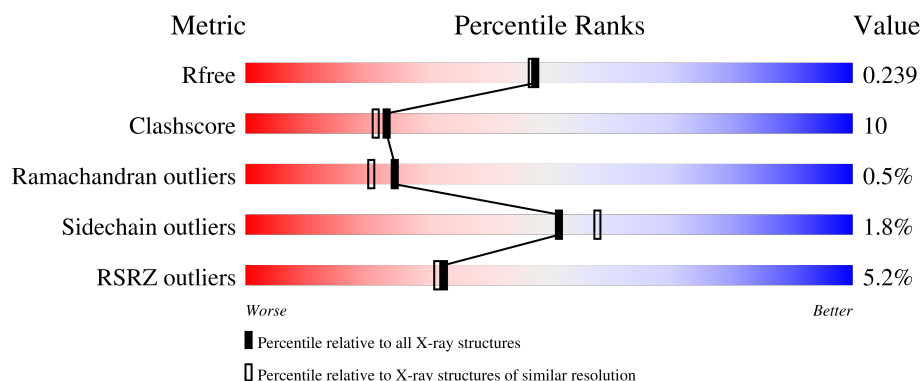
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	E	13	
1	F	13	
1	G	13	
1	H	13	
2	I	18	

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Mol	Chain	Length	Quality of chain
2	J	18	11% 72% 22% 6%
2	K	18	11% 67% 22% 6% 6%
2	L	18	6% 67% 28% 6%
3	A	352	3% 78% 17%
3	B	352	5% 76% 20%
3	C	352	7% 74% 22%
3	D	352	5% 74% 21%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14599 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			
1	F	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			
1	G	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			
1	H	13	Total	C	N	O	P	0	0	0
			274	129	60	73	12			

- Molecule 2 is a DNA chain called 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			
2	J	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			
2	K	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			
2	L	17	Total	C	N	O	P	0	0	0
			335	162	54	103	16			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2733	1754	468	504	7			
3	B	341	Total	C	N	O	S	0	0	0
			2739	1757	471	504	7			
3	C	341	Total	C	N	O	S	0	0	0
			2733	1755	469	502	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	341	Total	C	N	O	S	0	0	0
			2729	1752	468	502	7			

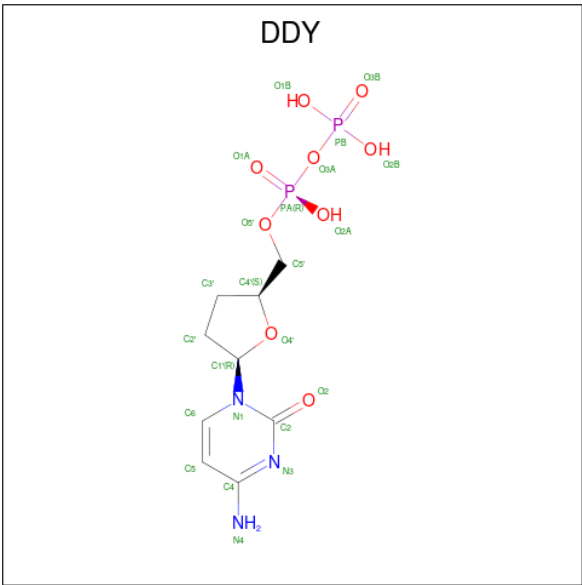
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2',3'-DIDEOXYCYTOSINE-5'-DIPHOSPHATE (CCD ID: DDY) (formula: C₉H₁₅N₃O₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			23	9	3	9	2		
6	B	1	Total	C	N	O	P	0	0
			23	9	3	9	2		
6	C	1	Total	C	N	O	P	0	0
			23	9	3	9	2		
6	D	1	Total	C	N	O	P	0	0
			23	9	3	9	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	36	Total	O	0	0
			36	36		
7	I	36	Total	O	0	0
			36	36		
7	F	49	Total	O	0	0
			49	49		
7	J	32	Total	O	0	0
			32	32		
7	G	35	Total	O	0	0
			35	35		
7	K	51	Total	O	0	0
			51	51		
7	H	33	Total	O	0	0
			33	33		
7	L	50	Total	O	0	0
			50	50		

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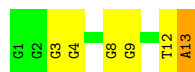
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	240	Total 240	O 240	0	0
7	B	180	Total 180	O 180	0	0
7	C	181	Total 181	O 181	0	0
7	D	206	Total 206	O 206	0	0

3 Residue-property plots [i](#)

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

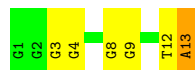
- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain E: 



- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain F: 



- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain G: 



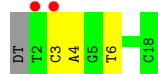
- Molecule 1: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*CP*TP*A)-3'

Chain H: 



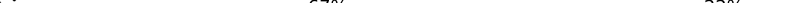
- Molecule 2: 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'

Chain I: 

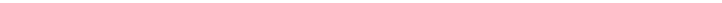


- Molecule 2: 5'-D(*T*TP*CP*AP*GP*TP*AP*GP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'

A diagram of a chromosome with six bands labeled DT, T2, C3, A4, G8, and C18. The bands are represented by colored rectangles: DT is grey, T2 is green, C3 is yellow, A4 is yellow, G8 is yellow, and C18 is yellow. Red dots are placed on the T2 and C3 bands.

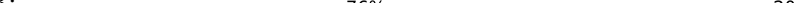
Chain K: 

Category	Count
DT	1
T2	2
C3	2
A4	2
G5	2
T6	2
A7	2
G8	2
C18	2

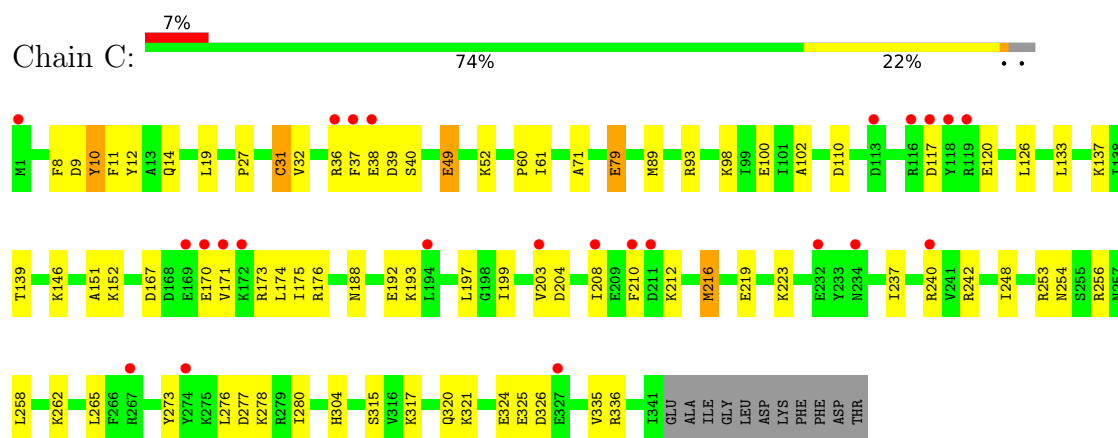
Chain L:  6% 67% 28% 6%

Chain A:  3% 78% 17% ..

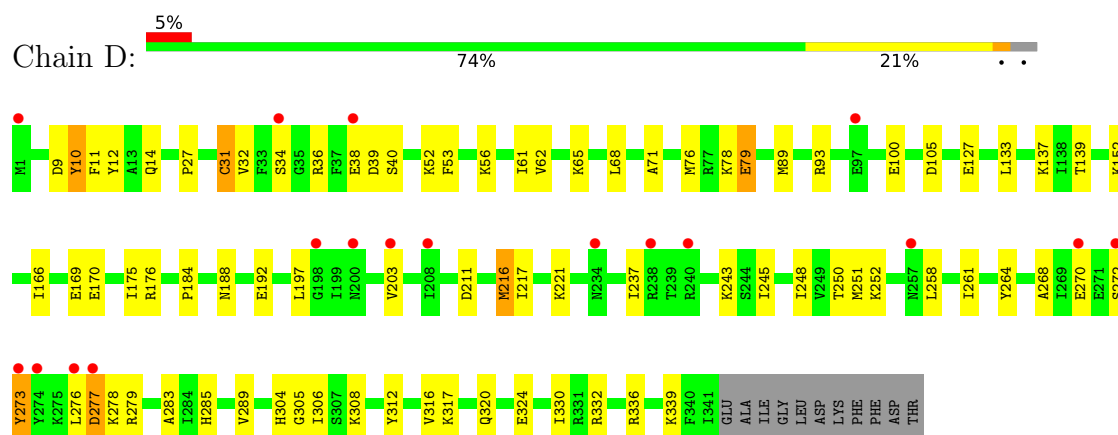
Residue	Position	Category	Score
ASP	1	Red	0.95
LYS	1180	Green	0.85
PHE	1181	Green	0.85
PHE	1190	Yellow	0.75
ASP	1191	Yellow	0.75
THR	1194	Yellow	0.75
	1195	Yellow	0.75
	1198	Red	0.95
	1208	Red	0.95
	1212	Green	0.85
	1214	Yellow	0.75
	1219	Green	0.85
	1220	Green	0.85
	1221	Orange	0.90
	1245	Yellow	0.75
	1252	Green	0.85
	1253	Green	0.85
	1256	Green	0.85
	1257	Orange	0.90
	1258	Yellow	0.75
	1259	Yellow	0.75
	1276	Green	0.85
	1277	Orange	0.90
	1278	Yellow	0.75
	1289	Yellow	0.75
	1294	Yellow	0.75
	1304	Green	0.85
	1305	Green	0.85
	1317	Yellow	0.75
	1320	Yellow	0.75
	1321	Yellow	0.75
	1324	Yellow	0.75
	1325	Yellow	0.75
	1326	Yellow	0.75
	1327	Red	0.95
	1332	Yellow	0.75
	1341	Red	0.95
GLU	1342	Green	0.85
ALA	1166	Yellow	0.75
ILE	1167	Yellow	0.75
GLY	1168	Yellow	0.75
LEU	1169	Yellow	0.75
	1171	Red	0.95
	1176	Green	0.85
	1177	Green	0.85
	1178	Orange	0.90
	1188	Yellow	0.75
	1189	Yellow	0.75
	1190	Yellow	0.75
	1196	Green	0.85
	1197	Green	0.85
	1202	Green	0.85
	1297	Yellow	0.75
	1298	Yellow	0.75
	1299	Yellow	0.75
	1306	Yellow	0.75
	1307	Green	0.85
	1308	Yellow	0.75
	1309	Yellow	0.75
	1312	Yellow	0.75
	1313	Yellow	0.75
	1319	Yellow	0.75
	1351	Yellow	0.75
	1358	Yellow	0.75
	1364	Orange	0.90
	1365	Yellow	0.75
	1366	Yellow	0.75
	1367	Yellow	0.75
	1368	Yellow	0.75
	1369	Yellow	0.75
	1370	Yellow	0.75
	1371	Yellow	0.75
	1372	Yellow	0.75
	1373	Yellow	0.75
	1374	Yellow	0.75
	1375	Yellow	0.75
	1376	Yellow	0.75
	1377	Yellow	0.75
	1378	Yellow	0.75
	1379	Yellow	0.75
	1380	Yellow	0.75
	1381	Yellow	0.75
	1382	Yellow	0.75
	1383	Yellow	0.75
	1384	Yellow	0.75
	1385	Yellow	0.75
	1386	Yellow	0.75
	1387	Yellow	0.75
	1388	Yellow	0.75
	1389	Yellow	0.75
	1390	Yellow	0.75
	1391	Yellow	0.75
	1392	Yellow	0.75
	1393	Yellow	0.75
	1394	Yellow	0.75
	1395	Yellow	0.75
	1396	Yellow	0.75
	1397	Yellow	0.75
	1398	Yellow	0.75
	1399	Yellow	0.75
	1400	Yellow	0.75
	1401	Yellow	0.75
	1402	Yellow	0.75
	1403	Yellow	0.75
	1404	Yellow	0.75
	1405	Yellow	0.75
	1406	Yellow	0.75
	1407	Yellow	0.75
	1408	Yellow	0.75
	1409	Yellow	0.75
	1410	Yellow	0.75
	1411	Yellow	0.75
	1412	Yellow	0.75
	1413	Yellow	0.75
	1414	Yellow	0.75
	1415	Yellow	0.75
	1416	Yellow	0.75
	1417	Yellow	0.75
	1418	Yellow	0.75
	1419	Yellow	0.75
	1420	Yellow	0.75
	1421	Yellow	0.75</

Chain B:  5% 76% 20% ..

● Molecule 3: DNA polymerase IV



● Molecule 3: DNA polymerase IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.80Å 100.30Å 110.80Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	44.6 (30.00-2.00) 93.5 (30.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.239 0.204 , 0.239	Depositor DCC
R_{free} test set	3529 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14599	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.91% 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: CA, DDY, 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	E	0.27	0/310	0.66	1/479 (0.2%)
1	F	0.26	0/310	0.72	1/479 (0.2%)
1	G	0.26	0/310	0.69	1/479 (0.2%)
1	H	0.27	0/310	0.72	1/479 (0.2%)
2	I	0.27	0/372	0.70	0/570
2	J	0.28	0/372	0.75	0/570
2	K	0.28	0/372	0.75	0/570
2	L	0.28	0/372	0.70	0/570
3	A	0.39	0/2772	0.85	4/3725 (0.1%)
3	B	0.37	0/2778	0.83	1/3732 (0.0%)
3	C	0.38	0/2772	0.83	3/3724 (0.1%)
3	D	0.39	0/2768	0.85	2/3720 (0.1%)
All	All	0.36	0/13818	0.81	14/19097 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
2	K	0	1
All	All	0	3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	DA	C2'-C3'-O3'	-8.68	98.48	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	13	DA	C2'-C3'-O3'	-8.25	99.13	111.50
3	A	11	PHE	N-CA-C	6.97	122.81	111.37
1	G	13	DA	C2'-C3'-O3'	-6.90	101.15	111.50
1	E	13	DA	C2'-C3'-O3'	-6.26	102.11	111.50
3	C	11	PHE	N-CA-C	6.10	123.80	110.80
3	B	11	PHE	N-CA-C	6.08	121.33	111.37
3	D	11	PHE	N-CA-C	5.81	123.18	110.80
3	A	294	ASP	N-CA-C	-5.77	102.77	110.55
3	A	31	CYS	N-CA-C	5.67	118.96	109.95
3	D	31	CYS	N-CA-C	5.57	118.80	109.95
3	C	151	ALA	N-CA-C	-5.41	105.47	111.36
3	A	151	ALA	N-CA-C	-5.36	105.52	111.36
3	C	31	CYS	N-CA-C	5.36	118.29	109.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	12	DT	Sidechain
1	F	12	DT	Sidechain
2	K	8	DG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	274	0	146	9	0
1	F	274	0	146	7	0
1	G	274	0	146	3	0
1	H	274	0	146	4	0
2	I	335	0	194	5	0
2	J	335	0	194	7	0
2	K	335	0	194	10	0
2	L	335	0	194	7	0
3	A	2733	0	2867	51	0
3	B	2739	0	2878	64	0
3	C	2733	0	2874	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2729	0	2863	62	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	23	0	12	2	0
6	B	23	0	12	4	0
6	C	23	0	12	1	0
6	D	23	0	12	1	0
7	A	240	0	0	4	0
7	B	180	0	0	6	0
7	C	181	0	0	2	0
7	D	206	0	0	6	0
7	E	36	0	0	0	0
7	F	49	0	0	1	0
7	G	35	0	0	0	0
7	H	33	0	0	0	0
7	I	36	0	0	0	0
7	J	32	0	0	0	0
7	K	51	0	0	1	0
7	L	50	0	0	0	0
All	All	14599	0	12890	271	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 10.

All (271) 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:D:14:GLN:HE22	3:D:139:THR:H	1.06	1.03
3:C:14:GLN:HE22	3:C:139:THR:H	0.97	0.95
2:L:16:DC:H2''	2:L:17:DC:H5'	1.46	0.95
3:B:176:ARG:HG2	3:B:203:VAL:HG21	1.50	0.93
3:C:176:ARG:HG2	3:C:203:VAL:HG11	1.49	0.93
3:A:14:GLN:HE22	3:A:139:THR:H	0.99	0.92
3:D:176:ARG:HG2	3:D:203:VAL:HG11	1.55	0.89
2:K:8:DG:H2'	3:C:336:ARG:HH21	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:197:LEU:HD11	3:B:216:MET:HG3	1.58	0.84
3:C:79:GLU:H	3:C:79:GLU:CD	1.82	0.83
3:A:79:GLU:CD	3:A:79:GLU:H	1.86	0.83
2:J:18:DC:H6	2:J:18:DC:H5'	1.46	0.81
2:L:16:DC:H2''	2:L:17:DC:C5'	2.10	0.80
1:H:3:DG:H2''	1:H:4:DG:H5'	1.63	0.80
3:A:88:ILE:HD11	3:A:138:ILE:HD12	1.64	0.80
3:B:79:GLU:CD	3:B:79:GLU:H	1.90	0.80
1:F:13:DA:H2''	6:B:4011:DDY:H4'	1.64	0.79
3:C:36:ARG:HH22	3:C:254:ASN:ND2	1.81	0.78
3:D:316:VAL:O	3:D:320:GLN:HG3	1.85	0.76
1:E:3:DG:H2''	1:E:4:DG:H5'	1.68	0.76
2:K:8:DG:H2'	3:C:336:ARG:NH2	2.00	0.76
3:D:14:GLN:NE2	3:D:139:THR:H	1.83	0.75
3:C:175:ILE:HG22	3:C:203:VAL:HG13	1.69	0.74
3:D:79:GLU:CD	3:D:79:GLU:H	1.92	0.74
3:B:175:ILE:O	3:B:203:VAL:HG23	1.88	0.73
3:C:14:GLN:HE22	3:C:139:THR:N	1.81	0.72
3:A:14:GLN:HE22	3:A:139:THR:N	1.83	0.71
3:A:320:GLN:O	3:A:324:GLU:HG3	1.92	0.70
3:C:12:TYR:CE2	6:C:4012:DDY:H2'1	2.26	0.70
3:D:34:SER:HB2	3:D:40:SER:OG	1.93	0.68
1:E:8:DG:H2''	1:E:9:DG:C5'	2.24	0.68
3:A:304:HIS:HD2	3:A:305:GLY:O	1.77	0.67
3:B:216:MET:HE2	3:B:216:MET:HA	1.78	0.66
2:I:3:DC:H4'	3:A:62:VAL:HG21	1.78	0.65
1:E:8:DG:H2''	1:E:9:DG:H5'	1.79	0.65
3:A:257:ASN:C	3:A:257:ASN:HD22	2.02	0.65
3:A:317:LYS:HA	3:A:320:GLN:HE21	1.61	0.64
3:B:175:ILE:HG22	3:B:203:VAL:HG22	1.80	0.64
3:D:270:GLU:OE2	3:D:308:LYS:HE2	1.97	0.64
3:C:36:ARG:NH2	3:C:254:ASN:ND2	2.46	0.64
3:C:117:ASP:OD2	3:C:120:GLU:HG3	1.98	0.64
3:B:316:VAL:O	3:B:320:GLN:HG3	1.99	0.63
3:A:12:TYR:CE2	6:A:4010:DDY:H2'1	2.34	0.63
3:A:214:LYS:HD2	3:A:219:GLU:HB2	1.79	0.63
3:B:257:ASN:C	3:B:257:ASN:HD22	2.06	0.63
2:J:18:DC:H5'	2:J:18:DC:C6	2.33	0.63
3:D:12:TYR:CE2	6:D:4013:DDY:H2'1	2.34	0.63
3:D:320:GLN:O	3:D:324:GLU:HG3	1.98	0.62
2:J:8:DG:P	3:B:336:ARG:HH22	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:304:HIS:HD2	3:D:305:GLY:O	1.81	0.62
3:A:289:VAL:HB	3:A:332:ARG:HB2	1.82	0.61
3:C:133:LEU:O	3:C:137:LYS:HD2	2.00	0.61
3:D:188:ASN:O	3:D:192:GLU:HG2	2.01	0.61
3:A:164:LYS:HD3	3:A:165:VAL:N	2.16	0.61
3:B:14:GLN:HE22	3:B:139:THR:H	1.48	0.61
3:B:285:HIS:HD2	7:B:4095:HOH:O	1.84	0.60
3:C:49:GLU:OE1	3:C:52:LYS:HE2	2.02	0.60
3:B:133:LEU:O	3:B:137:LYS:HD2	2.01	0.60
3:C:242:ARG:HH11	3:C:242:ARG:HG2	1.67	0.60
3:B:122:TYR:O	3:B:126:LEU:HD13	2.02	0.59
3:C:102:ALA:HA	3:C:240:ARG:NH1	2.18	0.59
3:A:69:PRO:CG	3:B:309:GLU:HG2	2.32	0.59
3:C:175:ILE:HG22	3:C:203:VAL:CG1	2.32	0.59
3:B:88:ILE:HD11	3:B:138:ILE:HD12	1.85	0.59
3:B:126:LEU:HD12	3:B:163:ILE:HD13	1.84	0.59
3:A:76:MET:HE3	3:A:78:LYS:HE3	1.83	0.58
3:C:304:HIS:HB3	7:C:4021:HOH:O	2.04	0.58
3:C:265:LEU:HD21	3:C:315:SER:HB3	1.86	0.58
3:C:321:LYS:O	3:C:325:GLU:HG3	2.03	0.58
3:D:261:ILE:HD13	3:D:330:ILE:HD12	1.86	0.57
3:D:268:ALA:O	3:D:272:SER:HB2	2.04	0.57
1:F:8:DG:H2''	1:F:9:DG:H5'	1.85	0.57
3:C:256:ARG:NH2	3:C:326:ASP:O	2.38	0.57
3:D:175:ILE:O	3:D:203:VAL:HG13	2.05	0.57
3:D:175:ILE:HG22	3:D:203:VAL:HG13	1.87	0.57
3:D:336:ARG:HD2	7:D:4191:HOH:O	2.05	0.56
2:L:10:DC:OP2	3:D:243:LYS:HD2	2.05	0.56
3:B:277:ASP:O	3:B:278:LYS:HB2	2.06	0.56
3:B:9:ASP:O	3:B:10:TYR:C	2.49	0.56
3:C:240:ARG:HG2	3:C:240:ARG:HH11	1.71	0.56
1:F:13:DA:H5''	3:B:106:GLU:CD	2.31	0.55
3:A:257:ASN:C	3:A:257:ASN:ND2	2.65	0.55
3:B:82:GLN:HB2	7:B:4138:HOH:O	2.06	0.55
3:B:289:VAL:HB	3:B:332:ARG:HB2	1.89	0.54
1:F:8:DG:H2''	1:F:9:DG:C5'	2.36	0.54
3:C:188:ASN:O	3:C:192:GLU:HG2	2.08	0.54
3:B:175:ILE:HG22	3:B:203:VAL:CG2	2.36	0.54
3:D:216:MET:HE2	3:D:216:MET:HA	1.89	0.54
3:B:21:PRO:O	3:B:24:LYS:HG2	2.07	0.54
3:A:2:ILE:H	3:A:112:SER:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:GLU:HB2	3:C:237:ILE:HG23	1.89	0.54
3:B:219:GLU:O	3:B:223:LYS:HG3	2.08	0.54
3:A:327:GLU:HG3	7:A:4157:HOH:O	2.08	0.54
3:D:9:ASP:O	3:D:10:TYR:C	2.51	0.54
2:I:3:DC:H4'	3:A:62:VAL:CG2	2.38	0.53
3:D:258:LEU:HD13	3:D:258:LEU:C	2.32	0.53
3:A:69:PRO:HG3	3:B:309:GLU:HG2	1.90	0.53
3:C:9:ASP:O	3:C:10:TYR:C	2.51	0.53
3:D:252:LYS:HE3	7:D:4193:HOH:O	2.08	0.53
3:B:142:VAL:HG22	3:B:163:ILE:HG13	1.90	0.53
3:B:169:GLU:HG2	7:B:4145:HOH:O	2.08	0.53
3:D:317:LYS:HA	3:D:320:GLN:HE21	1.74	0.53
3:C:199:ILE:HD11	3:C:208:ILE:HG13	1.90	0.53
3:D:39:ASP:CG	3:D:65:LYS:HE3	2.34	0.53
3:A:158:ALA:HB2	3:A:164:LYS:HB2	1.91	0.52
3:B:180:ILE:HD13	3:B:194:LEU:HD13	1.91	0.52
3:D:89:MET:O	3:D:93:ARG:HG3	2.09	0.52
3:A:9:ASP:O	3:A:10:TYR:C	2.52	0.52
3:B:14:GLN:NE2	3:B:139:THR:H	2.05	0.52
3:C:280:ILE:HD12	3:D:52:LYS:HD3	1.91	0.52
3:C:175:ILE:O	3:C:203:VAL:HG13	2.10	0.52
3:A:257:ASN:HD22	3:A:258:LEU:N	2.07	0.51
3:C:277:ASP:O	3:C:278:LYS:HB2	2.10	0.51
3:B:153:ILE:O	3:B:157:MET:HG3	2.10	0.51
3:D:248:ILE:HG23	3:D:332:ARG:NH2	2.26	0.51
3:B:116:ARG:NH2	7:B:4126:HOH:O	2.44	0.51
3:B:320:GLN:O	3:B:324:GLU:HG3	2.11	0.51
3:B:317:LYS:HA	3:B:320:GLN:HE21	1.75	0.51
3:C:193:LYS:HB3	3:C:216:MET:SD	2.50	0.51
3:D:27:PRO:HG2	3:D:71:ALA:HA	1.92	0.51
3:C:219:GLU:O	3:C:223:LYS:HG3	2.10	0.51
3:D:175:ILE:HG22	3:D:203:VAL:CG1	2.40	0.51
3:C:317:LYS:HA	3:C:320:GLN:HE21	1.75	0.51
3:D:38:GLU:O	3:D:39:ASP:HB2	2.11	0.51
3:B:27:PRO:HG2	3:B:71:ALA:HA	1.92	0.50
3:C:210:PHE:HZ	3:C:219:GLU:HG3	1.76	0.50
3:B:171:VAL:O	3:B:175:ILE:HG13	2.10	0.50
2:I:6:DT:H5'	3:A:32:VAL:HG11	1.94	0.50
1:H:13:DA:OP1	3:D:152:LYS:HE2	2.11	0.50
3:C:38:GLU:O	3:C:39:ASP:HB2	2.11	0.50
3:D:197:LEU:HD21	3:D:216:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:219:GLU:HG2	3:B:223:LYS:HD2	1.94	0.50
1:F:13:DA:H2''	6:B:4011:DDY:C4'	2.40	0.50
3:A:69:PRO:HG2	3:B:309:GLU:HG2	1.92	0.50
3:A:221:LYS:NZ	3:A:221:LYS:HB2	2.26	0.50
3:B:158:ALA:HB2	3:B:164:LYS:HB2	1.94	0.50
3:A:12:TYR:OH	3:A:78:LYS:HE2	2.11	0.49
3:A:252:LYS:HE3	7:A:4199:HOH:O	2.12	0.49
2:I:3:DC:H2''	2:I:4:DA:O5'	2.12	0.49
2:L:6:DT:H5'	3:D:32:VAL:HG11	1.94	0.49
3:A:277:ASP:O	3:A:278:LYS:HB2	2.12	0.49
3:A:27:PRO:HG2	3:A:71:ALA:HA	1.93	0.49
3:B:257:ASN:C	3:B:257:ASN:ND2	2.68	0.49
3:C:197:LEU:HD11	3:C:216:MET:HG3	1.95	0.49
3:D:251:MET:HG2	3:D:264:TYR:CD2	2.48	0.48
3:C:100:GLU:HG3	3:C:240:ARG:HD3	1.93	0.48
3:A:253:ARG:HD2	7:A:4095:HOH:O	2.12	0.48
3:B:100:GLU:HB2	3:B:237:ILE:HG23	1.95	0.47
3:C:170:GLU:O	3:C:174:LEU:HG	2.14	0.47
3:C:258:LEU:HD11	3:C:262:LYS:HD2	1.95	0.47
3:A:180:ILE:HD13	3:A:194:LEU:HD13	1.95	0.47
2:L:16:DC:C2'	2:L:17:DC:C5'	2.87	0.47
1:H:13:DA:OP1	3:D:152:LYS:CE	2.62	0.47
3:C:14:GLN:NE2	3:C:139:THR:H	1.83	0.47
3:C:304:HIS:CD2	3:D:53:PHE:O	2.68	0.47
3:B:8:PHE:CD1	3:B:8:PHE:N	2.81	0.47
3:B:126:LEU:CD1	3:B:163:ILE:HD13	2.45	0.47
3:B:199:ILE:HG23	3:B:204:ASP:HB2	1.96	0.47
3:C:27:PRO:HG2	3:C:71:ALA:HA	1.97	0.47
3:C:197:LEU:HD22	3:C:212:LYS:HE2	1.96	0.47
1:G:3:DG:H2''	1:G:4:DG:H5'	1.96	0.47
3:A:190:THR:HG21	3:A:221:LYS:HD3	1.96	0.46
3:B:283:ALA:HB2	3:B:339:LYS:HD2	1.97	0.46
3:A:191:ALA:O	3:A:195:LYS:HD3	2.15	0.46
2:K:8:DG:H5''	3:C:242:ARG:NH2	2.31	0.46
3:B:36:ARG:HH22	3:B:254:ASN:ND2	2.14	0.46
6:B:4011:DDY:H2'1	7:B:4094:HOH:O	2.16	0.46
3:C:199:ILE:HG23	3:C:204:ASP:HB2	1.97	0.46
2:J:3:DC:H6	2:J:3:DC:H5'	1.81	0.46
3:C:171:VAL:O	3:C:175:ILE:HG13	2.16	0.46
3:D:283:ALA:HB2	3:D:339:LYS:HD2	1.98	0.46
3:D:285:HIS:HD2	7:D:4119:HOH:O	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:320:GLN:O	3:C:324:GLU:HG3	2.16	0.46
3:B:168:ASP:O	3:B:172:LYS:HG3	2.15	0.45
1:E:3:DG:H2''	1:E:4:DG:C5'	2.43	0.45
2:I:6:DT:H5'	3:A:32:VAL:CG1	2.46	0.45
3:D:169:GLU:CD	3:D:169:GLU:H	2.23	0.45
3:D:76:MET:HE3	3:D:78:LYS:HD3	1.98	0.45
3:D:100:GLU:HB2	3:D:237:ILE:HG23	1.97	0.45
3:D:276:LEU:O	3:D:277:ASP:O	2.35	0.45
3:D:248:ILE:HG21	7:D:4043:HOH:O	2.17	0.45
2:K:3:DC:O2	3:C:60:PRO:HG2	2.17	0.45
3:B:13:ALA:O	3:B:17:GLU:HG3	2.16	0.45
3:A:257:ASN:ND2	3:A:259:GLU:H	2.14	0.45
3:C:240:ARG:NH1	3:C:240:ARG:HG2	2.31	0.45
3:D:217:ILE:HD12	3:D:221:LYS:HB3	1.98	0.45
1:G:13:DA:OP1	3:C:152:LYS:HE2	2.17	0.45
3:C:8:PHE:CD1	3:C:8:PHE:N	2.84	0.45
3:C:31:CYS:HB3	3:C:61:ILE:HD11	1.98	0.45
3:C:324:GLU:HG3	7:C:4140:HOH:O	2.17	0.45
3:D:245:ILE:CD1	3:D:279:ARG:HH21	2.30	0.45
2:K:3:DC:H2''	2:K:4:DA:O5'	2.17	0.45
2:K:2:DT:H72	3:C:253:ARG:HB3	1.99	0.44
7:K:455:HOH:O	3:C:248:ILE:HG22	2.16	0.44
3:B:176:ARG:CG	3:B:203:VAL:HG21	2.35	0.44
3:C:242:ARG:HG2	3:C:242:ARG:NH1	2.32	0.44
2:J:8:DG:OP2	3:B:336:ARG:NH2	2.44	0.44
3:A:97:GLU:HA	3:A:97:GLU:OE1	2.18	0.44
1:E:8:DG:C2'	1:E:9:DG:H5''	2.47	0.44
3:D:36:ARG:HD2	3:D:250:THR:CG2	2.48	0.44
3:D:133:LEU:O	3:D:137:LYS:HD2	2.18	0.44
2:L:3:DC:H4'	3:D:62:VAL:HG21	2.00	0.43
1:E:8:DG:H2''	1:E:9:DG:H5''	1.99	0.43
3:A:79:GLU:CD	3:A:79:GLU:N	2.65	0.43
3:B:79:GLU:CD	3:B:79:GLU:N	2.68	0.43
3:D:68:LEU:HD13	3:D:71:ALA:HB2	2.00	0.43
3:D:273:TYR:OH	3:D:306:ILE:O	2.32	0.43
3:D:277:ASP:O	3:D:278:LYS:HB2	2.17	0.43
2:J:8:DG:O5'	3:B:336:ARG:NH2	2.51	0.43
2:K:2:DT:H72	3:C:253:ARG:CB	2.49	0.43
3:B:180:ILE:HD11	3:B:225:LEU:HD13	2.01	0.43
1:E:13:DA:H2''	6:A:4010:DDY:O4'	2.19	0.43
7:F:489:HOH:O	3:B:189:ILE:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:8:PHE:N	3:A:8:PHE:CD1	2.83	0.43
2:L:16:DC:H1'	2:L:17:DC:H5''	2.00	0.43
3:B:108:TYR:C	3:B:109:LEU:HD12	2.44	0.43
3:B:167:ASP:O	3:B:171:VAL:HG23	2.17	0.43
3:C:173:ARG:HH11	3:C:173:ARG:HG2	1.84	0.43
3:D:166:ILE:HG23	3:D:170:GLU:HB3	2.00	0.43
3:A:108:TYR:C	3:A:109:LEU:HD12	2.44	0.42
3:A:167:ASP:HB2	7:A:4195:HOH:O	2.19	0.42
3:C:273:TYR:HA	3:C:276:LEU:HD12	2.01	0.42
3:C:89:MET:O	3:C:93:ARG:HG3	2.19	0.42
3:A:245:ILE:HD12	3:A:276:LEU:HD23	2.00	0.42
3:A:256:ARG:NH2	3:A:326:ASP:O	2.44	0.42
3:A:276:LEU:O	3:A:277:ASP:C	2.62	0.42
3:D:289:VAL:HB	3:D:332:ARG:HB2	2.00	0.42
3:A:208:ILE:HD11	3:A:212:LYS:HG2	2.02	0.42
3:C:167:ASP:O	3:C:171:VAL:HG23	2.20	0.42
3:C:335:VAL:HG22	3:C:336:ARG:N	2.34	0.42
2:K:8:DG:H5''	3:C:242:ARG:CZ	2.49	0.42
3:D:39:ASP:OD1	3:D:65:LYS:HE3	2.19	0.42
3:D:245:ILE:HD11	3:D:279:ARG:HH21	1.84	0.42
3:C:98:LYS:CB	3:C:110:ASP:HB3	2.50	0.42
3:B:258:LEU:CD1	3:B:262:LYS:HD2	2.50	0.41
1:E:8:DG:H1'	1:E:9:DG:H5''	2.02	0.41
1:G:3:DG:H2''	1:G:4:DG:C5'	2.50	0.41
3:B:176:ARG:NH1	3:B:176:ARG:HB2	2.35	0.41
3:C:197:LEU:CD2	3:C:212:LYS:HE2	2.49	0.41
3:D:31:CYS:HB3	3:D:61:ILE:CD1	2.51	0.41
1:F:13:DA:H5''	3:B:106:GLU:OE1	2.19	0.41
2:K:2:DT:O2	3:C:37:PHE:HB3	2.21	0.41
1:H:3:DG:C2'	1:H:4:DG:H5'	2.44	0.41
6:B:4011:DDY:H5'2	7:B:4168:HOH:O	2.20	0.41
3:D:31:CYS:HB3	3:D:61:ILE:HD11	2.03	0.41
3:B:39:ASP:CG	3:B:65:LYS:HE3	2.46	0.41
3:C:37:PHE:CD2	3:C:40:SER:HB3	2.56	0.41
3:D:184:PRO:HG3	7:D:4209:HOH:O	2.21	0.41
1:F:3:DG:H2''	1:F:4:DG:H5'	2.02	0.41
2:J:3:DC:H2''	2:J:4:DA:O5'	2.21	0.41
3:A:88:ILE:HD11	3:A:138:ILE:CD1	2.43	0.41
3:B:189:ILE:N	3:B:189:ILE:HD12	2.36	0.41
3:C:280:ILE:HD12	3:D:52:LYS:CD	2.50	0.41
3:D:221:LYS:HE2	7:D:4200:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:ILE:CD1	3:D:330:ILE:HD12	2.51	0.41
2:K:6:DT:H5'	3:C:32:VAL:HG11	2.03	0.41
3:B:122:TYR:CZ	3:B:126:LEU:HD11	2.56	0.41
3:B:126:LEU:HD12	3:B:163:ILE:CD1	2.51	0.41
1:E:13:DA:H5''	3:A:106:GLU:CD	2.46	0.40
3:A:7:ASP:OD2	3:A:7:ASP:C	2.64	0.40
3:D:270:GLU:OE2	3:D:312:TYR:OH	2.33	0.40
3:B:83:GLN:O	3:B:87:ARG:HG3	2.22	0.40
3:A:4:LEU:C	3:A:4:LEU:HD23	2.46	0.40
3:C:79:GLU:CD	3:C:79:GLU:N	2.62	0.40
3:C:258:LEU:CD1	3:C:262:LYS:HD2	2.52	0.40
3:D:176:ARG:CG	3:D:203:VAL:HG11	2.40	0.40
3:C:31:CYS:HB3	3:C:61:ILE:CD1	2.51	0.40
3:C:173:ARG:HG2	3:C:173:ARG:NH1	2.36	0.40
3:A:13:ALA:O	3:A:17:GLU:HG3	2.20	0.40
3:A:321:LYS:O	3:A:325:GLU:HG3	2.22	0.40
3:B:166:ILE:HG23	3:B:170:GLU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	339/352 (96%)	329 (97%)	8 (2%)	2 (1%)	21	17
3	B	339/352 (96%)	331 (98%)	6 (2%)	2 (1%)	21	17
3	C	339/352 (96%)	322 (95%)	16 (5%)	1 (0%)	36	35
3	D	339/352 (96%)	328 (97%)	9 (3%)	2 (1%)	21	17
All	All	1356/1408 (96%)	1310 (97%)	39 (3%)	7 (0%)	24	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	277	ASP
3	D	277	ASP
3	B	277	ASP
3	C	10	TYR
3	D	10	TYR
3	A	10	TYR
3	B	10	TYR

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	298/309 (96%)	294 (99%)	4 (1%)	61	68
3	B	299/309 (97%)	295 (99%)	4 (1%)	61	68
3	C	298/309 (96%)	292 (98%)	6 (2%)	48	54
3	D	297/309 (96%)	290 (98%)	7 (2%)	43	47
All	All	1192/1236 (96%)	1171 (98%)	21 (2%)	51	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	79	GLU
3	A	164	LYS
3	A	221	LYS
3	A	257	ASN
3	B	142	VAL
3	B	164	LYS
3	B	256	ARG
3	B	257	ASN
3	C	19	LEU
3	C	49	GLU
3	C	79	GLU
3	C	126	LEU
3	C	146	LYS
3	C	216	MET
3	D	56	LYS

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Mol	Chain	Res	Type
3	D	79	GLU
3	D	105	ASP
3	D	127	GLU
3	D	211	ASP
3	D	216	MET
3	D	273	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	70	ASN
3	A	83	GLN
3	A	161	ASN
3	A	200	ASN
3	A	254	ASN
3	A	257	ASN
3	A	304	HIS
3	A	320	GLN
3	B	14	GLN
3	B	70	ASN
3	B	83	GLN
3	B	161	ASN
3	B	188	ASN
3	B	200	ASN
3	B	254	ASN
3	B	257	ASN
3	B	285	HIS
3	B	320	GLN
3	C	14	GLN
3	C	70	ASN
3	C	82	GLN
3	C	130	ASN
3	C	161	ASN
3	C	254	ASN
3	C	304	HIS
3	C	320	GLN
3	D	14	GLN
3	D	70	ASN
3	D	82	GLN
3	D	83	GLN
3	D	161	ASN

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Mol	Chain	Res	Type
3	D	254	ASN
3	D	257	ASN
3	D	285	HIS
3	D	304	HIS
3	D	320	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 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	$\# Z > 2$
6	DDY	C	4012	4	23,24,24	3.02	9 (39%)	32,36,36	2.15	6 (18%)
6	DDY	B	4011	4	23,24,24	3.02	8 (34%)	32,36,36	2.22	5 (15%)
6	DDY	A	4010	4	23,24,24	3.02	8 (34%)	32,36,36	2.18	6 (18%)
6	DDY	D	4013	4	23,24,24	3.01	8 (34%)	32,36,36	2.15	6 (18%)

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
6	DDY	C	4012	4	-	3/16/25/25	0/2/2/2
6	DDY	B	4011	4	-	2/16/25/25	0/2/2/2
6	DDY	A	4010	4	-	3/16/25/25	0/2/2/2
6	DDY	D	4013	4	-	3/16/25/25	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	4013	DDY	C2'-C1'	-8.54	1.33	1.52
6	A	4010	DDY	C2'-C1'	-8.53	1.33	1.52
6	C	4012	DDY	C2'-C1'	-8.52	1.33	1.52
6	B	4011	DDY	C2'-C1'	-8.21	1.33	1.52
6	D	4013	DDY	C2'-C3'	-8.00	1.32	1.54
6	B	4011	DDY	C2'-C3'	-7.95	1.32	1.54
6	A	4010	DDY	C2'-C3'	-7.93	1.32	1.54
6	C	4012	DDY	C2'-C3'	-7.89	1.32	1.54
6	B	4011	DDY	C3'-C4'	-3.79	1.33	1.52
6	C	4012	DDY	C3'-C4'	-3.67	1.33	1.52
6	D	4013	DDY	C3'-C4'	-3.65	1.33	1.52
6	A	4010	DDY	C3'-C4'	-3.61	1.33	1.52
6	B	4011	DDY	C4-N3	3.54	1.41	1.34
6	C	4012	DDY	C4-N3	3.54	1.41	1.34
6	D	4013	DDY	C4-N3	3.52	1.41	1.34
6	B	4011	DDY	PA-O3A	3.41	1.63	1.59
6	B	4011	DDY	PB-O3B	3.34	1.60	1.50
6	A	4010	DDY	C4-N3	3.26	1.41	1.34
6	D	4013	DDY	PB-O3B	3.18	1.60	1.50
6	C	4012	DDY	PB-O3B	3.11	1.60	1.50
6	A	4010	DDY	PB-O3B	3.09	1.60	1.50
6	A	4010	DDY	PA-O3A	3.04	1.62	1.59
6	C	4012	DDY	PA-O3A	2.95	1.62	1.59
6	D	4013	DDY	PA-O3A	2.75	1.62	1.59
6	A	4010	DDY	C6-C5	2.43	1.40	1.35
6	B	4011	DDY	C2-N3	2.41	1.41	1.36
6	D	4013	DDY	C2-N3	2.38	1.41	1.36
6	B	4011	DDY	C6-C5	2.32	1.40	1.35
6	A	4010	DDY	C2-N3	2.32	1.40	1.36
6	C	4012	DDY	C2-N3	2.19	1.40	1.36
6	C	4012	DDY	PB-O1B	-2.19	1.46	1.54
6	D	4013	DDY	C6-C5	2.15	1.40	1.35
6	C	4012	DDY	C6-C5	2.15	1.40	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	4011	DDY	C3'-C2'-C1'	7.69	111.73	102.87
6	C	4012	DDY	C3'-C2'-C1'	7.68	111.71	102.87
6	A	4010	DDY	C3'-C2'-C1'	7.48	111.48	102.87
6	D	4013	DDY	C3'-C2'-C1'	7.40	111.40	102.87
6	B	4011	DDY	C4'-O4'-C1'	-5.75	104.38	109.81
6	D	4013	DDY	C4'-O4'-C1'	-5.72	104.41	109.81
6	A	4010	DDY	C4'-O4'-C1'	-5.47	104.65	109.81
6	C	4012	DDY	C4'-O4'-C1'	-5.03	105.06	109.81
6	A	4010	DDY	C2'-C3'-C4'	4.94	111.92	102.75
6	C	4012	DDY	C2'-C3'-C4'	4.92	111.89	102.75
6	D	4013	DDY	C2'-C3'-C4'	4.74	111.56	102.75
6	B	4011	DDY	C2'-C3'-C4'	4.44	111.00	102.75
6	A	4010	DDY	O4'-C1'-N1	3.10	113.36	107.86
6	B	4011	DDY	O4'-C1'-C2'	-2.93	102.95	106.41
6	B	4011	DDY	O2B-PB-O1B	2.91	118.71	107.80
6	D	4013	DDY	O4'-C1'-N1	2.75	112.75	107.86
6	A	4010	DDY	O2B-PB-O1B	2.68	117.83	107.80
6	C	4012	DDY	O4'-C1'-N1	2.64	112.55	107.86
6	D	4013	DDY	O2B-PB-O1B	2.64	117.69	107.80
6	C	4012	DDY	O2B-PB-O1B	2.59	117.51	107.80
6	C	4012	DDY	O4'-C1'-C2'	-2.32	103.67	106.41
6	D	4013	DDY	O4'-C1'-C2'	-2.25	103.75	106.41
6	A	4010	DDY	O4'-C1'-C2'	-2.18	103.83	106.41

There are no chirality outliers.

All (11) torsion outliers are listed below:

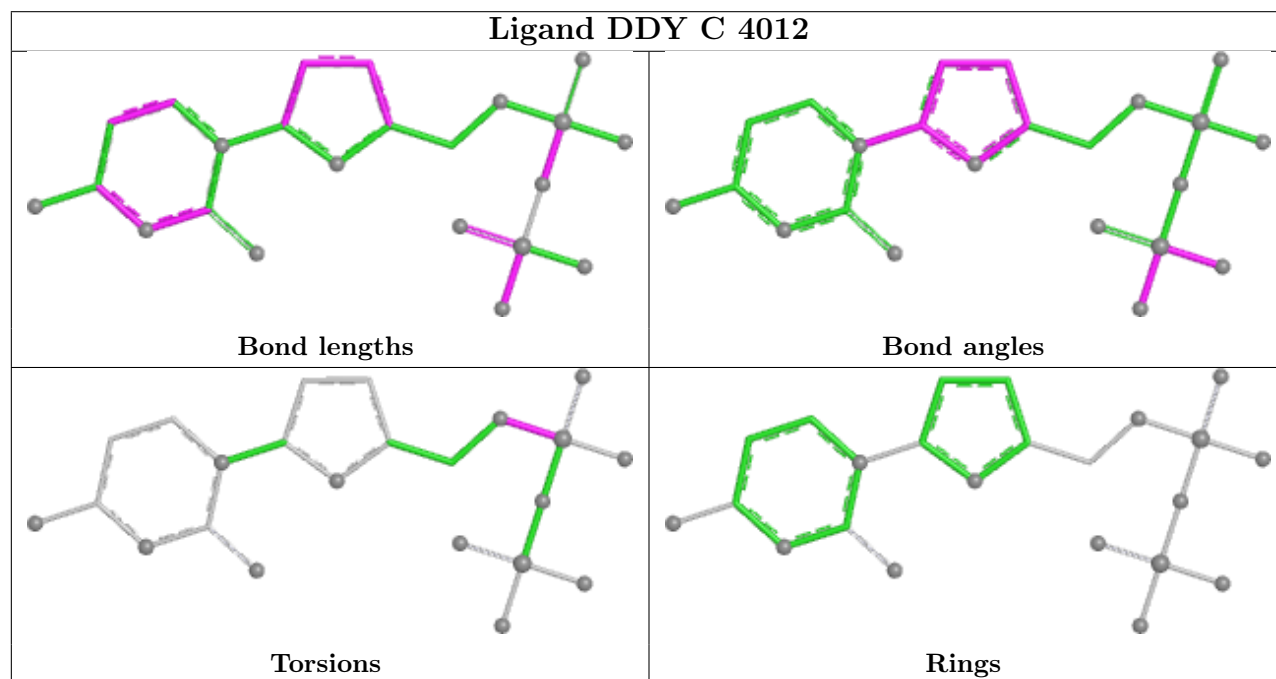
Mol	Chain	Res	Type	Atoms
6	A	4010	DDY	C5'-O5'-PA-O3A
6	A	4010	DDY	C5'-O5'-PA-O1A
6	A	4010	DDY	C5'-O5'-PA-O2A
6	B	4011	DDY	PA-O3A-PB-O1B
6	C	4012	DDY	C5'-O5'-PA-O3A
6	C	4012	DDY	C5'-O5'-PA-O1A
6	C	4012	DDY	C5'-O5'-PA-O2A
6	D	4013	DDY	C5'-O5'-PA-O3A
6	D	4013	DDY	C5'-O5'-PA-O1A
6	D	4013	DDY	C5'-O5'-PA-O2A
6	B	4011	DDY	PA-O3A-PB-O3B

There are no ring outliers.

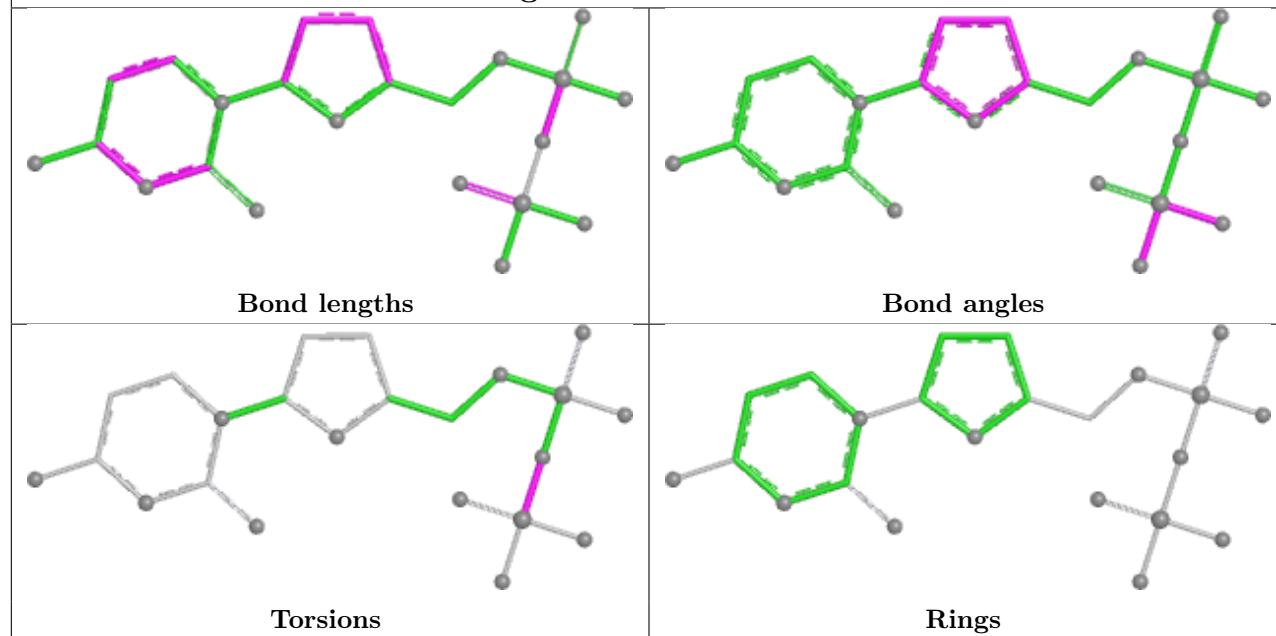
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	4012	DDY	1	0
6	B	4011	DDY	4	0
6	A	4010	DDY	2	0
6	D	4013	DDY	1	0

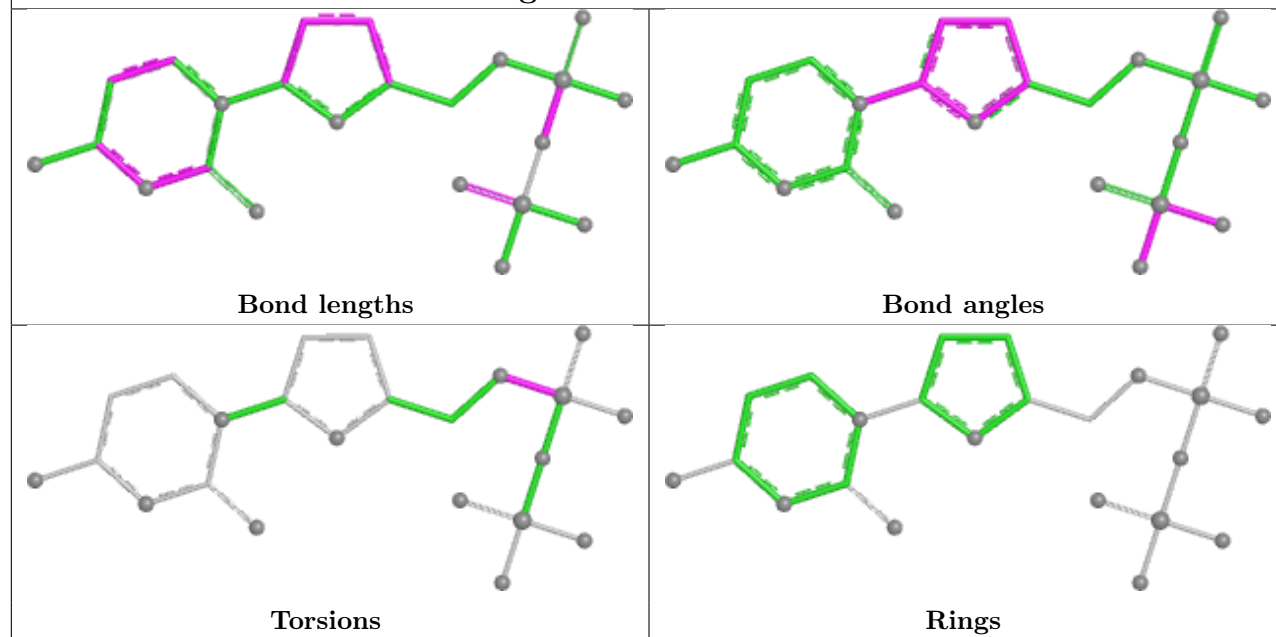
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

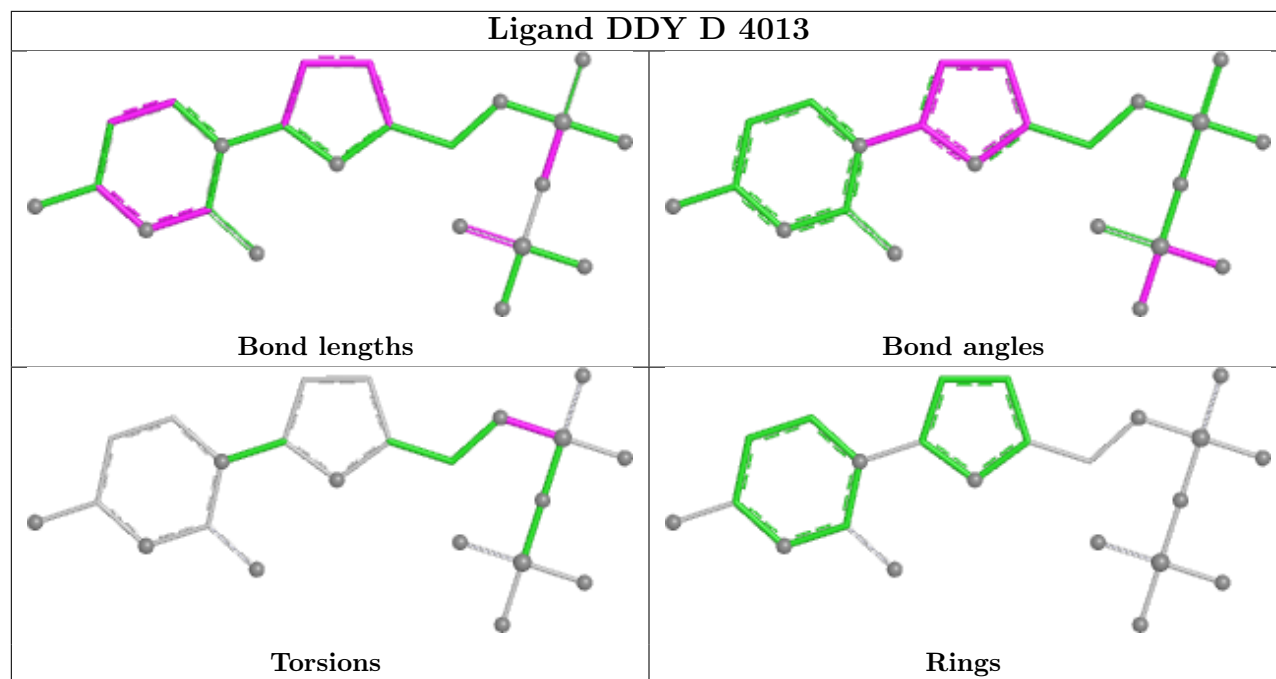


Ligand DDY B 4011



Ligand DDY A 4010





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	13/13 (100%)	0.11	0 100 100	27, 32, 40, 40	0
1	F	13/13 (100%)	-0.01	0 100 100	24, 32, 39, 43	0
1	G	13/13 (100%)	-0.00	0 100 100	24, 29, 35, 37	0
1	H	13/13 (100%)	0.17	0 100 100	27, 33, 43, 48	0
2	I	17/18 (94%)	0.26	2 (11%) 9 8	26, 34, 92, 103	0
2	J	17/18 (94%)	0.31	2 (11%) 9 8	24, 32, 70, 90	0
2	K	17/18 (94%)	0.18	2 (11%) 9 8	22, 32, 64, 82	0
2	L	17/18 (94%)	0.17	1 (5%) 28 27	25, 33, 58, 69	0
3	A	341/352 (96%)	0.19	10 (2%) 53 52	13, 29, 47, 54	1 (0%)
3	B	341/352 (96%)	0.45	18 (5%) 32 31	18, 33, 50, 59	1 (0%)
3	C	341/352 (96%)	0.50	24 (7%) 22 21	17, 31, 52, 61	1 (0%)
3	D	341/352 (96%)	0.24	18 (5%) 32 31	10, 29, 47, 62	1 (0%)
All	All	1484/1532 (96%)	0.33	77 (5%) 33 31	10, 31, 49, 103	4 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	1	MET	8.4
3	C	1	MET	6.9
3	A	1	MET	6.3
3	D	1	MET	6.2
3	D	273	TYR	4.8
2	J	2	DT	4.6
2	K	2	DT	4.1
3	D	274	TYR	3.7
2	I	2	DT	3.7
3	B	240	ARG	3.6
3	C	203	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	38	GLU	3.5
3	D	276	LEU	3.4
3	D	272	SER	3.4
3	D	34	SER	3.3
3	C	327	GLU	3.2
2	J	3	DC	3.0
3	B	207	SER	3.0
2	I	3	DC	3.0
3	D	277	ASP	3.0
3	C	113	ASP	2.8
3	B	234	ASN	2.8
3	C	234	ASN	2.7
3	C	274	TYR	2.7
3	D	203	VAL	2.7
2	L	2	DT	2.6
3	C	37	PHE	2.6
3	C	194	LEU	2.6
3	C	210	PHE	2.6
2	K	3	DC	2.6
3	C	208	ILE	2.6
3	A	169	GLU	2.5
3	C	240	ARG	2.5
3	D	200	ASN	2.5
3	D	270	GLU	2.5
3	C	172	LYS	2.5
3	A	327	GLU	2.4
3	C	232	GLU	2.4
3	B	113	ASP	2.4
3	B	203	VAL	2.4
3	A	112	SER	2.4
3	D	257	ASN	2.4
3	B	115	VAL	2.3
3	B	171	VAL	2.3
3	D	240	ARG	2.3
3	D	97	GLU	2.3
3	B	274	TYR	2.3
3	C	169	GLU	2.3
3	A	208	ILE	2.3
3	B	237	ILE	2.2
3	A	79	GLU	2.2
3	C	170	GLU	2.2
3	B	112	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	B	231	ASP	2.2
3	A	198	GLY	2.2
3	C	38	GLU	2.2
3	D	198	GLY	2.2
3	C	117	ASP	2.2
3	C	211	ASP	2.2
3	A	67	ILE	2.1
3	A	341	ILE	2.1
3	B	63	GLU	2.1
3	B	210	PHE	2.1
3	C	171	VAL	2.1
3	D	208	ILE	2.1
3	C	36	ARG	2.1
3	B	206	LEU	2.1
3	D	234	ASN	2.1
3	C	118	TYR	2.1
3	B	116	ARG	2.1
3	A	102	ALA	2.1
3	B	127	GLU	2.0
3	C	119	ARG	2.0
3	D	238	ARG	2.0
3	B	277	ASP	2.0
3	C	116	ARG	2.0
3	C	267	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

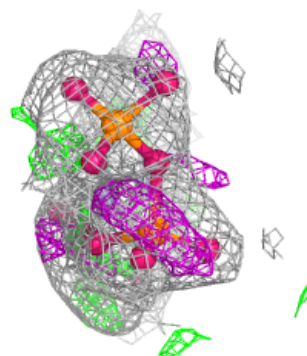
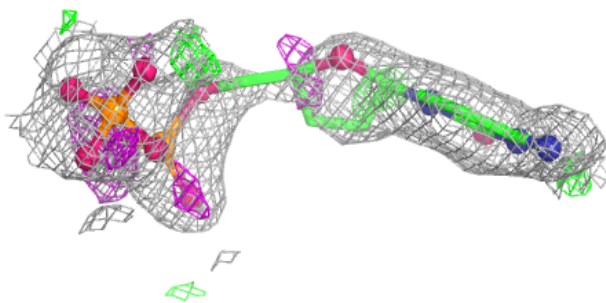
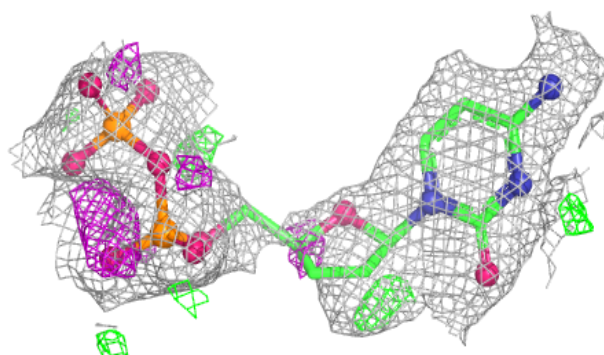
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	DDY	B	4011	23/23	0.89	0.13	40,44,48,49	0
5	MG	B	4008	1/1	0.92	0.10	39,39,39,39	0
5	MG	C	4005	1/1	0.94	0.06	28,28,28,28	0
4	CA	B	4002	1/1	0.94	0.07	44,44,44,44	0
6	DDY	C	4012	23/23	0.96	0.08	20,26,29,31	0
6	DDY	D	4013	23/23	0.96	0.07	17,22,27,28	0
6	DDY	A	4010	23/23	0.97	0.08	21,27,32,32	0
5	MG	D	4006	1/1	0.97	0.04	35,35,35,35	0
5	MG	A	4007	1/1	0.98	0.04	38,38,38,38	0
4	CA	C	4003	1/1	0.98	0.03	26,26,26,26	0
4	CA	A	4001	1/1	0.99	0.02	22,22,22,22	0
4	CA	D	4004	1/1	1.00	0.01	19,19,19,19	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.

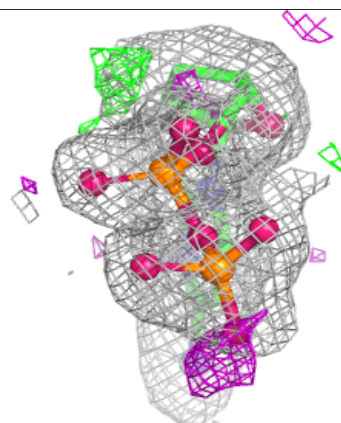
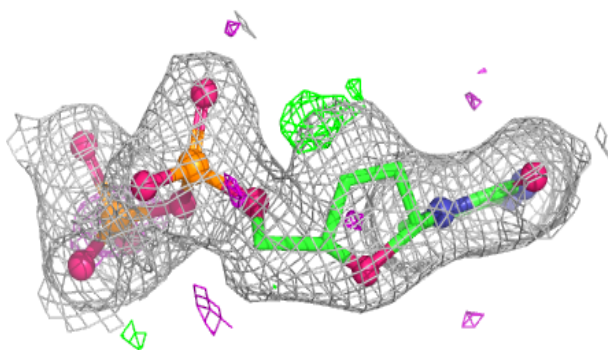
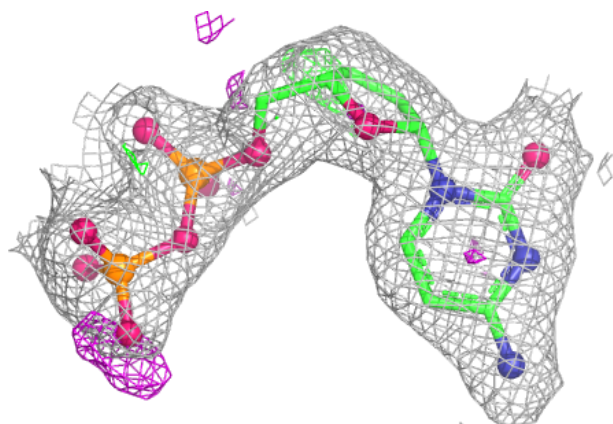
Electron density around DDY B 4011:

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

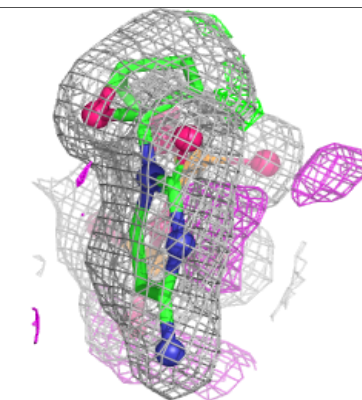
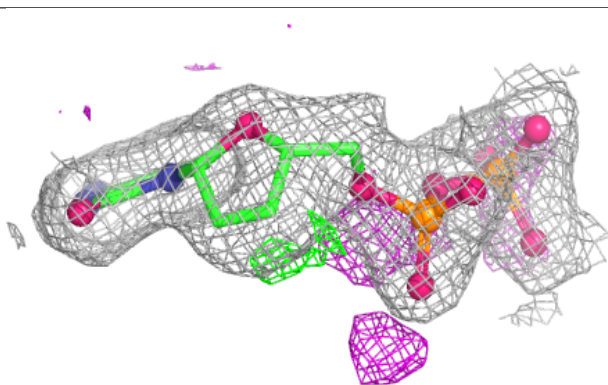
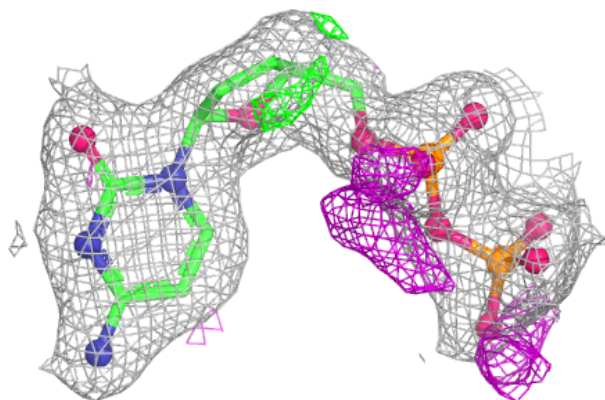


Electron density around DDY C 4012:

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

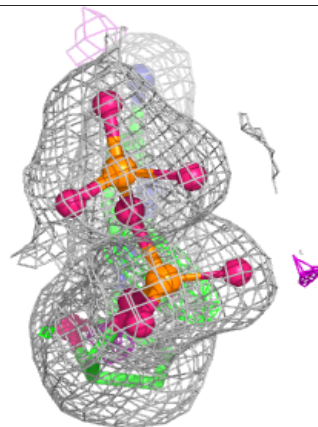
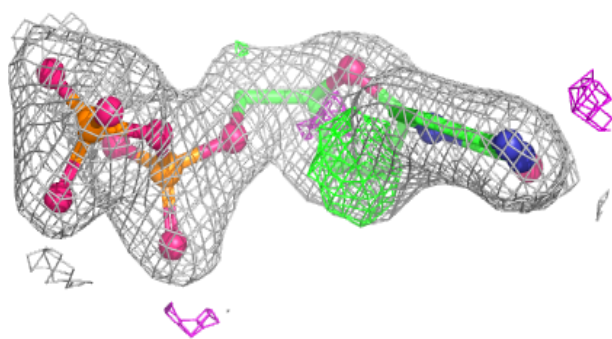
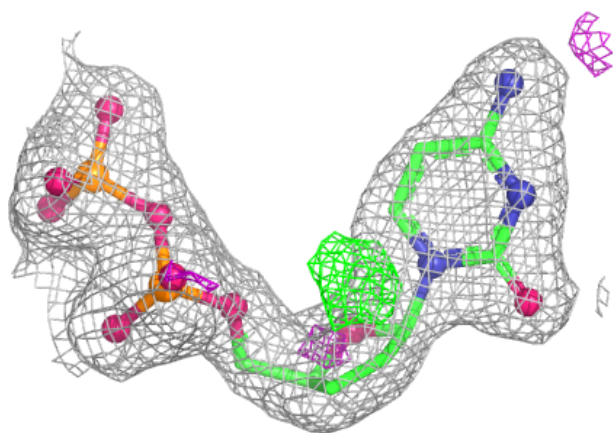
**Electron density around DDY D 4013:**

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



Electron density around DDY A 4010:

$2mF_o - DF_c$ (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.