Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 02:25 PM EDT

PDB ID	:	3GV5
Title	:	Human DNA polymerase iota in complex with T template DNA and incoming ddADP
Authors	:	Kirouac, K.N.; Ling, H.
Deposited on	:	2009-03-30
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 (i) 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 (i)) were used in the production of this report:

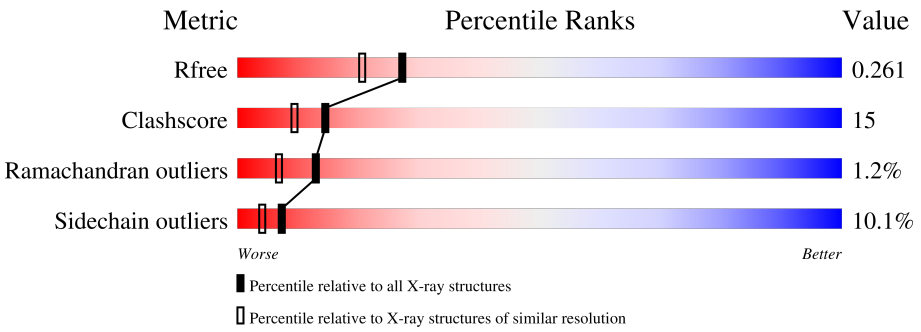
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Mol	Chain	Length	Quality of chain
1	B	420	62% 20% 8% 10%
1	D	420	65% 20% 6% • 9%
2	E	9	44% 22% 33%
2	P	9	33% 44% 22%
3	F	13	46% 54%
3	T	13	62% 31% 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7703 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 protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	B	379	2990	1892	521	555	11	11	0	0	0
1	D	383	3020	1909	526	562	11	12	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	9	189	90	39	52	8	0	0	0
2	E	9	189	90	39	52	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	13	257	124	41	79	13	0	0	0
3	F	13	257	124	41	79	13	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	B	3	3	3	0	0
4	P	1	1	1	0	0
4	D	3	3	3	0	0

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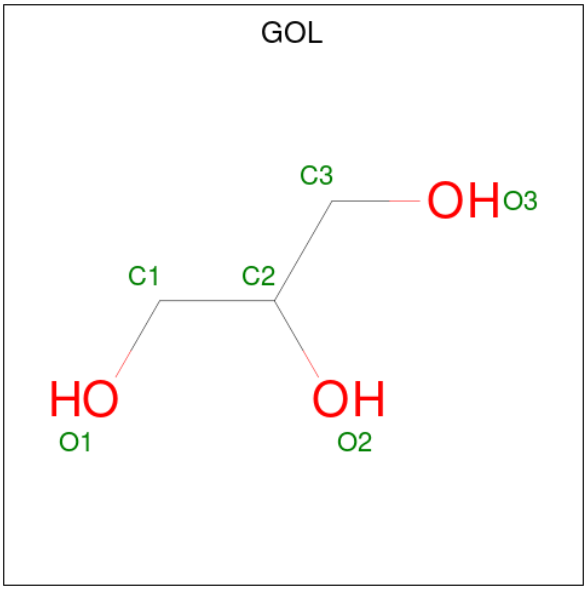
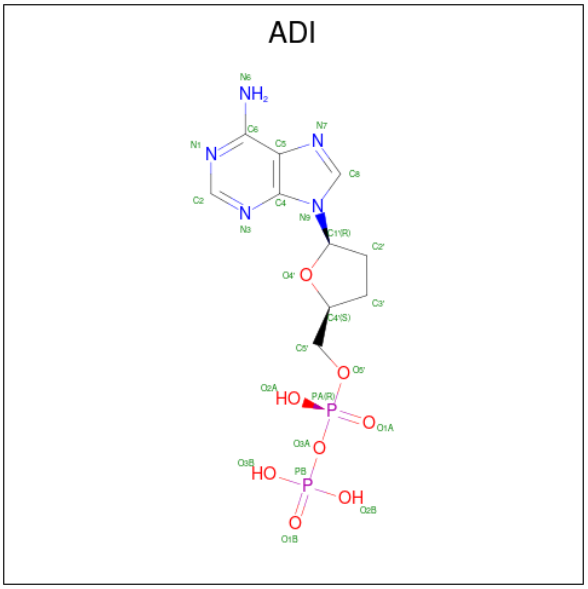
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	F	1	1	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	6	3	3	0	0

- Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-DIPHOSPHATE (three-letter code: ADI) (formula: $C_{10}H_{15}N_5O_8P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	25	10	5	8	2	0	0
			Total	C	N	O	P		
6	D	1	25	10	5	8	2	0	0

- Molecule 7 is water.

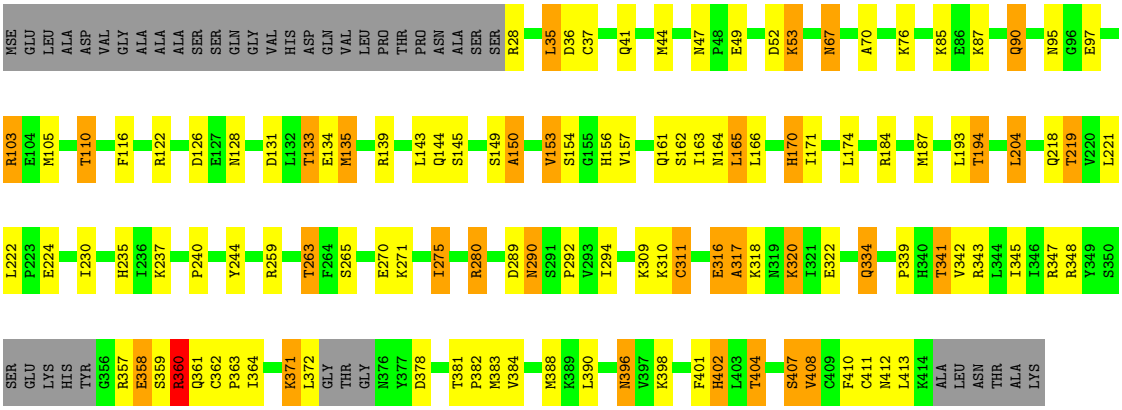
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	303	303	303	0	0
			Total	O		
7	P	32	32	32	0	0
			Total	O		
7	T	39	39	39	0	0
			Total	O		
7	D	306	306	306	0	0
			Total	O		
7	E	23	23	23	0	0
			Total	O		
7	F	34	34	34	0	0

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. 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. 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.

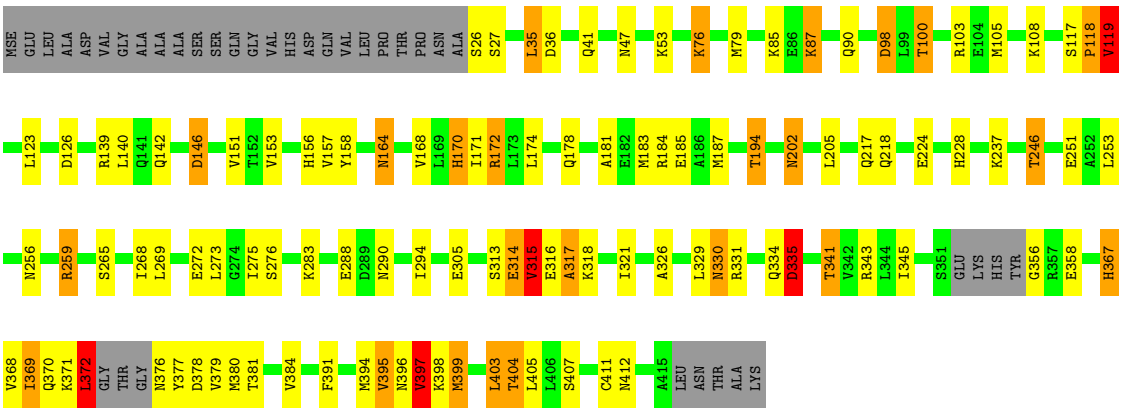
• Molecule 1: DNA polymerase iota

Chain B:



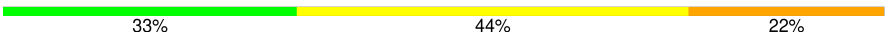
• Molecule 1: DNA polymerase iota

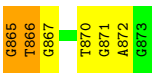
Chain D:



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

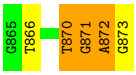
Chain P:





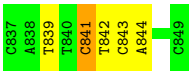
- Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'

Chain E:



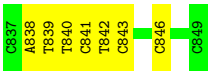
- Molecule 3: 5'-D(P*CP*AP*TP*TP*CP*TP*CP*AP*TP*CP*CP*AP*C)-3'

Chain T:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.16Å 71.75Å 127.42Å 90.00° 112.53° 90.00°	Depositor
Resolution (Å)	51.57 – 2.00 51.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (51.57-2.00) 95.4 (51.54-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.253 0.216 , 0.261	Depositor DCC
R_{free} test set	1551 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: GOL, CA, ADI

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	B	0.59	1/3022 (0.0%)	0.81	7/4055 (0.2%)
1	D	0.95	8/3052 (0.3%)	0.91	16/4095 (0.4%)
2	E	1.07	0/213	1.90	8/329 (2.4%)
2	P	1.10	0/213	1.74	5/329 (1.5%)
3	F	1.11	0/285	1.84	12/435 (2.8%)
3	T	1.16	0/285	1.77	8/435 (1.8%)
All	All	0.85	9/7070 (0.1%)	1.07	56/9678 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	8
1	D	0	13
All	All	0	21

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	358	GLU	CG-CD	-27.52	1.10	1.51
1	D	358	GLU	CA-CB	-13.59	1.24	1.53
1	D	358	GLU	CD-OE1	12.00	1.38	1.25
1	D	358	GLU	CB-CG	11.19	1.73	1.52
1	D	358	GLU	CD-OE2	10.34	1.37	1.25
1	D	98	ASP	CB-CG	-7.46	1.36	1.51
1	D	315	VAL	N-CA	6.51	1.59	1.46
1	D	335	ASP	N-CA	5.68	1.57	1.46
1	B	334	GLN	CA-C	5.55	1.67	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	358	GLU	OE1-CD-OE2	-16.94	102.98	123.30
2	E	866	DT	O4'-C1'-N1	-10.12	100.92	108.00
1	D	318	LYS	N-CA-C	-9.64	84.97	111.00
2	P	866	DT	O4'-C1'-N1	-9.43	101.40	108.00
1	B	358	GLU	N-CA-C	8.86	134.92	111.00
1	B	311	CYS	N-CA-C	8.60	134.23	111.00
3	F	843	DC	O4'-C1'-N1	8.35	113.84	108.00
1	D	405	LEU	CA-CB-CG	8.29	134.37	115.30
3	T	839	DT	O4'-C4'-C3'	-7.97	101.22	106.00
3	T	841	DC	O4'-C1'-N1	7.30	113.11	108.00
1	D	397	VAL	N-CA-C	-7.29	91.32	111.00
3	T	839	DT	C1'-O4'-C4'	-7.17	102.93	110.10
1	D	98	ASP	CB-CG-OD1	7.01	124.61	118.30
1	D	331	ARG	N-CA-C	-7.00	92.11	111.00
3	F	842	DT	O4'-C1'-N1	6.77	112.74	108.00
1	B	103	ARG	NE-CZ-NH1	6.69	123.64	120.30
3	F	839	DT	O4'-C1'-N1	6.67	112.67	108.00
1	D	119	VAL	N-CA-C	-6.67	93.00	111.00
1	B	408	VAL	N-CA-C	6.57	128.74	111.00
1	B	103	ARG	NE-CZ-NH2	-6.55	117.02	120.30
3	F	841	DC	O4'-C1'-N1	6.50	112.55	108.00
3	F	838	DA	P-O3'-C3'	6.49	127.49	119.70
1	B	360	ARG	N-CA-C	6.37	128.19	111.00
3	F	842	DT	N3-C2-O2	-6.16	118.61	122.30
2	P	867	DG	N1-C6-O6	-6.16	116.21	119.90
3	T	839	DT	O4'-C1'-N1	6.15	112.30	108.00
1	D	404	THR	N-CA-CB	-6.11	98.70	110.30
1	D	404	THR	CB-CA-C	-6.08	95.17	111.60
2	E	872	DA	O4'-C1'-N9	6.04	112.22	108.00
1	D	98	ASP	OD1-CG-OD2	-6.02	111.86	123.30
3	F	846	DC	O4'-C1'-N1	-5.96	103.83	108.00
1	D	103	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	D	395	VAL	N-CA-C	-5.80	95.34	111.00
3	F	840	DT	C6-C5-C7	-5.76	119.44	122.90
3	T	843	DC	O4'-C1'-N1	5.75	112.03	108.00
2	P	866	DT	N1-C1'-C2'	5.74	123.50	112.60
3	F	840	DT	C4-C5-C7	5.67	122.40	119.00
1	D	372	LEU	CA-CB-CG	5.61	128.21	115.30
1	D	358	GLU	N-CA-C	-5.61	95.86	111.00
3	T	844	DA	O4'-C1'-N9	5.56	111.89	108.00
3	F	838	DA	C1'-O4'-C4'	-5.53	104.57	110.10
2	P	865	DG	O4'-C1'-N9	5.52	111.87	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	404	THR	N-CA-C	5.51	125.89	111.00
2	E	871	DG	C4'-C3'-C2'	-5.51	98.14	103.10
2	E	873	DG	C5-C6-O6	-5.51	125.29	128.60
3	F	839	DT	C1'-O4'-C4'	-5.50	104.59	110.10
2	E	870	DT	O4'-C1'-N1	5.46	111.82	108.00
3	F	843	DC	P-O3'-C3'	5.40	126.18	119.70
1	B	318	LYS	N-CA-C	5.32	125.37	111.00
3	T	842	DT	N3-C2-O2	-5.32	119.11	122.30
3	T	842	DT	O4'-C1'-N1	5.32	111.72	108.00
2	E	866	DT	N1-C1'-C2'	5.21	122.50	112.60
2	E	870	DT	C4-C5-C7	5.20	122.12	119.00
1	D	98	ASP	CB-CG-OD2	5.19	122.97	118.30
2	E	870	DT	C1'-O4'-C4'	-5.14	104.95	110.10
2	P	870	DT	O4'-C1'-N1	5.03	111.52	108.00

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	LYS	Peptide
1	B	316	GLU	Peptide
1	B	317	ALA	Peptide
1	B	334	GLN	Peptide
1	B	357	ARG	Peptide
1	B	359	SER	Peptide
1	B	401	PHE	Peptide
1	B	407	SER	Peptide
1	D	118	PRO	Peptide
1	D	313	SER	Peptide
1	D	314	GLU	Peptide
1	D	315	VAL	Peptide
1	D	317	ALA	Peptide
1	D	329	LEU	Peptide
1	D	330	ASN	Peptide
1	D	334	GLN	Peptide
1	D	367	HIS	Peptide
1	D	394	MSE	Peptide
1	D	396	ASN	Peptide
1	D	403	LEU	Peptide
1	D	404	THR	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	B	2990	0	3082	108	0
1	D	3020	0	3112	96	0
2	E	189	0	103	4	0
2	P	189	0	103	2	0
3	F	257	0	148	0	0
3	T	257	0	148	1	0
4	B	3	0	0	0	1
4	D	3	0	0	0	1
4	F	1	0	0	0	0
4	P	1	0	0	0	0
5	B	6	0	8	3	0
6	B	25	0	12	1	0
6	D	25	0	12	1	0
7	B	303	0	0	19	0
7	D	306	0	0	15	0
7	E	23	0	0	0	0
7	F	34	0	0	0	0
7	P	32	0	0	0	0
7	T	39	0	0	0	0
All	All	7703	0	6728	211	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (211) 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)
1:B:47:ASN:HD21	1:B:49:GLU:HG2	1.16	1.08
1:D:172:ARG:HG3	1:D:172:ARG:HH11	0.93	1.07
1:D:35:LEU:HD21	1:D:187:MSE:HE1	1.38	1.02
1:D:172:ARG:HG3	1:D:172:ARG:NH1	1.46	1.01
1:D:87:LYS:HB2	7:D:645:HOH:O	1.59	1.00
1:D:153:VAL:HG22	1:D:174:LEU:HD22	1.45	0.97
1:D:305:GLU:HB3	1:D:407:SER:HB3	1.46	0.96
1:B:47:ASN:ND2	1:B:49:GLU:HG2	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:OD2	1:B:194:THR:HG23	1.68	0.93
1:B:41:GLN:HE22	1:B:194:THR:H	1.08	0.93
1:D:36:ASP:OD1	1:D:194:THR:HG22	1.68	0.93
1:D:172:ARG:HH11	1:D:172:ARG:CG	1.76	0.93
1:B:164:ASN:H	1:B:170:HIS:HD2	1.19	0.89
1:B:342:VAL:HG21	1:B:383:MSE:HE1	1.56	0.88
1:B:184:ARG:HE	1:B:218:GLN:HE21	1.19	0.88
1:D:123:LEU:HD21	2:E:872:DA:H2"	1.53	0.88
1:D:36:ASP:OD1	1:D:194:THR:CG2	2.22	0.87
1:B:347:ARG:HE	1:B:404:THR:CG2	1.89	0.85
1:D:372:LEU:HG	1:D:377:TYR:H	1.41	0.85
1:D:35:LEU:CD2	1:D:187:MSE:HE1	2.09	0.82
1:D:140:LEU:HD11	1:D:172:ARG:HD2	1.61	0.81
1:B:35:LEU:HD11	1:B:187:MSE:HE1	1.62	0.81
1:D:275:ILE:H	1:D:275:ILE:HD12	1.43	0.81
1:B:290:ASN:HB3	7:B:480:HOH:O	1.82	0.80
1:D:398:LYS:H	1:D:399[B]:MSE:HB2	1.47	0.80
1:B:90:GLN:H	1:B:90:GLN:HE21	1.30	0.80
1:B:371:LYS:HG2	1:B:372:LEU:H	1.47	0.79
1:D:153:VAL:HG22	1:D:174:LEU:CD2	2.13	0.79
1:B:163:ILE:HG21	1:B:174:LEU:HD11	1.64	0.78
1:B:149:SER:HB2	1:B:150:ALA:HB2	1.64	0.78
6:B:425:ADI:H1'	7:B:572:HOH:O	1.83	0.77
1:D:246:THR:HG23	2:E:871:DG:OP1	1.84	0.77
1:B:131:ASP:OD2	1:B:133:THR:HG23	1.85	0.76
6:D:424:ADI:H5'1	7:D:480:HOH:O	1.86	0.75
1:D:184:ARG:HH21	1:D:218:GLN:HE21	1.34	0.75
1:B:131:ASP:OD2	1:B:133:THR:CG2	2.35	0.75
1:B:347:ARG:HE	1:B:404:THR:HG22	1.51	0.75
1:B:343:ARG:HH21	1:B:361:GLN:HE22	1.34	0.74
1:B:47:ASN:HD21	1:B:49:GLU:CG	1.98	0.74
1:D:370:GLN:HA	1:D:371:LYS:HB3	1.69	0.74
1:D:341:THR:HG23	1:D:412:ASN:HB3	1.68	0.73
1:D:164:ASN:H	1:D:170:HIS:HD2	1.37	0.72
1:B:404:THR:HG21	7:B:473:HOH:O	1.90	0.71
1:D:118:PRO:HB2	1:D:119:VAL:HG13	1.72	0.70
1:B:170:HIS:HE1	1:B:224:GLU:OE2	1.73	0.70
1:B:371:LYS:HG2	1:B:372:LEU:N	2.05	0.70
1:B:110:THR:CG2	1:B:122:ARG:HH11	2.05	0.70
1:D:259:ARG:H	1:D:259:ARG:HD2	1.57	0.70
1:B:184:ARG:HE	1:B:218:GLN:NE2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:SER:HB2	1:B:150:ALA:CB	2.22	0.70
1:B:149:SER:N	1:B:150:ALA:HB3	2.06	0.70
1:B:343:ARG:NH2	1:B:361:GLN:HE22	1.90	0.69
1:B:153:VAL:HG13	1:B:174:LEU:HD22	1.74	0.69
1:B:348:ARG:HD2	1:B:358:GLU:OE1	1.93	0.69
1:B:35:LEU:CD1	1:B:187:MSE:HE1	2.22	0.69
1:B:164:ASN:H	1:B:170:HIS:CD2	2.09	0.68
1:B:28:ARG:N	7:B:603:HOH:O	2.28	0.66
1:D:98:ASP:OD1	1:D:100:THR:HG23	1.95	0.66
1:B:110:THR:HG21	1:B:122:ARG:HH11	1.59	0.66
1:B:381:THR:HG23	1:B:382:PRO:HD3	1.77	0.66
1:D:172:ARG:NH1	1:D:172:ARG:CG	2.31	0.66
1:B:388:MSE:HE1	7:B:503:HOH:O	1.97	0.65
1:D:168:VAL:O	1:D:172:ARG:HG2	1.95	0.65
1:B:317:ALA:HB3	7:B:503:HOH:O	1.96	0.65
1:B:347:ARG:NE	1:B:404:THR:CG2	2.60	0.65
1:B:52:ASP:O	7:B:464:HOH:O	2.14	0.65
1:D:290:ASN:ND2	1:D:290:ASN:H	1.95	0.65
1:D:251:GLU:HG3	1:D:256:ASN:HD21	1.61	0.64
1:B:90:GLN:H	1:B:90:GLN:NE2	1.94	0.64
1:B:116:PHE:HB3	1:B:135:MSE:HE1	1.80	0.64
1:B:35:LEU:HD11	1:B:187:MSE:CE	2.28	0.63
1:B:110:THR:HG21	1:B:122:ARG:HG2	1.81	0.63
1:B:259:ARG:O	1:B:263:THR:HB	1.99	0.63
1:D:305:GLU:CB	1:D:407:SER:HB3	2.26	0.63
1:B:103:ARG:NH2	7:B:684:HOH:O	2.32	0.63
1:D:140:LEU:CD1	1:D:172:ARG:HD2	2.27	0.62
1:D:123:LEU:C	1:D:123:LEU:HD23	2.20	0.62
1:B:52:ASP:HB3	7:B:590:HOH:O	1.99	0.62
1:D:398:LYS:N	1:D:399[B]:MSE:HB2	2.15	0.61
1:D:202:ASN:ND2	1:D:205:LEU:H	1.98	0.61
1:B:144:GLN:HG3	1:B:145:SER:H	1.66	0.61
1:D:156:HIS:HE1	1:D:217:GLN:HE21	1.46	0.60
1:D:98:ASP:OD1	1:D:100:THR:CG2	2.49	0.60
1:D:253:LEU:HD21	1:D:272:GLU:HG2	1.82	0.60
1:B:184:ARG:NE	1:B:218:GLN:HE21	1.97	0.59
1:B:41:GLN:HA	1:B:44:MSE:HE3	1.85	0.59
1:D:305:GLU:HB3	1:D:407:SER:CB	2.29	0.58
1:B:371:LYS:HG2	1:B:372:LEU:HD12	1.85	0.58
1:D:140:LEU:HD21	1:D:171:ILE:HG13	1.86	0.58
1:D:367:HIS:HA	1:D:370:GLN:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:THR:HG23	1:D:412:ASN:CB	2.34	0.57
1:B:156:HIS:HB2	1:B:219:THR:HB	1.85	0.57
1:B:41:GLN:HE22	1:B:194:THR:N	1.91	0.56
1:B:341:THR:HG23	1:B:412:ASN:CB	2.35	0.56
1:B:161:GLN:HG3	1:B:222:LEU:HD12	1.88	0.56
1:B:309:LYS:O	1:B:402:HIS:HE1	1.87	0.56
1:D:151:VAL:HG11	1:D:171:ILE:HD12	1.86	0.56
1:D:202:ASN:C	1:D:202:ASN:HD22	2.08	0.56
1:D:372:LEU:HB2	1:D:376:ASN:HA	1.87	0.56
1:D:345:ILE:HB	1:D:407:SER:OG	2.05	0.56
1:B:170:HIS:CE1	1:B:224:GLU:OE2	2.57	0.56
1:B:345:ILE:HB	1:B:407:SER:HB3	1.87	0.56
1:B:342:VAL:HG23	1:B:364:ILE:CG1	2.37	0.55
7:B:435:HOH:O	1:D:156:HIS:HD2	1.89	0.55
1:D:172:ARG:NH1	7:D:598:HOH:O	2.40	0.55
1:B:347:ARG:HE	1:B:404:THR:HG23	1.71	0.54
1:D:146:ASP:HB2	7:D:444:HOH:O	2.06	0.54
1:B:131:ASP:OD2	1:B:133:THR:HG22	2.08	0.54
5:B:422:GOL:H12	7:B:479:HOH:O	2.07	0.54
1:B:348:ARG:NH2	7:B:544:HOH:O	2.41	0.53
1:D:35:LEU:HD21	1:D:187:MSE:CE	2.26	0.53
1:B:90:GLN:HG2	7:D:604:HOH:O	2.09	0.53
1:B:280:ARG:NH2	1:B:289:ASP:OD1	2.41	0.53
1:D:290:ASN:H	1:D:290:ASN:HD22	1.55	0.53
1:B:292:PRO:HG2	1:B:294:ILE:HD11	1.89	0.53
1:B:290:ASN:HD22	1:B:290:ASN:H	1.57	0.53
1:B:341:THR:HG23	1:B:412:ASN:HB2	1.90	0.53
1:B:270:GLU:HG2	1:B:275:ILE:HA	1.91	0.53
1:D:47:ASN:HB2	7:D:541:HOH:O	2.09	0.52
1:B:204:LEU:HD23	1:B:240:PRO:HG2	1.91	0.52
1:D:181:ALA:O	1:D:185:GLU:HG3	2.08	0.52
1:D:356:GLY:N	7:D:583:HOH:O	2.43	0.52
5:B:422:GOL:H11	3:T:841:DC:H5”	1.92	0.52
1:B:110:THR:HB	1:B:128:ASN:OD1	2.09	0.52
1:B:320:LYS:HG3	7:B:432:HOH:O	2.09	0.52
1:B:347:ARG:HH11	1:B:404:THR:HG23	1.74	0.52
1:B:396:ASN:HD21	1:B:398:LYS:HB2	1.76	0.51
1:D:164:ASN:H	1:D:170:HIS:CD2	2.25	0.51
1:B:153:VAL:CG1	1:B:174:LEU:HD22	2.39	0.51
1:D:368:VAL:O	1:D:371:LYS:HB2	2.11	0.51
1:B:157:VAL:HG11	1:B:161:GLN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LYS:HE2	1:B:244:TYR:HA	1.92	0.51
1:D:371:LYS:HD3	1:D:379:VAL:HG11	1.93	0.50
1:D:369:ILE:HG22	1:D:369:ILE:O	2.10	0.50
1:D:178:GLN:NE2	7:D:481:HOH:O	2.45	0.50
1:D:251:GLU:HG3	1:D:256:ASN:ND2	2.27	0.50
1:D:151:VAL:HG11	1:D:171:ILE:CD1	2.42	0.49
1:D:384:VAL:HG22	7:D:626:HOH:O	2.13	0.49
1:B:322:GLU:HG2	1:B:384:VAL:HG11	1.94	0.49
1:B:378:ASP:HA	7:B:695:HOH:O	2.13	0.49
1:D:183:MSE:O	1:D:187:MSE:HG3	2.11	0.49
1:B:360:ARG:HB3	1:B:390:LEU:HD22	1.95	0.49
2:P:865:DG:H2'	2:P:866:DT:H71	1.95	0.49
1:D:275:ILE:H	1:D:275:ILE:CD1	2.16	0.49
1:D:391:PHE:CZ	1:D:395:VAL:HG11	2.47	0.49
1:D:53:LYS:HE2	7:D:627:HOH:O	2.12	0.49
1:B:358:GLU:H	1:B:358:GLU:HG3	1.22	0.49
1:B:342:VAL:HG23	1:B:364:ILE:HG12	1.95	0.48
1:D:36:ASP:OD1	1:D:194:THR:HG23	2.12	0.48
1:D:321:ILE:HG22	7:D:626:HOH:O	2.13	0.48
1:D:372:LEU:H	1:D:372:LEU:HD23	1.78	0.48
1:B:230:ILE:HD11	7:B:589:HOH:O	2.13	0.48
1:B:360:ARG:HD3	1:B:360:ARG:N	2.29	0.48
1:B:372:LEU:H	1:B:372:LEU:HD12	1.78	0.48
1:D:343:ARG:HD2	1:D:345:ILE:HD11	1.95	0.47
1:D:370:GLN:HA	1:D:371:LYS:CB	2.40	0.47
1:D:380:MSE:O	1:D:384:VAL:HG23	2.14	0.47
1:D:172:ARG:HG2	1:D:172:ARG:H	1.38	0.47
1:D:184:ARG:NH2	1:D:218:GLN:HE21	2.08	0.47
1:B:149:SER:CA	1:B:150:ALA:HB3	2.44	0.47
1:D:275:ILE:HD12	1:D:275:ILE:N	2.21	0.47
1:B:95:ASN:ND2	1:B:97:GLU:H	2.13	0.47
1:D:123:LEU:C	1:D:123:LEU:CD2	2.83	0.47
1:B:396:ASN:C	1:B:396:ASN:HD22	2.18	0.46
1:B:316:GLU:O	1:B:320:LYS:HD3	2.14	0.46
1:D:76:LYS:HE3	7:D:510:HOH:O	2.15	0.46
1:D:158:TYR:OH	1:D:228:HIS:HD2	1.99	0.46
1:D:76:LYS:HE2	1:D:76:LYS:HB2	1.73	0.45
1:D:283:LYS:HG2	1:D:288:GLU:HG3	1.97	0.45
1:D:391:PHE:O	1:D:395:VAL:HB	2.17	0.45
1:D:202:ASN:HD21	1:D:205:LEU:H	1.62	0.45
1:D:316:GLU:O	1:D:317:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:SER:CB	1:B:150:ALA:CB	2.94	0.45
1:B:165:LEU:HD23	1:B:171:ILE:HD11	1.97	0.45
1:B:347:ARG:NH1	1:B:404:THR:HG23	2.32	0.45
1:B:67:ASN:ND2	1:B:70:ALA:H	2.15	0.45
1:D:168:VAL:O	1:D:171:ILE:HG22	2.17	0.45
1:B:411:CYS:HB2	7:B:678:HOH:O	2.16	0.45
1:B:53:LYS:HD2	7:B:590:HOH:O	2.16	0.44
1:B:35:LEU:HB2	1:B:126:ASP:HB2	2.00	0.44
1:B:341:THR:HG23	1:B:412:ASN:HB3	1.99	0.44
1:D:26:SER:HA	1:D:27:SER:HA	1.55	0.44
1:D:156:HIS:CE1	1:D:217:GLN:HE21	2.30	0.44
1:B:67:ASN:C	1:B:67:ASN:HD22	2.21	0.44
1:B:342:VAL:HG21	1:B:383:MSE:CE	2.37	0.44
1:D:153:VAL:HG21	1:D:157:VAL:CG2	2.48	0.44
1:D:315:VAL:HG23	7:D:667:HOH:O	2.18	0.44
1:D:411:CYS:HB2	7:D:643:HOH:O	2.18	0.44
1:B:339:PRO:HB3	1:B:410:PHE:HB3	1.99	0.43
1:B:347:ARG:NE	1:B:404:THR:HG23	2.31	0.43
1:D:397:VAL:HG22	7:D:449:HOH:O	2.18	0.43
2:P:871:DG:H2'	2:P:872:DA:C8	2.53	0.43
2:E:870:DT:H2"	2:E:871:DG:H8	1.83	0.43
1:B:362:CYS:HB2	1:B:363:PRO:HD2	2.00	0.43
1:D:76:LYS:HD3	1:D:79:MSE:HE3	2.00	0.43
1:D:253:LEU:CD2	1:D:272:GLU:HG2	2.47	0.43
1:B:105:MSE:CG	1:B:193:LEU:HD11	2.48	0.43
1:D:326:ALA:HB2	1:D:380:MSE:HE1	2.00	0.43
1:D:398:LYS:H	1:D:399[A]:MSE:HB2	1.83	0.43
1:B:97:GLU:HB3	5:B:422:GOL:H11	2.01	0.42
1:B:110:THR:CG2	1:B:122:ARG:NH1	2.78	0.42
1:B:35:LEU:HD12	1:B:35:LEU:HA	1.86	0.42
1:B:162:SER:HB3	7:B:652:HOH:O	2.19	0.42
1:B:235:HIS:HD2	7:B:433:HOH:O	2.03	0.41
1:D:170:HIS:HE1	1:D:224:GLU:OE2	2.04	0.41
1:D:378:ASP:OD2	1:D:381:THR:HG23	2.21	0.41
1:B:41:GLN:NE2	1:B:194:THR:H	1.92	0.41
1:B:396:ASN:C	1:B:396:ASN:ND2	2.75	0.41
1:B:139:ARG:O	1:B:143:LEU:HD13	2.21	0.41
1:D:372:LEU:HD23	1:D:372:LEU:N	2.35	0.41
1:D:246:THR:CG2	2:E:871:DG:OP1	2.61	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:421:CA:CA	4:D:423:CA:CA[1_565]	0.43	1.77

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	373/420 (89%)	363 (97%)	7 (2%)	3 (1%)	19 13
1	D	378/420 (90%)	359 (95%)	12 (3%)	7 (2%)	8 3
All	All	751/840 (89%)	722 (96%)	19 (2%)	10 (1%)	13 6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	315	VAL
1	D	330	ASN
1	D	335	ASP
1	D	397	VAL
1	B	150	ALA
1	B	37	CYS
1	B	402	HIS
1	D	399[A]	MSE
1	D	399[B]	MSE
1	D	369	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	344/364 (94%)	309 (90%)	35 (10%)	7 4
1	D	348/364 (96%)	313 (90%)	35 (10%)	7 4
All	All	692/728 (95%)	622 (90%)	70 (10%)	7 4

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	LEU
1	B	53	LYS
1	B	67	ASN
1	B	76	LYS
1	B	85	LYS
1	B	87	LYS
1	B	90	GLN
1	B	110	THR
1	B	133	THR
1	B	134	GLU
1	B	135	MSE
1	B	153	VAL
1	B	154	SER
1	B	165	LEU
1	B	166	LEU
1	B	170	HIS
1	B	194	THR
1	B	204	LEU
1	B	219	THR
1	B	221	LEU
1	B	263	THR
1	B	265	SER
1	B	271	LYS
1	B	275	ILE
1	B	280	ARG
1	B	290	ASN
1	B	311	CYS
1	B	320	LYS
1	B	341	THR
1	B	360	ARG
1	B	371	LYS
1	B	396	ASN
1	B	404	THR
1	B	408	VAL
1	B	413	LEU

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Mol	Chain	Res	Type
1	D	35	LEU
1	D	41	GLN
1	D	76	LYS
1	D	85	LYS
1	D	87	LYS
1	D	90	GLN
1	D	100	THR
1	D	105	MSE
1	D	108	LYS
1	D	117	SER
1	D	119	VAL
1	D	126	ASP
1	D	139	ARG
1	D	142	GLN
1	D	146	ASP
1	D	164	ASN
1	D	170	HIS
1	D	172	ARG
1	D	194	THR
1	D	202	ASN
1	D	237	LYS
1	D	246	THR
1	D	259	ARG
1	D	265	SER
1	D	268	ILE
1	D	269	LEU
1	D	273	LEU
1	D	276	SER
1	D	294	ILE
1	D	314	GLU
1	D	335	ASP
1	D	341	THR
1	D	372	LEU
1	D	397	VAL
1	D	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	67	ASN
1	B	90	GLN
1	B	95	ASN
1	B	156	HIS
1	B	170	HIS
1	B	217	GLN
1	B	218	GLN
1	B	227	GLN
1	B	228	HIS
1	B	290	ASN
1	B	330	ASN
1	B	361	GLN
1	B	396	ASN
1	B	402	HIS
1	D	58	GLN
1	D	142	GLN
1	D	156	HIS
1	D	161	GLN
1	D	164	ASN
1	D	170	HIS
1	D	178	GLN
1	D	202	ASN
1	D	216	ASN
1	D	218	GLN
1	D	227	GLN
1	D	228	HIS
1	D	256	ASN
1	D	290	ASN
1	D	330	ASN
1	D	412	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	ADI	D	424	4	23,27,27	1.10	2 (8%)	26,41,41	2.26	8 (30%)
6	ADI	B	425	4	23,27,27	1.08	2 (8%)	26,41,41	2.03	6 (23%)
5	GOL	B	422	-	5,5,5	0.56	0	5,5,5	0.39	0

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	ADI	D	424	4	-	5/12/25/25	0/3/3/3
6	ADI	B	425	4	-	4/12/25/25	0/3/3/3
5	GOL	B	422	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	425	ADI	PA-O3A	3.09	1.62	1.59
6	D	424	ADI	PA-O3A	3.02	1.62	1.59
6	D	424	ADI	C2-N3	2.36	1.35	1.32
6	B	425	ADI	C2-N3	2.08	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	424	ADI	O4'-C1'-N9	8.44	119.94	108.75
6	B	425	ADI	O4'-C1'-N9	5.26	115.72	108.75
6	B	425	ADI	N3-C2-N1	-4.67	122.33	128.67
6	D	424	ADI	N3-C2-N1	-3.50	123.92	128.67
6	B	425	ADI	C4'-O4'-C1'	-3.44	106.56	109.81
6	B	425	ADI	C2'-C1'-N9	-3.23	106.40	112.48
6	B	425	ADI	O4'-C1'-C2'	-2.98	102.88	106.41
6	D	424	ADI	C3'-C2'-C1'	2.94	106.26	102.87
6	D	424	ADI	O4'-C1'-C2'	-2.53	103.42	106.41
6	D	424	ADI	C4'-O4'-C1'	-2.49	107.46	109.81
6	B	425	ADI	C3'-C2'-C1'	2.49	105.74	102.87
6	D	424	ADI	C4-C5-N7	-2.24	106.97	109.34
6	D	424	ADI	C2'-C1'-N9	-2.14	108.44	112.48
6	D	424	ADI	O4'-C4'-C5'	2.14	113.20	109.34

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	422	GOL	C1-C2-C3-O3
6	B	425	ADI	PA-O3A-PB-O3B
6	D	424	ADI	PA-O3A-PB-O2B
6	D	424	ADI	PA-O3A-PB-O3B
6	D	424	ADI	O4'-C4'-C5'-O5'
6	B	425	ADI	C4'-C5'-O5'-PA
5	B	422	GOL	O2-C2-C3-O3
6	D	424	ADI	C4'-C5'-O5'-PA
6	B	425	ADI	PA-O3A-PB-O1B
6	D	424	ADI	PA-O3A-PB-O1B
6	B	425	ADI	PA-O3A-PB-O2B

There are no ring outliers.

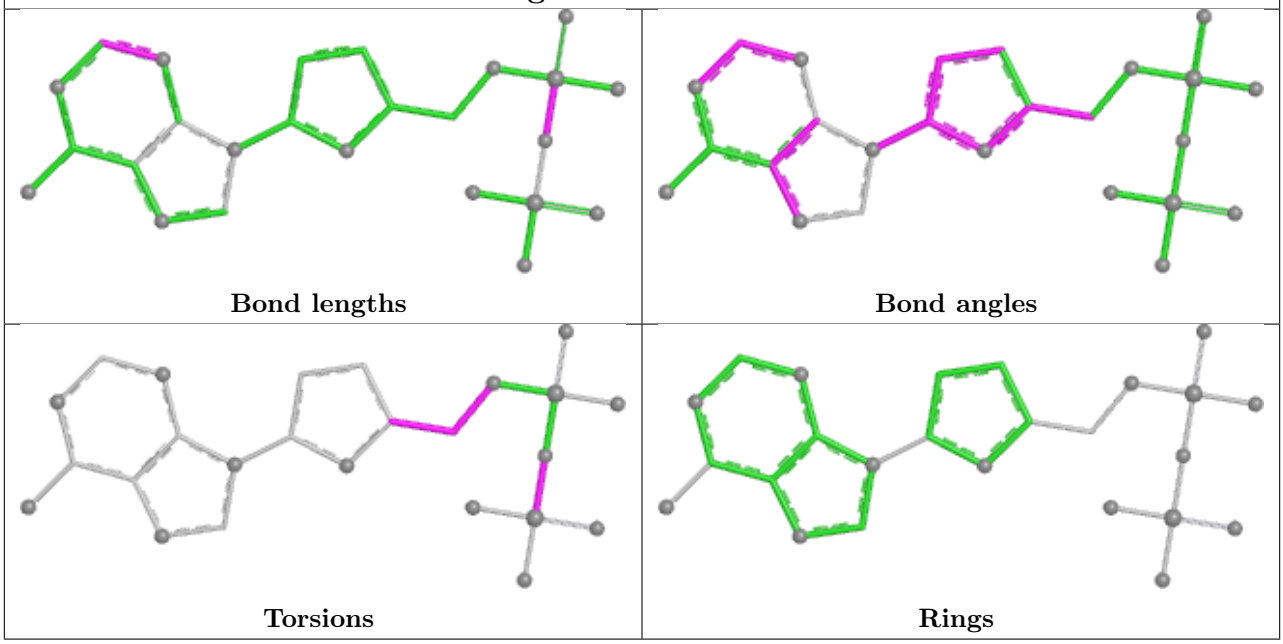
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	424	ADI	1	0
6	B	425	ADI	1	0
5	B	422	GOL	3	0

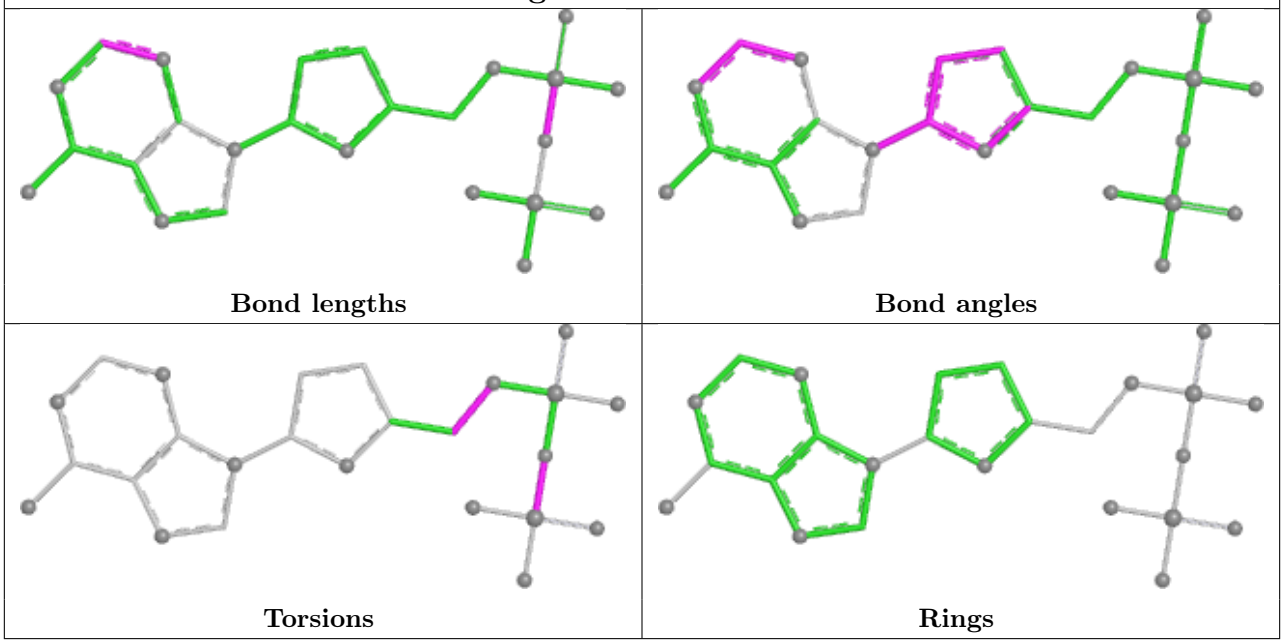
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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 ADI D 424



Ligand ADI B 425



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

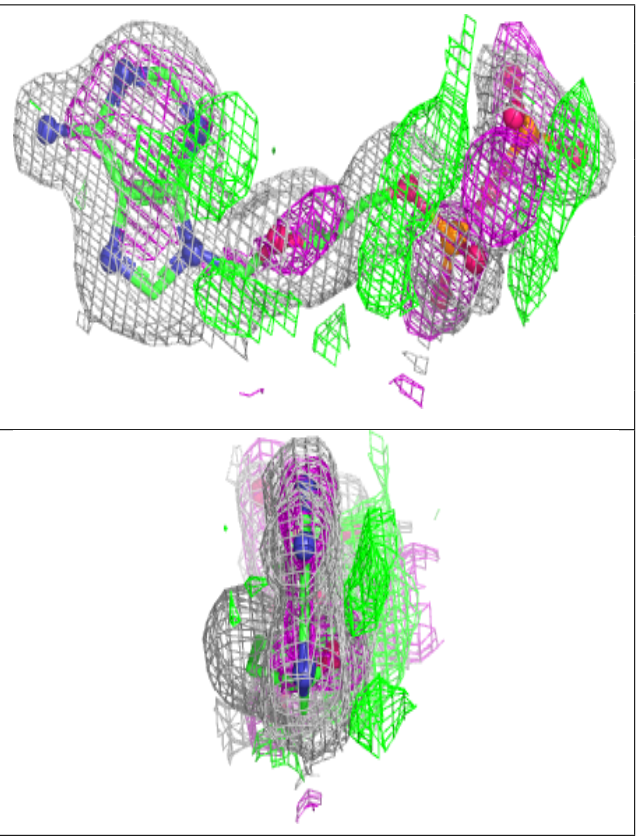
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

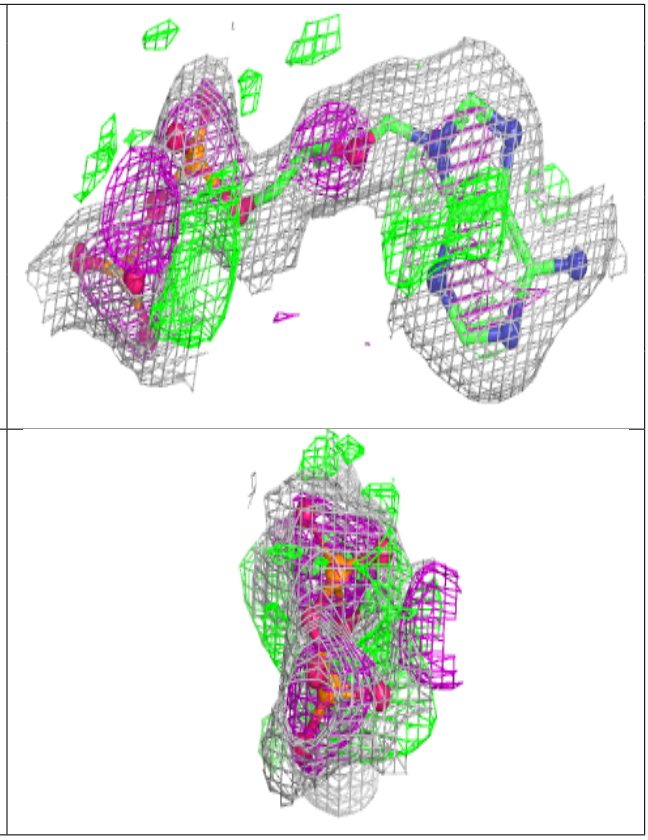
Electron density around ADI B 425:

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



Electron density around ADI D 424:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.