



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 06:11 PM EST

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 ⓘ 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

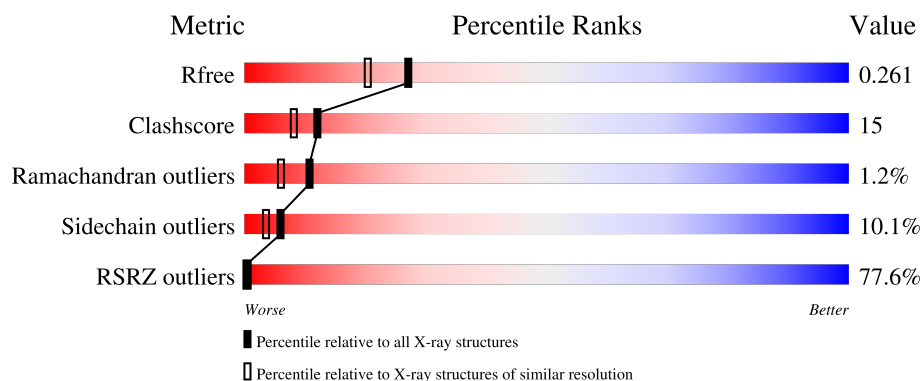
1 Overall quality at a glance

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	420	<div> <div>70%</div> <div>62%</div> <div>20%</div> <div>8%</div> <div>10%</div> </div>
1	D	420	<div> <div>72%</div> <div>65%</div> <div>20%</div> <div>6%</div> <div>9%</div> </div>
2	E	9	<div> <div>44%</div> <div>22%</div> <div>33%</div> </div>
2	P	9	<div> <div>22%</div> <div>33%</div> <div>44%</div> <div>22%</div> </div>
3	F	13	<div> <div>15%</div> <div>46%</div> <div>54%</div> </div>
3	T	13	<div> <div>31%</div> <div>62%</div> <div>31%</div> <div>8%</div> </div>

2 Entry composition

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
1	B	379	Total	C	N	O	S	Se	0	0	0
			2990	1892	521	555	11	11			
1	D	383	Total	C	N	O	S	Se	0	1	0
			3020	1909	526	562	11	12			

- 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
2	P	9	Total	C	N	O	P	0	0	0
			189	90	39	52	8			
2	E	9	Total	C	N	O	P	0	0	0
			189	90	39	52	8			

- 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
3	T	13	Total	C	N	O	P	0	0	0
			257	124	41	79	13			
3	F	13	Total	C	N	O	P	0	0	0
			257	124	41	79	13			

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

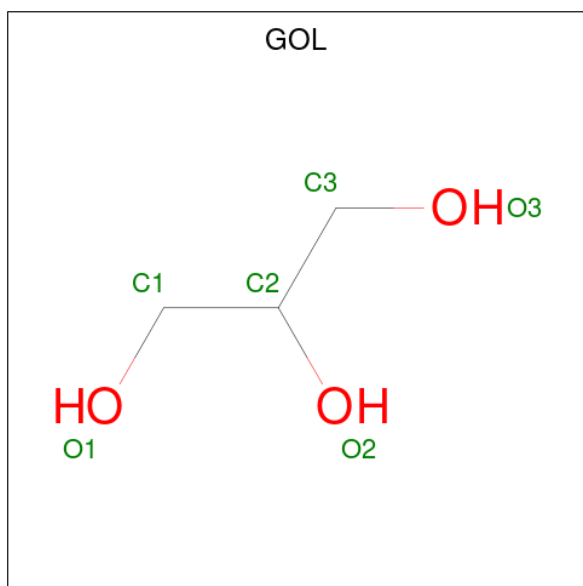
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Ca	0	0
			3	3		
4	P	1	Total	Ca	0	0
			1	1		
4	D	3	Total	Ca	0	0
			3	3		

Continued on next page...

Continued from previous page...

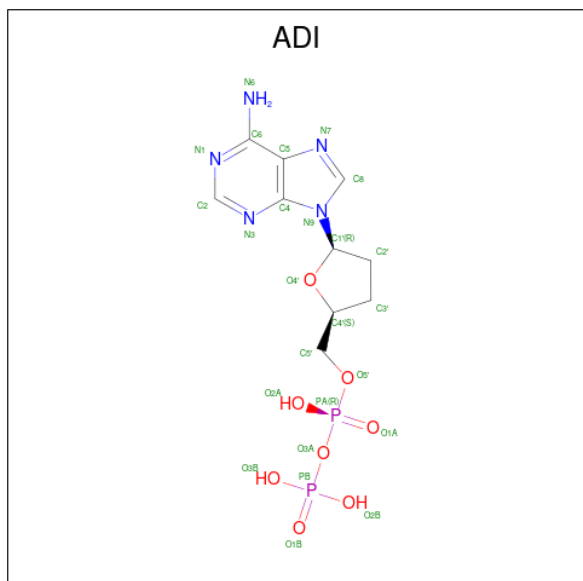
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	Ca	0	0
			1	1		

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



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

- 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
6	B	1	Total	C	N	O	P	0	0
			25	10	5	8	2		
6	D	1	Total	C	N	O	P	0	0
			25	10	5	8	2		

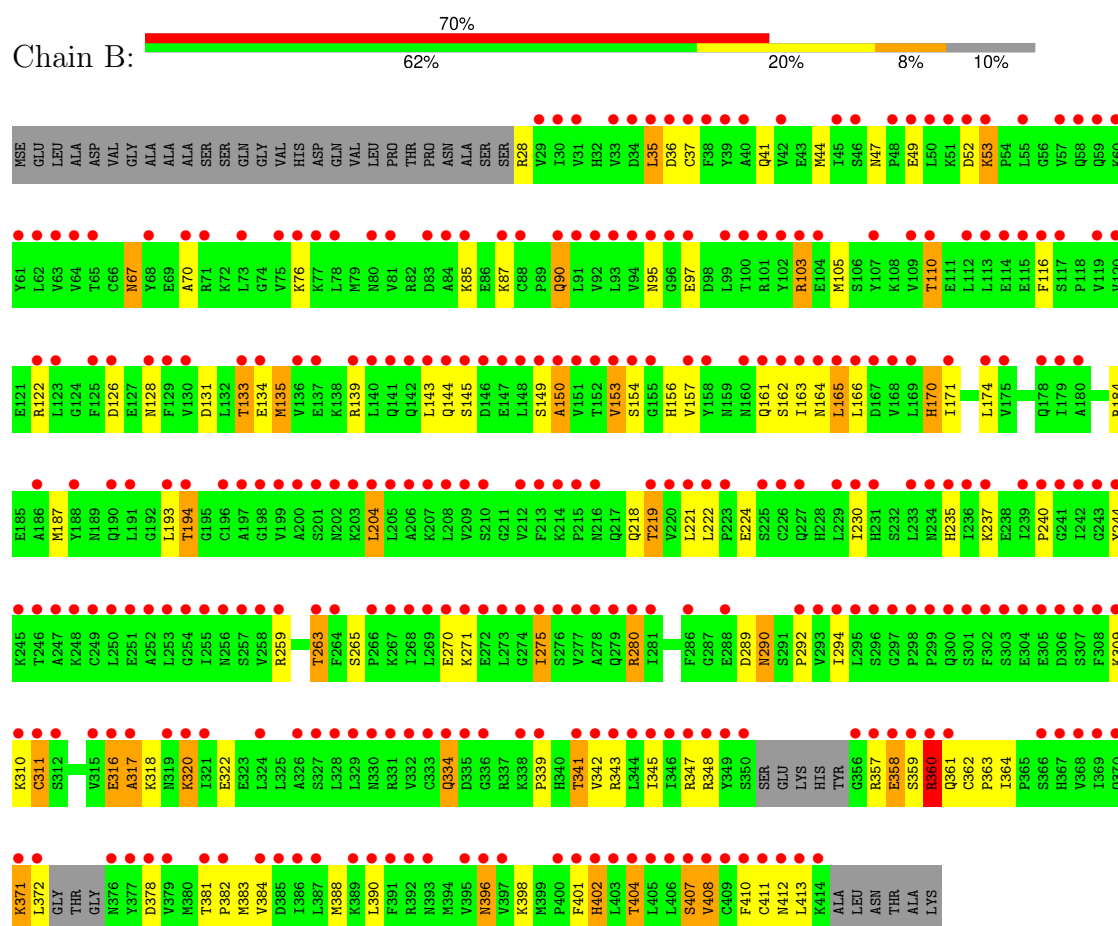
- Molecule 7 is water.

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

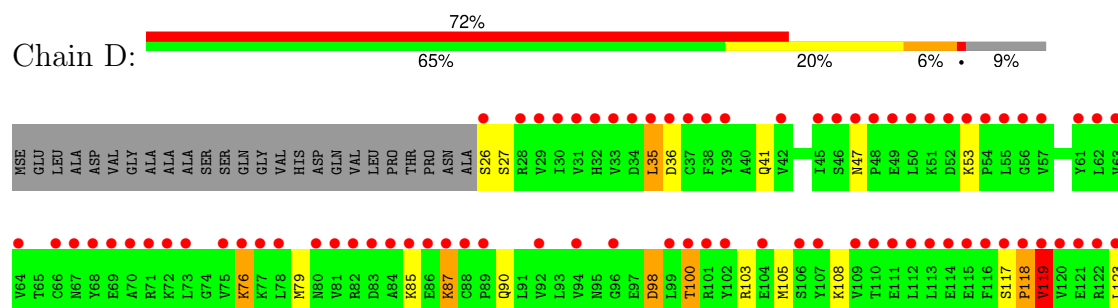
3 Residue-property plots

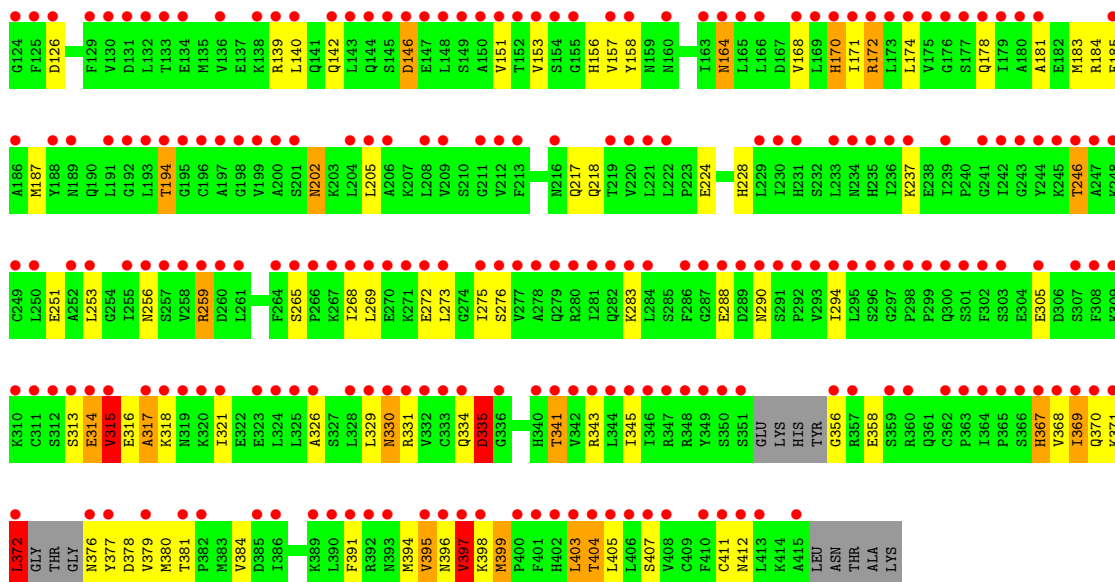
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

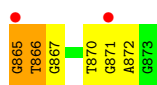


• Molecule 1: DNA polymerase iota





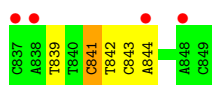
• Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'



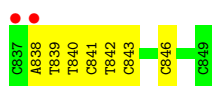
• Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'



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



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



4 Data and refinement statistics

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 51.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (51.57-2.00) 95.4 (51.57-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	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.*

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: ADI, CA, GOL

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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	16	12
1	D	378/420 (90%)	359 (95%)	12 (3%)	7 (2%)	6	3
All	All	751/840 (89%)	722 (96%)	19 (2%)	10 (1%)	11	5

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%)	6	3
1	D	348/364 (96%)	313 (90%)	35 (10%)	6	3
All	All	692/728 (95%)	622 (90%)	70 (10%)	6	3

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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%)
5	GOL	B	422	-	5,5,5	0.56	0	5,5,5	0.39	0
6	ADI	B	425	4	23,27,27	1.08	2 (8%)	26,41,41	2.03	6 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADI	D	424	4	-	5/12/25/25	0/3/3/3
5	GOL	B	422	-	-	2/4/4/4	-
6	ADI	B	425	4	-	4/12/25/25	0/3/3/3

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(°)	Ideal(°)
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

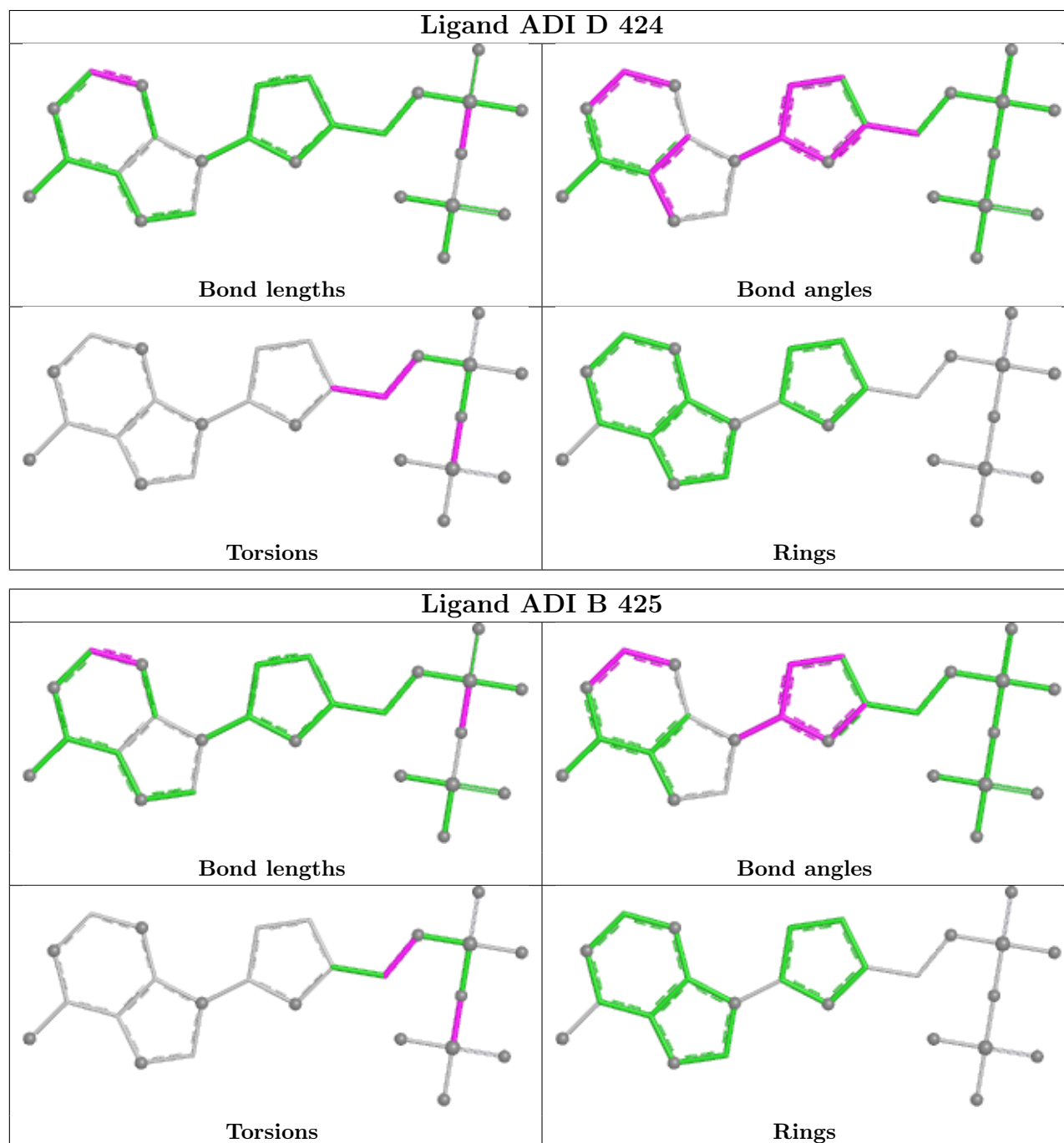
There are no ring outliers.

3 monomers are involved in 5 short contacts:

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



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 ⓘ

Warning: The R factor obtained from EDS is 0.3928, which does not match the depositor's R factor of 0.205. Please interpret the results in this section carefully.

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	B	368/420 (87%)	2.88	296 (80%) 0 0	45, 56, 69, 80	0
1	D	372/420 (88%)	2.81	304 (81%) 0 0	17, 54, 66, 88	0
2	E	9/9 (100%)	1.28	0 100 100	34, 37, 40, 41	0
2	P	9/9 (100%)	1.84	2 (22%) 3 2	49, 51, 55, 57	0
3	F	13/13 (100%)	1.30	2 (15%) 6 5	31, 38, 52, 68	0
3	T	13/13 (100%)	1.87	4 (30%) 1 1	45, 54, 68, 85	0
All	All	784/884 (88%)	2.77	608 (77%) 0 0	17, 55, 68, 88	0

All (608) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	LEU	7.4
1	D	372	LEU	7.1
1	D	356	GLY	7.0
1	B	150	ALA	6.9
1	B	149	SER	6.8
1	B	145	SER	6.6
1	D	315	VAL	6.2
1	D	119	VAL	5.9
1	B	143	LEU	5.7
1	B	372	LEU	5.7
1	D	152	THR	5.6
1	B	356	GLY	5.6
1	B	146	ASP	5.5
1	B	349	TYR	5.1
1	D	395	VAL	5.1
1	B	243	GLY	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	237	LYS	5.1
1	B	168	VAL	5.1
1	B	242	ILE	5.0
1	D	397	VAL	5.0
1	D	136	VAL	4.9
1	D	370	GLN	4.8
1	D	35	LEU	4.8
1	B	107	TYR	4.8
1	D	357	ARG	4.8
1	D	311	CYS	4.8
1	D	146	ASP	4.8
1	B	151	VAL	4.7
1	B	302	PHE	4.6
1	B	249	CYS	4.6
1	B	207	LYS	4.6
1	D	84	ALA	4.6
1	D	376	ASN	4.6
1	B	204	LEU	4.6
1	D	403	LEU	4.6
1	B	300	GLN	4.6
1	B	405	LEU	4.6
1	B	61	TYR	4.5
1	B	188	TYR	4.5
1	B	324	LEU	4.5
1	B	236	ILE	4.5
1	B	379	VAL	4.5
1	D	85	LYS	4.4
1	B	268	ILE	4.4
1	D	26	SER	4.4
1	D	255	ILE	4.4
1	B	271	LYS	4.4
1	D	369	ILE	4.4
1	B	333	CYS	4.3
1	D	367	HIS	4.3
1	D	319	ASN	4.3
1	D	250	LEU	4.3
1	D	278	ALA	4.3
1	B	110	THR	4.3
1	B	308	PHE	4.3
1	B	350	SER	4.2
1	B	295	LEU	4.2
1	D	244	TYR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	351	SER	4.2
1	B	298	PRO	4.2
1	B	273	LEU	4.2
1	B	62	LEU	4.2
1	D	268	ILE	4.1
1	B	404	THR	4.1
1	B	296	SER	4.1
1	D	118	PRO	4.1
1	B	193	LEU	4.1
1	B	345	ILE	4.1
1	D	243	GLY	4.1
1	B	244	TYR	4.1
1	B	125	PHE	4.0
1	D	36	ASP	4.0
1	D	117	SER	4.0
1	D	359	SER	4.0
1	D	30	ILE	4.0
1	D	237	LYS	4.0
1	D	165	LEU	4.0
1	B	92	VAL	4.0
1	B	247	ALA	4.0
1	D	336	GLY	4.0
1	B	221	LEU	4.0
1	B	332	VAL	4.0
1	B	303	SER	4.0
1	D	346	ILE	4.0
1	B	241	GLY	4.0
1	D	142	GLN	3.9
1	B	384	VAL	3.9
1	B	240	PRO	3.9
1	B	395	VAL	3.9
1	D	48	PRO	3.9
1	B	309	LYS	3.9
1	D	377	TYR	3.9
1	B	315	VAL	3.9
1	B	163	ILE	3.8
1	D	45	ILE	3.8
1	B	208	LEU	3.8
1	D	401	PHE	3.8
1	B	246	THR	3.8
1	D	279	GLN	3.8
1	D	406	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	77	LYS	3.8
1	B	225	SER	3.8
1	B	367	HIS	3.8
1	D	286	PHE	3.8
1	D	290	ASN	3.7
1	B	194	THR	3.7
1	B	120	VAL	3.7
1	B	226	CYS	3.7
1	B	144	GLN	3.7
1	D	273	LEU	3.7
1	B	317	ALA	3.7
1	D	116	PHE	3.7
1	D	120	VAL	3.7
1	B	255	ILE	3.7
1	B	346	ILE	3.7
1	D	78	LEU	3.7
1	D	169	LEU	3.7
1	D	241	GLY	3.7
1	D	247	ALA	3.7
1	B	212	VAL	3.7
1	B	235	HIS	3.7
1	B	311	CYS	3.7
1	B	359	SER	3.7
1	B	203	LYS	3.7
1	D	245	LYS	3.7
1	D	248	LYS	3.7
1	D	325	LEU	3.7
1	B	321	ILE	3.6
1	B	250	LEU	3.6
1	D	405	LEU	3.6
1	B	400	PRO	3.6
1	B	277	VAL	3.6
1	D	258	VAL	3.6
1	D	76	LYS	3.6
1	B	239	ILE	3.6
1	D	277	VAL	3.6
1	D	293	VAL	3.6
1	B	270	GLU	3.6
1	D	236	ILE	3.6
1	D	297	GLY	3.6
1	B	78	LEU	3.6
1	B	328	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	403	LEU	3.6
1	D	390	LEU	3.6
1	B	102	TYR	3.6
1	B	206	ALA	3.6
1	B	178	GLN	3.5
1	D	269	LEU	3.5
1	B	39	TYR	3.5
1	B	377	TYR	3.5
1	D	320	LYS	3.5
1	D	185	GLU	3.5
1	D	87	LYS	3.5
1	B	305	GLU	3.5
1	D	259	ARG	3.5
1	B	397	VAL	3.5
1	D	294	ILE	3.5
1	B	85	LYS	3.5
1	D	398	LYS	3.5
1	D	86	GLU	3.5
1	B	68	TYR	3.5
1	D	68	TYR	3.5
1	D	75	VAL	3.5
1	D	81	VAL	3.5
1	B	37	CYS	3.5
1	B	269	LEU	3.5
1	D	111	GLU	3.5
1	D	181	ALA	3.4
1	D	186	ALA	3.4
1	D	317	ALA	3.4
1	B	81	VAL	3.4
1	B	45	ILE	3.4
1	B	191	LEU	3.4
1	D	143	LEU	3.4
1	D	415	ALA	3.4
1	D	61	TYR	3.4
1	B	109	VAL	3.4
1	B	157	VAL	3.4
1	B	371	LYS	3.4
1	D	220	VAL	3.4
1	B	253	LEU	3.4
1	D	178	GLN	3.4
1	B	153	VAL	3.4
1	B	199	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	837	DC	3.4
1	B	171	ILE	3.4
1	B	413	LEU	3.4
1	D	62	LEU	3.4
1	D	266	PRO	3.4
1	D	267	LYS	3.4
1	B	281	ILE	3.3
1	B	390	LEU	3.3
1	D	163	ILE	3.3
1	D	275	ILE	3.3
1	D	345	ILE	3.3
1	D	89	PRO	3.3
1	D	271	LYS	3.3
1	B	357	ARG	3.3
1	B	42	VAL	3.3
1	B	401	PHE	3.3
1	D	153	VAL	3.3
1	D	123	LEU	3.3
1	D	324	LEU	3.3
1	B	245	LYS	3.3
1	B	310	LYS	3.3
1	D	51	LYS	3.3
1	B	299	PRO	3.3
1	B	335	ASP	3.3
1	D	83	ASP	3.3
1	B	80	ASN	3.3
1	B	133	THR	3.3
1	B	233	LEU	3.3
1	D	148	LEU	3.3
1	B	307	SER	3.3
1	D	252	ALA	3.3
1	B	126	ASP	3.3
1	B	254	GLY	3.3
1	B	258	VAL	3.3
1	B	293	VAL	3.3
1	D	314	GLU	3.3
1	B	165	LEU	3.3
1	D	208	LEU	3.3
1	D	301	SER	3.3
1	D	350	SER	3.3
1	B	414	LYS	3.2
1	D	64	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	132	LEU	3.2
1	D	149	SER	3.2
1	D	191	LEU	3.2
1	D	37	CYS	3.2
1	D	150	ALA	3.2
1	D	175	VAL	3.2
1	D	379	VAL	3.2
1	D	308	PHE	3.2
1	D	100	THR	3.2
1	D	110	THR	3.2
1	D	46	SER	3.2
1	D	396	ASN	3.2
1	B	147	GLU	3.2
1	D	360	ARG	3.2
1	B	35	LEU	3.2
1	D	253	LEU	3.2
1	B	275	ILE	3.2
1	D	230	ILE	3.2
1	D	411	CYS	3.2
1	B	103	ARG	3.2
1	B	160	ASN	3.2
1	B	360	ARG	3.2
1	D	168	VAL	3.1
1	B	52	ASP	3.1
1	D	174	LEU	3.1
1	B	297	GLY	3.1
1	B	336	GLY	3.1
1	B	369	ILE	3.1
1	D	288	GLU	3.1
1	B	63	VAL	3.1
1	B	119	VAL	3.1
1	B	276	SER	3.1
1	B	327	SER	3.1
1	D	310	LYS	3.1
1	D	328	LEU	3.1
1	B	36	ASP	3.1
1	B	162	SER	3.1
1	D	31	VAL	3.1
1	D	33	VAL	3.1
1	B	166	LEU	3.1
1	D	295	LEU	3.1
1	B	230	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	281	ILE	3.1
1	B	409	CYS	3.1
1	B	402	HIS	3.0
1	D	55	LEU	3.0
1	D	99	LEU	3.0
1	B	294	ILE	3.0
1	D	364	ILE	3.0
1	D	386	ILE	3.0
1	B	301	SER	3.0
1	D	407	SER	3.0
1	B	164	ASN	3.0
1	B	213	PHE	3.0
1	B	412	ASN	3.0
1	D	113	LEU	3.0
1	B	70	ALA	3.0
1	B	158	TYR	3.0
1	D	349	TYR	3.0
1	B	316	GLU	3.0
1	D	151	VAL	3.0
1	D	199	VAL	3.0
1	B	205	LEU	3.0
1	B	343	ARG	3.0
1	B	104	GLU	3.0
1	D	124	GLY	3.0
1	D	92	VAL	3.0
1	B	99	LEU	3.0
1	D	221	LEU	3.0
1	B	331	ARG	3.0
1	B	347	ARG	3.0
1	B	83	ASP	2.9
1	D	242	ILE	2.9
1	D	321	ILE	2.9
1	D	362	CYS	2.9
1	D	133	THR	2.9
1	D	246	THR	2.9
1	D	157	VAL	2.9
1	D	368	VAL	2.9
1	D	129	PHE	2.9
1	B	60	LYS	2.9
1	D	107	TYR	2.9
1	D	188	TYR	2.9
2	P	871	DG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	298	PRO	2.9
1	B	31	VAL	2.9
1	B	64	VAL	2.9
1	B	304	GLU	2.9
1	B	93	LEU	2.9
1	B	174	LEU	2.9
1	B	222	LEU	2.9
1	B	329	LEU	2.9
1	D	138	LYS	2.9
1	B	278	ALA	2.9
1	D	126	ASP	2.9
1	D	330	ASN	2.9
1	B	49	GLU	2.9
1	B	214	LYS	2.9
1	D	50	LEU	2.9
1	D	344	LEU	2.9
1	D	38	PHE	2.9
1	D	391	PHE	2.9
1	B	84	ALA	2.9
1	B	200	ALA	2.9
1	B	279	GLN	2.9
1	B	234	ASN	2.9
1	D	47	ASN	2.9
1	D	280	ARG	2.9
1	D	392	ARG	2.9
1	D	194	THR	2.9
1	D	381	THR	2.9
1	D	404	THR	2.9
1	B	358	GLU	2.9
1	B	389	LYS	2.9
1	B	223	PRO	2.8
1	D	109	VAL	2.8
1	D	222	LEU	2.8
1	D	229	LEU	2.8
1	B	197	ALA	2.8
1	D	197	ALA	2.8
1	D	300	GLN	2.8
1	B	46	SER	2.8
3	T	838	DA	2.8
1	B	320	LYS	2.8
1	B	91	LEU	2.8
1	D	63	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	252	ALA	2.8
1	B	122	ARG	2.8
1	D	213	PHE	2.8
1	B	312	SER	2.8
1	B	216	ASN	2.8
1	D	160	ASN	2.8
1	D	114	GLU	2.8
1	B	198	GLY	2.8
1	D	333	CYS	2.8
1	D	32	HIS	2.8
1	D	402	HIS	2.8
1	B	209	VAL	2.8
1	B	186	ALA	2.8
1	B	201	SER	2.8
1	B	248	LYS	2.8
1	D	292	PRO	2.8
1	D	28	ARG	2.8
1	B	50	LEU	2.8
1	D	205	LEU	2.8
1	D	413	LEU	2.8
1	B	137	GLU	2.8
1	D	332	VAL	2.8
1	B	180	ALA	2.7
1	D	145	SER	2.8
1	D	296	SER	2.8
1	B	100	THR	2.7
1	B	334	GLN	2.7
1	D	158	TYR	2.7
1	B	406	LEU	2.7
1	D	189	ASN	2.7
1	D	209	VAL	2.7
1	B	65	THR	2.7
1	B	386	ILE	2.7
1	D	71	ARG	2.7
1	D	82	ARG	2.7
1	B	77	LYS	2.7
1	B	55	LEU	2.7
1	D	329	LEU	2.7
1	D	130	VAL	2.7
1	D	195	GLY	2.7
1	B	280	ARG	2.7
1	B	348	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	101	ARG	2.7
1	B	87	LYS	2.7
1	D	88	CYS	2.7
1	B	123	LEU	2.7
1	B	210	SER	2.7
1	D	173	LEU	2.7
1	D	204	LEU	2.7
1	D	284	LEU	2.7
1	B	40	ALA	2.7
1	D	212	VAL	2.7
1	B	96	GLY	2.7
1	B	274	GLY	2.7
1	B	38	PHE	2.7
1	B	101	ARG	2.7
1	B	259	ARG	2.7
1	B	231	HIS	2.7
1	B	152	THR	2.7
1	D	299	PRO	2.6
1	D	256	ASN	2.6
1	B	229	LEU	2.6
1	D	73	LEU	2.6
1	B	33	VAL	2.6
1	B	392	ARG	2.6
1	B	408	VAL	2.6
1	D	348	ARG	2.6
1	D	155	GLY	2.6
1	B	129	PHE	2.6
1	D	125	PHE	2.6
1	D	302	PHE	2.6
1	B	167	ASP	2.6
1	B	306	ASP	2.6
1	D	34	ASP	2.6
1	B	53	LYS	2.6
1	B	338	LYS	2.6
1	D	389	LYS	2.6
1	D	196	CYS	2.6
1	D	106	SER	2.6
1	B	140	LEU	2.6
1	D	261	LEU	2.6
1	B	57	VAL	2.6
1	B	94	VAL	2.6
1	B	410	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	260	ASP	2.6
1	B	330	ASN	2.6
1	D	154	SER	2.6
1	D	343	ARG	2.6
1	B	112	LEU	2.6
1	B	220	VAL	2.6
1	D	29	VAL	2.6
1	D	39	TYR	2.6
1	B	396	ASN	2.6
1	D	171	ILE	2.6
1	D	291	SER	2.6
1	B	113	LEU	2.6
1	D	249	CYS	2.6
1	D	121	GLU	2.6
1	D	287	GLY	2.5
1	B	368	VAL	2.5
1	D	131	ASP	2.5
1	B	264	PHE	2.5
1	B	190	GLN	2.5
1	D	239	ILE	2.5
1	D	147	GLU	2.5
1	D	231	HIS	2.5
1	B	75	VAL	2.5
1	B	130	VAL	2.5
1	B	219	THR	2.5
1	B	48	PRO	2.5
1	B	169	LEU	2.5
1	D	198	GLY	2.5
1	B	393	ASN	2.5
1	D	216	ASN	2.5
1	D	305	GLU	2.5
1	B	257	SER	2.5
1	B	366	SER	2.5
1	B	407	SER	2.5
1	D	283	LYS	2.5
1	D	309	LYS	2.5
1	B	385	ASP	2.5
1	B	251	GLU	2.4
1	D	363	PRO	2.4
1	B	391	PHE	2.4
1	D	307	SER	2.4
1	B	344	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	166	LEU	2.4
1	D	144	GLN	2.4
1	D	180	ALA	2.4
1	B	256	ASN	2.4
1	B	134	GLU	2.4
1	D	54	PRO	2.4
1	D	235	HIS	2.4
1	B	286	PHE	2.4
1	D	264	PHE	2.4
1	B	179	ILE	2.4
1	D	347	ARG	2.4
1	B	142	GLN	2.4
1	D	140	LEU	2.4
1	B	196	CYS	2.4
1	B	95	ASN	2.4
1	B	76	LYS	2.4
1	B	342	VAL	2.4
1	D	318	LYS	2.4
1	D	400	PRO	2.4
1	D	179	ILE	2.4
1	B	141	GLN	2.4
1	D	193	LEU	2.4
1	B	288	GLU	2.4
1	D	49	GLU	2.4
1	D	80	ASN	2.4
1	D	371	LYS	2.4
1	B	266	PRO	2.4
1	B	382	PRO	2.4
1	D	96	GLY	2.4
3	T	837	DC	2.3
1	D	164	ASN	2.3
1	D	42	VAL	2.3
1	D	312	SER	2.3
1	D	342	VAL	2.3
1	D	382	PRO	2.3
1	D	408	VAL	2.3
1	B	370	GLN	2.3
1	D	192	GLY	2.3
3	T	844	DA	2.3
1	D	257	SER	2.3
1	D	282	GLN	2.3
1	B	116	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	340	HIS	2.3
1	D	233	LEU	2.3
1	D	265	SER	2.3
1	D	303	SER	2.3
1	D	313	SER	2.3
1	D	366	SER	2.3
1	B	175	VAL	2.3
1	D	57	VAL	2.3
1	D	270	GLU	2.3
1	D	72	LYS	2.3
1	B	202	ASN	2.3
1	B	88	CYS	2.2
1	B	215	PRO	2.2
1	D	104	GLU	2.2
1	D	122	ARG	2.2
1	D	102	TYR	2.2
1	B	263	THR	2.2
1	D	115	GLU	2.2
1	D	272	GLU	2.2
1	D	326	ALA	2.2
1	B	292	PRO	2.2
1	B	378	ASP	2.2
1	D	52	ASP	2.2
1	D	211	GLY	2.2
1	D	94	VAL	2.2
1	B	376	ASN	2.2
1	B	30	ILE	2.2
1	B	161	GLN	2.2
1	B	387	LEU	2.2
1	D	200	ALA	2.2
1	D	201	SER	2.2
1	B	339	PRO	2.2
1	B	59	GLN	2.2
1	B	227	GLN	2.2
3	F	838	DA	2.2
1	B	136	VAL	2.2
1	B	115	GLU	2.1
1	D	219	THR	2.1
1	D	177	SER	2.1
1	B	326	ALA	2.1
1	D	365	PRO	2.1
2	P	865	DG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	412	ASN	2.1
1	B	90	GLN	2.1
1	D	334	GLN	2.1
1	B	97	GLU	2.1
1	D	69	GLU	2.1
1	B	154	SER	2.1
1	D	289	ASP	2.1
1	D	341	THR	2.1
1	B	155	GLY	2.1
1	B	319	ASN	2.1
1	D	234	ASN	2.1
1	D	134	GLU	2.1
1	D	66	CYS	2.1
1	B	29	VAL	2.1
1	B	267	LYS	2.1
1	D	139	ARG	2.1
1	D	112	LEU	2.1
1	D	410	PHE	2.1
1	B	117	SER	2.1
1	B	341	THR	2.1
1	D	276	SER	2.1
1	D	70	ALA	2.1
1	D	206	ALA	2.1
1	D	56	GLY	2.1
1	D	393	ASN	2.1
1	B	411	CYS	2.1
1	B	51	LYS	2.1
1	D	53	LYS	2.1
1	B	71	ARG	2.1
1	B	139	ARG	2.1
1	D	331	ARG	2.1
1	B	34	ASP	2.1
1	B	381	THR	2.1
1	D	170	HIS	2.1
1	B	361	GLN	2.1
1	D	176	GLY	2.0
1	D	67	ASN	2.0
3	T	848	DA	2.0
1	D	172	ARG	2.0
1	D	385	ASP	2.0
1	B	58	GLN	2.0
1	B	73	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	114	GLU	2.0
1	B	272	GLU	2.0
1	D	323	GLU	2.0
1	B	128	ASN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

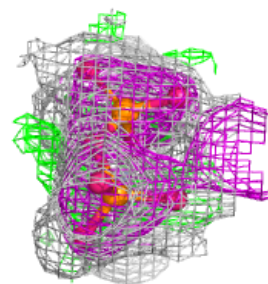
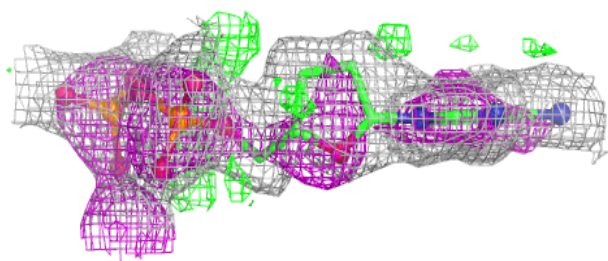
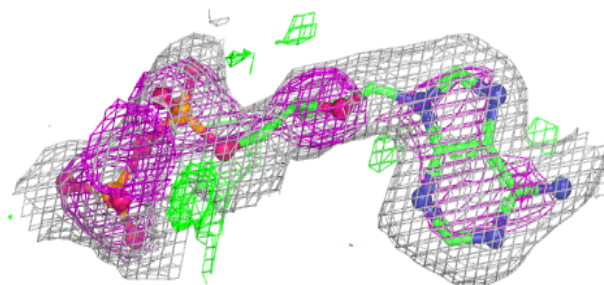
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	422	6/6	0.85	0.18	32,34,34,35	0
6	ADI	D	424	25/25	0.86	0.14	19,24,29,30	0
6	ADI	B	425	25/25	0.88	0.12	15,21,24,26	0
4	CA	D	422	1/1	0.91	0.27	43,43,43,43	0
4	CA	F	1	1/1	0.96	0.20	19,19,19,19	0
4	CA	P	1	1/1	0.97	0.15	31,31,31,31	0
4	CA	B	423	1/1	0.97	0.23	28,28,28,28	0
4	CA	D	421	1/1	0.98	0.21	14,14,14,14	0
4	CA	B	421	1/1	0.99	0.37	35,35,35,35	0
4	CA	D	423	1/1	0.99	0.37	36,36,36,36	0
4	CA	B	424	1/1	0.99	0.20	13,13,13,13	0

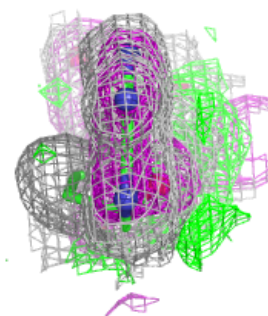
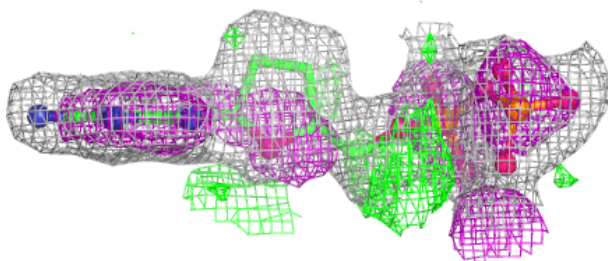
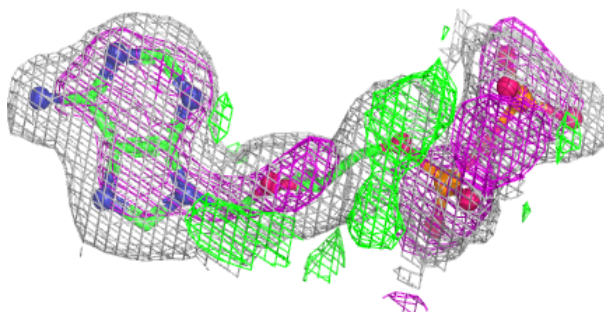
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.