



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 11:19 AM UTC

PDB ID : 3GV5 / pdb_00003gv5
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:

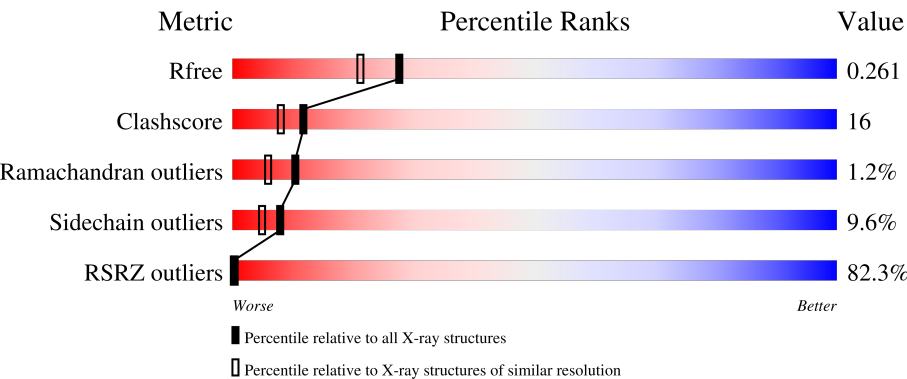
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 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}	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	B	420	74% 61%21%7%10%
1	D	420	76% 64%20%6%9%
2	E	9	11% 56%44%
2	P	9	56% 56%33%11%
3	F	13	15% 92%8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	T	13	54% 92% 8%

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 (CCD ID: 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...

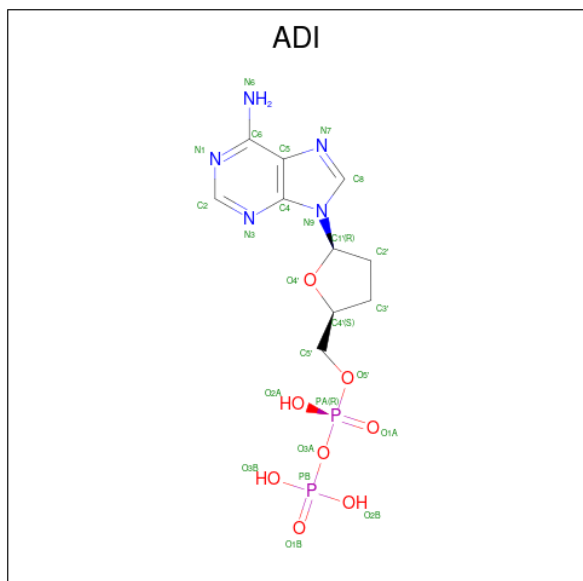
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	Ca	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: 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 (CCD ID: 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		

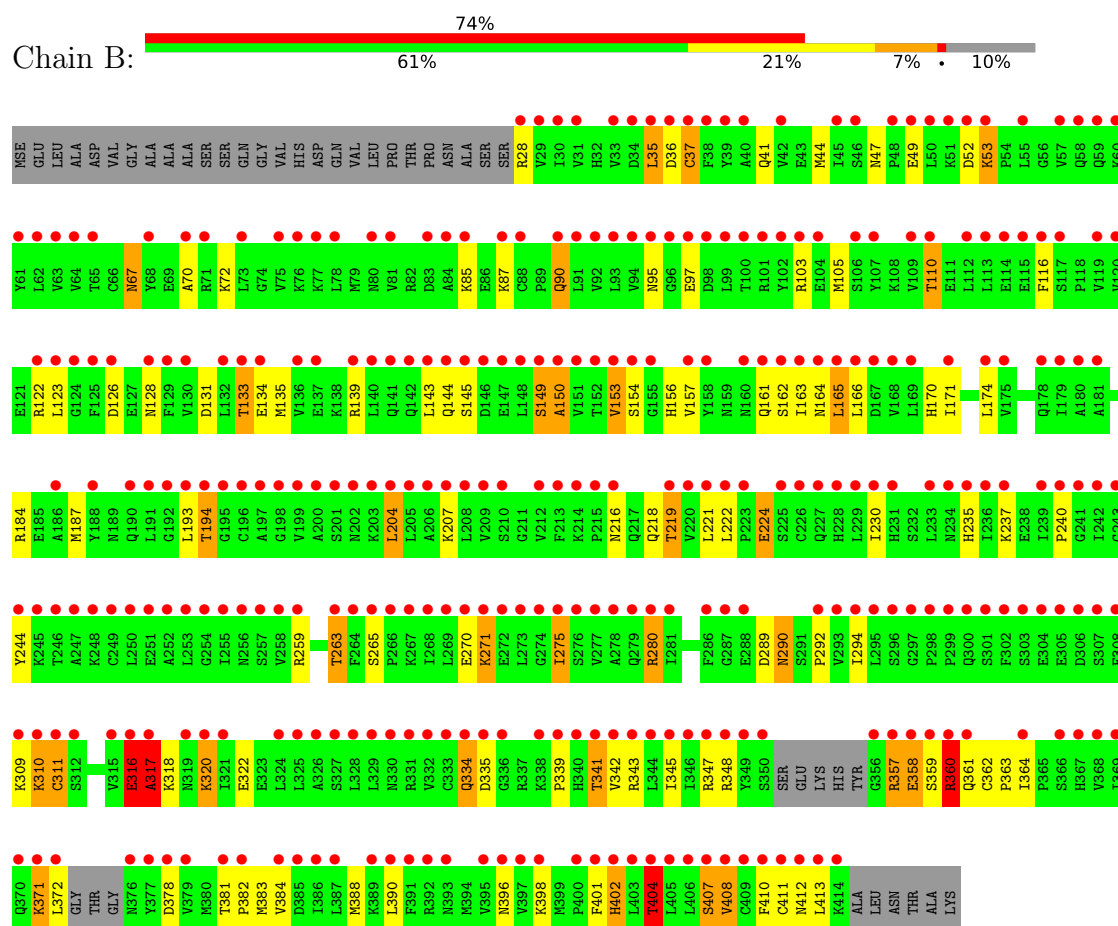
- Molecule 7 is water.

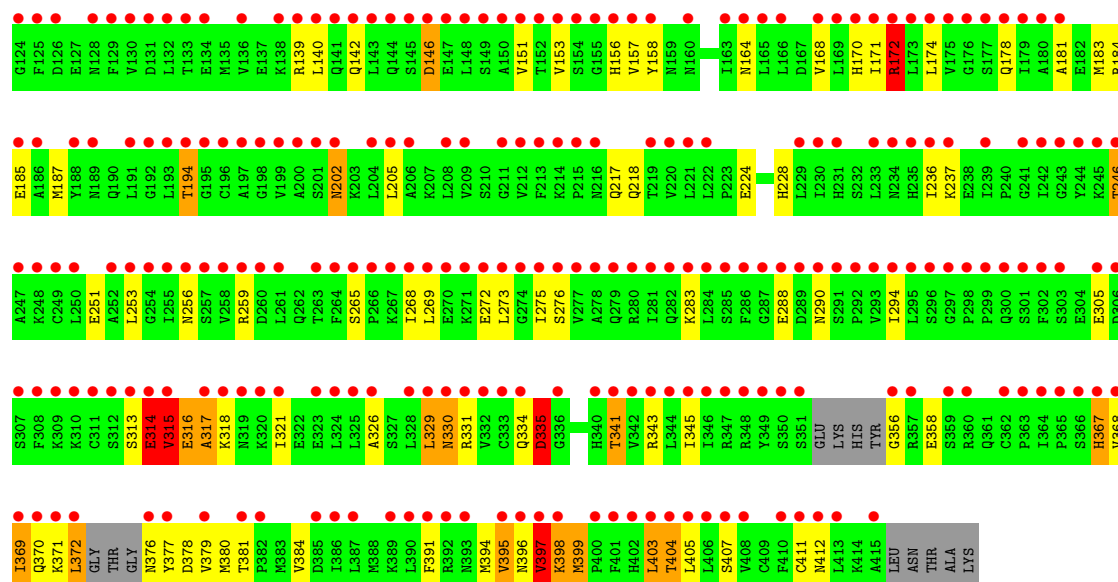
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	303	Total	O	0	0
			303	303		
7	P	32	Total	O	0	0
			32	32		
7	T	39	Total	O	0	0
			39	39		
7	D	306	Total	O	0	0
			306	306		
7	E	23	Total	O	0	0
			23	23		
7	F	34	Total	O	0	0
			34	34		

3 Residue-property plots

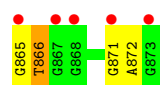
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase iota

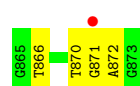




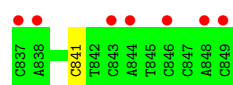
• Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'



• 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 , 43.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ADI, 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	0.81	2/3022 (0.1%)	1.17	20/4055 (0.5%)
1	D	1.01	14/3052 (0.5%)	1.24	22/4095 (0.5%)
2	E	0.49	0/213	1.18	1/329 (0.3%)
2	P	0.47	0/213	1.18	1/329 (0.3%)
3	F	0.48	0/285	1.26	1/435 (0.2%)
3	T	0.52	0/285	1.14	0/435
All	All	0.87	16/7070 (0.2%)	1.20	45/9678 (0.5%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	358	GLU	CG-CD	-16.55	1.10	1.52
1	D	358	GLU	CA-CB	-12.80	1.24	1.53
1	B	334	GLN	CA-C	10.80	1.67	1.52
1	D	315	VAL	N-CA	10.41	1.59	1.46
1	D	335	ASP	N-CA	8.93	1.57	1.46
1	D	172	ARG	C-O	-7.49	1.15	1.24
1	D	358	GLU	CD-OE1	7.10	1.38	1.25
1	D	358	GLU	CB-CG	6.99	1.73	1.52
1	D	358	GLU	CA-C	6.66	1.60	1.52
1	D	358	GLU	N-CA	6.53	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	ASP	CB-CG	-6.38	1.36	1.52
1	D	358	GLU	CD-OE2	6.14	1.37	1.25
1	D	36	ASP	C-O	-5.66	1.17	1.23
1	D	331	ARG	N-CA	5.61	1.53	1.46
1	B	317	ALA	N-CA	5.07	1.52	1.46
1	D	97	GLU	C-O	-5.05	1.18	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	318	LYS	N-CA-C	-22.68	84.97	113.55
1	D	331	ARG	N-CA-C	-17.46	92.11	113.41
1	B	311	CYS	N-CA-C	16.76	134.23	109.59
1	B	408	VAL	N-CA-C	14.36	128.74	109.21
1	B	358	GLU	N-CA-C	11.32	134.92	110.80
1	B	360	ARG	N-CA-C	11.24	128.19	110.32
1	B	317	ALA	N-CA-C	-10.48	100.62	113.41
1	D	316	GLU	N-CA-C	-10.46	97.91	112.45
1	D	404	THR	N-CA-C	10.38	125.89	111.56
1	D	404	THR	CB-CA-C	-10.26	95.17	111.18
1	D	314	GLU	N-CA-C	-9.42	101.68	113.55
1	D	404	THR	N-CA-CB	-8.86	98.70	111.54
1	D	397	VAL	N-CA-C	-8.67	91.32	109.34
1	D	358	GLU	N-CA-C	-8.66	95.86	109.72
1	D	395	VAL	N-CA-C	-8.35	95.34	107.78
1	D	358	GLU	OE1-CD-OE2	-8.30	102.98	122.90
1	D	329	LEU	N-CA-C	8.02	121.55	111.69
1	D	119	VAL	N-CA-C	-7.86	93.00	109.34
1	B	310	LYS	CA-C-N	7.29	131.73	121.24
1	B	310	LYS	C-N-CA	7.29	131.73	121.24
1	B	149	SER	N-CA-C	6.97	119.53	111.02
1	B	357	ARG	N-CA-C	-6.92	97.96	109.24
1	B	318	LYS	N-CA-C	6.84	125.37	110.80
1	D	47	ASN	CA-C-N	6.68	128.19	119.84
1	D	47	ASN	C-N-CA	6.68	128.19	119.84
2	P	866	DT	N1-C1'-C2'	6.66	123.50	113.50
1	D	405	LEU	N-CA-CB	-6.61	101.12	111.56
1	D	405	LEU	N-CA-C	6.37	118.45	108.96
1	B	335	ASP	N-CA-C	-6.36	105.53	113.55
1	B	357	ARG	CA-C-N	6.22	133.43	121.54
1	B	357	ARG	C-N-CA	6.22	133.43	121.54
1	B	149	SER	CA-C-N	6.02	132.53	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	SER	C-N-CA	6.02	132.53	121.70
2	E	866	DT	N1-C1'-C2'	6.00	122.50	113.50
1	D	398	LYS	N-CA-C	5.85	123.26	110.80
1	D	119	VAL	N-CA-CB	5.70	120.63	111.23
1	B	357	ARG	CB-CA-C	5.68	119.12	109.75
1	B	404	THR	CB-CA-C	5.59	117.73	109.29
3	F	838	DA	N9-C1'-C2'	5.30	121.45	113.50
1	B	335	ASP	CA-C-O	5.27	125.73	119.67
1	D	38	PHE	N-CA-C	5.25	116.68	111.07
1	D	397	VAL	N-CA-CB	5.20	119.81	111.23
1	D	405	LEU	CA-CB-CG	5.16	134.37	116.30
1	B	316	GLU	CA-C-N	-5.02	113.10	122.09
1	B	316	GLU	C-N-CA	-5.02	113.10	122.09

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	112	0
1	D	3020	0	3112	99	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	20	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	218	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 16.

All (218) 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:D:123:LEU:C	1:D:123:LEU:HD23	2.20	0.67
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: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:202:ASN:C	1:D:202:ASN:HD22	2.08	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:HIS:HA	1:D:370:GLN:H	1.70	0.57
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: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:123:LEU:C	1:D:123:LEU:CD2	2.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:HG11	1:B:161:GLN:O	2.11	0.51
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:B:396:ASN:C	1:B:396:ASN:HD22	2.18	0.50
1:D:316:GLU:O	1:D:317:ALA:C	2.55	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:B:67:ASN:HD22	1:B:67:ASN:C	2.21	0.47
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: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:B:396:ASN:C	1:B:396:ASN:ND2	2.75	0.45
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:271:LYS:C	7:B:502:HOH:O	2.61	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: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:36:ASP:O	1:B:37:CYS:C	2.61	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:D:36:ASP:O	1:D:37:CYS:C	2.60	0.43
1:B:97:GLU:HB3	5:B:422:GOL:H11	2.01	0.42
1:B:194:THR:OG1	1:B:216:ASN:CG	2.62	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:D:164:ASN:C	1:D:164:ASN:HD22	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HD21	1:B:207:LYS:HZ2	1.86	0.41
1:B:139:ARG:O	1:B:143:LEU:HD13	2.21	0.41
1:D:202:ASN:ND2	1:D:202:ASN:C	2.78	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 ⓘ

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	
1	B	373/420 (89%)	363 (97%)	7 (2%)	3 (1%)	16	11
1	D	378/420 (90%)	359 (95%)	12 (3%)	7 (2%)	6	3
All	All	751/840 (89%)	722 (96%)	19 (2%)	10 (1%)	10	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	399[B]	MSE
1	D	369	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	344/364 (94%)	311 (90%)	33 (10%)	8	5
1	D	348/364 (96%)	315 (90%)	33 (10%)	8	5
All	All	692/728 (95%)	626 (90%)	66 (10%)	8	5

All (66) 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	72	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	153	VAL
1	B	154	SER
1	B	165	LEU
1	B	166	LEU
1	B	194	THR
1	B	204	LEU
1	B	219	THR
1	B	221	LEU
1	B	224	GLU
1	B	263	THR
1	B	265	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	404	THR
1	B	408	VAL
1	B	413	LEU
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	123	LEU
1	D	139	ARG
1	D	142	GLN
1	D	146	ASP
1	D	172	ARG
1	D	194	THR
1	D	202	ASN
1	D	236	ILE
1	D	237	LYS
1	D	246	THR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN
1	B	67	ASN
1	B	90	GLN
1	B	95	ASN
1	B	156	HIS
1	B	170	HIS
1	B	218	GLN
1	B	228	HIS
1	B	256	ASN
1	B	290	ASN
1	B	330	ASN
1	B	340	HIS
1	B	361	GLN
1	B	396	ASN
1	B	402	HIS
1	B	412	ASN
1	D	58	GLN
1	D	144	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	217	GLN
1	D	218	GLN
1	D	227	GLN
1	D	228	HIS
1	D	256	ASN
1	D	282	GLN
1	D	290	ASN
1	D	396	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 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	B	425	4	26,27,27	1.67	6 (23%)	37,41,41	2.24	14 (37%)
6	ADI	D	424	4	26,27,27	1.64	6 (23%)	37,41,41	2.38	12 (32%)
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	B	425	4	-	6/16/25/25	0/3/3/3
6	ADI	D	424	4	-	6/16/25/25	0/3/3/3
5	GOL	B	422	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	425	ADI	C5-C4	5.17	1.48	1.39
6	D	424	ADI	C5-C4	4.82	1.47	1.39
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	C5-N7	-2.85	1.33	1.39
6	D	424	ADI	C5-C6	2.83	1.48	1.41
6	B	425	ADI	C5-C6	2.57	1.48	1.41
6	B	425	ADI	C5-N7	-2.50	1.34	1.39
6	B	425	ADI	C8-N7	2.25	1.36	1.31
6	B	425	ADI	C4-N9	-2.20	1.33	1.37
6	D	424	ADI	C1'-N9	2.10	1.50	1.46
6	D	424	ADI	C8-N7	2.07	1.35	1.31

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	424	ADI	O4'-C1'-N9	6.67	119.94	107.96
6	D	424	ADI	C5-C4-N3	-6.47	117.81	126.72
6	D	424	ADI	N3-C4-N9	5.16	135.95	127.17
6	B	425	ADI	C5-C4-N3	-5.10	119.70	126.72
6	B	425	ADI	N3-C4-N9	4.51	134.84	127.17
6	B	425	ADI	O4'-C1'-N9	4.32	115.72	107.96
6	B	425	ADI	N3-C2-N1	-4.13	122.33	128.58
6	D	424	ADI	C2-N3-C4	3.81	121.13	111.83
6	B	425	ADI	C2-N3-C4	3.73	120.94	111.83
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	D	424	ADI	C4-C5-N7	-3.16	106.97	110.58
6	D	424	ADI	N3-C2-N1	-3.08	123.92	128.58
6	B	425	ADI	O4'-C1'-C2'	-2.98	102.88	106.41
6	B	425	ADI	C4-N9-C8	2.95	108.83	105.74
6	D	424	ADI	C3'-C2'-C1'	2.94	106.26	102.87
6	B	425	ADI	C4-C5-N7	-2.62	107.58	110.58
6	D	424	ADI	C5-N7-C8	2.59	107.52	103.45
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	B	425	ADI	C2-N1-C6	2.40	122.68	118.73
6	B	425	ADI	C6-C5-N7	2.31	136.55	132.09
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
6	B	425	ADI	C5-N7-C8	2.02	106.63	103.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

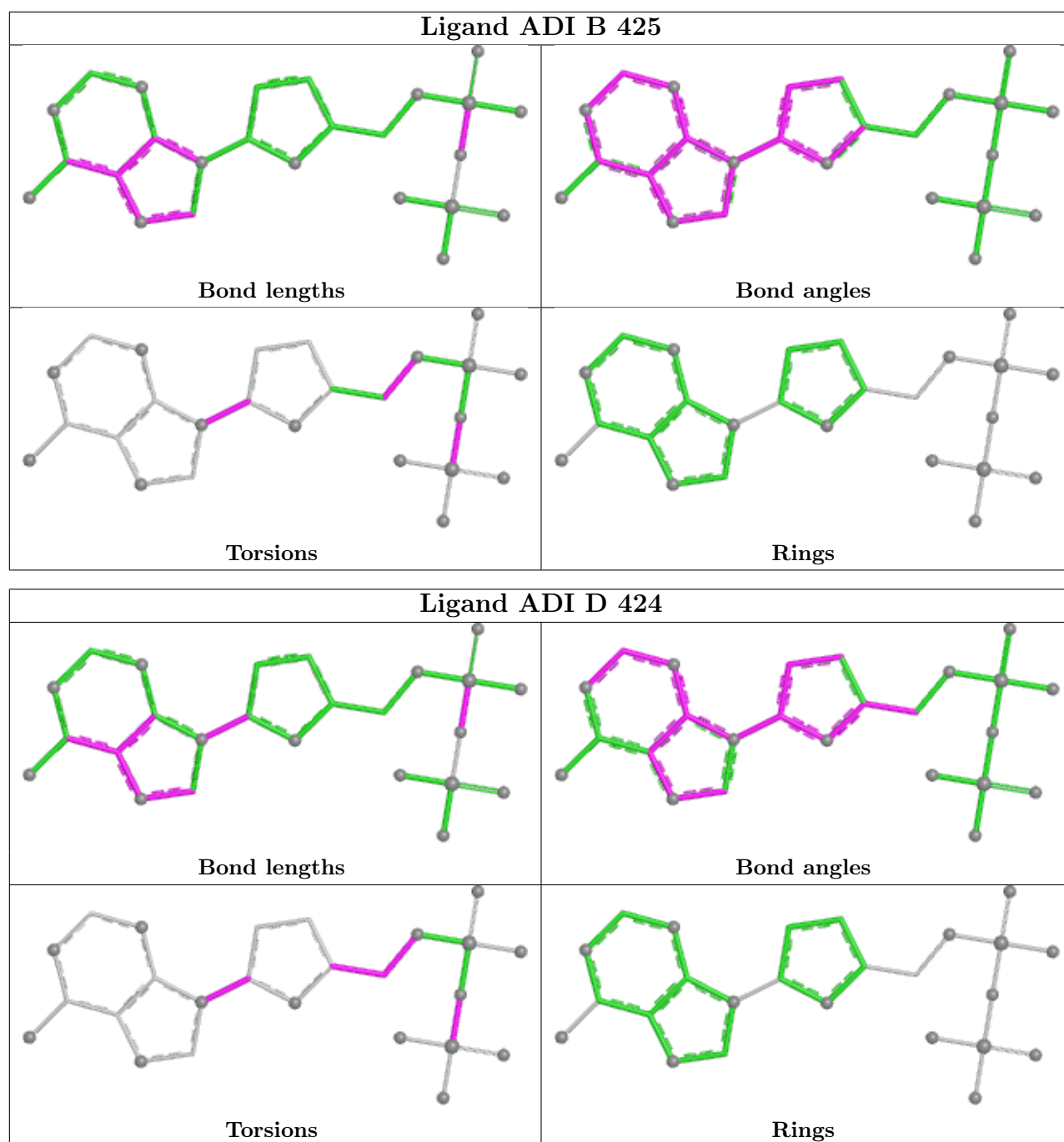
Mol	Chain	Res	Type	Atoms
5	B	422	GOL	C1-C2-C3-O3
6	B	425	ADI	PA-O3A-PB-O3B
6	D	424	ADI	PA-O3A-PB-O2B
6	D	424	ADI	PA-O3A-PB-O3B
6	D	424	ADI	O4'-C4'-C5'-O5'
6	B	425	ADI	C4'-C5'-O5'-PA
5	B	422	GOL	O2-C2-C3-O3
6	D	424	ADI	C4'-C5'-O5'-PA
6	B	425	ADI	O4'-C1'-N9-C8
6	D	424	ADI	O4'-C1'-N9-C8
6	B	425	ADI	PA-O3A-PB-O1B
6	D	424	ADI	PA-O3A-PB-O1B
6	B	425	ADI	PA-O3A-PB-O2B
6	B	425	ADI	O4'-C1'-N9-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	425	ADI	1	0
6	D	424	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 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

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%)	3.01	311 (84%) 0 0	45, 56, 69, 80	0
1	D	372/420 (88%)	2.93	319 (85%) 0 0	17, 54, 66, 88	0
2	E	9/9 (100%)	1.52	1 (11%) 10 9	34, 37, 40, 41	0
2	P	9/9 (100%)	2.13	5 (55%) 0 0	49, 51, 55, 57	0
3	F	13/13 (100%)	1.54	2 (15%) 5 4	31, 38, 52, 68	0
3	T	13/13 (100%)	2.14	7 (53%) 0 0	45, 54, 68, 85	0
All	All	784/884 (88%)	2.90	645 (82%) 0 0	17, 55, 68, 88	0

All (645) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	LEU	7.6
1	D	372	LEU	7.3
1	D	356	GLY	7.3
1	B	150	ALA	7.1
1	B	149	SER	7.0
1	B	145	SER	6.7
1	D	315	VAL	6.4
1	D	119	VAL	6.1
1	B	143	LEU	5.9
1	B	372	LEU	5.9
1	D	152	THR	5.8
1	B	356	GLY	5.8
1	B	146	ASP	5.6
1	B	349	TYR	5.3
1	B	243	GLY	5.3
1	D	395	VAL	5.3
1	B	168	VAL	5.2
1	D	397	VAL	5.2
1	B	242	ILE	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	136	VAL	5.1
1	B	237	LYS	5.1
1	D	35	LEU	5.0
1	B	107	TYR	5.0
1	D	311	CYS	4.9
1	D	370	GLN	4.9
1	B	151	VAL	4.9
1	B	302	PHE	4.9
1	D	146	ASP	4.8
1	B	249	CYS	4.8
1	D	84	ALA	4.8
1	D	357	ARG	4.8
1	B	204	LEU	4.8
1	D	403	LEU	4.8
1	B	405	LEU	4.7
1	D	376	ASN	4.7
1	B	61	TYR	4.7
1	B	188	TYR	4.7
1	B	300	GLN	4.7
1	B	324	LEU	4.7
1	B	207	LYS	4.7
1	B	379	VAL	4.6
1	B	236	ILE	4.6
1	B	268	ILE	4.6
1	D	255	ILE	4.6
1	D	26	SER	4.5
1	D	369	ILE	4.5
1	D	85	LYS	4.5
1	B	333	CYS	4.5
1	B	308	PHE	4.5
1	D	278	ALA	4.5
1	D	250	LEU	4.5
1	B	271	LYS	4.4
1	D	367	HIS	4.4
1	B	295	LEU	4.4
1	D	244	TYR	4.4
1	B	110	THR	4.4
1	D	319	ASN	4.4
1	B	298	PRO	4.4
1	B	273	LEU	4.4
1	B	350	SER	4.4
1	D	351	SER	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	62	LEU	4.3
1	D	268	ILE	4.3
1	B	404	THR	4.3
1	B	193	LEU	4.3
1	D	243	GLY	4.3
1	B	244	TYR	4.3
1	D	118	PRO	4.3
1	B	296	SER	4.3
1	B	125	PHE	4.2
1	B	345	ILE	4.2
1	B	247	ALA	4.2
1	D	165	LEU	4.2
1	B	92	VAL	4.2
1	D	336	GLY	4.2
1	D	30	ILE	4.2
1	B	221	LEU	4.2
1	B	332	VAL	4.2
1	B	241	GLY	4.1
1	D	117	SER	4.1
1	D	359	SER	4.1
1	B	384	VAL	4.1
1	D	36	ASP	4.1
1	D	346	ILE	4.1
1	B	395	VAL	4.1
1	B	303	SER	4.1
1	B	240	PRO	4.1
1	D	377	TYR	4.1
1	D	237	LYS	4.1
1	D	48	PRO	4.1
1	D	142	GLN	4.0
1	B	315	VAL	4.0
1	D	401	PHE	4.0
1	B	208	LEU	4.0
1	B	163	ILE	4.0
1	D	45	ILE	4.0
1	D	406	LEU	4.0
1	B	246	THR	4.0
1	D	286	PHE	4.0
1	B	309	LYS	3.9
1	B	120	VAL	3.9
1	D	116	PHE	3.9
1	D	279	GLN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	367	HIS	3.9
1	B	226	CYS	3.9
1	B	317	ALA	3.9
1	B	225	SER	3.9
1	D	273	LEU	3.9
1	B	194	THR	3.9
1	D	120	VAL	3.9
1	D	241	GLY	3.9
1	D	247	ALA	3.9
1	D	78	LEU	3.9
1	D	169	LEU	3.9
1	D	290	ASN	3.9
1	B	212	VAL	3.8
1	B	255	ILE	3.8
1	B	346	ILE	3.8
1	B	311	CYS	3.8
1	D	77	LYS	3.8
1	D	325	LEU	3.8
1	B	144	GLN	3.8
1	B	250	LEU	3.8
1	D	405	LEU	3.8
1	B	235	HIS	3.8
1	B	277	VAL	3.8
1	D	258	VAL	3.8
3	F	837	DC	3.8
1	B	321	ILE	3.8
1	B	359	SER	3.8
1	B	400	PRO	3.8
1	D	277	VAL	3.8
1	D	293	VAL	3.8
1	D	297	GLY	3.8
1	B	239	ILE	3.7
1	B	102	TYR	3.7
1	B	206	ALA	3.7
1	B	78	LEU	3.7
1	B	328	LEU	3.7
1	B	403	LEU	3.7
1	D	390	LEU	3.7
1	D	236	ILE	3.7
1	B	39	TYR	3.7
1	B	377	TYR	3.7
1	D	269	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	203	LYS	3.7
1	D	245	LYS	3.7
1	D	248	LYS	3.7
1	B	397	VAL	3.7
1	D	76	LYS	3.7
1	B	68	TYR	3.7
1	D	68	TYR	3.7
1	D	75	VAL	3.6
1	D	81	VAL	3.6
1	B	270	GLU	3.6
1	B	178	GLN	3.6
1	D	294	ILE	3.6
1	D	181	ALA	3.6
1	D	186	ALA	3.6
1	D	317	ALA	3.6
1	B	269	LEU	3.6
1	B	37	CYS	3.6
1	B	81	VAL	3.6
1	D	415	ALA	3.6
1	B	191	LEU	3.6
1	D	143	LEU	3.6
1	D	61	TYR	3.6
1	D	185	GLU	3.6
1	D	320	LYS	3.6
1	B	109	VAL	3.6
1	B	157	VAL	3.6
1	D	220	VAL	3.6
1	B	45	ILE	3.6
1	B	253	LEU	3.6
1	B	305	GLU	3.6
1	D	259	ARG	3.6
1	D	87	LYS	3.6
1	B	153	VAL	3.5
1	B	199	VAL	3.5
1	D	86	GLU	3.5
1	B	85	LYS	3.5
1	D	398	LYS	3.5
1	B	413	LEU	3.5
1	D	62	LEU	3.5
1	D	111	GLU	3.5
1	B	171	ILE	3.5
1	B	401	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	266	PRO	3.5
1	B	390	LEU	3.5
1	B	42	VAL	3.5
1	D	153	VAL	3.5
1	D	178	GLN	3.5
1	B	281	ILE	3.5
1	D	163	ILE	3.5
1	D	275	ILE	3.5
1	D	345	ILE	3.5
1	D	89	PRO	3.5
1	D	123	LEU	3.5
1	D	324	LEU	3.5
1	B	371	LYS	3.5
1	B	299	PRO	3.4
1	D	252	ALA	3.4
1	B	254	GLY	3.4
1	B	233	LEU	3.4
1	D	148	LEU	3.4
1	B	133	THR	3.4
1	B	258	VAL	3.4
1	B	293	VAL	3.4
1	B	165	LEU	3.4
1	D	208	LEU	3.4
1	D	267	LYS	3.4
1	B	80	ASN	3.4
1	D	64	VAL	3.4
1	B	307	SER	3.4
1	B	335	ASP	3.4
1	B	357	ARG	3.4
1	D	83	ASP	3.4
1	D	150	ALA	3.4
1	D	132	LEU	3.4
1	D	191	LEU	3.4
1	D	271	LYS	3.4
1	D	308	PHE	3.4
1	D	37	CYS	3.4
1	D	175	VAL	3.4
1	D	379	VAL	3.4
1	B	126	ASP	3.4
1	D	301	SER	3.4
1	D	350	SER	3.4
1	B	245	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	310	LYS	3.4
1	D	51	LYS	3.4
1	D	100	THR	3.3
1	D	110	THR	3.3
1	D	149	SER	3.3
1	B	35	LEU	3.3
1	D	253	LEU	3.3
2	P	871	DG	3.3
1	D	314	GLU	3.3
1	D	411	CYS	3.3
1	D	46	SER	3.3
1	B	297	GLY	3.3
1	B	336	GLY	3.3
1	D	168	VAL	3.3
1	B	275	ILE	3.3
1	D	230	ILE	3.3
1	D	174	LEU	3.3
1	D	396	ASN	3.3
1	B	414	LYS	3.3
1	B	63	VAL	3.3
1	B	119	VAL	3.3
1	D	328	LEU	3.3
1	B	160	ASN	3.3
1	D	31	VAL	3.2
1	D	33	VAL	3.2
1	D	360	ARG	3.2
1	B	147	GLU	3.2
1	B	369	ILE	3.2
1	B	166	LEU	3.2
1	D	295	LEU	3.2
1	B	52	ASP	3.2
1	B	276	SER	3.2
1	B	327	SER	3.2
1	B	103	ARG	3.2
1	B	360	ARG	3.2
1	B	409	CYS	3.2
1	B	230	ILE	3.2
1	D	55	LEU	3.2
1	D	281	ILE	3.2
1	B	213	PHE	3.2
1	B	162	SER	3.2
1	D	288	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	70	ALA	3.2
1	B	158	TYR	3.2
1	B	294	ILE	3.2
1	D	99	LEU	3.2
1	D	113	LEU	3.2
1	D	349	TYR	3.2
1	D	364	ILE	3.2
1	D	386	ILE	3.2
1	B	36	ASP	3.2
1	B	402	HIS	3.2
1	D	310	LYS	3.2
3	T	838	DA	3.2
1	D	151	VAL	3.1
1	D	199	VAL	3.1
1	B	205	LEU	3.1
1	B	301	SER	3.1
1	D	407	SER	3.1
1	D	124	GLY	3.1
1	B	164	ASN	3.1
1	B	412	ASN	3.1
1	D	92	VAL	3.1
1	B	99	LEU	3.1
1	D	221	LEU	3.1
1	D	129	PHE	3.1
1	D	362	CYS	3.1
1	D	157	VAL	3.1
1	D	368	VAL	3.1
1	D	242	ILE	3.1
1	D	321	ILE	3.1
1	D	107	TYR	3.1
1	D	188	TYR	3.1
1	D	133	THR	3.1
1	D	246	THR	3.1
1	B	316	GLU	3.1
1	B	278	ALA	3.1
1	B	31	VAL	3.1
1	B	64	VAL	3.1
1	B	93	LEU	3.1
1	B	174	LEU	3.1
1	B	222	LEU	3.1
1	B	329	LEU	3.1
1	B	343	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	38	PHE	3.0
1	D	298	PRO	3.0
1	D	391	PHE	3.0
1	B	104	GLU	3.0
1	B	83	ASP	3.0
1	B	84	ALA	3.0
1	B	200	ALA	3.0
1	D	50	LEU	3.0
1	D	344	LEU	3.0
1	B	331	ARG	3.0
1	B	347	ARG	3.0
1	B	197	ALA	3.0
1	D	197	ALA	3.0
1	D	109	VAL	3.0
1	D	222	LEU	3.0
1	D	229	LEU	3.0
1	D	330	ASN	3.0
1	D	194	THR	3.0
1	D	381	THR	3.0
1	D	404	THR	3.0
1	B	223	PRO	3.0
1	D	126	ASP	3.0
1	B	60	LYS	3.0
1	D	213	PHE	3.0
1	B	252	ALA	3.0
1	B	91	LEU	3.0
1	D	63	VAL	3.0
1	B	234	ASN	3.0
1	B	304	GLU	3.0
1	D	47	ASN	3.0
1	D	138	LYS	3.0
1	B	279	GLN	2.9
1	B	46	SER	2.9
1	B	49	GLU	2.9
1	B	186	ALA	2.9
1	D	333	CYS	2.9
1	B	209	VAL	2.9
1	B	198	GLY	2.9
1	B	214	LYS	2.9
1	D	300	GLN	2.9
1	D	280	ARG	2.9
1	D	392	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	358	GLU	2.9
1	B	312	SER	2.9
1	B	180	ALA	2.9
1	B	216	ASN	2.9
1	D	160	ASN	2.9
1	B	389	LYS	2.9
1	D	205	LEU	2.9
1	D	413	LEU	2.9
1	D	332	VAL	2.9
1	D	32	HIS	2.9
1	D	402	HIS	2.9
1	D	292	PRO	2.9
1	D	158	TYR	2.9
1	B	201	SER	2.9
1	B	320	LYS	2.9
1	B	50	LEU	2.9
1	B	406	LEU	2.9
1	D	209	VAL	2.9
1	B	100	THR	2.9
1	B	122	ARG	2.9
1	D	114	GLU	2.9
1	D	145	SER	2.9
1	D	296	SER	2.9
1	D	195	GLY	2.9
1	B	55	LEU	2.8
1	D	329	LEU	2.8
1	D	130	VAL	2.8
1	B	65	THR	2.8
1	B	386	ILE	2.8
1	B	248	LYS	2.8
1	D	189	ASN	2.8
1	B	38	PHE	2.8
1	B	334	GLN	2.8
1	D	28	ARG	2.8
1	B	40	ALA	2.8
1	B	96	GLY	2.8
1	B	274	GLY	2.8
1	B	123	LEU	2.8
1	D	173	LEU	2.8
1	D	204	LEU	2.8
1	D	284	LEU	2.8
1	B	137	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	88	CYS	2.8
1	D	212	VAL	2.8
1	B	129	PHE	2.8
1	D	125	PHE	2.8
1	D	302	PHE	2.8
1	D	155	GLY	2.8
1	B	229	LEU	2.8
1	D	73	LEU	2.8
1	B	152	THR	2.8
1	B	33	VAL	2.8
1	B	408	VAL	2.8
1	D	299	PRO	2.8
1	B	210	SER	2.8
1	D	71	ARG	2.8
1	D	82	ARG	2.8
1	B	231	HIS	2.8
1	B	410	PHE	2.8
1	B	140	LEU	2.8
1	D	261	LEU	2.8
1	B	77	LYS	2.8
1	B	57	VAL	2.8
1	B	94	VAL	2.8
1	D	196	CYS	2.8
1	B	280	ARG	2.7
1	B	348	ARG	2.7
1	D	101	ARG	2.7
1	D	256	ASN	2.7
1	D	34	ASP	2.7
1	B	87	LYS	2.7
1	B	112	LEU	2.7
1	D	39	TYR	2.7
1	B	101	ARG	2.7
1	B	259	ARG	2.7
1	B	220	VAL	2.7
1	D	29	VAL	2.7
1	D	106	SER	2.7
1	B	167	ASP	2.7
1	B	306	ASP	2.7
1	D	287	GLY	2.7
1	B	264	PHE	2.7
1	B	113	LEU	2.7
1	B	392	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	348	ARG	2.7
1	B	330	ASN	2.7
1	B	368	VAL	2.7
1	D	171	ILE	2.7
1	D	154	SER	2.7
1	D	249	CYS	2.7
1	D	260	ASP	2.7
1	B	338	LYS	2.7
1	D	389	LYS	2.7
3	T	837	DC	2.7
1	B	396	ASN	2.7
1	B	75	VAL	2.7
1	B	130	VAL	2.7
1	D	291	SER	2.7
1	D	239	ILE	2.7
1	B	53	LYS	2.7
1	D	198	GLY	2.7
1	D	343	ARG	2.7
1	B	169	LEU	2.6
1	B	219	THR	2.6
1	B	48	PRO	2.6
1	D	231	HIS	2.6
1	D	131	ASP	2.6
1	B	190	GLN	2.6
1	D	121	GLU	2.6
1	B	391	PHE	2.6
3	T	844	DA	2.6
1	D	147	GLU	2.6
1	B	393	ASN	2.6
1	D	216	ASN	2.6
1	D	180	ALA	2.6
1	B	344	LEU	2.6
1	D	166	LEU	2.6
1	D	363	PRO	2.6
1	B	257	SER	2.6
1	B	286	PHE	2.6
1	B	366	SER	2.6
1	B	407	SER	2.6
1	D	264	PHE	2.6
1	B	385	ASP	2.6
1	D	54	PRO	2.6
1	D	140	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	307	SER	2.6
1	D	305	GLU	2.5
1	B	179	ILE	2.5
1	B	342	VAL	2.5
1	B	196	CYS	2.5
1	D	235	HIS	2.5
1	B	256	ASN	2.5
1	D	283	LYS	2.5
1	D	309	LYS	2.5
1	D	400	PRO	2.5
1	D	144	GLN	2.5
1	D	193	LEU	2.5
1	B	251	GLU	2.5
1	D	96	GLY	2.5
1	D	179	ILE	2.5
1	B	95	ASN	2.5
1	B	142	GLN	2.5
1	B	134	GLU	2.5
1	B	266	PRO	2.5
1	B	382	PRO	2.5
1	D	192	GLY	2.5
1	D	42	VAL	2.5
1	D	342	VAL	2.5
1	D	347	ARG	2.5
1	D	408	VAL	2.5
1	D	80	ASN	2.5
1	B	141	GLN	2.5
2	P	865	DG	2.5
1	D	382	PRO	2.5
1	B	76	LYS	2.5
1	B	116	PHE	2.5
1	D	318	LYS	2.5
3	F	838	DA	2.5
1	D	164	ASN	2.5
1	B	288	GLU	2.4
1	D	49	GLU	2.4
1	D	312	SER	2.4
1	D	233	LEU	2.4
1	D	371	LYS	2.4
1	B	370	GLN	2.4
1	B	175	VAL	2.4
1	D	57	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	257	SER	2.4
1	D	340	HIS	2.4
1	D	282	GLN	2.4
1	D	265	SER	2.4
1	D	303	SER	2.4
1	D	313	SER	2.4
1	D	366	SER	2.4
1	B	88	CYS	2.4
1	B	215	PRO	2.4
1	D	102	TYR	2.4
1	D	326	ALA	2.4
1	B	202	ASN	2.4
1	D	211	GLY	2.4
1	D	94	VAL	2.4
1	B	263	THR	2.4
1	B	292	PRO	2.4
1	D	200	ALA	2.3
1	D	270	GLU	2.3
1	B	387	LEU	2.3
1	D	72	LYS	2.3
1	B	30	ILE	2.3
3	T	848	DA	2.3
1	B	339	PRO	2.3
1	D	104	GLU	2.3
1	B	376	ASN	2.3
1	B	378	ASP	2.3
1	D	52	ASP	2.3
1	D	122	ARG	2.3
1	D	201	SER	2.3
1	B	136	VAL	2.3
1	D	115	GLU	2.3
1	D	272	GLU	2.3
1	B	161	GLN	2.3
1	B	326	ALA	2.3
1	B	59	GLN	2.3
1	B	227	GLN	2.3
1	D	219	THR	2.3
1	D	365	PRO	2.3
1	B	155	GLY	2.3
1	D	177	SER	2.2
1	D	410	PHE	2.2
1	B	29	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	341	THR	2.2
1	D	412	ASN	2.2
1	D	56	GLY	2.2
1	D	66	CYS	2.2
1	D	70	ALA	2.2
1	D	206	ALA	2.2
1	D	112	LEU	2.2
2	P	868	DG	2.2
2	E	871	DG	2.2
1	B	115	GLU	2.2
1	B	90	GLN	2.2
1	D	334	GLN	2.2
1	B	154	SER	2.2
1	B	319	ASN	2.2
1	B	341	THR	2.2
1	D	234	ASN	2.2
1	D	289	ASP	2.2
1	D	176	GLY	2.2
1	B	97	GLU	2.2
1	B	411	CYS	2.2
1	D	69	GLU	2.2
1	B	117	SER	2.2
1	D	276	SER	2.2
3	T	846	DC	2.2
3	T	849	DC	2.2
1	D	393	ASN	2.2
1	B	381	THR	2.2
1	D	134	GLU	2.2
1	D	170	HIS	2.2
1	B	73	LEU	2.2
1	D	139	ARG	2.2
1	B	267	LYS	2.2
1	D	67	ASN	2.2
1	B	34	ASP	2.2
1	B	361	GLN	2.1
1	D	274	GLY	2.1
1	B	71	ARG	2.1
1	B	132	LEU	2.1
1	B	139	ARG	2.1
1	B	325	LEU	2.1
1	D	331	ARG	2.1
1	B	51	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	53	LYS	2.1
1	B	128	ASN	2.1
1	D	385	ASP	2.1
1	B	58	GLN	2.1
1	D	172	ARG	2.1
1	B	181	ALA	2.1
1	B	265	SER	2.1
1	D	387	LEU	2.1
1	B	114	GLU	2.1
1	B	272	GLU	2.1
1	D	323	GLU	2.1
1	D	156	HIS	2.1
1	B	287	GLY	2.1
1	B	364	ILE	2.1
1	D	254	GLY	2.1
2	P	867	DG	2.1
1	B	106	SER	2.1
1	D	93	LEU	2.1
1	D	128	ASN	2.1
1	D	202	ASN	2.1
1	B	98	ASP	2.1
1	B	340	HIS	2.1
1	D	65	THR	2.1
1	B	192	GLY	2.1
1	D	74	GLY	2.1
1	D	285	SER	2.1
1	B	28	ARG	2.0
1	B	228	HIS	2.0
1	D	263	THR	2.0
2	P	873	DG	2.0
1	D	141	GLN	2.0
1	D	306	ASP	2.0
1	B	398	LYS	2.0
1	D	214	LYS	2.0
3	T	843	DC	2.0
1	D	215	PRO	2.0
1	B	124	GLY	2.0
1	B	195	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

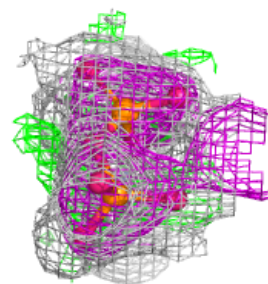
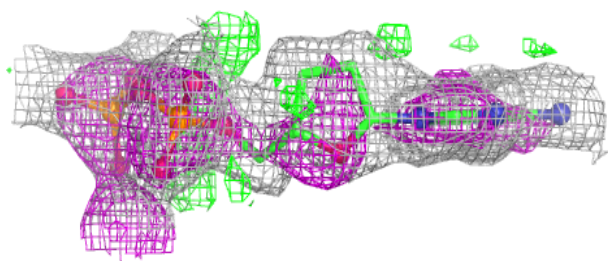
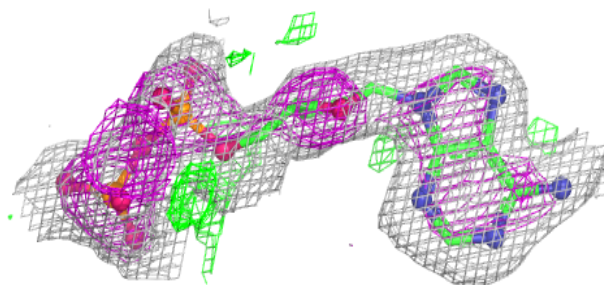
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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	0.90	0.26	43,43,43,43	0
4	CA	F	1	1/1	0.95	0.20	19,19,19,19	0
4	CA	B	423	1/1	0.96	0.23	28,28,28,28	0
4	CA	P	1	1/1	0.97	0.15	31,31,31,31	0
4	CA	D	421	1/1	0.98	0.21	14,14,14,14	0
4	CA	B	421	1/1	0.99	0.36	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

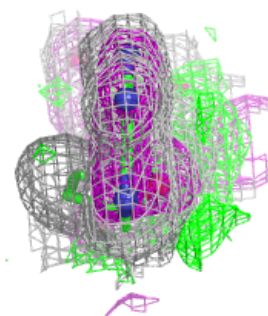
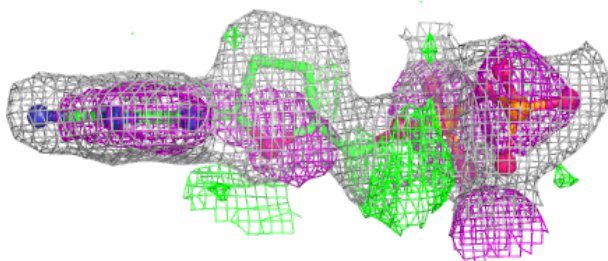
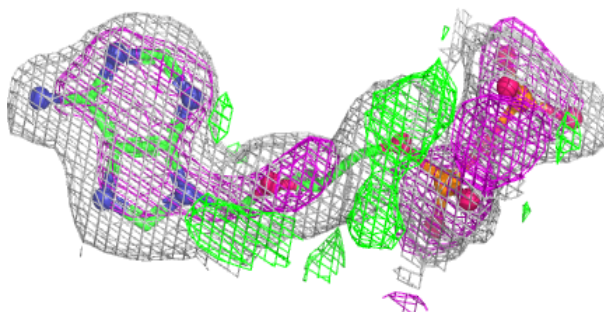
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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