



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:16 AM UTC

PDB ID : 2Y65 / pdb_00002y65
Title : Crystal structure of Drosophila melanogaster kinesin-1 motor domain dimer-tail complex
Authors : Kaan, H.Y.K.; Hackney, D.D.; Kozielski, F.
Deposited on : 2011-01-19
Resolution : 2.20 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:

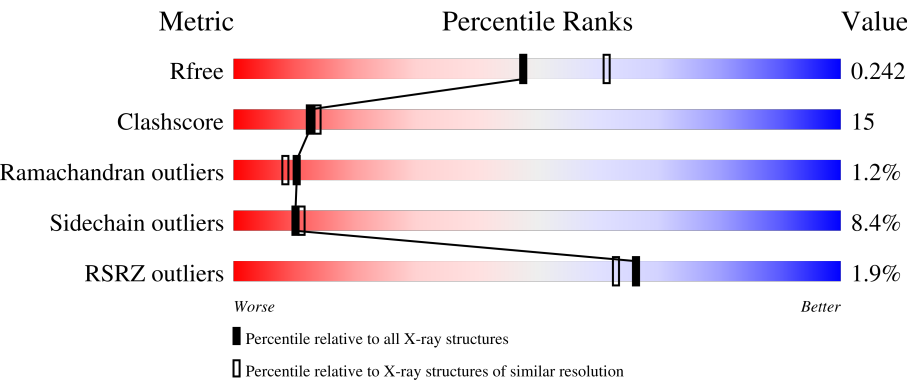
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	A	365	10% 66%19%10%
1	B	365	63%27%7%
1	C	365	2%71%19%6%
1	D	365	2%65%22%5%7%
2	W	20	10%10%35%20%35%

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Mol	Chain	Length	Quality of chain
2	X	20	
2	Y	20	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11750 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 KINESIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	10	0
			2598	1640	450	499	9			
1	B	341	Total	C	N	O	S	0	6	0
			2681	1692	460	519	10			
1	C	343	Total	C	N	O	S	0	3	0
			2694	1693	471	521	9			
1	D	338	Total	C	N	O	S	0	6	0
			2654	1672	457	516	9			

- Molecule 2 is a protein called KINESIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	13	Total	C	N	O	0	13	0
			174	108	36	30			
2	X	13	Total	C	N	O	0	0	0
			93	58	19	16			
2	Y	12	Total	C	N	O	0	0	0
			88	55	18	15			

There are 12 discrepancies between the modelled and reference sequences:

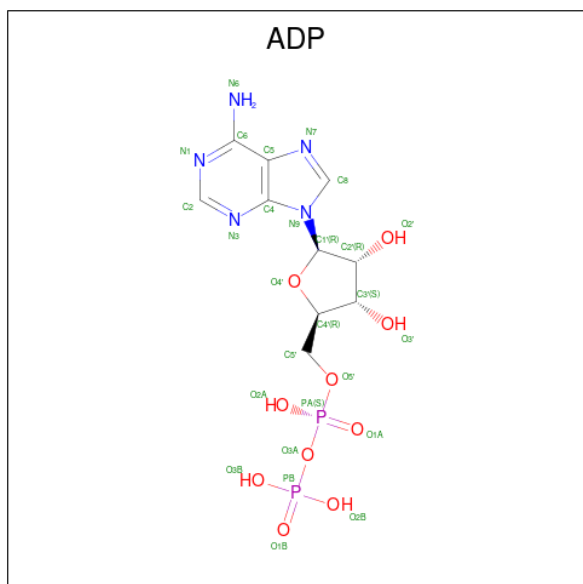
Chain	Residue	Modelled	Actual	Comment	Reference
W	935	GLY	-	expression tag	UNP P17210
W	936	SER	-	expression tag	UNP P17210
W	953	THR	-	expression tag	UNP P17210
W	954	SER	-	expression tag	UNP P17210
X	935	GLY	-	expression tag	UNP P17210
X	936	SER	-	expression tag	UNP P17210
X	953	THR	-	expression tag	UNP P17210
X	954	SER	-	expression tag	UNP P17210
Y	935	GLY	-	expression tag	UNP P17210
Y	936	SER	-	expression tag	UNP P17210

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	953	THR	-	expression tag	UNP P17210
Y	954	SER	-	expression tag	UNP P17210

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

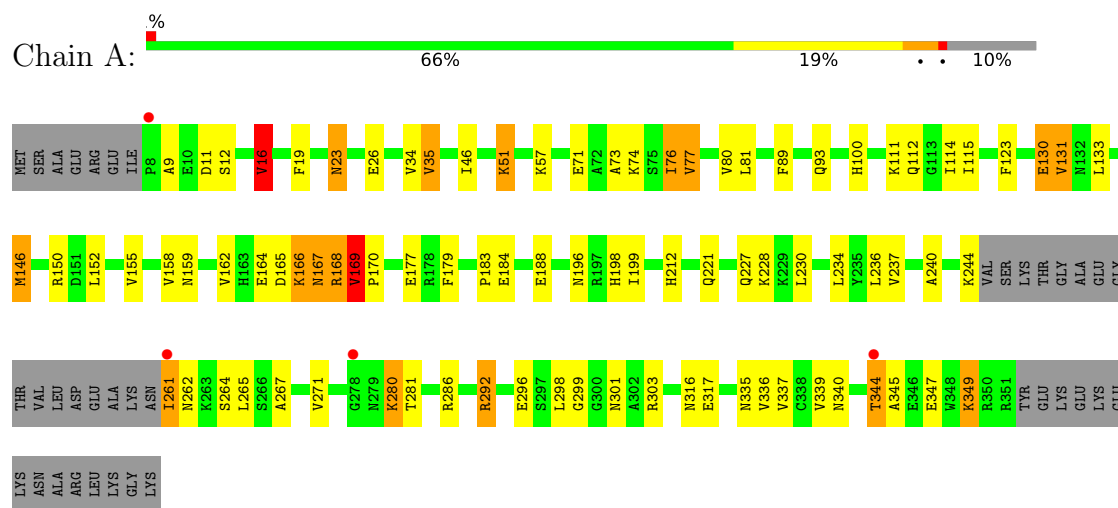
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	196	Total 196	O 196	0	0
5	B	175	Total 175	O 175	0	0
5	C	180	Total 180	O 180	0	0
5	D	96	Total 96	O 96	0	0
5	W	2	Total 2	O 2	0	0
5	X	6	Total 6	O 6	0	0
5	Y	1	Total 1	O 1	0	0

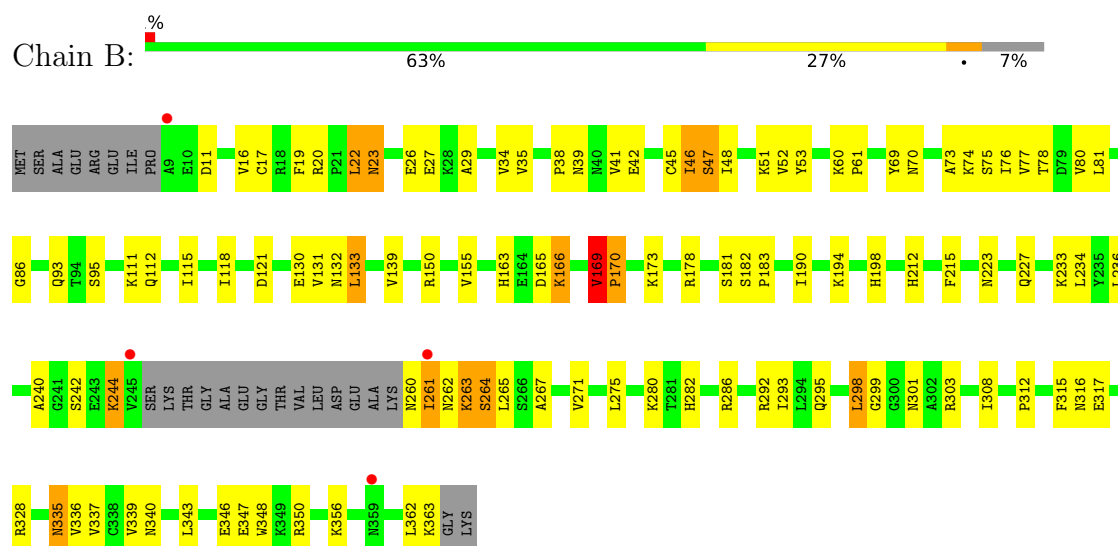
3 Residue-property plots

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: KINESIN HEAVY CHAIN

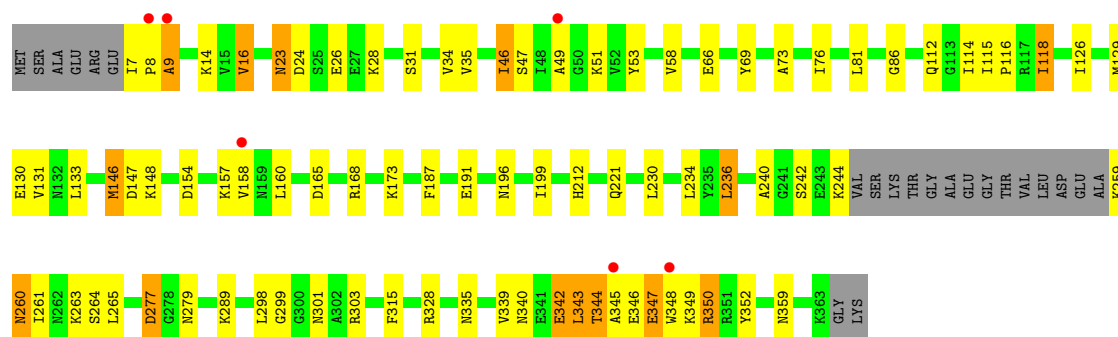


• Molecule 1: KINESIN HEAVY CHAIN

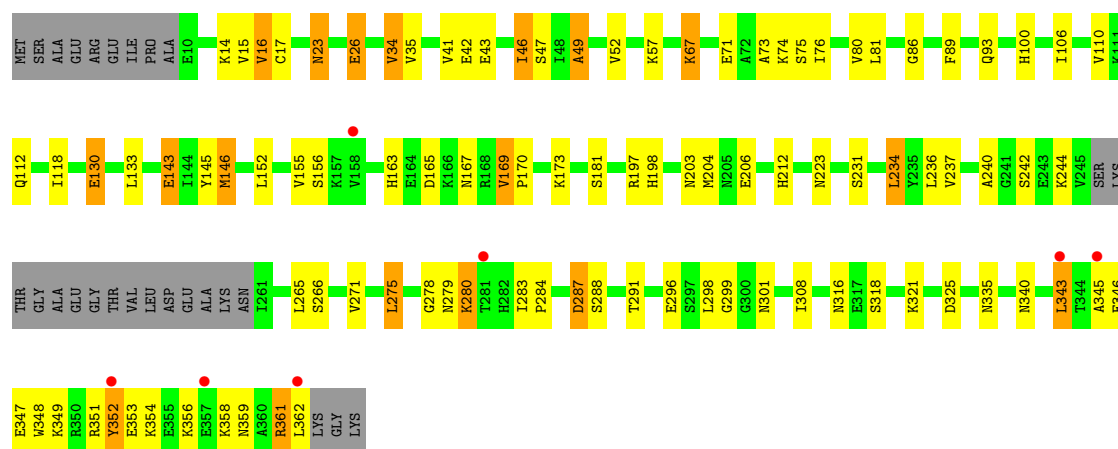


• Molecule 1: KINESIN HEAVY CHAIN

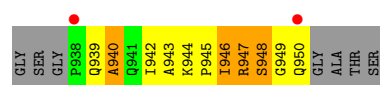




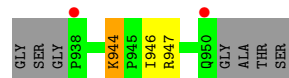
• Molecule 1: KINESIN HEAVY CHAIN



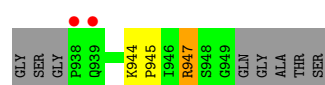
• Molecule 2: KINESIN HEAVY CHAIN



• Molecule 2: KINESIN HEAVY CHAIN



• Molecule 2: KINESIN HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.77Å 190.71Å 145.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.20) 99.8 (50.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.252 (Not available) , 0.242	Depositor DCC
R_{free} test set	4044 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11750	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8708e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.76	1/2669 (0.0%)	1.14	5/3604 (0.1%)
1	B	0.69	0/2741	1.12	7/3699 (0.2%)
1	C	0.71	1/2745 (0.0%)	1.15	7/3702 (0.2%)
1	D	0.57	0/2713	1.07	7/3661 (0.2%)
2	W	0.28	0/174	0.63	0/229
2	X	0.55	0/94	1.38	2/125 (1.6%)
2	Y	0.60	0/89	1.07	0/118
All	All	0.68	2/11225 (0.0%)	1.12	28/15138 (0.2%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	ILE	CA-CB	5.22	1.57	1.54
1	C	115	ILE	CA-C	5.05	1.57	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	944	LYS	CA-C-N	8.23	128.73	119.92
2	X	944	LYS	C-N-CA	8.23	128.73	119.92
1	A	114	ILE	N-CA-C	8.00	118.10	110.42
1	D	169	VAL	N-CA-C	7.53	115.66	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	49	ALA	N-CA-C	7.03	120.94	111.24
1	A	167	ASN	N-CA-C	6.93	121.64	111.87
1	B	169	VAL	CA-C-N	6.65	128.16	119.84
1	B	169	VAL	C-N-CA	6.65	128.16	119.84
1	C	118	ILE	CB-CA-C	-6.56	103.58	111.97
1	B	169	VAL	N-CA-C	6.41	114.88	107.89
1	C	7	ILE	CA-C-N	6.20	125.88	119.56
1	C	7	ILE	C-N-CA	6.20	125.88	119.56
1	C	173	LYS	N-CA-C	6.09	118.00	111.36
1	A	16	VAL	CB-CA-C	5.85	119.50	110.50
1	C	16	VAL	N-CA-CB	-5.75	101.38	111.39
1	D	198	HIS	N-CA-C	5.63	119.32	112.23
1	D	15	VAL	N-CA-C	5.61	115.97	108.11
1	C	34	VAL	N-CA-C	5.56	117.45	112.17
1	B	335	ASN	N-CA-C	-5.51	101.18	109.95
1	D	26	GLU	N-CA-C	-5.49	105.29	111.28
1	A	34	VAL	N-CA-C	5.46	117.45	111.77
1	A	34	VAL	CB-CA-C	-5.46	105.20	112.46
1	C	263	LYS	N-CA-C	5.43	117.95	111.71
1	B	115	ILE	CA-C-N	-5.39	113.35	119.28
1	B	115	ILE	C-N-CA	-5.39	113.35	119.28
1	D	325	ASP	N-CA-C	-5.24	105.65	111.36
1	D	43	GLU	N-CA-C	5.22	118.79	110.70
1	B	121	ASP	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	49	ALA	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	A	2598	0	2613	80	0
1	B	2681	0	2663	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2694	0	2679	77	0
1	D	2654	0	2637	84	0
2	W	174	0	188	30	0
2	X	93	0	98	4	0
2	Y	88	0	96	3	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	196	0	0	9	0
5	B	175	0	0	8	0
5	C	180	0	0	6	0
5	D	96	0	0	9	0
5	W	2	0	0	0	0
5	X	6	0	0	4	0
5	Y	1	0	0	0	0
All	All	11750	0	11022	338	0

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

All (338) 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:A:168:ARG:HG3	1:A:168:ARG:HH11	1.04	1.18
2:W:943[A]:ALA:HB3	2:W:944[A]:LYS:CG	1.79	1.12
2:W:945[B]:PRO:C	2:W:946[B]:ILE:HD13	1.74	1.11
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:HA	1.30	1.07
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:HG2	1.88	1.03
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:CG	2.39	0.99
2:W:943[A]:ALA:HB3	2:W:944[A]:LYS:HG3	1.43	0.98
2:X:947:ARG:NH1	5:X:2004:HOH:O	1.94	0.98
1:D:80:VAL:HG21	1:D:234[B]:LEU:HD21	1.46	0.98
1:D:80:VAL:HG21	1:D:234[B]:LEU:CD2	1.95	0.96
1:C:46[A]:ILE:HD13	1:C:46[A]:ILE:H	1.32	0.94
1:B:39:ASN:H	1:C:196:ASN:HD21	1.17	0.92
1:D:343:LEU:HD12	1:D:343:LEU:H	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:CA	1.99	0.92
1:A:168:ARG:HG3	1:A:168:ARG:NH1	1.77	0.92
1:C:348:TRP:CD1	1:D:345:ALA:HB1	2.06	0.91
1:D:299:GLY:H	1:D:335:ASN:HD21	1.16	0.89
2:W:943[A]:ALA:HB3	2:W:944[A]:LYS:HG2	1.48	0.88
2:W:939[B]:GLN:HG3	2:W:940[B]:ALA:H	1.39	0.86
2:W:947[B]:ARG:O	2:W:948[B]:SER:OG	1.94	0.85
1:A:167:ASN:N	1:A:168:ARG:HA	1.91	0.84
1:C:343:LEU:HD23	1:C:347:GLU:HB3	1.59	0.84
1:D:100:HIS:HD2	5:D:2094:HOH:O	1.60	0.84
1:C:348:TRP:HD1	1:D:345:ALA:HB1	1.40	0.83
1:C:212:HIS:CD2	1:C:240:ALA:H	1.98	0.81
1:A:262:ASN:HD21	1:A:264:SER:HB2	1.44	0.81
1:B:51:LYS:HE2	1:B:328:ARG:HH22	1.44	0.81
1:C:187:PHE:O	1:C:191[A]:GLU:HG2	1.80	0.80
1:C:46[A]:ILE:HD11	1:C:53:TYR:HB2	1.64	0.80
1:A:299:GLY:H	1:A:335:ASN:HD21	1.26	0.79
1:C:299:GLY:H	1:C:335:ASN:HD21	1.29	0.78
1:C:259:LYS:O	1:C:260:ASN:HB2	1.81	0.78
1:A:23:ASN:C	1:A:23:ASN:HD22	1.91	0.78
1:A:74:LYS:O	1:A:77[B]:VAL:HG12	1.83	0.78
1:D:80:VAL:CG2	1:D:234[B]:LEU:HD21	2.14	0.78
1:A:162:VAL:HG11	1:A:292:ARG:HG2	1.65	0.77
1:A:73:ALA:O	1:A:76:ILE:HG22	1.84	0.76
1:C:51:LYS:HE2	1:C:328:ARG:HH22	1.51	0.76
1:B:299:GLY:H	1:B:335:ASN:ND2	1.83	0.75
1:B:181:SER:HB3	2:X:944:LYS:HG3	1.68	0.75
1:D:181:SER:HB3	2:W:943[A]:ALA:HB2	1.67	0.75
1:D:106:ILE:O	5:D:2048:HOH:O	2.05	0.74
1:C:342:GLU:O	5:C:2172:HOH:O	2.06	0.74
1:B:23:ASN:C	1:B:23:ASN:HD22	1.95	0.74
1:C:301:ASN:HD21	1:C:340:ASN:HD21	1.35	0.73
1:D:41:VAL:HG22	1:D:42:GLU:O	1.88	0.73
1:D:57:LYS:NZ	1:D:71:GLU:HG3	2.03	0.73
1:D:343:LEU:HD12	1:D:343:LEU:N	2.03	0.72
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:CA	2.66	0.72
1:D:353:GLU:HB3	5:D:2090:HOH:O	1.87	0.72
1:A:158:VAL:O	5:A:2108:HOH:O	2.08	0.72
1:D:299:GLY:H	1:D:335:ASN:ND2	1.87	0.71
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:HG2	1.72	0.71
1:A:345:ALA:HB1	1:A:349:LYS:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASN:HD21	1:B:264:SER:HB2	1.55	0.71
1:C:31:SER:OG	1:C:315:PHE:HB2	1.91	0.71
1:C:299:GLY:H	1:C:335:ASN:ND2	1.89	0.71
1:C:344:THR:CG2	1:C:347:GLU:HB2	2.21	0.70
1:B:299:GLY:H	1:B:335:ASN:HD21	1.36	0.70
1:A:196:ASN:ND2	5:A:2136:HOH:O	2.25	0.70
2:W:939[B]:GLN:O	2:W:940[B]:ALA:HB3	1.92	0.70
1:D:112:GLN:NE2	5:D:2048:HOH:O	2.24	0.69
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:CG	2.21	0.69
1:A:165:ASP:OD1	1:A:168:ARG:O	2.11	0.68
1:B:262:ASN:HD21	1:B:264:SER:CB	2.07	0.68
1:C:343:LEU:CD2	1:C:347:GLU:HB3	2.23	0.68
1:A:280:LYS:HD2	1:A:281:THR:H	1.60	0.67
1:C:154:ASP:OD2	1:C:157:LYS:HE3	1.95	0.67
1:C:66:GLU:OE2	5:C:2049:HOH:O	2.12	0.67
2:X:947:ARG:NH2	5:X:2006:HOH:O	2.22	0.67
1:C:344:THR:HG22	1:C:347:GLU:HB2	1.75	0.67
1:C:23:ASN:ND2	1:C:26:GLU:H	1.92	0.66
1:A:57:LYS:HG2	1:A:71[B]:GLU:HG2	1.77	0.66
1:B:45[B]:CYS:SG	1:B:52:VAL:HG13	2.36	0.66
1:B:267:ALA:O	1:B:271:VAL:HG23	1.95	0.66
1:D:354:LYS:O	1:D:358:LYS:HB2	1.94	0.66
1:C:328:ARG:HD2	5:C:2166:HOH:O	1.96	0.66
1:D:100:HIS:CD2	5:D:2094:HOH:O	2.42	0.65
1:A:299:GLY:H	1:A:335:ASN:ND2	1.92	0.65
2:W:946[B]:ILE:HD13	2:W:946[B]:ILE:N	2.12	0.65
1:B:23:ASN:ND2	1:B:26:GLU:H	1.95	0.64
1:C:23:ASN:C	1:C:23:ASN:HD22	2.06	0.64
1:B:227:GLN:HG3	1:B:350:ARG:HH22	1.62	0.64
1:C:277:ASP:HB3	1:C:279:ASN:ND2	2.12	0.64
1:D:23:ASN:HD22	1:D:23:ASN:C	2.06	0.64
1:A:11:ASP:OD2	1:A:303[B]:ARG:HD2	1.97	0.63
1:A:317:GLU:OE1	5:A:2175:HOH:O	2.14	0.63
1:A:212:HIS:CD2	1:A:240:ALA:H	2.16	0.63
1:A:16:VAL:HG22	1:A:57:LYS:HB3	1.81	0.63
1:A:301:ASN:HD21	1:A:340:ASN:HD21	1.46	0.63
1:A:23:ASN:ND2	1:A:26:GLU:H	1.96	0.63
1:B:39:ASN:H	1:C:196:ASN:ND2	1.94	0.63
1:C:46[B]:ILE:HG12	1:C:47:SER:N	2.09	0.62
2:W:945[B]:PRO:O	2:W:946[B]:ILE:HD13	1.98	0.62
1:B:212:HIS:CD2	1:B:240:ALA:H	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASP:OD2	1:B:303:ARG:HG2	1.99	0.62
1:B:299:GLY:HA2	1:B:335:ASN:HD22	1.65	0.62
1:D:345:ALA:C	1:D:347:GLU:H	2.07	0.62
1:A:112:GLN:NE2	5:A:2089:HOH:O	2.33	0.61
1:B:73:ALA:O	1:B:74:LYS:C	2.42	0.61
2:W:939[B]:GLN:O	2:W:940[B]:ALA:CB	2.48	0.61
1:D:343:LEU:H	1:D:343:LEU:CD1	2.09	0.61
1:C:51:LYS:HE2	1:C:328:ARG:NH2	2.15	0.61
1:A:168:ARG:HG3	1:A:169:VAL:H	1.65	0.61
1:D:345:ALA:O	1:D:347:GLU:N	2.34	0.61
1:A:168:ARG:HH11	1:A:168:ARG:CG	1.93	0.60
1:B:45[B]:CYS:SG	1:B:52:VAL:CG1	2.89	0.60
1:D:57:LYS:HZ1	1:D:71:GLU:HG3	1.64	0.60
1:C:51:LYS:CE	1:C:328:ARG:HH22	2.13	0.60
1:B:73:ALA:O	1:B:76:ILE:HG22	2.02	0.59
1:A:93:GLN:HE22	1:A:316:ASN:HB3	1.66	0.59
1:C:35:VAL:HG13	1:C:46[B]:ILE:HG13	1.85	0.59
1:D:23:ASN:ND2	1:D:26:GLU:H	2.00	0.59
1:C:147:ASP:O	1:C:289:LYS:HE3	2.03	0.59
1:C:259:LYS:O	1:C:260:ASN:CB	2.50	0.59
1:A:179:PHE:CE1	2:Y:945:PRO:HG2	2.38	0.58
1:A:339:VAL:HG12	5:A:2184:HOH:O	2.03	0.58
1:C:244:LYS:HA	1:C:260:ASN:HA	1.85	0.58
1:A:80[B]:VAL:HG21	1:A:234[B]:LEU:HG	1.86	0.58
1:B:299:GLY:N	1:B:335:ASN:ND2	2.50	0.58
1:D:80:VAL:CG2	1:D:234[B]:LEU:CD2	2.78	0.58
1:C:165:ASP:HB2	5:C:2103:HOH:O	2.04	0.58
1:D:163:HIS:O	1:D:170:PRO:HA	2.02	0.58
1:D:143:GLU:HG2	1:D:152:LEU:HD21	1.86	0.57
1:C:348:TRP:HD1	1:D:345:ALA:CB	2.15	0.57
1:A:234[A]:LEU:CD2	1:A:236:LEU:HD21	2.34	0.57
1:D:242:SER:HA	1:D:265:LEU:HD13	1.87	0.57
1:B:346[A]:GLU:CD	1:B:346[A]:GLU:H	2.10	0.57
1:D:16:VAL:HG22	1:D:57:LYS:HB2	1.86	0.57
1:A:234[A]:LEU:HD21	1:A:236:LEU:HD21	1.86	0.57
1:C:46[A]:ILE:HG23	1:C:58:VAL:HG11	1.87	0.56
1:C:301:ASN:ND2	1:C:340:ASN:HD21	2.02	0.56
1:B:29:ALA:O	1:B:315[B]:PHE:HE2	1.87	0.56
1:C:277:ASP:HB3	1:C:279:ASN:HD21	1.69	0.56
1:D:106:ILE:HG12	5:D:2049:HOH:O	2.04	0.56
1:D:181:SER:HB3	2:W:943[A]:ALA:CB	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASN:HD22	1:B:26:GLU:H	1.51	0.56
1:D:80:VAL:HG21	1:D:234[B]:LEU:CG	2.35	0.56
1:A:100:HIS:HD2	5:A:2188:HOH:O	1.89	0.56
1:D:361:ARG:O	1:D:362:LEU:C	2.49	0.56
1:D:279:ASN:O	1:D:280:LYS:HB2	2.05	0.56
2:W:939[B]:GLN:HG3	2:W:940[B]:ALA:N	2.17	0.56
1:A:198:HIS:HD2	1:B:111:LYS:NZ	2.05	0.55
1:D:146:MET:HA	1:D:146:MET:HE2	1.88	0.55
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:CB	2.36	0.55
1:A:158:VAL:CG1	5:A:2109:HOH:O	2.55	0.55
2:W:942[A]:ILE:HG22	2:W:943[A]:ALA:N	2.21	0.55
1:C:114:ILE:O	1:C:118:ILE:HG12	2.06	0.55
1:B:244:LYS:HA	1:B:260:ASN:O	2.07	0.55
1:D:133:LEU:HD23	1:D:223:ASN:HA	1.90	0.54
1:D:212:HIS:CD2	1:D:240:ALA:H	2.24	0.54
1:C:242:SER:HA	1:C:265:LEU:HD13	1.88	0.54
1:B:69:TYR:HE1	1:B:118:ILE:HG13	1.71	0.54
1:D:57:LYS:HZ2	1:D:71:GLU:HG3	1.72	0.54
1:A:23:ASN:C	1:A:23:ASN:ND2	2.65	0.54
1:C:342:GLU:HG2	5:C:2135:HOH:O	2.07	0.54
1:C:212:HIS:HE1	1:C:264:SER:OG	1.91	0.54
1:B:343:LEU:HD13	1:B:347:GLU:HG3	1.90	0.54
1:C:69:TYR:HE1	1:C:118:ILE:HD13	1.72	0.54
1:A:345:ALA:O	1:A:349:LYS:N	2.27	0.53
1:D:93:GLN:HE22	1:D:316:ASN:HB3	1.72	0.53
1:D:296[A]:GLU:HG3	1:D:301:ASN:H	1.73	0.53
1:D:343:LEU:CD2	1:D:351:ARG:HH12	2.21	0.53
1:A:158:VAL:HG12	1:A:159:ASN:H	1.73	0.53
1:C:349:LYS:HB2	1:D:348:TRP:CE2	2.42	0.53
1:B:233:LYS:HE3	5:B:2132:HOH:O	2.09	0.53
2:W:947[B]:ARG:C	2:W:948[B]:SER:OG	2.52	0.52
1:B:39:ASN:N	1:C:196:ASN:HD21	1.96	0.52
1:D:89:PHE:HB3	1:D:237:VAL:HB	1.91	0.52
1:D:284:PRO:HB2	1:D:287:ASP:OD2	2.10	0.52
1:B:182:SER:HB2	1:B:183:PRO:HD2	1.92	0.52
1:B:299:GLY:HA2	1:B:335:ASN:ND2	2.25	0.52
1:A:168:ARG:C	1:A:169:VAL:HG13	2.35	0.51
1:A:184:GLU:O	1:A:188:GLU:HG3	2.09	0.51
1:B:170:PRO:HG2	1:B:295:GLN:HG2	1.92	0.51
1:A:280:LYS:HD2	1:A:281:THR:N	2.26	0.51
1:C:157:LYS:HB3	1:C:160:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:HD12	1:B:223:ASN:HA	1.92	0.51
1:D:155:VAL:HG22	1:D:155:VAL:O	2.11	0.51
1:C:212:HIS:HD2	1:C:240:ALA:H	1.52	0.51
1:D:352:TYR:CE2	1:D:353:GLU:HG3	2.45	0.50
1:B:34:VAL:O	1:B:34:VAL:HG22	2.10	0.50
1:D:75:SER:OG	5:D:2039:HOH:O	2.19	0.50
1:D:100:HIS:HE1	5:D:2003:HOH:O	1.93	0.50
1:D:73:ALA:O	1:D:74:LYS:C	2.53	0.50
1:B:23:ASN:C	1:B:23:ASN:ND2	2.67	0.50
1:B:301:ASN:ND2	1:B:340:ASN:HD21	2.10	0.50
1:C:46[A]:ILE:CD1	1:C:53:TYR:HB2	2.40	0.50
1:A:168:ARG:HH11	1:A:169:VAL:H	1.58	0.50
1:B:163:HIS:CD2	1:B:173:LYS:HD2	2.47	0.50
2:X:947:ARG:NE	5:X:2003:HOH:O	2.43	0.50
1:C:73:ALA:O	1:C:76:ILE:HG22	2.11	0.49
2:W:942[A]:ILE:HG22	2:W:943[A]:ALA:HB2	1.94	0.49
1:A:130:GLU:O	1:A:131:VAL:C	2.55	0.49
1:B:48:ILE:HD11	1:B:317:GLU:HG3	1.95	0.49
1:A:267:ALA:O	1:A:271:VAL:HG23	2.13	0.49
1:D:359:ASN:HA	1:D:362:LEU:HD12	1.93	0.49
1:C:46[A]:ILE:HD13	1:C:53:TYR:O	2.12	0.49
1:C:346:GLU:O	1:C:349:LYS:HB3	2.13	0.49
2:W:949[B]:GLY:HA3	2:W:950[B]:GLN:HB2	1.94	0.49
1:A:23:ASN:HD22	1:A:26:GLU:H	1.61	0.49
1:A:19:PHE:CE2	1:A:35:VAL:HG21	2.48	0.49
1:A:262:ASN:HD22	1:A:265:LEU:H	1.60	0.48
1:A:158:VAL:HG12	1:A:159:ASN:N	2.28	0.48
1:B:22:LEU:HD23	1:B:27:GLU:HG3	1.95	0.48
1:B:299:GLY:CA	1:B:335:ASN:ND2	2.76	0.48
1:C:46[A]:ILE:CG2	1:C:58:VAL:HG11	2.43	0.48
1:A:9:ALA:HB1	1:A:337:VAL:O	2.13	0.48
1:C:126:ILE:O	1:C:129:MET:HB2	2.14	0.48
1:A:158:VAL:HG13	5:A:2109:HOH:O	2.12	0.48
1:B:262:ASN:HB2	5:B:2049:HOH:O	2.12	0.48
1:A:111:LYS:NZ	1:B:198:HIS:HD2	2.10	0.48
1:B:242:SER:HA	1:B:265:LEU:HD13	1.95	0.48
1:D:203:ASN:HD22	1:D:206:GLU:HB2	1.78	0.48
1:A:301:ASN:ND2	1:A:340:ASN:HD21	2.12	0.48
1:B:165:ASP:OD2	1:B:169:VAL:HG23	2.13	0.48
1:C:24:ASP:OD1	1:C:28:LYS:HE3	2.14	0.47
1:D:278:GLY:HA2	5:D:2079:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLN:HB3	1:A:344:THR:HG21	1.96	0.47
1:B:301:ASN:HD21	1:B:340:ASN:HD21	1.62	0.47
1:D:271:VAL:O	1:D:275:LEU:HD12	2.15	0.47
1:A:168:ARG:HG3	1:A:169:VAL:N	2.28	0.47
1:B:150:ARG:HD2	1:B:155:VAL:HB	1.96	0.47
1:D:17:CYS:HA	1:D:308:ILE:HG13	1.97	0.47
1:D:197:ARG:O	1:D:204:MET:HE1	2.14	0.47
1:D:34:VAL:O	1:D:34:VAL:HG13	2.15	0.47
1:D:352:TYR:CD1	1:D:356:LYS:HD3	2.49	0.47
2:W:946[B]:ILE:N	2:W:946[B]:ILE:CD1	2.76	0.47
1:A:179:PHE:CD1	2:Y:945:PRO:HD2	2.50	0.47
1:C:344:THR:O	1:C:345:ALA:C	2.57	0.47
1:D:296[A]:GLU:HG3	1:D:301:ASN:N	2.30	0.46
1:B:275:LEU:HD11	1:B:298:LEU:O	2.13	0.46
1:B:299:GLY:N	1:B:335:ASN:HD21	2.09	0.46
1:C:344:THR:HG23	1:C:347:GLU:HB2	1.97	0.46
1:D:67:LYS:HA	1:D:67:LYS:CE	2.45	0.46
1:D:345:ALA:C	1:D:347:GLU:N	2.73	0.46
1:C:146:MET:HE3	1:C:146:MET:HA	1.97	0.46
1:A:262:ASN:ND2	1:A:264:SER:HB2	2.22	0.46
1:B:170:PRO:HG3	1:B:295:GLN:OE1	2.16	0.46
1:D:67:LYS:HA	1:D:67:LYS:HE3	1.97	0.46
1:A:286:ARG:HB2	5:A:2166:HOH:O	2.15	0.46
1:A:166:LYS:C	1:A:168:ARG:HA	2.41	0.46
1:A:168:ARG:NH1	1:A:168:ARG:CG	2.59	0.46
1:A:177:GLU:H	2:Y:947:ARG:NH2	2.14	0.46
1:A:51:LYS:HB3	1:A:51:LYS:HE3	1.63	0.45
1:C:112:GLN:HB2	1:C:116:PRO:HG2	1.98	0.45
1:D:275:LEU:HG	1:D:283:ILE:HD12	1.97	0.45
1:C:359:ASN:HB2	1:D:359:ASN:OD1	2.16	0.45
1:B:261:ILE:O	1:B:262:ASN:C	2.58	0.45
2:W:942[A]:ILE:CG2	2:W:943[A]:ALA:N	2.79	0.45
1:B:47:SER:HB2	1:B:52:VAL:HG22	1.97	0.45
1:B:78:THR:HG23	5:B:2038:HOH:O	2.16	0.45
1:B:198:HIS:HE1	5:B:2040:HOH:O	1.99	0.45
1:A:168:ARG:HH11	1:A:169:VAL:N	2.15	0.45
1:B:70:ASN:ND2	5:B:2035:HOH:O	2.24	0.45
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:HA	2.10	0.45
1:A:221:GLN:HG2	1:A:230:LEU:HB2	2.00	0.44
1:B:112:GLN:NE2	5:B:2066:HOH:O	2.50	0.44
1:A:89:PHE:HB3	1:A:237:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.77	0.44
1:C:349:LYS:HG2	1:C:350:ARG:HD3	1.99	0.44
1:D:165:ASP:CB	1:D:167:ASN:H	2.30	0.44
1:D:23:ASN:HD22	1:D:26:GLU:H	1.63	0.44
1:C:234:LEU:HD11	1:C:236:LEU:HD11	1.99	0.44
1:B:51:LYS:CE	1:B:328:ARG:HH22	2.23	0.44
1:B:139[A]:VAL:HG21	1:B:215:PHE:CZ	2.53	0.44
1:C:221:GLN:HG2	1:C:230:LEU:HB2	2.00	0.44
1:B:280:LYS:HE3	1:B:282:HIS:O	2.18	0.44
1:B:86:GLY:O	1:B:234:LEU:HA	2.18	0.43
1:D:288:SER:OG	1:D:291:THR:OG1	2.33	0.43
1:C:8:PRO:O	1:C:9:ALA:CB	2.66	0.43
1:D:145:TYR:O	1:D:146:MET:C	2.60	0.43
1:B:362:LEU:O	1:B:363:LYS:C	2.61	0.43
1:C:345:ALA:HA	1:D:345:ALA:HB2	2.01	0.43
1:D:80:VAL:HG21	1:D:234[B]:LEU:HG	2.00	0.43
1:A:123:PHE:CG	1:A:183:PRO:HD3	2.53	0.43
1:D:165:ASP:HB2	1:D:167:ASN:H	1.83	0.43
1:D:301:ASN:HD21	1:D:340:ASN:HD21	1.65	0.43
1:A:244:LYS:HA	1:A:261:ILE:HG13	2.00	0.43
1:D:46:ILE:C	1:D:46:ILE:HD13	2.43	0.43
1:C:346:GLU:HB2	1:C:350:ARG:NH1	2.33	0.43
1:A:73:ALA:O	1:A:76:ILE:CG2	2.64	0.43
1:B:131:VAL:HG12	1:B:132:ASN:N	2.34	0.43
1:B:356:LYS:HB3	1:B:356:LYS:HE2	1.69	0.43
1:C:23:ASN:HD21	1:C:26:GLU:HG3	1.84	0.43
1:B:262:ASN:ND2	1:B:264:SER:CB	2.80	0.43
1:B:93:GLN:HE22	1:B:316:ASN:HB3	1.84	0.42
1:A:261:ILE:O	1:A:262:ASN:C	2.62	0.42
1:B:45[B]:CYS:HA	1:B:53:TYR:O	2.20	0.42
1:C:279:ASN:ND2	1:C:279:ASN:H	2.17	0.42
1:B:182:SER:HB2	1:B:183:PRO:CD	2.49	0.42
1:B:262:ASN:O	1:B:263:LYS:C	2.62	0.42
1:C:230:LEU:HD22	1:C:339:VAL:HG22	2.02	0.42
1:D:23:ASN:ND2	1:D:26:GLU:HG3	2.34	0.42
2:W:945[B]:PRO:C	2:W:946[B]:ILE:CD1	2.67	0.42
1:C:86:GLY:O	1:C:234:LEU:HA	2.20	0.42
1:B:19:PHE:CE1	1:B:46:ILE:HG13	2.54	0.42
1:C:349:LYS:HD3	1:D:348:TRP:CZ2	2.55	0.42
1:B:165:ASP:HB2	1:B:166:LYS:HE3	2.02	0.42
1:B:20:ARG:O	1:B:312:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HB2	1:B:348:TRP:NE1	2.35	0.42
1:A:168:ARG:NH1	1:A:169:VAL:H	2.18	0.42
1:A:228:LYS:HB2	1:A:228:LYS:HE2	1.81	0.42
1:B:17:CYS:HA	1:B:308:ILE:HG13	2.02	0.42
1:B:316:ASN:ND2	5:B:2154:HOH:O	2.47	0.42
1:D:352:TYR:CE1	1:D:356:LYS:HD3	2.55	0.42
1:A:80[B]:VAL:HB	1:A:234[B]:LEU:HD21	2.02	0.41
1:A:146:MET:HE2	1:A:146:MET:HA	2.02	0.41
1:B:39:ASN:HD21	1:B:42:GLU:HG3	1.85	0.41
1:B:38:PRO:HB3	1:C:199:ILE:HD11	2.01	0.41
1:A:169:VAL:O	1:A:169:VAL:CG2	2.68	0.41
1:A:164:GLU:HA	1:A:170:PRO:HA	2.02	0.41
1:A:198:HIS:HD2	1:B:111:LYS:HZ2	1.67	0.41
1:B:130:GLU:N	5:B:2074:HOH:O	2.12	0.41
1:B:178:ARG:NE	5:X:2006:HOH:O	2.47	0.41
1:D:169:VAL:HA	1:D:170:PRO:HD3	1.96	0.41
1:D:203:ASN:ND2	1:D:206:GLU:HB2	2.35	0.41
1:A:296:GLU:HG3	1:A:301:ASN:N	2.35	0.41
1:D:86:GLY:O	1:D:234[A]:LEU:HA	2.21	0.41
1:A:296:GLU:HG3	1:A:301:ASN:H	1.85	0.41
1:C:14:LYS:CE	5:C:2003:HOH:O	2.68	0.41
1:D:130:GLU:HA	2:W:949[B]:GLY:O	2.20	0.41
1:A:150:ARG:HH11	1:A:150:ARG:HD2	1.68	0.41
1:C:212:HIS:CE1	1:C:264:SER:OG	2.71	0.41
1:C:343:LEU:O	1:C:344:THR:HB	2.21	0.41
1:B:190:ILE:O	1:B:194:LYS:HG3	2.21	0.40
1:C:230:LEU:HD22	1:C:339:VAL:CG2	2.51	0.40
1:B:60:LYS:HB3	1:B:61:PRO:HD2	2.03	0.40
1:D:23:ASN:HD21	1:D:26:GLU:HG3	1.86	0.40
1:A:155[A]:VAL:HG11	1:A:199:ILE:CD1	2.51	0.40
1:D:299:GLY:N	1:D:335:ASN:ND2	2.62	0.40
1:A:234[A]:LEU:HD22	1:A:236:LEU:HG	2.04	0.40
1:D:73:ALA:O	1:D:76:ILE:HG22	2.22	0.40
1:B:262:ASN:HD22	1:B:265:LEU:HG	1.87	0.40
1:B:286:ARG:HG2	1:B:292:ARG:HD2	2.04	0.40
1:C:348:TRP:HB2	1:D:348:TRP:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/365 (92%)	320 (96%)	11 (3%)	3 (1%)	14	14
1	B	343/365 (94%)	327 (95%)	15 (4%)	1 (0%)	36	42
1	C	342/365 (94%)	329 (96%)	7 (2%)	6 (2%)	6	4
1	D	340/365 (93%)	316 (93%)	20 (6%)	4 (1%)	10	8
2	W	21/20 (105%)	11 (52%)	6 (29%)	4 (19%)	0	0
2	X	11/20 (55%)	9 (82%)	2 (18%)	0	100	100
2	Y	10/20 (50%)	9 (90%)	1 (10%)	0	100	100
All	All	1401/1520 (92%)	1321 (94%)	62 (4%)	18 (1%)	10	8

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	9	ALA
1	C	260	ASN
1	C	344	THR
1	D	280	LYS
1	D	346	GLU
1	A	344	THR
1	A	169	VAL
1	C	49	ALA
1	C	130	GLU
2	W	948[A]	SER
2	W	948[B]	SER
1	A	131	VAL
1	D	244	LYS
2	W	940[A]	ALA
2	W	940[B]	ALA
1	B	75	SER
1	D	361	ARG
1	C	131	VAL

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	A	293/321 (91%)	270 (92%)	23 (8%)	11	13
1	B	297/321 (92%)	271 (91%)	26 (9%)	9	10
1	C	298/321 (93%)	278 (93%)	20 (7%)	15	17
1	D	295/321 (92%)	265 (90%)	30 (10%)	7	7
2	W	18/13 (138%)	14 (78%)	4 (22%)	1	1
2	X	9/13 (69%)	8 (89%)	1 (11%)	6	6
2	Y	9/13 (69%)	7 (78%)	2 (22%)	1	1
All	All	1219/1323 (92%)	1113 (91%)	106 (9%)	10	10

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	16	VAL
1	A	23	ASN
1	A	35	VAL
1	A	46	ILE
1	A	51	LYS
1	A	76	ILE
1	A	77[A]	VAL
1	A	77[B]	VAL
1	A	81	LEU
1	A	130	GLU
1	A	133	LEU
1	A	146	MET
1	A	166	LYS
1	A	168	ARG
1	A	169	VAL
1	A	261	ILE
1	A	280	LYS
1	A	292	ARG
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	336	VAL
1	A	347	GLU
1	A	349	LYS
1	B	16	VAL
1	B	22	LEU
1	B	23	ASN
1	B	35	VAL
1	B	41	VAL
1	B	46	ILE
1	B	47	SER
1	B	77	VAL
1	B	80	VAL
1	B	81	LEU
1	B	95	SER
1	B	133	LEU
1	B	166	LYS
1	B	169	VAL
1	B	170	PRO
1	B	236	LEU
1	B	244	LYS
1	B	261	ILE
1	B	263	LYS
1	B	264	SER
1	B	293[A]	ILE
1	B	293[B]	ILE
1	B	298	LEU
1	B	336	VAL
1	B	337	VAL
1	B	339	VAL
1	C	16	VAL
1	C	23	ASN
1	C	46[A]	ILE
1	C	46[B]	ILE
1	C	81	LEU
1	C	133	LEU
1	C	146	MET
1	C	148	LYS
1	C	158	VAL
1	C	168	ARG
1	C	236	LEU
1	C	261	ILE
1	C	277	ASP

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Mol	Chain	Res	Type
1	C	298	LEU
1	C	303	ARG
1	C	342	GLU
1	C	343	LEU
1	C	347	GLU
1	C	350	ARG
1	C	352	TYR
1	D	14	LYS
1	D	16	VAL
1	D	23	ASN
1	D	34	VAL
1	D	35	VAL
1	D	46	ILE
1	D	47	SER
1	D	52	VAL
1	D	67	LYS
1	D	81	LEU
1	D	110	VAL
1	D	118	ILE
1	D	130	GLU
1	D	143	GLU
1	D	146	MET
1	D	156	SER
1	D	173	LYS
1	D	231	SER
1	D	234[A]	LEU
1	D	234[B]	LEU
1	D	236	LEU
1	D	266	SER
1	D	275	LEU
1	D	287	ASP
1	D	298	LEU
1	D	318	SER
1	D	321	LYS
1	D	343	LEU
1	D	349	LYS
1	D	352	TYR
2	W	946[A]	ILE
2	W	946[B]	ILE
2	W	947[A]	ARG
2	W	947[B]	ARG
2	X	946	ILE

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Mol	Chain	Res	Type
2	Y	944	LYS
2	Y	947	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	44	ASN
1	A	70	ASN
1	A	93	GLN
1	A	100	HIS
1	A	132	ASN
1	A	159	ASN
1	A	163	HIS
1	A	196	ASN
1	A	198	HIS
1	A	205	ASN
1	A	212	HIS
1	A	262	ASN
1	A	316	ASN
1	A	335	ASN
1	A	340	ASN
1	B	23	ASN
1	B	40	ASN
1	B	70	ASN
1	B	93	GLN
1	B	112	GLN
1	B	125	HIS
1	B	167	ASN
1	B	198	HIS
1	B	205	ASN
1	B	212	HIS
1	B	227	GLN
1	B	262	ASN
1	B	282	HIS
1	B	316	ASN
1	B	335	ASN
1	B	340	ASN
1	C	23	ASN
1	C	70	ASN
1	C	93	GLN
1	C	112	GLN

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Mol	Chain	Res	Type
1	C	125	HIS
1	C	196	ASN
1	C	198	HIS
1	C	212	HIS
1	C	221	GLN
1	C	227	GLN
1	C	279	ASN
1	C	295	GLN
1	C	316	ASN
1	C	335	ASN
1	C	340	ASN
1	D	23	ASN
1	D	70	ASN
1	D	93	GLN
1	D	100	HIS
1	D	112	GLN
1	D	132	ASN
1	D	163	HIS
1	D	196	ASN
1	D	205	ASN
1	D	207	HIS
1	D	212	HIS
1	D	295	GLN
1	D	316	ASN
1	D	335	ASN
1	D	340	ASN
2	X	939	GLN
2	Y	941	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	D	603	4	28,29,29	1.79	5 (17%)	43,45,45	1.86	13 (30%)
3	ADP	C	603	4	28,29,29	1.70	4 (14%)	43,45,45	2.11	13 (30%)
3	ADP	B	603	4	28,29,29	1.38	4 (14%)	43,45,45	2.32	12 (27%)
3	ADP	A	603	4	28,29,29	1.46	4 (14%)	43,45,45	1.89	9 (20%)

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
3	ADP	D	603	4	-	3/16/32/32	0/3/3/3
3	ADP	C	603	4	-	2/16/32/32	0/3/3/3
3	ADP	B	603	4	-	2/16/32/32	0/3/3/3
3	ADP	A	603	4	-	3/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	ADP	C5-C4	6.08	1.49	1.39
3	D	603	ADP	C5-C4	5.49	1.48	1.39
3	D	603	ADP	PA-O3A	4.66	1.64	1.59
3	B	603	ADP	C5-C4	4.60	1.47	1.39
3	A	603	ADP	C5-C4	4.45	1.47	1.39
3	C	603	ADP	PA-O3A	3.72	1.63	1.59
3	D	603	ADP	C5-N7	-3.21	1.33	1.39
3	B	603	ADP	C5-C6	2.94	1.49	1.41
3	A	603	ADP	C5-C6	2.80	1.48	1.41
3	C	603	ADP	C5-C6	2.74	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	ADP	PA-O3A	2.74	1.62	1.59
3	D	603	ADP	C5-C6	2.63	1.48	1.41
3	C	603	ADP	C8-N7	2.43	1.36	1.31
3	D	603	ADP	C8-N7	2.24	1.36	1.31
3	A	603	ADP	C8-N7	2.24	1.36	1.31
3	B	603	ADP	C8-N7	2.17	1.35	1.31
3	B	603	ADP	C5-N7	-2.01	1.35	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	ADP	C5-C4-N3	-7.59	116.27	126.72
3	C	603	ADP	C5-C4-N3	-6.24	118.12	126.72
3	A	603	ADP	C5-C4-N3	-5.91	118.58	126.72
3	B	603	ADP	N3-C4-N9	5.54	136.59	127.17
3	A	603	ADP	N3-C4-N9	4.94	135.56	127.17
3	B	603	ADP	C4-C5-N7	-4.93	104.95	110.58
3	D	603	ADP	C5-C4-N3	-4.90	119.97	126.72
3	C	603	ADP	N3-C4-N9	4.88	135.47	127.17
3	B	603	ADP	C2-N3-C4	4.72	123.36	111.83
3	C	603	ADP	C4-C5-N7	-4.36	105.59	110.58
3	D	603	ADP	C4-C5-N7	-4.06	105.94	110.58
3	D	603	ADP	N3-C4-N9	3.98	133.94	127.17
3	B	603	ADP	N3-C2-N1	-3.76	122.89	128.58
3	C	603	ADP	C2-N3-C4	3.60	120.63	111.83
3	B	603	ADP	C5-N7-C8	3.57	109.06	103.45
3	A	603	ADP	C4-C5-N7	-3.42	106.68	110.58
3	C	603	ADP	N3-C2-N1	-3.34	123.52	128.58
3	C	603	ADP	C5-N7-C8	3.34	108.69	103.45
3	A	603	ADP	C2-N3-C4	3.25	119.76	111.83
3	D	603	ADP	C2'-C1'-N9	-3.20	105.36	113.30
3	D	603	ADP	C5-N7-C8	3.14	108.38	103.45
3	B	603	ADP	O2A-PA-O3A	3.11	115.67	107.27
3	A	603	ADP	C4-N9-C8	3.08	108.97	105.74
3	C	603	ADP	C4-N9-C8	3.04	108.93	105.74
3	D	603	ADP	C2-N1-C6	2.97	123.62	118.73
3	C	603	ADP	C2-N1-C6	2.85	123.41	118.73
3	C	603	ADP	O3B-PB-O2B	2.84	118.44	107.80
3	D	603	ADP	C4-N9-C8	2.75	108.62	105.74
3	A	603	ADP	C5-N7-C8	2.71	107.71	103.45
3	A	603	ADP	N3-C2-N1	-2.70	124.50	128.58
3	B	603	ADP	C6-C5-N7	2.63	137.16	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	603	ADP	C2-N3-C4	2.60	118.17	111.83
3	D	603	ADP	N3-C2-N1	-2.58	124.68	128.58
3	B	603	ADP	N9-C8-N7	-2.48	110.42	113.94
3	B	603	ADP	O3B-PB-O2B	2.48	117.09	107.80
3	C	603	ADP	N9-C8-N7	-2.47	110.43	113.94
3	B	603	ADP	C4-N9-C8	2.37	108.23	105.74
3	A	603	ADP	N9-C8-N7	-2.30	110.67	113.94
3	A	603	ADP	O3'-C3'-C2'	-2.25	104.60	111.82
3	C	603	ADP	C4'-O4'-C1'	2.24	114.42	109.47
3	C	603	ADP	O3A-PA-O1A	-2.21	104.04	110.70
3	B	603	ADP	O4'-C1'-N9	-2.21	103.85	108.09
3	D	603	ADP	O2A-PA-O3A	2.19	113.20	107.27
3	D	603	ADP	C6-C5-N7	2.18	136.29	132.09
3	D	603	ADP	N9-C8-N7	-2.15	110.88	113.94
3	D	603	ADP	O3'-C3'-C2'	-2.13	105.00	111.82
3	C	603	ADP	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

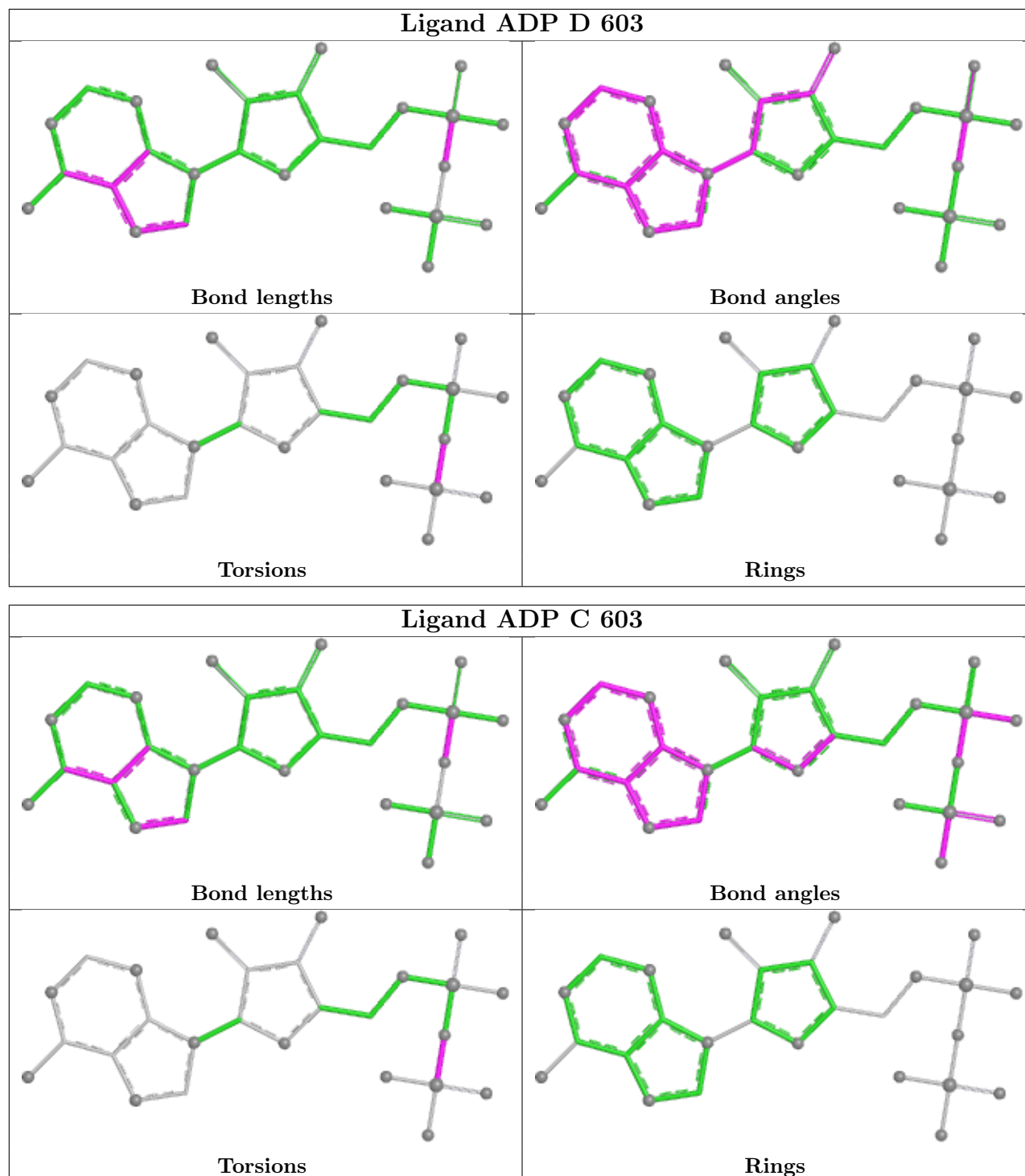
Mol	Chain	Res	Type	Atoms
3	A	603	ADP	PA-O3A-PB-O2B
3	B	603	ADP	PA-O3A-PB-O2B
3	C	603	ADP	PA-O3A-PB-O2B
3	D	603	ADP	PA-O3A-PB-O2B
3	C	603	ADP	PA-O3A-PB-O3B
3	A	603	ADP	PA-O3A-PB-O1B
3	A	603	ADP	PA-O3A-PB-O3B
3	B	603	ADP	PA-O3A-PB-O3B
3	D	603	ADP	PA-O3A-PB-O3B
3	D	603	ADP	PA-O3A-PB-O1B

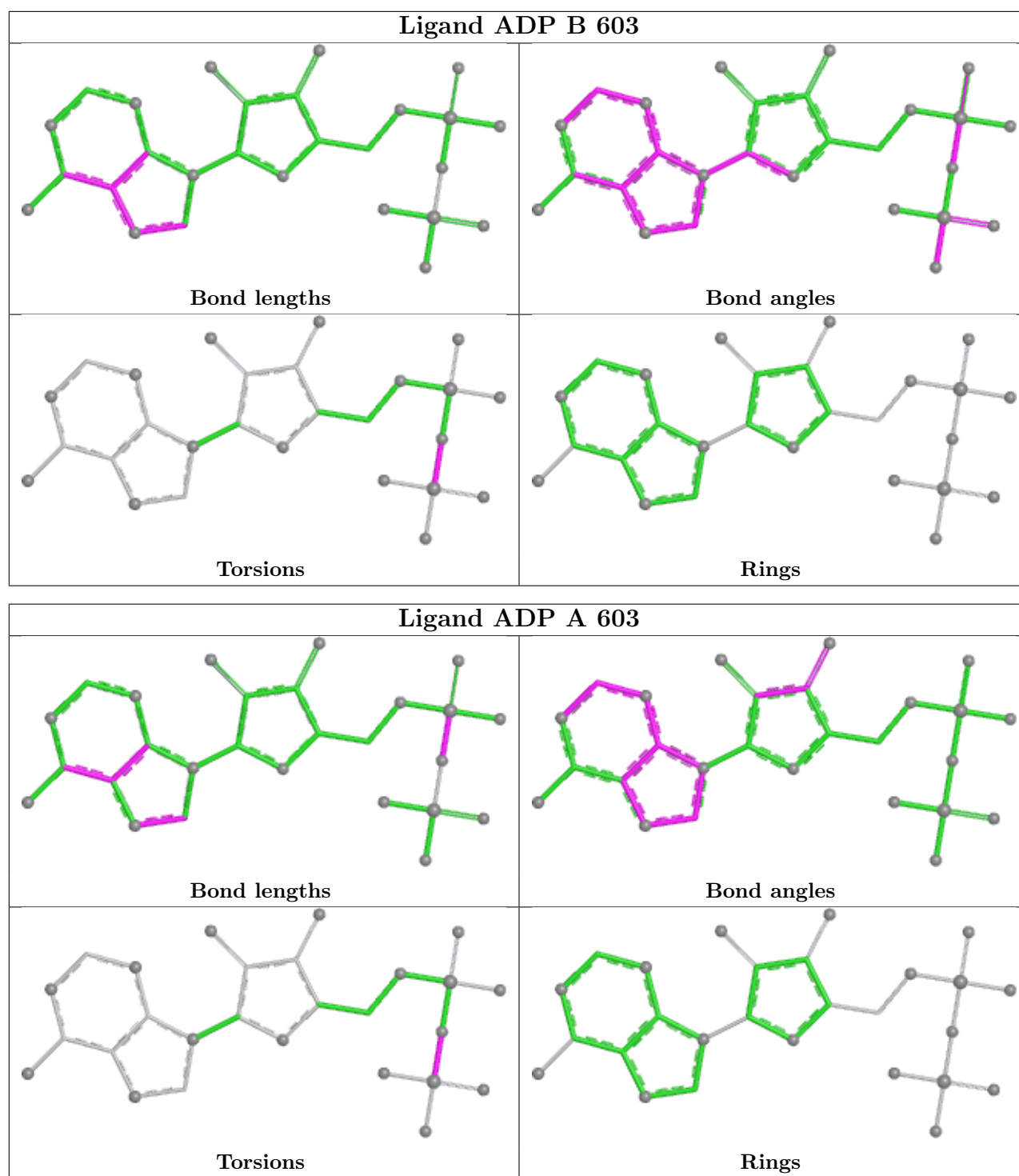
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	328/365 (89%)	-0.35	4 (1%) 76 74	15, 31, 67, 99	10 (3%)
1	B	341/365 (93%)	-0.14	4 (1%) 76 74	17, 39, 70, 96	6 (1%)
1	C	343/365 (93%)	-0.25	6 (1%) 69 66	18, 36, 70, 91	3 (0%)
1	D	338/365 (92%)	0.22	7 (2%) 63 60	23, 50, 82, 95	6 (1%)
2	W	13/20 (65%)	1.07	2 (15%) 5 4	22, 25, 34, 57	13 (100%)
2	X	13/20 (65%)	1.00	2 (15%) 5 4	20, 22, 35, 53	13 (100%)
2	Y	12/20 (60%)	0.73	2 (16%) 4 3	14, 17, 23, 23	12 (100%)
All	All	1388/1520 (91%)	-0.10	27 (1%) 66 63	14, 38, 75, 99	63 (4%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	938	PRO	5.7
1	D	352	TYR	5.1
1	C	8	PRO	4.5
2	W	938[A]	PRO	3.6
1	A	261	ILE	3.2
2	Y	938	PRO	3.2
1	D	158	VAL	2.9
1	B	359	ASN	2.9
1	C	345	ALA	2.8
1	B	9	ALA	2.8
1	A	344	THR	2.8
2	Y	939	GLN	2.5
1	D	343	LEU	2.4
1	A	8	PRO	2.4
1	D	357[A]	GLU	2.4
1	D	362	LEU	2.4
1	C	158	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	X	950	GLN	2.3
1	C	9	ALA	2.2
1	B	261	ILE	2.2
2	W	950[B]	GLN	2.2
1	C	49	ALA	2.2
1	C	348	TRP	2.1
1	A	278	GLY	2.1
1	D	345	ALA	2.1
1	B	245	VAL	2.1
1	D	281	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

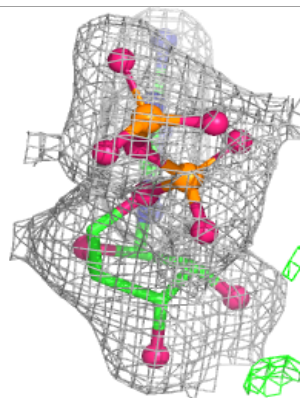
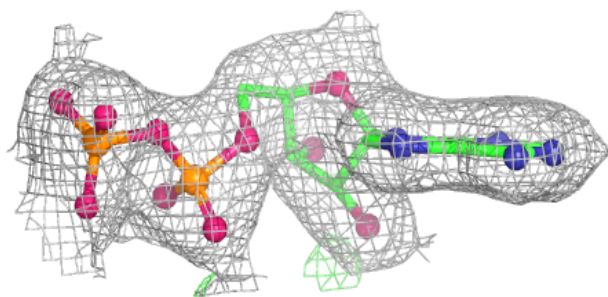
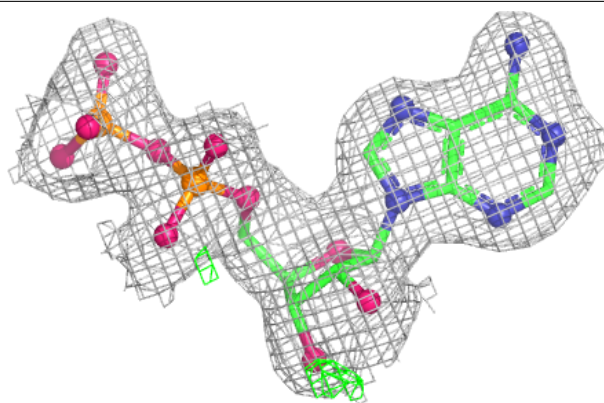
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	B	603	27/27	0.98	0.04	18,26,31,32	0
3	ADP	C	603	27/27	0.98	0.04	20,29,34,37	0
3	ADP	D	603	27/27	0.98	0.04	29,35,39,44	0
4	MG	C	800	1/1	0.98	0.03	28,28,28,28	0
4	MG	A	800	1/1	0.99	0.07	20,20,20,20	0
4	MG	B	800	1/1	0.99	0.03	20,20,20,20	0
3	ADP	A	603	27/27	0.99	0.04	14,23,28,30	0
4	MG	D	800	1/1	0.99	0.04	36,36,36,36	0

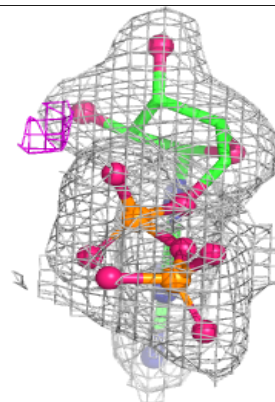
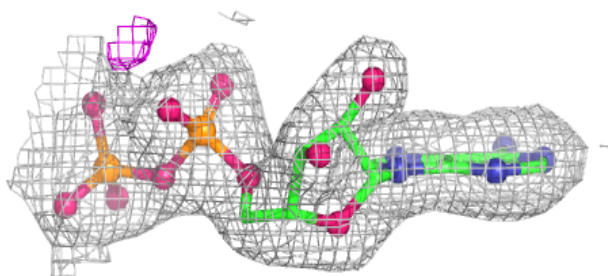
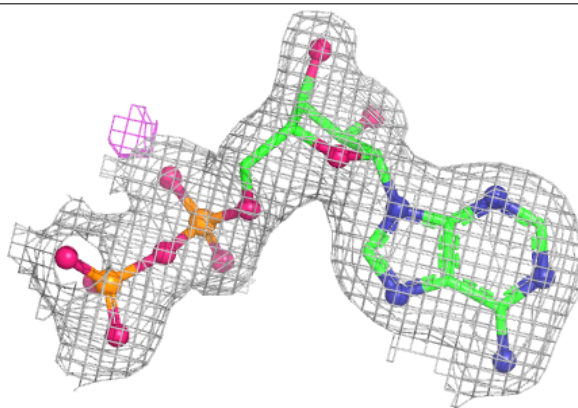
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 603:

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

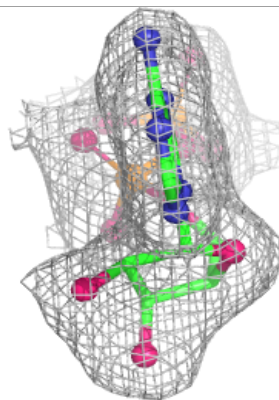
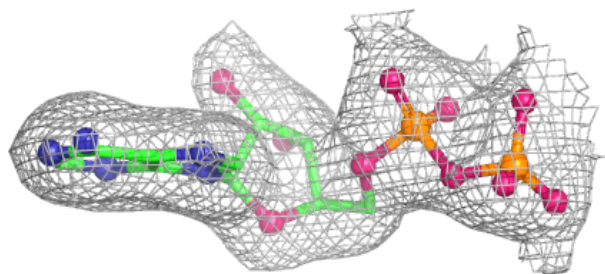
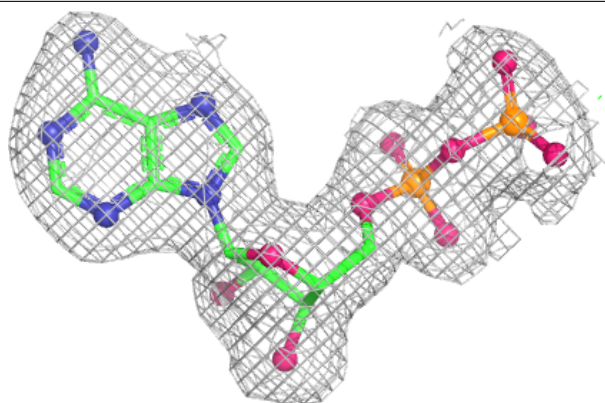
**Electron density around ADP C 603:**

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

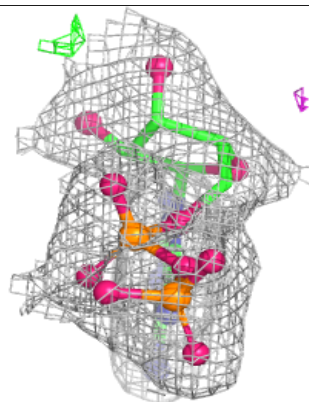
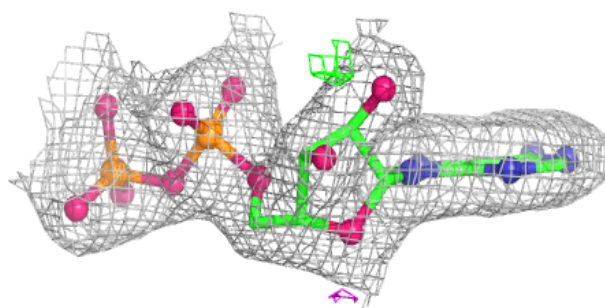
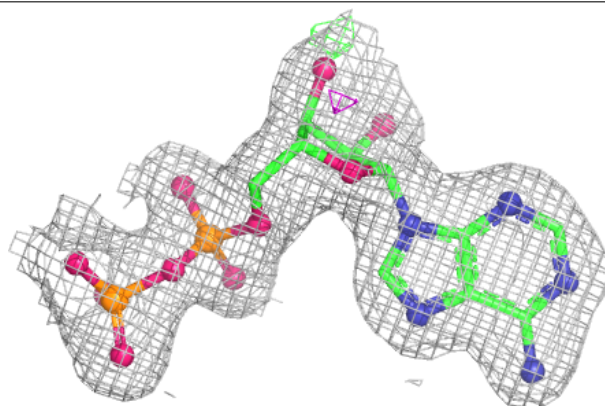


Electron density around ADP D 603:

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

**Electron density around ADP A 603:**

$2mF_o-DF_c$ (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.