



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:57 AM UTC

PDB ID : 4BN2 / pdb_00004bn2
Title : The crystal structure of kinesin-like protein KIF15
Authors : Klejnot, M.; Falnikar, A.; Ulaganathan, V.; Cross, R.; Baas, P.; Kozielski, F.
Deposited on : 2013-05-13
Resolution : 2.69 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

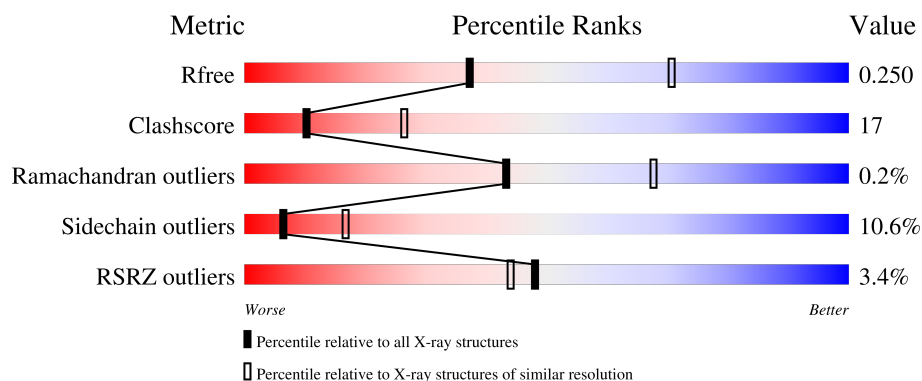
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	361	4% 58% 25% 7% 10%
1	B	361	3% 60% 24% 5% 10%
1	C	361	2% 59% 23% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7582 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-LIKE PROTEIN KIF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	3	0
			2473	1556	436	470	11			
1	B	324	Total	C	N	O	S	0	1	1
			2462	1544	431	475	12			
1	C	311	Total	C	N	O	S	1	1	0
			2360	1483	416	450	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9NS87
A	2	ALA	-	expression tag	UNP Q9NS87
A	3	MET	-	expression tag	UNP Q9NS87
A	4	GLY	-	expression tag	UNP Q9NS87
B	1	GLY	-	expression tag	UNP Q9NS87
B	2	ALA	-	expression tag	UNP Q9NS87
B	3	MET	-	expression tag	UNP Q9NS87
B	4	GLY	-	expression tag	UNP Q9NS87
C	1	GLY	-	expression tag	UNP Q9NS87
C	2	ALA	-	expression tag	UNP Q9NS87
C	3	MET	-	expression tag	UNP Q9NS87
C	4	GLY	-	expression tag	UNP Q9NS87

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

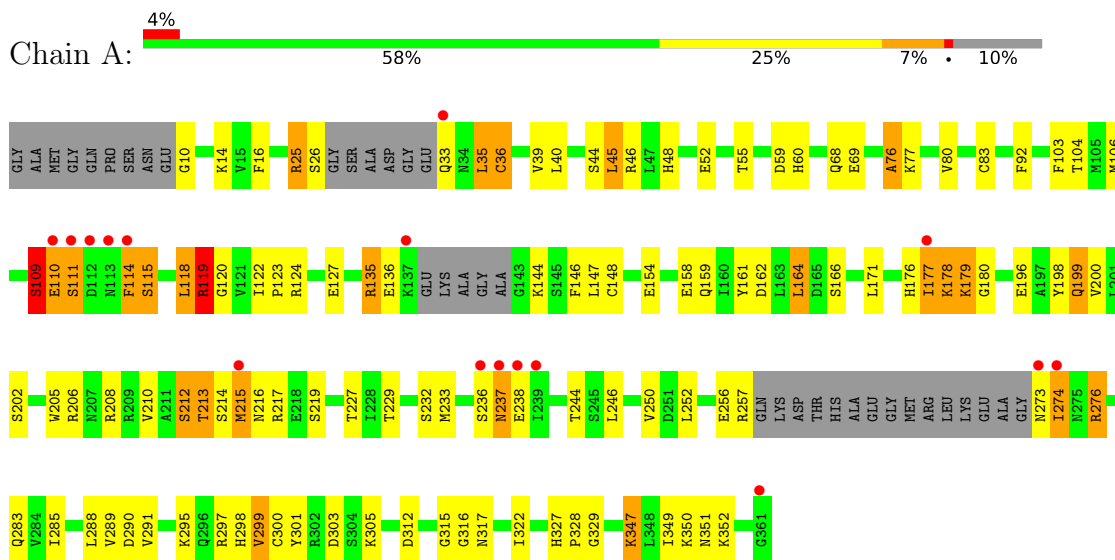
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	81	Total	O	0	0
			81	81		
4	C	54	Total	O	0	0
			54	54		

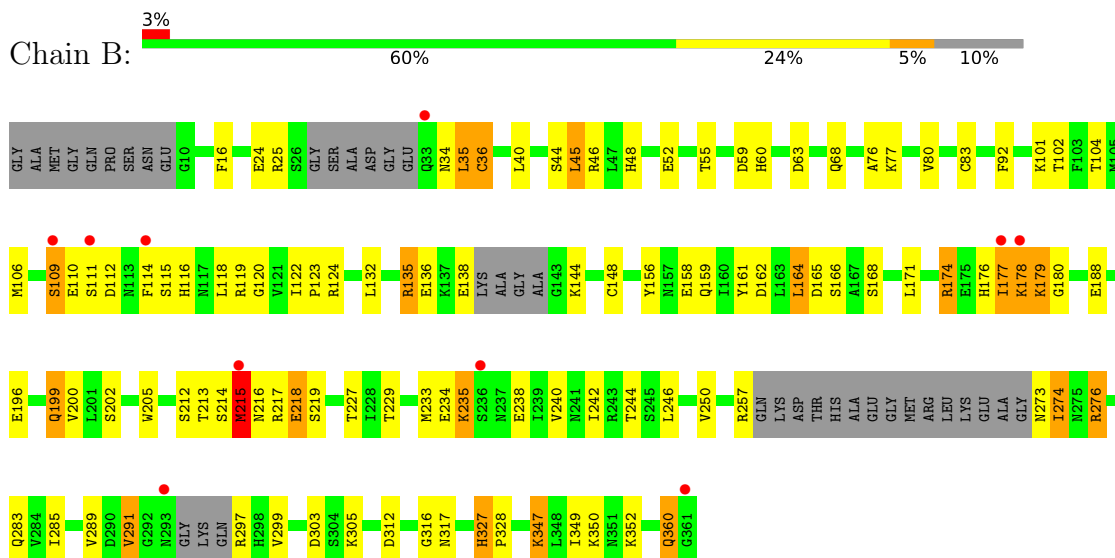
3 Residue-property plots [i](#)

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

• Molecule 1: KINESIN-LIKE PROTEIN KIF15

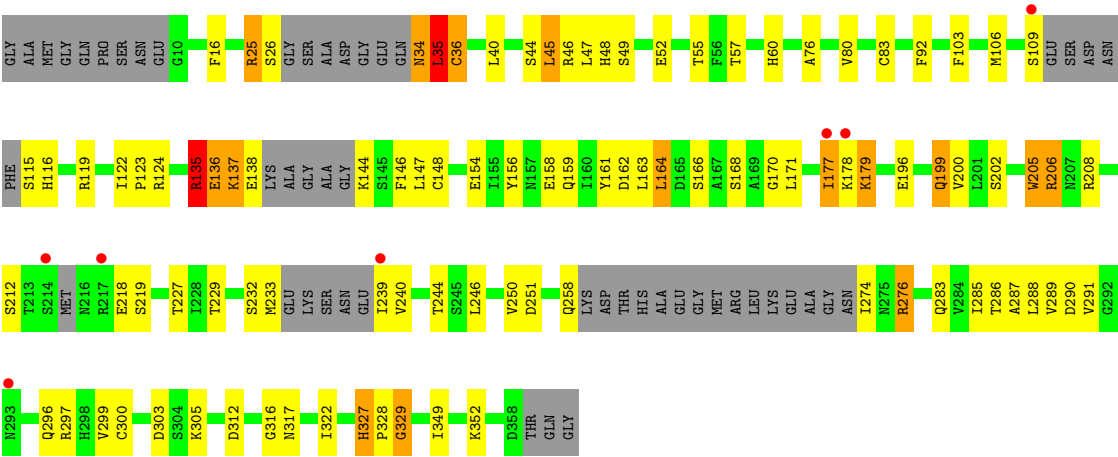


• Molecule 1: KINESIN-LIKE PROTEIN KIF15



• Molecule 1: KINESIN-LIKE PROTEIN KIF15





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.08Å 90.08Å 249.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.49 – 2.69 29.49 – 2.69	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.49-2.69) 85.7 (29.49-2.69)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.68Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.202 , 0.259 0.193 , 0.250	Depositor DCC
R_{free} test set	765 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7582	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 22.68 % 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 5.4253e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.82	2/2520 (0.1%)	1.22	23/3405 (0.7%)
1	B	0.81	0/2499	1.20	21/3370 (0.6%)
1	C	1.20	4/2392 (0.2%)	1.17	16/3230 (0.5%)
All	All	0.95	6/7411 (0.1%)	1.20	60/10005 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	5
1	C	0	3
All	All	0	15

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	ARG	C-N	-45.08	0.70	1.33
1	A	135	ARG	CA-CB	-6.85	1.42	1.53
1	C	205	TRP	C-N	5.71	1.41	1.33
1	A	135	ARG	N-CA	-5.16	1.39	1.46
1	C	200	VAL	CA-CB	-5.14	1.48	1.54
1	C	135	ARG	CG-CD	-5.05	1.37	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ARG	O-C-N	-16.36	100.84	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	LYS	N-CA-C	11.24	128.04	108.02
1	A	35	LEU	N-CA-C	9.03	123.61	112.23
1	A	212	SER	CA-C-N	-8.89	110.87	122.79
1	A	212	SER	C-N-CA	-8.89	110.87	122.79
1	A	119	ARG	NE-CZ-NH2	-8.66	111.41	119.20
1	A	119	ARG	CD-NE-CZ	8.42	136.18	124.40
1	A	213	THR	CB-CA-C	-8.36	98.93	111.72
1	B	35	LEU	N-CA-C	8.12	123.74	112.45
1	C	200	VAL	N-CA-C	-7.90	102.64	110.30
1	B	174	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	B	200	VAL	N-CA-C	-7.25	103.27	110.30
1	C	35	LEU	N-CA-C	7.22	122.36	112.90
1	B	34	ASN	N-CA-CB	-6.80	98.12	109.28
1	A	119	ARG	NE-CZ-NH1	6.65	128.15	121.50
1	B	174	ARG	CD-NE-CZ	6.54	133.56	124.40
1	C	327	HIS	CA-C-N	-6.49	114.04	120.98
1	C	327	HIS	C-N-CA	-6.49	114.04	120.98
1	A	200	VAL	N-CA-C	-6.48	104.02	110.30
1	B	234	GLU	CA-C-N	-6.45	113.70	122.86
1	B	234	GLU	C-N-CA	-6.45	113.70	122.86
1	B	174	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	C	135	ARG	CB-CG-CD	-6.27	96.88	111.30
1	A	135	ARG	CA-CB-CG	-6.12	101.87	114.10
1	B	135	ARG	CB-CG-CD	-6.00	97.51	111.30
1	C	135	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	B	178	LYS	N-CA-C	-5.72	106.01	112.87
1	C	135	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	104	THR	N-CA-C	5.69	117.16	111.07
1	A	295	LYS	CB-CA-C	-5.66	109.06	115.79
1	B	235	LYS	CB-CA-C	-5.61	102.14	110.62
1	A	119	ARG	CG-CD-NE	-5.59	99.69	112.00
1	B	109	SER	CA-C-N	-5.59	115.11	122.99
1	B	109	SER	C-N-CA	-5.59	115.11	122.99
1	B	135	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	C	299	VAL	CA-C-N	-5.55	115.04	122.42
1	C	299	VAL	C-N-CA	-5.55	115.04	122.42
1	A	114[A]	PHE	N-CA-C	5.52	116.36	108.74
1	A	114[B]	PHE	N-CA-C	5.52	116.36	108.74
1	A	252	LEU	N-CA-C	5.46	117.74	110.53
1	A	301	TYR	N-CA-C	-5.41	105.41	112.23
1	C	49	SER	N-CA-C	-5.41	101.35	109.95
1	B	135	ARG	NE-CZ-NH2	5.39	124.05	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	VAL	CA-C-N	-5.38	115.26	122.42
1	B	299	VAL	C-N-CA	-5.38	115.26	122.42
1	C	76	ALA	N-CA-C	5.37	118.99	112.23
1	A	178	LYS	N-CA-C	-5.33	106.48	112.87
1	C	47	LEU	CA-C-N	-5.32	113.83	122.34
1	C	47	LEU	C-N-CA	-5.32	113.83	122.34
1	A	135	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	C	178	LYS	N-CA-C	-5.25	106.57	112.87
1	A	135	ARG	CB-CG-CD	-5.21	99.33	111.30
1	B	327	HIS	CA-C-N	-5.20	113.35	119.84
1	B	327	HIS	C-N-CA	-5.20	113.35	119.84
1	A	198	TYR	N-CA-C	5.13	117.54	111.33
1	B	104	THR	N-CA-C	5.12	116.55	111.07
1	A	76	ALA	N-CA-C	5.11	118.66	112.23
1	A	299	VAL	CA-C-N	-5.10	114.91	122.41
1	A	299	VAL	C-N-CA	-5.10	114.91	122.41
1	C	136	GLU	N-CA-C	-5.09	106.76	112.87

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	SER	Peptide,Mainchain
1	A	213	THR	Peptide,Mainchain
1	A	215	MET	Peptide
1	A	33	GLN	Peptide
1	A	48	HIS	Mainchain
1	B	111	SER	Peptide
1	B	213	THR	Peptide
1	B	215	MET	Peptide
1	B	235	LYS	Peptide
1	B	48	HIS	Mainchain
1	C	206	ARG	Mainchain
1	C	329	GLY	Peptide
1	C	48	HIS	Mainchain

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	2473	0	2436	103	0
1	B	2462	0	2433	73	0
1	C	2360	0	2314	76	0
2	A	27	0	12	2	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	68	0	0	4	0
4	B	81	0	0	8	0
4	C	54	0	0	4	0
All	All	7582	0	7219	250	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 17.

All (250) 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:C:34:ASN:N	1:C:34:ASN:HD22	1.52	1.08
1:A:276:ARG:NH2	1:A:303:ASP:O	1.88	1.05
1:A:257:ARG:HA	1:A:273:ASN:C	1.79	1.05
1:B:276:ARG:NH2	1:B:303:ASP:O	1.91	1.02
1:C:276:ARG:NH2	1:C:303:ASP:O	1.91	1.02
1:B:165:ASP:OD2	4:B:2061:HOH:O	1.87	0.91
1:A:215:MET:HA	1:A:216:ASN:C	1.96	0.91
1:A:206:ARG:NH2	1:C:196:GLU:OE2	2.05	0.90
1:B:36:CYS:SG	4:B:2007:HOH:O	2.13	0.90
1:C:34:ASN:N	1:C:34:ASN:ND2	2.18	0.90
1:B:214:SER:O	1:B:215:MET:HG2	1.72	0.88
1:C:25:ARG:HG2	1:C:25:ARG:HH11	1.40	0.86
1:B:215:MET:HA	1:B:216:ASN:C	2.02	0.85
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.39	0.84
1:B:327:HIS:ND1	1:B:328:PRO:O	2.10	0.84
1:B:188:GLU:OE2	4:B:2066:HOH:O	1.97	0.83
1:C:327:HIS:ND1	1:C:328:PRO:O	2.11	0.82
1:C:179:LYS:HE3	1:C:317:ASN:HD22	1.48	0.79
1:A:327:HIS:ND1	1:A:328:PRO:O	2.15	0.79
1:A:114[A]:PHE:HD1	1:A:115:SER:H	1.27	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:HE3	1:A:317:ASN:HD22	1.48	0.77
1:C:179:LYS:HE3	1:C:317:ASN:ND2	2.01	0.76
1:B:179:LYS:HE3	1:B:317:ASN:HD22	1.51	0.75
1:A:25:ARG:HH11	1:A:25:ARG:CG	2.00	0.74
1:A:46:ARG:HE	1:A:55:THR:HG22	1.52	0.74
1:A:45:LEU:C	1:A:45:LEU:HD12	2.14	0.73
1:B:273:ASN:O	1:B:274:ILE:HG22	1.87	0.73
1:A:25:ARG:HG2	1:A:25:ARG:NH1	2.02	0.72
1:A:215:MET:CB	1:A:217:ARG:HG3	2.20	0.71
1:A:257:ARG:HA	1:A:273:ASN:O	1.90	0.71
1:C:45:LEU:C	1:C:45:LEU:HD12	2.14	0.71
1:C:25:ARG:HH11	1:C:25:ARG:CG	2.01	0.71
1:B:46:ARG:HE	1:B:55:THR:HG22	1.56	0.71
1:A:109:SER:C	1:A:111:SER:H	1.99	0.70
1:A:114[A]:PHE:CD1	1:A:115:SER:N	2.50	0.70
1:A:10:GLY:N	4:A:2001:HOH:O	2.24	0.70
1:A:162:ASP:HB2	1:A:171:LEU:HD11	1.75	0.69
1:A:109:SER:HB2	1:A:110:GLU:CB	2.23	0.68
1:C:45:LEU:HD12	1:C:45:LEU:O	1.93	0.68
1:A:206:ARG:HH22	1:C:196:GLU:CD	1.99	0.68
1:B:240:VAL:HG13	1:B:360:GLN:HG3	1.76	0.68
1:C:162:ASP:HB2	1:C:171:LEU:HD11	1.76	0.67
1:C:170:GLY:N	4:C:2035:HOH:O	2.26	0.67
1:C:251:ASP:OD1	4:C:2025:HOH:O	2.12	0.67
1:C:25:ARG:HG2	1:C:25:ARG:NH1	2.02	0.66
1:A:179:LYS:HE3	1:A:317:ASN:ND2	2.09	0.66
1:A:298:HIS:CE1	4:A:2059:HOH:O	2.49	0.66
1:C:285:ILE:HG23	1:C:349:ILE:HD11	1.79	0.65
1:A:237:ASN:C	1:A:237:ASN:OD1	2.39	0.65
1:C:46:ARG:HE	1:C:55:THR:HG22	1.62	0.65
1:B:162:ASP:HB2	1:B:171:LEU:HD11	1.78	0.64
1:A:109:SER:O	1:A:111:SER:N	2.20	0.64
1:B:179:LYS:HE3	1:B:317:ASN:ND2	2.12	0.64
1:B:46:ARG:HE	1:B:55:THR:CG2	2.10	0.63
1:B:285:ILE:HG23	1:B:349:ILE:HD11	1.80	0.63
1:A:46:ARG:HE	1:A:55:THR:CG2	2.11	0.62
1:C:57:THR:N	4:C:2011:HOH:O	2.26	0.62
1:A:45:LEU:HD12	1:A:45:LEU:O	1.99	0.62
1:C:179:LYS:CE	1:C:317:ASN:HD22	2.13	0.61
1:A:274:ILE:HG23	1:A:274:ILE:O	2.01	0.60
1:B:102:THR:OG1	4:B:2043:HOH:O	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:OD2	1:B:347[A]:LYS:HE2	2.02	0.59
1:A:215:MET:CA	1:A:216:ASN:C	2.74	0.58
1:A:178:LYS:HG3	1:A:180:GLY:H	1.69	0.58
1:B:110:GLU:HB3	4:B:2048:HOH:O	2.03	0.58
1:B:350:LYS:N	4:B:2078:HOH:O	2.35	0.58
1:A:285:ILE:HG23	1:A:349:ILE:HD11	1.85	0.57
1:B:214:SER:C	1:B:215:MET:HG2	2.29	0.57
1:A:176:HIS:ND1	1:A:178:LYS:HG2	2.20	0.57
1:B:122:ILE:HB	1:B:123:PRO:HD3	1.86	0.57
1:B:45:LEU:C	1:B:45:LEU:HD23	2.29	0.56
1:B:178:LYS:HG3	1:B:180:GLY:H	1.70	0.56
1:A:59:ASP:OD2	1:A:347[A]:LYS:HE2	2.05	0.56
1:A:285:ILE:HD12	1:A:349:ILE:CD1	2.34	0.56
1:A:92:PHE:HB3	1:A:250:VAL:HB	1.88	0.56
1:A:257:ARG:CA	1:A:273:ASN:C	2.62	0.56
1:C:26:SER:O	1:C:26:SER:OG	2.16	0.56
1:B:177:ILE:C	1:B:179:LYS:H	2.13	0.55
1:C:45:LEU:C	1:C:45:LEU:CD1	2.79	0.55
1:C:46:ARG:HE	1:C:55:THR:CG2	2.19	0.55
1:B:92:PHE:HB3	1:B:250:VAL:HB	1.89	0.55
1:C:116:HIS:O	1:C:119:ARG:HD3	2.07	0.55
1:C:122:ILE:HB	1:C:123:PRO:HD3	1.87	0.55
1:B:317:ASN:HA	1:B:352:LYS:O	2.06	0.55
1:C:177:ILE:C	1:C:179:LYS:H	2.13	0.55
1:C:92:PHE:CB	1:C:250:VAL:HB	2.38	0.54
1:A:45:LEU:C	1:A:45:LEU:CD1	2.80	0.54
1:C:258:GLN:H	1:C:274:ILE:N	2.06	0.54
1:B:159:GLN:HG2	1:B:161:TYR:CE1	2.43	0.54
1:B:285:ILE:HD12	1:B:349:ILE:CD1	2.38	0.53
1:B:92:PHE:CB	1:B:250:VAL:HB	2.38	0.53
1:A:46:ARG:NE	1:A:55:THR:HG22	2.21	0.53
1:A:80:VAL:O	1:A:83:CYS:HB2	2.08	0.53
1:A:177:ILE:C	1:A:179:LYS:H	2.15	0.53
1:A:52:GLU:O	1:A:52:GLU:HG2	2.08	0.53
1:A:122:ILE:HB	1:A:123:PRO:HD3	1.91	0.53
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.75	0.52
1:B:46:ARG:NE	1:B:55:THR:HG22	2.23	0.52
1:A:179:LYS:CE	1:A:317:ASN:HD22	2.19	0.52
1:A:92:PHE:CB	1:A:250:VAL:HB	2.40	0.52
1:A:159:GLN:HG2	1:A:161:TYR:CE1	2.44	0.51
1:B:215:MET:CA	1:B:216:ASN:C	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:C	1:C:137:LYS:N	2.65	0.51
1:C:179:LYS:HG3	1:C:312:ASP:OD2	2.10	0.51
1:A:290:ASP:HB2	1:A:297:ARG:HG3	1.93	0.51
1:A:109:SER:C	1:A:111:SER:N	2.64	0.51
1:B:312:ASP:HA	1:B:316:GLY:HA3	1.92	0.51
1:C:136:GLU:OE1	1:C:136:GLU:HA	2.09	0.51
1:C:227:THR:HG21	1:C:246:LEU:HD11	1.93	0.51
1:B:45:LEU:C	1:B:45:LEU:CD2	2.84	0.51
1:C:159:GLN:HG2	1:C:161:TYR:CE1	2.46	0.51
1:C:317:ASN:HA	1:C:352:LYS:O	2.11	0.51
1:A:178:LYS:HZ2	1:A:180:GLY:HA3	1.76	0.51
1:A:179:LYS:HG3	1:A:312:ASP:OD2	2.11	0.50
1:C:80:VAL:O	1:C:83:CYS:HB2	2.12	0.50
1:C:158:GLU:OE2	1:C:305:LYS:HG3	2.11	0.50
1:A:215:MET:HA	1:A:217:ARG:N	2.27	0.50
1:A:35:LEU:O	1:A:329:GLY:N	2.36	0.50
1:C:92:PHE:HB3	1:C:250:VAL:HB	1.92	0.50
1:C:196:GLU:HA	1:C:199:GLN:HE21	1.77	0.50
1:C:285:ILE:HD12	1:C:349:ILE:CD1	2.42	0.50
1:B:116:HIS:O	1:B:119:ARG:HD3	2.11	0.49
1:C:291:VAL:HG23	1:C:297:ARG:HB2	1.93	0.49
1:A:26:SER:O	1:A:26:SER:OG	2.25	0.49
1:A:256:GLU:O	1:A:273:ASN:O	2.30	0.49
1:B:177:ILE:C	1:B:179:LYS:N	2.69	0.49
1:B:179:LYS:HG3	1:B:312:ASP:OD2	2.13	0.49
1:B:215:MET:SD	1:B:217:ARG:CB	3.00	0.48
1:A:35:LEU:O	1:A:36:CYS:HB3	2.12	0.48
1:B:176:HIS:ND1	1:B:178:LYS:HG2	2.29	0.48
1:B:242:ILE:HD12	1:B:360:GLN:OE1	2.14	0.48
1:A:103:PHE:CE2	2:A:600:ADP:C6	3.01	0.48
1:A:227:THR:HG21	1:A:246:LEU:HD11	1.95	0.48
1:A:196:GLU:HA	1:A:199:GLN:HE21	1.78	0.48
1:C:290:ASP:HB2	1:C:297:ARG:HG3	1.95	0.48
1:B:179:LYS:CE	1:B:317:ASN:HD22	2.22	0.48
1:C:137:LYS:O	1:C:138:GLU:CB	2.62	0.48
1:A:317:ASN:HA	1:A:352:LYS:O	2.14	0.48
1:B:52:GLU:O	1:B:52:GLU:HG2	2.13	0.47
1:B:215:MET:HA	1:B:217:ARG:N	2.29	0.47
1:C:196:GLU:HA	1:C:199:GLN:NE2	2.29	0.47
1:A:16:PHE:HD1	1:A:60:HIS:HB3	1.79	0.47
1:A:35:LEU:O	1:A:36:CYS:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:O	1:B:36:CYS:HB3	2.14	0.47
1:A:164:LEU:N	1:A:164:LEU:CD1	2.77	0.47
1:A:14:LYS:HE3	4:A:2002:HOH:O	2.15	0.47
1:C:35:LEU:O	1:C:329:GLY:N	2.38	0.47
1:A:92:PHE:CE1	1:A:322:ILE:HG12	2.50	0.46
1:A:177:ILE:C	1:A:179:LYS:N	2.71	0.46
1:B:16:PHE:HD1	1:B:60:HIS:HB3	1.80	0.46
1:A:291:VAL:HG23	1:A:297:ARG:HB2	1.98	0.46
1:C:16:PHE:HD1	1:C:60:HIS:HB3	1.81	0.46
1:C:146:PHE:CE2	1:C:232:SER:HB3	2.50	0.46
1:C:177:ILE:C	1:C:179:LYS:N	2.69	0.46
1:C:144:LYS:HA	1:C:233:MET:O	2.14	0.46
1:A:46:ARG:NH1	4:A:2009:HOH:O	2.48	0.46
1:B:227:THR:HG21	1:B:246:LEU:HD11	1.97	0.46
1:B:212:SER:OG	1:B:219:SER:HB2	2.16	0.46
1:C:46:ARG:HG2	1:C:46:ARG:HH11	1.81	0.46
1:A:205:TRP:O	1:A:205:TRP:CD1	2.69	0.46
1:C:52:GLU:HG2	1:C:52:GLU:O	2.15	0.46
1:C:285:ILE:O	1:C:289:VAL:HG23	2.15	0.45
1:C:164:LEU:N	1:C:164:LEU:CD1	2.79	0.45
1:A:285:ILE:O	1:A:289:VAL:HG23	2.16	0.45
1:B:80:VAL:O	1:B:83:CYS:HB2	2.16	0.45
1:B:114:PHE:O	1:B:118:LEU:HG	2.16	0.45
1:C:300:CYS:HB3	1:C:303:ASP:HB2	1.97	0.45
1:A:69:GLU:HB2	1:A:124:ARG:NH2	2.31	0.45
1:C:296:GLN:O	1:C:297:ARG:HG2	2.17	0.45
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.82	0.45
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.79	0.45
1:C:285:ILE:HG23	1:C:349:ILE:CD1	2.46	0.45
1:A:69:GLU:HB2	1:A:124:ARG:HH21	1.82	0.44
1:C:312:ASP:HA	1:C:316:GLY:HA3	1.99	0.44
1:A:298:HIS:NE2	1:A:300:CYS:SG	2.86	0.44
1:B:156:TYR:O	1:B:159:GLN:HB3	2.17	0.44
1:C:92:PHE:CE1	1:C:322:ILE:HG12	2.52	0.44
1:C:46:ARG:NE	1:C:55:THR:HG22	2.30	0.44
1:A:144:LYS:HA	1:A:233:MET:O	2.18	0.44
1:A:148:CYS:HA	1:A:229:THR:O	2.17	0.44
1:B:285:ILE:O	1:B:289:VAL:HG23	2.18	0.44
1:A:290:ASP:CB	1:A:297:ARG:HG3	2.47	0.44
1:C:177:ILE:H	1:C:177:ILE:HG12	1.36	0.44
1:A:119:ARG:HH11	1:A:127:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:CG2	1:A:246:LEU:HD11	2.48	0.43
1:C:290:ASP:CB	1:C:297:ARG:HG3	2.48	0.43
1:A:236:SER:O	1:A:237:ASN:C	2.61	0.43
1:A:312:ASP:HA	1:A:316:GLY:HA3	2.00	0.43
1:B:35:LEU:O	1:B:36:CYS:CB	2.66	0.43
1:B:164:LEU:N	1:B:164:LEU:CD1	2.81	0.43
1:A:196:GLU:HA	1:A:199:GLN:NE2	2.34	0.43
1:B:63:ASP:HB3	4:B:2021:HOH:O	2.17	0.43
1:A:135:ARG:O	1:A:135:ARG:HG2	2.18	0.43
1:A:158:GLU:OE2	1:A:305:LYS:HG3	2.18	0.43
1:B:52:GLU:OE1	1:B:52:GLU:N	2.49	0.43
1:C:212:SER:OG	1:C:219:SER:HB2	2.18	0.43
1:A:212:SER:OG	1:A:219:SER:HB2	2.19	0.43
1:A:315:GLY:N	1:A:351:ASN:OD1	2.50	0.43
1:B:176:HIS:HB3	1:B:178:LYS:HG2	2.01	0.43
1:B:178:LYS:HZ2	1:B:180:GLY:HA3	1.83	0.43
1:B:257:ARG:HD2	4:B:2072:HOH:O	2.18	0.43
1:B:101:LYS:HB2	1:B:101:LYS:HE2	1.85	0.43
1:C:156:TYR:O	1:C:159:GLN:HB3	2.19	0.43
1:B:196:GLU:HA	1:B:199:GLN:HE21	1.84	0.43
1:C:119:ARG:HG2	1:C:124:ARG:NH1	2.34	0.43
1:C:35:LEU:HD12	1:C:35:LEU:HA	1.63	0.42
1:C:55:THR:HG23	4:C:2009:HOH:O	2.19	0.42
1:B:119:ARG:HG2	1:B:124:ARG:NH1	2.34	0.42
1:A:114[A]:PHE:HD1	1:A:115:SER:N	2.01	0.42
1:C:52:GLU:OE1	1:C:52:GLU:N	2.51	0.42
1:B:291:VAL:HG12	1:B:297:ARG:HB2	2.02	0.42
1:C:35:LEU:O	1:C:36:CYS:HB3	2.19	0.42
1:A:76:ALA:O	1:A:77:LYS:C	2.62	0.42
1:C:103:PHE:CE2	2:C:600:ADP:C6	3.07	0.42
1:C:286:THR:O	1:C:287:ALA:C	2.63	0.42
1:A:288:LEU:HA	1:A:288:LEU:HD23	1.81	0.42
1:C:154:GLU:OE1	1:C:208:ARG:HG3	2.18	0.42
1:A:120:GLY:O	1:A:123:PRO:HD2	2.20	0.42
1:A:146:PHE:CE2	1:A:232:SER:HB3	2.55	0.42
1:B:136:GLU:OE1	1:B:136:GLU:HA	2.20	0.42
1:C:164:LEU:HA	1:C:164:LEU:HD12	1.83	0.42
1:A:68:GLN:HA	1:A:68:GLN:OE1	2.19	0.41
1:A:164:LEU:N	1:A:164:LEU:HD13	2.35	0.41
1:B:24:GLU:O	1:B:25:ARG:HB2	2.20	0.41
1:B:158:GLU:OE2	1:B:305:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLU:HA	1:A:136:GLU:OE1	2.20	0.41
1:A:154:GLU:OE1	1:A:208:ARG:HG3	2.19	0.41
1:A:178:LYS:NZ	1:A:180:GLY:HA3	2.34	0.41
1:B:76:ALA:O	1:B:77:LYS:C	2.63	0.41
1:C:35:LEU:O	1:C:36:CYS:CB	2.69	0.41
1:A:285:ILE:HD12	1:A:349:ILE:HD12	2.01	0.41
1:A:118:LEU:HD12	1:A:118:LEU:HA	1.92	0.41
1:A:52:GLU:OE1	1:A:52:GLU:N	2.51	0.41
1:A:103:PHE:CE2	2:A:600:ADP:N6	2.88	0.41
1:B:68:GLN:OE1	1:B:68:GLN:HA	2.20	0.41
1:B:120:GLY:O	1:B:123:PRO:HD2	2.21	0.41
1:B:205:TRP:O	1:B:205:TRP:CD1	2.74	0.41
1:B:217:ARG:C	1:B:218:GLU:HG2	2.45	0.41
1:C:148:CYS:HA	1:C:229:THR:O	2.20	0.41
1:A:285:ILE:HG23	1:A:349:ILE:CD1	2.51	0.41
1:B:144:LYS:HA	1:B:233:MET:O	2.21	0.41
1:B:148:CYS:HA	1:B:229:THR:O	2.19	0.41
1:C:205:TRP:O	1:C:205:TRP:CD1	2.74	0.41
1:C:288:LEU:HA	1:C:288:LEU:HD23	1.79	0.41
1:A:176:HIS:HB3	1:A:178:LYS:HG2	2.03	0.41
1:C:227:THR:CG2	1:C:246:LEU:HD11	2.51	0.40
1:B:178:LYS:O	1:B:179:LYS:CB	2.68	0.40
1:A:92:PHE:CZ	1:A:322:ILE:HG12	2.56	0.40
1:A:349:ILE:CG2	1:A:350:LYS:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	323/361 (90%)	303 (94%)	19 (6%)	1 (0%)	36 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	315/361 (87%)	297 (94%)	17 (5%)	1 (0%)	36	60
1	C	298/361 (82%)	286 (96%)	12 (4%)	0	100	100
All	All	936/1083 (86%)	886 (95%)	48 (5%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLU
1	B	274	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	A	266/303 (88%)	237 (89%)	29 (11%)	6	16
1	B	269/303 (89%)	240 (89%)	29 (11%)	6	16
1	C	254/303 (84%)	227 (89%)	27 (11%)	6	17
All	All	789/909 (87%)	704 (89%)	85 (11%)	6	16

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	36	CYS
1	A	39	VAL
1	A	40	LEU
1	A	44	SER
1	A	45	LEU
1	A	106	MET
1	A	109	SER
1	A	111	SER
1	A	115	SER
1	A	118	LEU
1	A	119	ARG

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	166	SER
1	A	177	ILE
1	A	179	LYS
1	A	199	GLN
1	A	202	SER
1	A	210	VAL
1	A	214	SER
1	A	237	ASN
1	A	238	GLU
1	A	244	THR
1	A	274	ILE
1	A	276	ARG
1	A	283	GLN
1	A	299	VAL
1	A	347[A]	LYS
1	A	347[B]	LYS
1	B	36	CYS
1	B	40	LEU
1	B	44	SER
1	B	45	LEU
1	B	106	MET
1	B	109	SER
1	B	112	ASP
1	B	115	SER
1	B	132	LEU
1	B	135	ARG
1	B	138	GLU
1	B	164	LEU
1	B	166	SER
1	B	168	SER
1	B	174	ARG
1	B	177	ILE
1	B	179	LYS
1	B	199	GLN
1	B	202	SER
1	B	215	MET
1	B	218	GLU
1	B	238	GLU
1	B	244	THR
1	B	276	ARG
1	B	283	GLN

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Mol	Chain	Res	Type
1	B	291	VAL
1	B	347[A]	LYS
1	B	347[B]	LYS
1	B	360	GLN
1	C	25	ARG
1	C	34	ASN
1	C	35	LEU
1	C	36	CYS
1	C	40	LEU
1	C	44	SER
1	C	45	LEU
1	C	106	MET
1	C	109	SER
1	C	115	SER
1	C	135	ARG
1	C	137	LYS
1	C	147	LEU
1	C	163	LEU
1	C	164	LEU
1	C	166	SER
1	C	168	SER
1	C	177	ILE
1	C	179	LYS
1	C	199	GLN
1	C	202	SER
1	C	218	GLU
1	C	239	ILE
1	C	240	VAL
1	C	244	THR
1	C	276	ARG
1	C	283	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	96	GLN
1	A	344	GLN
1	B	60	HIS
1	B	96	GLN
1	B	199	GLN
1	B	325	ASN

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Mol	Chain	Res	Type
1	C	325	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 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
2	ADP	C	600	3	28,29,29	1.57	6 (21%)	43,45,45	1.67	9 (20%)
2	ADP	A	600	3	28,29,29	1.61	6 (21%)	43,45,45	1.90	10 (23%)
2	ADP	B	600	3	28,29,29	1.56	6 (21%)	43,45,45	1.82	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	600	3	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	600	3	-	2/16/32/32	0/3/3/3
2	ADP	B	600	3	-	3/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ADP	C5-C4	4.74	1.47	1.39
2	B	600	ADP	C5-C4	4.70	1.47	1.39
2	C	600	ADP	C5-C4	4.42	1.47	1.39
2	A	600	ADP	PA-O3A	3.75	1.63	1.59
2	C	600	ADP	PA-O3A	3.20	1.63	1.59
2	B	600	ADP	C5-N7	-3.11	1.33	1.39
2	B	600	ADP	PA-O3A	3.01	1.62	1.59
2	C	600	ADP	C4-N9	-2.88	1.31	1.37
2	A	600	ADP	C5-C6	2.77	1.48	1.41
2	C	600	ADP	C8-N7	2.67	1.36	1.31
2	B	600	ADP	C5-C6	2.65	1.48	1.41
2	C	600	ADP	C5-N7	-2.54	1.34	1.39
2	A	600	ADP	C8-N7	2.54	1.36	1.31
2	C	600	ADP	C5-C6	2.42	1.47	1.41
2	A	600	ADP	C5-N7	-2.37	1.34	1.39
2	B	600	ADP	C8-N7	2.24	1.36	1.31
2	B	600	ADP	C4-N9	-2.24	1.33	1.37
2	A	600	ADP	C4-N9	-2.19	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ADP	C5-C4-N3	-5.88	118.62	126.72
2	A	600	ADP	C5-C4-N3	-5.67	118.91	126.72
2	C	600	ADP	C5-C4-N3	-4.67	120.28	126.72
2	A	600	ADP	C4-C5-N7	-4.28	105.69	110.58
2	B	600	ADP	C4-C5-N7	-4.13	105.86	110.58
2	B	600	ADP	N3-C4-N9	4.10	134.15	127.17
2	A	600	ADP	N3-C4-N9	3.88	133.76	127.17
2	C	600	ADP	N3-C4-N9	3.61	133.30	127.17
2	B	600	ADP	C2-N3-C4	3.36	120.03	111.83
2	A	600	ADP	C2-N3-C4	3.23	119.72	111.83
2	C	600	ADP	C4-N9-C8	3.07	108.96	105.74
2	C	600	ADP	C4-C5-N7	-3.02	107.13	110.58
2	C	600	ADP	C2-N3-C4	3.01	119.17	111.83
2	B	600	ADP	C5-N7-C8	2.92	108.04	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	ADP	N3-C2-N1	-2.89	124.20	128.58
2	A	600	ADP	C5-N7-C8	2.74	107.75	103.45
2	A	600	ADP	O2A-PA-O3A	2.74	114.67	107.27
2	A	600	ADP	O3B-PB-O2B	2.55	117.35	107.80
2	A	600	ADP	N3-C2-N1	-2.45	124.88	128.58
2	B	600	ADP	O3B-PB-O2B	2.40	116.80	107.80
2	C	600	ADP	C2-N1-C6	2.39	122.66	118.73
2	B	600	ADP	N3-C2-N1	-2.33	125.06	128.58
2	A	600	ADP	C6-C5-N7	2.28	136.49	132.09
2	A	600	ADP	C4-N9-C8	2.21	108.06	105.74
2	B	600	ADP	C6-C5-N7	2.16	136.26	132.09
2	C	600	ADP	N9-C8-N7	-2.16	110.88	113.94
2	C	600	ADP	C5-N7-C8	2.01	106.61	103.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	ADP	PA-O3A-PB-O2B
2	B	600	ADP	PA-O3A-PB-O2B
2	B	600	ADP	PA-O3A-PB-O3B
2	A	600	ADP	PA-O3A-PB-O3B
2	C	600	ADP	PA-O3A-PB-O3B
2	B	600	ADP	PA-O3A-PB-O1B

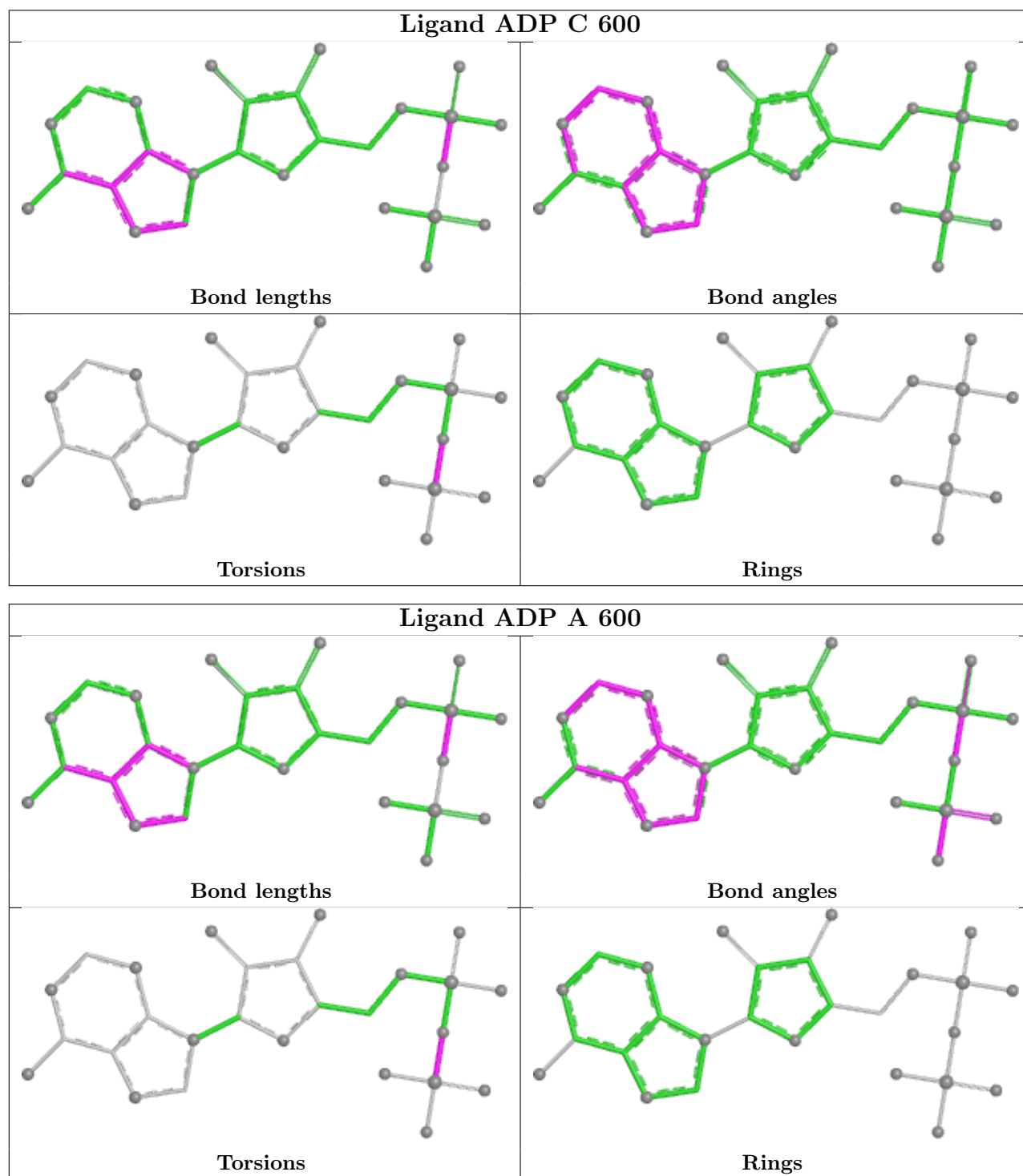
There are no ring outliers.

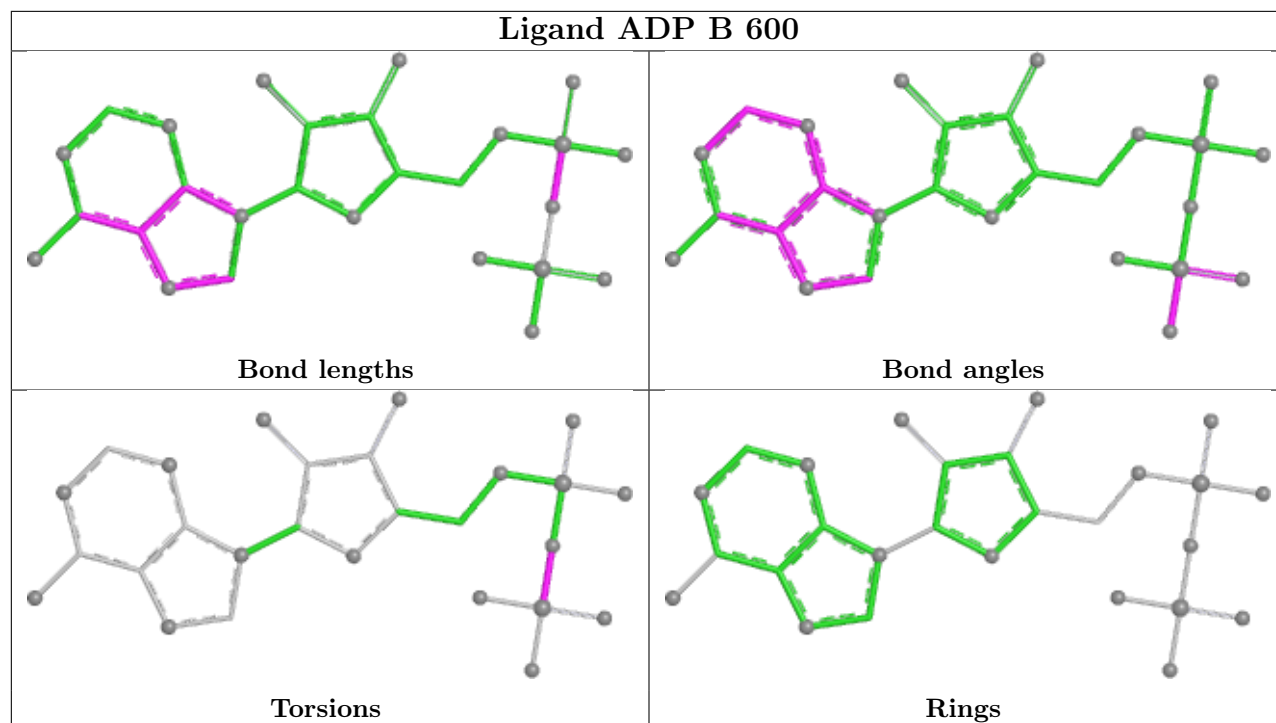
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	ADP	1	0
2	A	600	ADP	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	206:ARG	C	207:ASN	N	0.70

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	326/361 (90%)	-0.10	16 (4%) 35 31	15, 33, 81, 124	3 (0%)
1	B	324/361 (89%)	-0.20	10 (3%) 51 48	14, 31, 80, 105	1 (0%)
1	C	311/361 (86%)	-0.16	7 (2%) 61 58	14, 34, 73, 104	2 (0%)
All	All	961/1083 (88%)	-0.15	33 (3%) 48 44	14, 33, 80, 124	6 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	ASN	6.0
1	A	114[A]	PHE	5.9
1	A	110	GLU	5.4
1	A	237	ASN	4.9
1	B	33	GLN	3.8
1	A	112	ASP	3.3
1	A	137	LYS	3.3
1	C	178	LYS	3.3
1	C	109	SER	3.2
1	C	217	ARG	3.2
1	A	239	ILE	3.0
1	B	177	ILE	3.0
1	C	214	SER	3.0
1	A	361	GLY	2.8
1	A	33	GLN	2.7
1	C	239	ILE	2.7
1	B	114	PHE	2.7
1	A	113	ASN	2.6
1	A	274	ILE	2.5
1	A	238	GLU	2.5
1	A	111	SER	2.5
1	B	293	ASN	2.4
1	C	293	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	109	SER	2.4
1	B	236	SER	2.4
1	B	215	MET	2.4
1	B	361	GLY	2.4
1	A	177	ILE	2.2
1	B	178	LYS	2.1
1	C	177	ILE	2.1
1	A	236	SER	2.1
1	B	111	SER	2.0
1	A	215	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

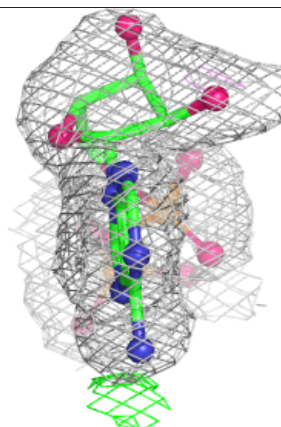
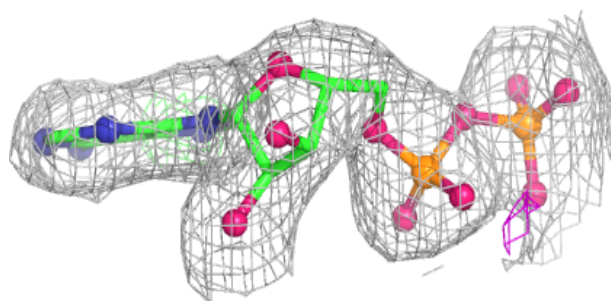
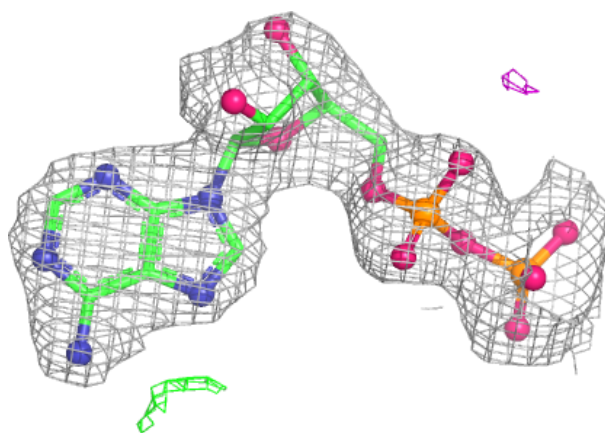
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	601	1/1	0.98	0.08	15,15,15,15	0
2	ADP	B	600	27/27	0.99	0.04	9,16,23,25	0
2	ADP	C	600	27/27	0.99	0.05	13,22,32,39	0
2	ADP	A	600	27/27	0.99	0.05	12,19,27,29	0
3	MG	B	601	1/1	0.99	0.14	24,24,24,24	0
3	MG	C	601	1/1	1.00	0.06	17,17,17,17	0

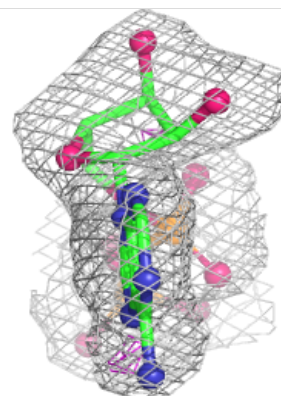
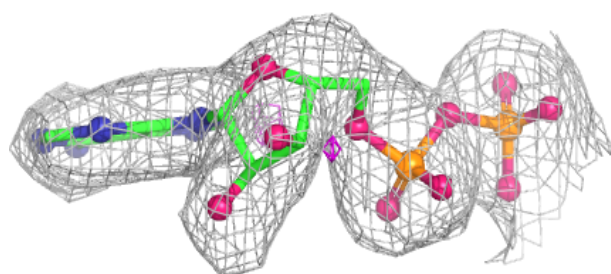
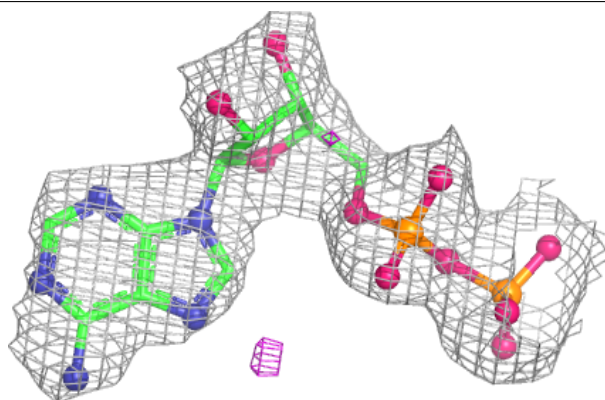
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 600:

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

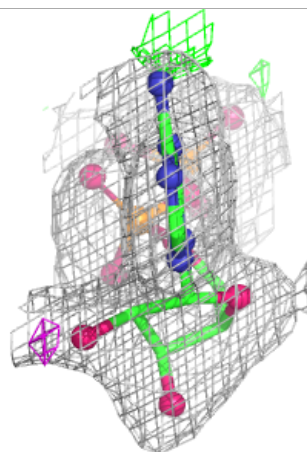
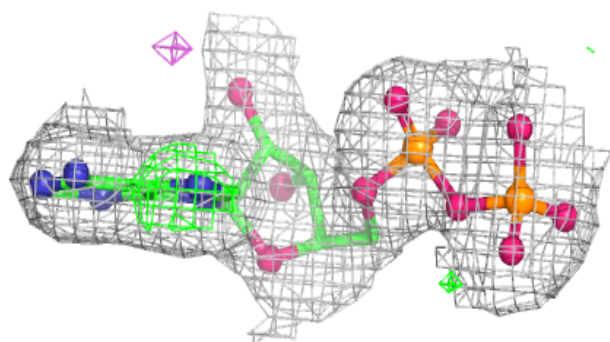
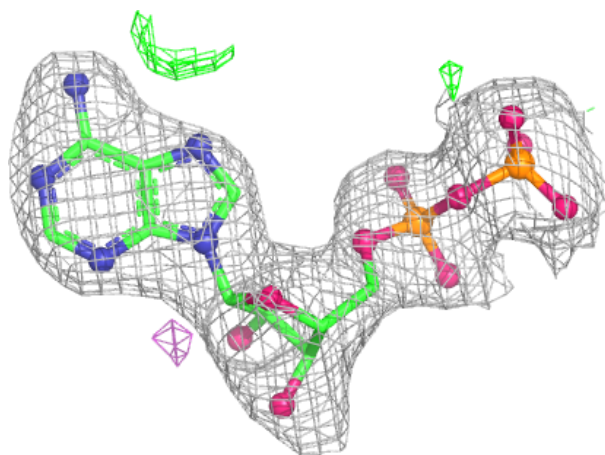
**Electron density around ADP C 600:**

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



Electron density around ADP A 600:

$2mF_o-DF_c$ (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.