WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 12:31 AM EST

PDB ID	:	3KX2
Title	:	Crystal structure of Prp43p in complex with ADP
Authors	:	Nielsen, K.H.; Andersen, G.R.; He, Y.
Deposited on	:	2009-12-02
Resolution	:	2.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
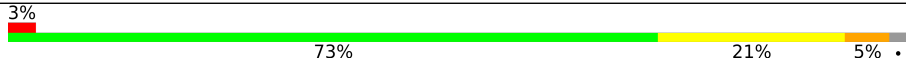*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.
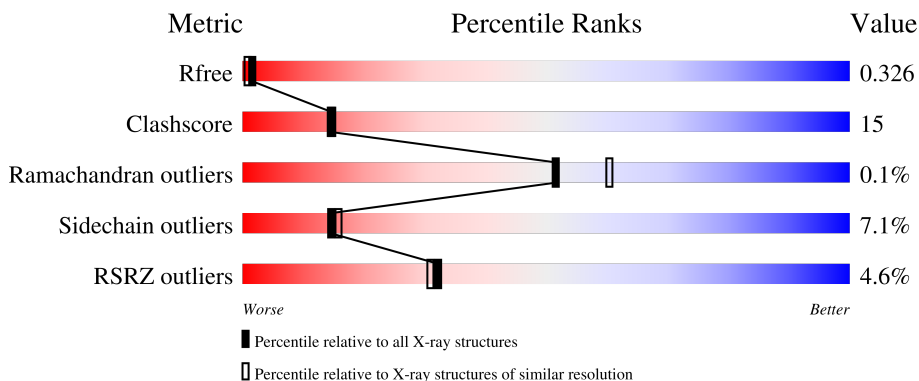
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	767	6% / 73% / 21% / · ·
1	B	767	3% / 73% / 21% / 5% ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13172 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 Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	755	Total	C	N	O	S	0	0	0
			6067	3841	1048	1153	25			
1	A	755	Total	C	N	O	S	0	0	0
			6067	3841	1048	1153	25			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
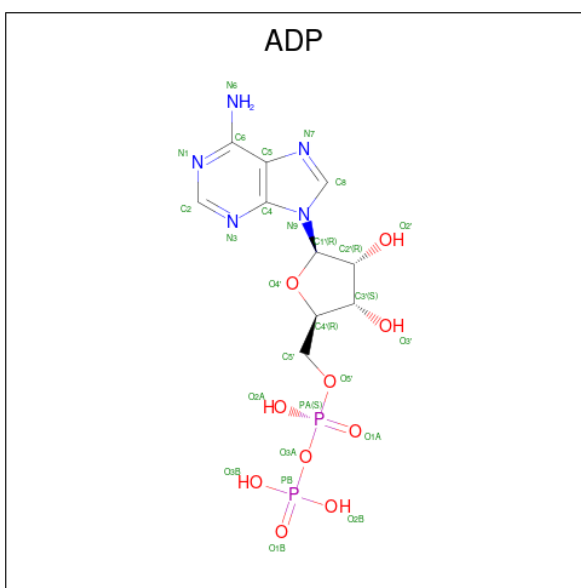
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	538	Total 538	O 538	0	0
4	A	444	Total 444	O 444	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: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43
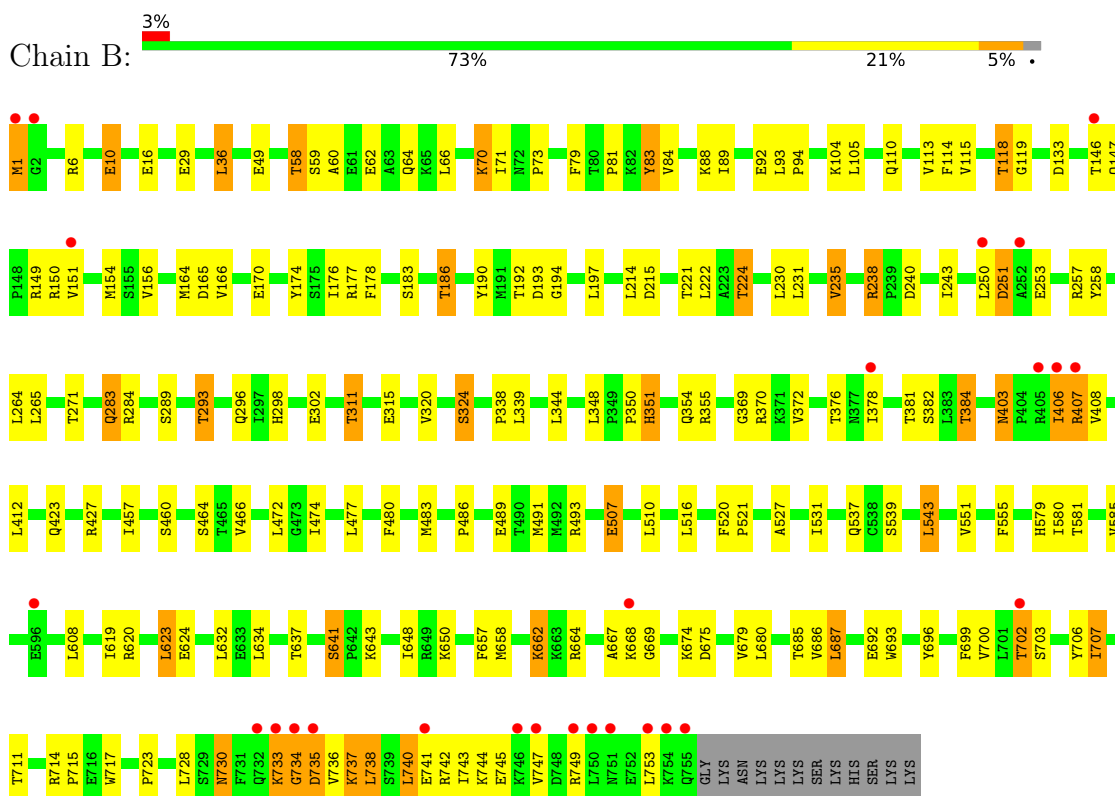
- Molecule 1: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43
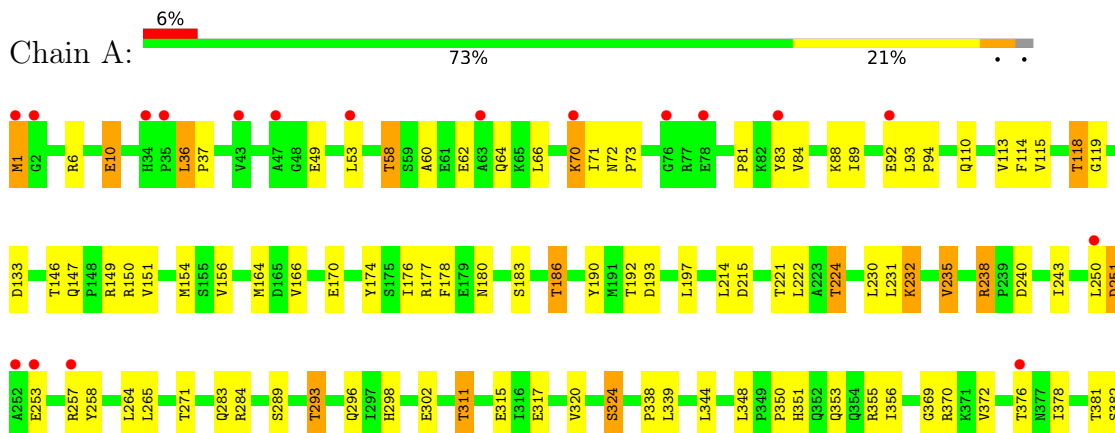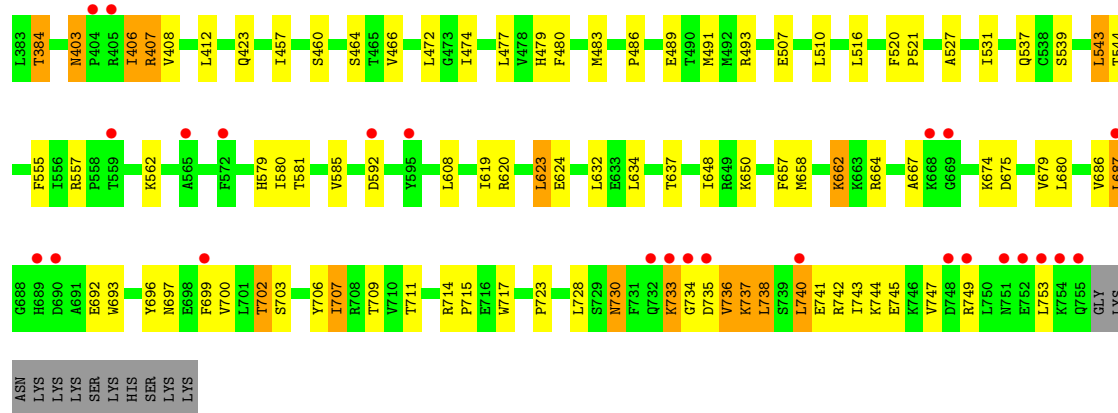
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.15Å 118.15Å 253.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.42 – 2.20 48.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.42-2.20) 99.8 (48.42-2.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.250 0.301 , 0.326	Depositor DCC
R_{free} test set	5221 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13172	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	0.71	18/6195 (0.3%)	0.58	6/8384 (0.1%)
1	B	0.59	16/6195 (0.3%)	0.61	9/8384 (0.1%)
All	All	0.65	34/12390 (0.3%)	0.59	15/16768 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	GLU	CD-OE2	-17.97	1.05	1.25
1	A	317	GLU	CD-OE1	-17.68	1.06	1.25
1	A	83	TYR	CE2-CZ	-17.41	1.16	1.38
1	B	83	TYR	CD1-CE1	-17.22	1.13	1.39
1	B	83	TYR	CD2-CE2	-15.92	1.15	1.39
1	A	83	TYR	CD2-CE2	-13.93	1.18	1.39
1	B	215	ASP	C-O	-13.37	0.97	1.23
1	A	544	THR	C-O	-12.34	0.99	1.23
1	A	83	TYR	CG-CD1	-11.01	1.24	1.39
1	A	83	TYR	CD1-CE1	-10.31	1.23	1.39
1	A	317	GLU	CG-CD	-10.04	1.36	1.51
1	A	317	GLU	CB-CG	-9.70	1.33	1.52
1	B	83	TYR	CE1-CZ	-9.05	1.26	1.38
1	A	317	GLU	C-O	-9.04	1.06	1.23
1	A	215	ASP	CG-OD2	-8.93	1.04	1.25
1	A	544	THR	CB-CG2	-8.74	1.23	1.52
1	B	271	THR	C-O	-8.50	1.07	1.23
1	A	215	ASP	C-O	-8.50	1.07	1.23
1	A	83	TYR	CZ-OH	-8.37	1.23	1.37
1	B	83	TYR	CZ-OH	-8.14	1.24	1.37
1	B	83	TYR	C-O	-8.13	1.07	1.23
1	B	83	TYR	CE2-CZ	-8.06	1.28	1.38
1	A	215	ASP	CG-OD1	-7.66	1.07	1.25
1	B	215	ASP	CG-OD2	-7.37	1.08	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	TYR	CG-CD1	-6.96	1.30	1.39
1	B	271	THR	CA-C	-6.05	1.37	1.52
1	B	685	THR	C-O	-6.03	1.11	1.23
1	B	215	ASP	CG-OD1	-5.96	1.11	1.25
1	B	685	THR	CB-CG2	-5.63	1.33	1.52
1	B	685	THR	CB-OG1	-5.61	1.32	1.43
1	A	271	THR	C-O	-5.43	1.13	1.23
1	A	544	THR	CA-C	-5.35	1.39	1.52
1	B	271	THR	CB-OG1	-5.18	1.32	1.43
1	A	83	TYR	CE1-CZ	-5.10	1.31	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	734	GLY	N-CA-C	12.59	144.58	113.10
1	B	215	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	232	LYS	CB-CA-C	9.33	129.06	110.40
1	B	733	LYS	N-CA-C	8.59	134.18	111.00
1	A	215	ASP	CB-CG-OD1	8.56	126.01	118.30
1	A	733	LYS	N-CA-C	8.45	133.82	111.00
1	B	351	HIS	CB-CA-C	7.79	125.98	110.40
1	B	733	LYS	CB-CA-C	-7.57	95.27	110.40
1	A	733	LYS	CB-CA-C	-7.32	95.77	110.40
1	A	734	GLY	N-CA-C	7.20	131.11	113.10
1	A	317	GLU	OE1-CD-OE2	-7.02	114.87	123.30
1	B	685	THR	CB-CA-C	-6.27	94.68	111.60
1	B	641	SER	CB-CA-C	-6.18	98.36	110.10
1	B	215	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	B	271	THR	CA-CB-CG2	5.71	120.39	112.40

There are no chirality outliers.

There are no planarity outliers.

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	6067	0	6035	184	0
1	B	6067	0	6035	185	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	3	0
4	A	444	0	0	14	0
4	B	538	0	0	19	0
All	All	13172	0	12094	374	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 (374) 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:70:LYS:H	1:A:70:LYS:HE2	1.13	1.13
1:B:70:LYS:HE2	1:B:70:LYS:H	1.13	1.13
1:B:735:ASP:HB2	1:B:737:LYS:HE3	1.27	1.13
1:A:737:LYS:HE2	1:A:737:LYS:H	1.10	1.12
1:B:737:LYS:H	1:B:737:LYS:HE2	1.10	1.11
1:B:407:ARG:HG3	1:B:407:ARG:HH11	1.17	1.05
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.18	1.05
1:B:693:TRP:CD1	1:B:715:PRO:HG3	1.97	0.99
1:A:693:TRP:CD1	1:A:715:PRO:HG3	1.98	0.99
1:A:737:LYS:HD2	1:A:738:LEU:H	1.26	0.97
1:B:679:VAL:HG21	1:B:707:ILE:HD12	1.45	0.96
1:A:679:VAL:HG21	1:A:707:ILE:HD12	1.48	0.95
1:B:737:LYS:HD2	1:B:738:LEU:H	1.28	0.94
1:B:146:THR:HG22	1:B:214:LEU:HA	1.56	0.86
1:A:146:THR:HG22	1:A:214:LEU:HA	1.55	0.86
1:B:700:VAL:HG13	1:B:706:TYR:HB2	1.57	0.85
1:A:700:VAL:HG13	1:A:706:TYR:HB2	1.57	0.85
1:B:728:LEU:HD12	1:B:728:LEU:H	1.43	0.84
1:A:115:VAL:HG11	1:A:250:LEU:HA	1.60	0.83
1:B:115:VAL:HG11	1:B:250:LEU:HA	1.60	0.83
1:B:735:ASP:HB2	1:B:737:LYS:CE	2.09	0.83
1:B:6:ARG:HB3	4:B:957:HOH:O	1.78	0.82
1:B:70:LYS:HE2	1:B:70:LYS:N	1.96	0.81
1:A:728:LEU:HD12	1:A:728:LEU:H	1.46	0.80
1:B:407:ARG:HH11	1:B:407:ARG:CG	1.94	0.80
1:A:737:LYS:HE2	1:A:737:LYS:N	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HH11	1:A:407:ARG:CG	1.95	0.79
1:B:555:PHE:CZ	1:B:585:VAL:HG21	2.17	0.78
1:A:183:SER:H	1:A:186:THR:HG23	1.47	0.78
1:B:737:LYS:HE2	1:B:737:LYS:N	1.94	0.78
1:B:183:SER:H	1:B:186:THR:HG23	1.50	0.77
1:B:311:THR:HB	1:B:315:GLU:OE1	1.86	0.75
1:A:555:PHE:CZ	1:A:585:VAL:HG21	2.21	0.75
1:B:555:PHE:HZ	1:B:585:VAL:HG21	1.53	0.74
1:B:687:LEU:H	1:B:687:LEU:HD23	1.53	0.74
1:A:311:THR:HB	1:A:315:GLU:OE1	1.86	0.74
1:A:183:SER:H	1:A:186:THR:CG2	2.00	0.73
1:A:70:LYS:HE2	1:A:70:LYS:N	1.96	0.72
1:B:70:LYS:H	1:B:70:LYS:CE	1.98	0.72
1:A:687:LEU:HD23	1:A:687:LEU:H	1.53	0.71
1:A:70:LYS:H	1:A:70:LYS:CE	1.99	0.71
1:A:735:ASP:HB2	1:A:737:LYS:HE3	1.71	0.71
3:B:1000:ADP:H5'1	3:B:1000:ADP:N3	2.06	0.71
1:B:183:SER:H	1:B:186:THR:CG2	2.03	0.71
1:A:736:VAL:H	1:A:737:LYS:HE2	1.56	0.70
1:A:376:THR:HG23	1:A:378:ILE:H	1.55	0.70
1:A:146:THR:OG1	1:A:193:ASP:HA	1.92	0.70
1:B:146:THR:OG1	1:B:193:ASP:HA	1.93	0.69
1:B:376:THR:HG23	1:B:378:ILE:H	1.57	0.69
1:A:737:LYS:CD	1:A:738:LEU:H	2.03	0.69
1:A:555:PHE:HZ	1:A:585:VAL:HG21	1.58	0.69
1:A:477:LEU:HB3	1:A:491:MET:CE	2.23	0.68
1:B:477:LEU:HB3	1:B:491:MET:CE	2.23	0.67
1:B:253:GLU:O	1:B:257:ARG:HG2	1.94	0.67
1:A:737:LYS:H	1:A:737:LYS:CE	2.00	0.67
1:A:407:ARG:HG3	1:A:407:ARG:NH1	1.99	0.67
1:A:537:GLN:HB2	4:A:804:HOH:O	1.95	0.66
1:A:49:GLU:HG3	1:A:73:PRO:HA	1.78	0.66
1:A:693:TRP:CZ2	1:A:740:LEU:HD11	2.30	0.66
1:B:221:THR:OG1	1:B:224:THR:HG23	1.96	0.66
1:B:737:LYS:CD	1:B:738:LEU:H	2.05	0.66
1:B:118:THR:HG21	1:B:381:THR:HA	1.78	0.66
1:B:693:TRP:CZ2	1:B:740:LEU:HD11	2.31	0.66
1:A:221:THR:OG1	1:A:224:THR:HG23	1.96	0.65
1:B:49:GLU:HG3	1:B:73:PRO:HA	1.78	0.65
1:B:477:LEU:HB3	1:B:491:MET:HE1	1.76	0.65
1:A:58:THR:HB	1:A:133:ASP:OD2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1000:ADP:N3	3:A:1000:ADP:H5'1	2.11	0.65
1:B:736:VAL:H	1:B:737:LYS:HE2	1.60	0.65
1:B:114:PHE:CE2	1:B:265:LEU:HD22	2.32	0.65
1:A:298:HIS:HD2	1:A:370:ARG:HD2	1.62	0.65
1:B:384:THR:HG23	4:B:836:HOH:O	1.96	0.65
1:A:702:THR:HG23	1:A:703:SER:H	1.62	0.65
1:B:527:ALA:O	1:B:531:ILE:HG12	1.97	0.64
1:A:170:GLU:O	1:A:186:THR:HG22	1.98	0.64
1:B:702:THR:HG23	1:B:703:SER:H	1.61	0.64
1:B:737:LYS:H	1:B:737:LYS:CE	2.00	0.64
1:B:298:HIS:HD2	1:B:370:ARG:HD2	1.61	0.64
1:A:537:GLN:O	1:A:637:THR:HG23	1.98	0.64
1:A:479:HIS:HE1	4:A:937:HOH:O	1.80	0.63
1:A:253:GLU:O	1:A:257:ARG:HG2	1.97	0.63
1:A:662:LYS:NZ	1:A:662:LYS:HB3	2.13	0.63
1:B:715:PRO:HB2	1:B:744:LYS:HD3	1.81	0.63
1:B:58:THR:HB	1:B:133:ASP:OD2	1.99	0.63
1:A:737:LYS:HD2	1:A:738:LEU:N	2.08	0.62
1:A:298:HIS:CD2	1:A:370:ARG:HD2	2.35	0.62
3:B:1000:ADP:H2'	4:B:1167:HOH:O	2.00	0.61
1:B:662:LYS:NZ	1:B:662:LYS:HB3	2.15	0.61
1:B:170:GLU:O	1:B:186:THR:HG22	2.00	0.61
1:A:114:PHE:CE2	1:A:265:LEU:HD22	2.36	0.61
1:A:715:PRO:HB2	1:A:744:LYS:HD3	1.81	0.61
1:B:320:VAL:O	1:B:324:SER:HB2	2.00	0.61
1:B:298:HIS:CD2	1:B:370:ARG:HD2	2.36	0.60
1:A:527:ALA:O	1:A:531:ILE:HG12	2.01	0.60
1:A:118:THR:HG21	1:A:381:THR:HA	1.82	0.60
1:A:298:HIS:HD2	1:A:370:ARG:HH11	1.50	0.60
1:A:407:ARG:HD2	1:A:493:ARG:HH11	1.67	0.60
1:A:477:LEU:HB3	1:A:491:MET:HE3	1.84	0.60
1:B:537:GLN:O	1:B:637:THR:HG23	2.02	0.60
3:B:1000:ADP:N3	3:B:1000:ADP:C5'	2.65	0.60
1:B:104:LYS:HG2	4:B:893:HOH:O	2.02	0.59
1:B:118:THR:HG23	4:B:792:HOH:O	2.01	0.59
1:A:662:LYS:HG3	1:A:693:TRP:CZ2	2.38	0.59
1:A:113:VAL:HG23	1:A:264:LEU:HD12	1.85	0.59
1:B:744:LYS:HE2	1:B:744:LYS:HA	1.85	0.59
1:B:298:HIS:HD2	1:B:370:ARG:HH11	1.50	0.58
1:B:407:ARG:HD2	1:B:493:ARG:HH11	1.68	0.58
1:A:320:VAL:O	1:A:324:SER:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LYS:HA	1:A:744:LYS:HE2	1.86	0.58
1:A:735:ASP:HB2	1:A:737:LYS:CE	2.33	0.58
1:B:384:THR:CG2	4:B:836:HOH:O	2.52	0.58
1:A:113:VAL:HG23	1:A:264:LEU:CD1	2.34	0.58
1:B:737:LYS:HD2	1:B:738:LEU:N	2.11	0.57
1:B:662:LYS:HG3	1:B:693:TRP:CZ2	2.39	0.57
1:A:662:LYS:HE3	1:A:740:LEU:CD1	2.34	0.57
1:B:193:ASP:OD2	1:B:224:THR:HG22	2.05	0.57
1:A:679:VAL:HG21	1:A:707:ILE:CD1	2.27	0.57
1:B:113:VAL:HG23	1:B:264:LEU:HD12	1.87	0.57
1:B:113:VAL:HG23	1:B:264:LEU:CD1	2.34	0.57
1:B:662:LYS:HE3	1:B:740:LEU:CD1	2.34	0.57
1:B:679:VAL:HG21	1:B:707:ILE:CD1	2.26	0.57
1:B:407:ARG:HG3	1:B:407:ARG:NH1	1.98	0.57
1:B:730:ASN:HD22	1:B:730:ASN:C	2.08	0.57
1:A:407:ARG:CG	1:A:407:ARG:NH1	2.61	0.57
1:A:592:ASP:HB3	4:A:1229:HOH:O	2.04	0.56
1:B:407:ARG:CG	1:B:407:ARG:NH1	2.60	0.56
1:A:1:MET:H1	1:A:1:MET:HE3	1.70	0.56
1:B:581:THR:O	1:B:585:VAL:HG23	2.06	0.56
1:B:403:ASN:HB3	1:B:406:ILE:HG23	1.87	0.56
1:A:53:LEU:HA	4:A:890:HOH:O	2.05	0.56
1:A:737:LYS:O	1:A:741:GLU:HG2	2.05	0.56
1:B:79:PHE:CE1	1:B:83:TYR:CE2	2.94	0.56
1:B:737:LYS:O	1:B:741:GLU:HG2	2.05	0.56
1:A:147:GLN:O	1:A:192:THR:HA	2.06	0.56
1:A:174:TYR:HA	1:A:190:TYR:O	2.05	0.56
1:A:477:LEU:HB3	1:A:491:MET:HE1	1.87	0.56
1:B:1:MET:HE3	1:B:1:MET:H1	1.71	0.56
1:B:147:GLN:O	1:B:192:THR:HA	2.06	0.55
1:A:581:THR:O	1:A:585:VAL:HG23	2.06	0.55
1:B:668:LYS:HG3	4:B:972:HOH:O	2.07	0.55
1:A:403:ASN:HB3	1:A:406:ILE:HG23	1.88	0.55
1:A:193:ASP:OD2	1:A:224:THR:HG22	2.07	0.54
1:B:83:TYR:CD2	1:B:165:ASP:HB2	2.42	0.54
1:A:730:ASN:C	1:A:730:ASN:HD22	2.09	0.54
1:B:289:SER:O	1:B:293:THR:HG22	2.06	0.54
1:A:81:PRO:O	1:A:84:VAL:HG22	2.08	0.54
1:A:423:GLN:HE21	1:A:423:GLN:HA	1.72	0.54
1:B:734:GLY:O	1:B:735:ASP:C	2.45	0.54
1:A:543:LEU:HD22	1:A:620:ARG:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PRO:O	1:B:84:VAL:HG22	2.08	0.54
1:B:174:TYR:HA	1:B:190:TYR:O	2.08	0.53
1:B:289:SER:O	1:B:293:THR:CG2	2.56	0.53
1:B:339:LEU:HD11	1:B:372:VAL:CG2	2.38	0.53
1:A:657:PHE:CE2	1:A:658:MET:HG3	2.43	0.53
3:A:1000:ADP:N3	3:A:1000:ADP:C5'	2.71	0.53
1:B:376:THR:CG2	1:B:378:ILE:HG13	2.38	0.53
1:A:355:ARG:HD2	4:A:945:HOH:O	2.08	0.53
1:A:230:LEU:HD21	1:A:472:LEU:HD13	1.91	0.53
1:A:289:SER:O	1:A:293:THR:HG22	2.08	0.53
1:A:728:LEU:HB3	1:A:738:LEU:HD21	1.90	0.53
1:B:423:GLN:HE21	1:B:423:GLN:HA	1.73	0.53
1:B:728:LEU:HB3	1:B:738:LEU:HD21	1.91	0.53
1:B:662:LYS:HE2	1:B:736:VAL:CG1	2.39	0.53
1:A:662:LYS:HE2	1:A:736:VAL:CG1	2.39	0.53
1:B:543:LEU:HD22	1:B:620:ARG:HG3	1.91	0.53
1:A:119:GLY:HA2	1:A:384:THR:HG21	1.91	0.53
1:A:579:HIS:HE1	4:A:913:HOH:O	1.91	0.53
1:B:36:LEU:H	1:B:36:LEU:CD2	2.21	0.52
1:A:302:GLU:O	1:A:370:ARG:NH2	2.42	0.52
1:B:170:GLU:O	1:B:186:THR:HA	2.10	0.52
1:A:339:LEU:HD11	1:A:372:VAL:CG2	2.40	0.52
1:B:406:ILE:O	1:B:406:ILE:HG13	2.10	0.52
1:A:516:LEU:HD22	4:A:1070:HOH:O	2.09	0.52
4:B:1020:HOH:O	1:A:351:HIS:HD2	1.93	0.51
1:A:338:PRO:HD2	1:A:369:GLY:HA2	1.92	0.51
1:B:298:HIS:CD2	1:B:370:ARG:HH11	2.29	0.51
1:B:657:PHE:CE2	1:B:658:MET:HG3	2.46	0.51
1:A:406:ILE:HG13	1:A:406:ILE:O	2.11	0.51
1:A:619:ILE:HG22	1:A:623:LEU:HD22	1.93	0.51
1:A:693:TRP:HZ2	1:A:740:LEU:HD11	1.71	0.51
1:A:289:SER:O	1:A:293:THR:CG2	2.59	0.51
1:A:36:LEU:CD2	1:A:36:LEU:H	2.24	0.51
1:B:693:TRP:HZ2	1:B:740:LEU:HD11	1.73	0.51
1:B:149:ARG:HD2	1:B:382:SER:OG	2.11	0.50
1:A:531:ILE:HD13	1:A:632:LEU:HD11	1.92	0.50
1:B:539:SER:O	1:B:543:LEU:HB2	2.11	0.50
1:A:150:ARG:NH2	1:A:348:LEU:O	2.44	0.50
1:B:423:GLN:HA	1:B:423:GLN:NE2	2.27	0.50
1:B:619:ILE:HG22	1:B:623:LEU:HD22	1.94	0.50
1:B:740:LEU:HD13	1:B:741:GLU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:O	1:A:232:LYS:C	2.49	0.50
1:A:674:LYS:O	1:A:675:ASP:HB2	2.12	0.50
1:B:60:ALA:O	1:B:64:GLN:HG3	2.12	0.50
1:B:119:GLY:HA2	1:B:384:THR:HG21	1.93	0.50
1:A:298:HIS:CD2	1:A:370:ARG:HH11	2.30	0.50
1:A:539:SER:O	1:A:543:LEU:HB2	2.12	0.50
1:A:692:GLU:HG3	1:A:693:TRP:HD1	1.77	0.50
1:A:423:GLN:HA	1:A:423:GLN:NE2	2.26	0.50
1:B:110:GLN:CD	1:B:235:VAL:HG22	2.32	0.50
1:B:738:LEU:HD13	1:B:742:ARG:NH2	2.27	0.50
1:A:180:ASN:HB2	4:A:1148:HOH:O	2.10	0.50
1:B:302:GLU:HG2	4:B:1095:HOH:O	2.12	0.49
1:A:231:LEU:HB3	1:A:243:ILE:HD13	1.94	0.49
1:B:150:ARG:HG3	1:B:176:ILE:HG21	1.94	0.49
1:A:193:ASP:OD2	1:A:224:THR:CG2	2.60	0.49
1:A:6:ARG:HG2	4:A:1203:HOH:O	2.13	0.49
1:B:79:PHE:CE1	1:B:83:TYR:CZ	3.00	0.49
1:A:580:ILE:CD1	1:A:648:ILE:HG21	2.42	0.49
1:A:60:ALA:O	1:A:64:GLN:HG3	2.13	0.48
1:A:170:GLU:O	1:A:186:THR:HA	2.12	0.48
1:B:230:LEU:HD21	1:B:472:LEU:HD13	1.96	0.48
1:A:150:ARG:HG3	1:A:176:ILE:HG21	1.96	0.48
1:A:231:LEU:HB3	1:A:243:ILE:CD1	2.43	0.48
1:A:110:GLN:CD	1:A:235:VAL:HG22	2.34	0.48
1:A:230:LEU:HD11	1:A:472:LEU:HD13	1.96	0.48
1:B:477:LEU:HB3	1:B:491:MET:HE3	1.96	0.48
1:B:302:GLU:O	1:B:370:ARG:NH2	2.47	0.48
1:B:674:LYS:O	1:B:675:ASP:HB2	2.14	0.48
1:B:692:GLU:HG3	1:B:693:TRP:HD1	1.77	0.48
1:A:662:LYS:HG3	1:A:693:TRP:CE2	2.49	0.48
1:B:537:GLN:HG2	1:B:637:THR:HG22	1.96	0.48
1:A:149:ARG:HD2	1:A:382:SER:OG	2.14	0.48
1:A:740:LEU:HD13	1:A:741:GLU:N	2.28	0.48
1:B:183:SER:O	1:B:186:THR:HG23	2.14	0.47
1:B:407:ARG:O	1:B:407:ARG:HG2	2.14	0.47
1:A:466:VAL:HG13	1:A:477:LEU:HD11	1.97	0.47
1:B:193:ASP:OD2	1:B:224:THR:CG2	2.61	0.47
1:B:696:TYR:CB	1:B:707:ILE:HG23	2.44	0.47
1:A:714:ARG:HB2	1:A:717:TRP:CD2	2.50	0.47
1:B:1:MET:HA	4:B:1055:HOH:O	2.15	0.47
1:A:738:LEU:HD13	1:A:742:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:CG2	1:A:214:LEU:HA	2.36	0.47
1:A:183:SER:O	1:A:186:THR:HG23	2.15	0.47
1:A:407:ARG:O	1:A:407:ARG:HG2	2.15	0.46
1:A:662:LYS:HB3	1:A:662:LYS:HZ3	1.80	0.46
1:A:696:TYR:CB	1:A:707:ILE:HG23	2.45	0.46
1:B:531:ILE:HD13	1:B:632:LEU:HD11	1.96	0.46
1:B:662:LYS:HG3	1:B:693:TRP:CE2	2.50	0.46
1:A:457:ILE:HD11	1:A:486:PRO:HG3	1.98	0.46
1:B:338:PRO:HD2	1:B:369:GLY:HA2	1.97	0.46
1:B:743:ILE:O	1:B:747:VAL:HG23	2.15	0.46
1:B:154:MET:CE	1:B:350:PRO:HG3	2.46	0.46
1:A:624:GLU:HG3	1:A:634:LEU:HD11	1.97	0.46
1:A:735:ASP:O	1:A:736:VAL:HG22	2.15	0.46
1:B:231:LEU:HB3	1:B:243:ILE:HD13	1.98	0.46
1:B:466:VAL:HG13	1:B:477:LEU:HD11	1.98	0.46
1:B:579:HIS:HD2	1:B:711:THR:OG1	1.99	0.46
1:A:537:GLN:HG2	1:A:637:THR:HG22	1.97	0.46
1:B:230:LEU:HD11	1:B:472:LEU:HD13	1.97	0.46
1:A:423:GLN:HE21	1:A:423:GLN:CA	2.28	0.46
1:B:238:ARG:HB2	1:B:240:ASP:OD1	2.16	0.45
1:A:693:TRP:CZ2	1:A:740:LEU:HD21	2.51	0.45
1:A:736:VAL:O	1:A:740:LEU:HD12	2.16	0.45
1:A:743:ILE:O	1:A:747:VAL:HG23	2.16	0.45
1:A:680:LEU:HD12	1:A:680:LEU:N	2.32	0.45
1:B:258:TYR:CG	1:B:483:MET:HE2	2.52	0.45
1:B:177:ARG:O	1:B:178:PHE:HB2	2.17	0.45
1:A:258:TYR:CG	1:A:483:MET:HE2	2.51	0.45
1:B:474:ILE:HD13	1:B:480:PHE:CE1	2.51	0.45
1:A:664:ARG:HD2	1:A:667:ALA:HB3	1.98	0.45
1:B:736:VAL:O	1:B:740:LEU:HD12	2.17	0.45
1:B:624:GLU:HG3	1:B:634:LEU:HD11	1.99	0.45
1:B:680:LEU:N	1:B:680:LEU:HD12	2.32	0.45
1:B:693:TRP:CZ2	1:B:740:LEU:HD21	2.52	0.45
1:B:714:ARG:HB2	1:B:717:TRP:CD2	2.52	0.45
1:A:474:ILE:HD13	1:A:480:PHE:CE1	2.52	0.45
1:A:579:HIS:HD2	1:A:711:THR:OG1	2.00	0.45
1:A:735:ASP:CB	1:A:737:LYS:HE3	2.43	0.45
1:B:146:THR:CG2	1:B:214:LEU:HA	2.39	0.44
1:B:579:HIS:HE1	4:B:994:HOH:O	2.00	0.44
1:A:177:ARG:O	1:A:178:PHE:HB2	2.17	0.44
1:A:376:THR:CG2	1:A:378:ILE:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ASP:O	1:A:736:VAL:CG2	2.65	0.44
1:B:664:ARG:HD2	1:B:667:ALA:HB3	2.00	0.44
1:B:740:LEU:HD13	1:B:740:LEU:C	2.38	0.44
1:A:238:ARG:HB2	1:A:240:ASP:OD1	2.18	0.44
1:A:118:THR:HG23	4:A:942:HOH:O	2.16	0.44
1:A:214:LEU:HD11	1:A:231:LEU:HD12	2.00	0.44
1:A:740:LEU:HD23	4:A:918:HOH:O	2.18	0.44
1:B:16:GLU:HB2	4:B:816:HOH:O	2.18	0.44
1:B:231:LEU:HB3	1:B:243:ILE:CD1	2.47	0.44
1:A:10:GLU:H	1:A:10:GLU:HG2	1.46	0.44
1:B:150:ARG:NH2	1:B:348:LEU:O	2.51	0.44
1:B:723:PRO:HD2	4:B:1243:HOH:O	2.18	0.44
1:B:62:GLU:O	1:B:66:LEU:HD22	2.18	0.43
1:B:214:LEU:HD11	1:B:231:LEU:HD12	2.00	0.43
1:B:650:LYS:HE2	1:B:717:TRP:CD1	2.54	0.43
1:B:580:ILE:CD1	1:B:648:ILE:HG21	2.49	0.43
1:B:662:LYS:HB3	1:B:662:LYS:HZ3	1.82	0.43
1:B:543:LEU:HD13	1:B:620:ARG:CZ	2.48	0.43
1:B:520:PHE:HA	1:B:521:PRO:HD3	1.91	0.43
1:A:115:VAL:CG1	1:A:250:LEU:HA	2.41	0.43
1:B:10:GLU:H	1:B:10:GLU:HG2	1.46	0.43
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.85	0.43
1:B:350:PRO:O	1:B:351:HIS:C	2.54	0.43
1:B:354:GLN:NE2	4:B:1127:HOH:O	2.51	0.43
1:B:737:LYS:CG	1:B:738:LEU:N	2.82	0.43
1:B:58:THR:HG23	1:B:59:SER:N	2.34	0.43
1:A:403:ASN:O	1:A:407:ARG:N	2.51	0.43
1:A:740:LEU:HD13	1:A:740:LEU:C	2.39	0.43
1:B:745:GLU:O	1:B:749:ARG:HG3	2.19	0.42
1:A:744:LYS:HA	1:A:744:LYS:CE	2.49	0.42
1:B:151:VAL:HG11	1:B:344:LEU:HD11	2.00	0.42
1:B:403:ASN:O	1:B:407:ARG:N	2.51	0.42
1:A:737:LYS:CG	1:A:738:LEU:N	2.82	0.42
1:A:296:GLN:HE21	1:A:296:GLN:HB2	1.67	0.42
1:B:88:LYS:HG3	1:B:89:ILE:N	2.34	0.42
1:B:355:ARG:HD2	4:B:1146:HOH:O	2.19	0.42
1:B:93:LEU:HA	1:B:94:PRO:HD3	1.93	0.42
1:B:296:GLN:HE21	1:B:296:GLN:HB2	1.67	0.42
1:B:302:GLU:HG2	1:B:302:GLU:H	1.65	0.42
1:B:715:PRO:HB2	1:B:744:LYS:CD	2.48	0.42
1:A:338:PRO:HD2	1:A:369:GLY:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:HIS:CE1	4:A:937:HOH:O	2.63	0.42
1:B:339:LEU:HD11	1:B:372:VAL:HG23	2.02	0.42
1:B:662:LYS:HE2	1:B:736:VAL:HG12	2.01	0.42
1:A:93:LEU:HA	1:A:94:PRO:HD3	1.93	0.42
1:A:537:GLN:NE2	4:A:1128:HOH:O	2.52	0.42
1:B:744:LYS:HA	1:B:744:LYS:CE	2.49	0.42
1:A:251:ASP:OD2	1:A:251:ASP:C	2.57	0.42
1:A:520:PHE:HA	1:A:521:PRO:HD3	1.93	0.42
1:A:723:PRO:HD2	4:A:912:HOH:O	2.20	0.42
1:B:164:MET:O	1:B:166:VAL:HG13	2.20	0.41
1:A:88:LYS:HG3	1:A:89:ILE:N	2.35	0.41
1:A:733:LYS:N	1:A:733:LYS:HE2	2.35	0.41
1:B:457:ILE:HD11	1:B:486:PRO:HG3	2.03	0.41
1:A:119:GLY:CA	1:A:384:THR:HG21	2.49	0.41
1:B:641:SER:O	1:B:643:LYS:N	2.53	0.41
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.84	0.41
1:A:177:ARG:HG2	1:A:178:PHE:CD2	2.55	0.41
1:A:696:TYR:CD1	1:A:707:ILE:HD13	2.55	0.41
1:B:516:LEU:CD2	1:B:531:ILE:HD12	2.51	0.41
1:B:733:LYS:HE2	1:B:733:LYS:N	2.36	0.41
1:B:734:GLY:HA2	4:B:1319:HOH:O	2.21	0.41
1:A:353:GLN:O	1:A:356:ILE:HG12	2.21	0.41
1:A:697:ASN:HB3	1:A:709:THR:HB	2.02	0.41
1:B:29:GLU:HB3	4:B:1190:HOH:O	2.20	0.41
1:B:283:GLN:HE21	1:B:283:GLN:CA	2.33	0.41
1:B:507:GLU:HG3	4:B:1361:HOH:O	2.20	0.41
1:A:580:ILE:HD11	1:A:648:ILE:HG21	2.01	0.41
1:A:693:TRP:HZ2	1:A:740:LEU:HD21	1.85	0.41
1:A:745:GLU:O	1:A:749:ARG:HG3	2.19	0.41
1:B:88:LYS:HB2	1:B:88:LYS:HE2	1.90	0.41
1:A:737:LYS:HZ3	1:A:737:LYS:HB3	1.86	0.41
1:B:664:ARG:HB2	1:B:669:GLY:O	2.20	0.41
1:A:62:GLU:O	1:A:66:LEU:HD22	2.21	0.41
1:B:423:GLN:HE21	1:B:423:GLN:CA	2.29	0.41
1:B:740:LEU:O	1:B:740:LEU:HD22	2.20	0.41
1:B:36:LEU:N	1:B:36:LEU:HD23	2.36	0.41
1:B:251:ASP:OD2	1:B:251:ASP:C	2.59	0.41
1:A:154:MET:CE	1:A:350:PRO:HG3	2.51	0.41
1:A:715:PRO:HB2	1:A:744:LYS:CD	2.48	0.41
1:B:696:TYR:CD1	1:B:707:ILE:HD13	2.56	0.41
1:A:72:ASN:HA	1:A:73:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:O	1:A:166:VAL:HG13	2.21	0.41
1:A:557:ARG:NH1	1:A:562:LYS:HD3	2.36	0.41
1:A:623:LEU:HD12	1:A:623:LEU:HA	1.89	0.41
1:A:662:LYS:HE2	1:A:736:VAL:HG12	2.01	0.41
1:A:151:VAL:HG11	1:A:344:LEU:HD11	2.03	0.40
1:B:36:LEU:H	1:B:36:LEU:HD23	1.87	0.40
1:B:194:GLY:HA3	4:B:838:HOH:O	2.20	0.40
1:A:537:GLN:CG	1:A:637:THR:HG22	2.52	0.40
1:B:537:GLN:CG	1:B:637:THR:HG22	2.51	0.40
1:B:177:ARG:HG2	1:B:178:PHE:CD2	2.56	0.40
1:B:516:LEU:HG	1:B:531:ILE:CD1	2.51	0.40
1:A:176:ILE:HG22	1:A:177:ARG:N	2.37	0.40
1:A:650:LYS:HE2	1:A:717:TRP:CD1	2.57	0.40
1:B:119:GLY:CA	1:B:384:THR:HG21	2.50	0.40
1:B:579:HIS:CD2	1:B:711:THR:OG1	2.74	0.40
1:A:230:LEU:HD11	1:A:472:LEU:CD1	2.52	0.40
1:A:516:LEU:CD2	1:A:531:ILE:HD12	2.51	0.40
1:A:579:HIS:CD2	1:A:711:THR:OG1	2.75	0.40
1:A:735:ASP:H	1:A:737:LYS:HE3	1.86	0.40
1:A:740:LEU:O	1:A:740:LEU:HD22	2.22	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	753/767 (98%)	723 (96%)	29 (4%)	1 (0%)	51	60
1	B	753/767 (98%)	722 (96%)	31 (4%)	0	100	100
All	All	1506/1534 (98%)	1445 (96%)	60 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	668/679 (98%)	622 (93%)	46 (7%)	15	16
1	B	668/679 (98%)	619 (93%)	49 (7%)	14	15
All	All	1336/1358 (98%)	1241 (93%)	95 (7%)	14	16

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	10	GLU
1	B	36	LEU
1	B	58	THR
1	B	70	LYS
1	B	71	ILE
1	B	92	GLU
1	B	118	THR
1	B	156	VAL
1	B	186	THR
1	B	197	LEU
1	B	222	LEU
1	B	224	THR
1	B	235	VAL
1	B	238	ARG
1	B	251	ASP
1	B	283	GLN
1	B	284	ARG
1	B	293	THR
1	B	311	THR
1	B	324	SER
1	B	384	THR
1	B	403	ASN

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Mol	Chain	Res	Type
1	B	406	ILE
1	B	407	ARG
1	B	408	VAL
1	B	412	LEU
1	B	427	ARG
1	B	460	SER
1	B	464	SER
1	B	489	GLU
1	B	507	GLU
1	B	510	LEU
1	B	543	LEU
1	B	551	VAL
1	B	608	LEU
1	B	623	LEU
1	B	662	LYS
1	B	686	VAL
1	B	687	LEU
1	B	699	PHE
1	B	702	THR
1	B	707	ILE
1	B	730	ASN
1	B	735	ASP
1	B	737	LYS
1	B	738	LEU
1	B	740	LEU
1	B	753	LEU
1	A	1	MET
1	A	10	GLU
1	A	36	LEU
1	A	58	THR
1	A	70	LYS
1	A	71	ILE
1	A	92	GLU
1	A	118	THR
1	A	156	VAL
1	A	186	THR
1	A	197	LEU
1	A	222	LEU
1	A	224	THR
1	A	235	VAL
1	A	238	ARG
1	A	251	ASP

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Mol	Chain	Res	Type
1	A	283	GLN
1	A	284	ARG
1	A	293	THR
1	A	311	THR
1	A	324	SER
1	A	384	THR
1	A	403	ASN
1	A	406	ILE
1	A	407	ARG
1	A	408	VAL
1	A	412	LEU
1	A	460	SER
1	A	464	SER
1	A	489	GLU
1	A	507	GLU
1	A	510	LEU
1	A	543	LEU
1	A	608	LEU
1	A	623	LEU
1	A	662	LYS
1	A	686	VAL
1	A	687	LEU
1	A	699	PHE
1	A	702	THR
1	A	707	ILE
1	A	730	ASN
1	A	737	LYS
1	A	738	LEU
1	A	740	LEU
1	A	753	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	GLN
1	B	260	ASN
1	B	283	GLN
1	B	296	GLN
1	B	298	HIS
1	B	353	GLN
1	B	403	ASN
1	B	422	GLN

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Mol	Chain	Res	Type
1	B	423	GLN
1	B	452	GLN
1	B	579	HIS
1	B	647	ASN
1	B	659	GLN
1	B	730	ASN
1	A	54	GLN
1	A	283	GLN
1	A	296	GLN
1	A	298	HIS
1	A	353	GLN
1	A	403	ASN
1	A	422	GLN
1	A	423	GLN
1	A	452	GLN
1	A	579	HIS
1	A	647	ASN
1	A	730	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	A	1000	2	24,29,29	1.38	4 (16%)	29,45,45	1.42	3 (10%)
3	ADP	B	1000	2	24,29,29	1.39	4 (16%)	29,45,45	1.39	3 (10%)

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	A	1000	2	-	3/12/32/32	0/3/3/3
3	ADP	B	1000	2	-	3/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	ADP	O4'-C1'	3.99	1.46	1.41
3	B	1000	ADP	O4'-C1'	3.94	1.46	1.41
3	A	1000	ADP	C5-C4	2.59	1.47	1.40
3	A	1000	ADP	C2-N3	2.52	1.36	1.32
3	B	1000	ADP	C5-C4	2.46	1.47	1.40
3	B	1000	ADP	C2-N3	2.44	1.36	1.32
3	A	1000	ADP	C2'-C1'	2.18	1.57	1.53
3	B	1000	ADP	C2'-C1'	2.10	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1000	ADP	C3'-C2'-C1'	4.25	107.37	100.98
3	B	1000	ADP	C3'-C2'-C1'	4.10	107.16	100.98
3	A	1000	ADP	O5'-C5'-C4'	-2.91	98.97	108.99
3	B	1000	ADP	O5'-C5'-C4'	-2.85	99.19	108.99
3	A	1000	ADP	O4'-C1'-C2'	-2.31	103.55	106.93
3	B	1000	ADP	O4'-C4'-C3'	2.29	109.64	105.11

There are no chirality outliers.
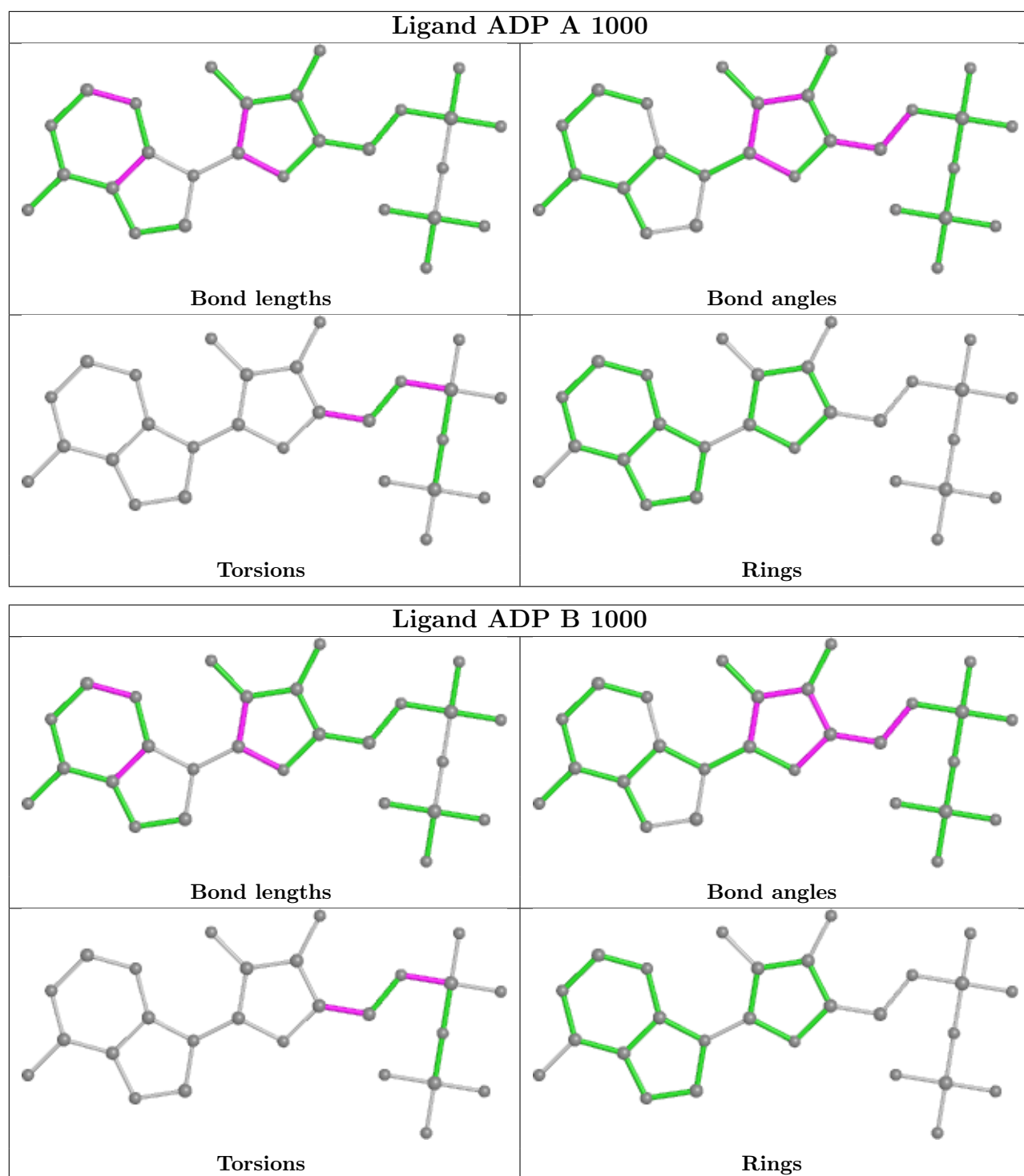
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1000	ADP	O4'-C4'-C5'-O5'
3	A	1000	ADP	O4'-C4'-C5'-O5'
3	B	1000	ADP	C3'-C4'-C5'-O5'
3	A	1000	ADP	C3'-C4'-C5'-O5'
3	B	1000	ADP	C5'-O5'-PA-O2A
3	A	1000	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	ADP	2	0
3	B	1000	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 1000

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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	A	755/767 (98%)	0.19	43 (5%)	23	22	23, 48, 100, 191	0
1	B	755/767 (98%)	0.02	26 (3%)	45	43	22, 44, 100, 191	0
All	All	1510/1534 (98%)	0.11	69 (4%)	32	31	22, 46, 100, 191	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	14.5
1	A	1	MET	13.5
1	B	755	GLN	9.7
1	B	754	LYS	9.6
1	A	754	LYS	8.3
1	A	753	LEU	7.9
1	A	755	GLN	7.1
1	B	668	LYS	5.9
1	B	735	ASP	5.6
1	B	751	ASN	5.5
1	A	734	GLY	5.4
1	B	405	ARG	4.6
1	A	404	PRO	4.6
1	A	690	ASP	4.3
1	A	733	LYS	4.3
1	B	733	LYS	4.2
1	A	748	ASP	4.0
1	A	252	ALA	3.9
1	A	735	ASP	3.9
1	B	702	THR	3.8
1	B	753	LEU	3.7
1	A	689	HIS	3.5
1	B	732	GLN	3.4
1	A	732	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	668	LYS	3.3
1	A	669	GLY	3.3
1	A	34	HIS	3.2
1	A	250	LEU	3.2
1	B	2	GLY	3.2
1	B	747	VAL	3.2
1	B	734	GLY	3.1
1	A	740	LEU	3.1
1	B	407	ARG	3.1
1	A	405	ARG	3.1
1	A	2	GLY	3.1
1	A	751	ASN	3.0
1	B	406	ILE	3.0
1	B	250	LEU	2.9
1	A	559	THR	2.9
1	A	749	ARG	2.8
1	A	595	TYR	2.8
1	B	252	ALA	2.7
1	B	749	ARG	2.6
1	B	741	GLU	2.6
1	A	78	GLU	2.6
1	A	63	ALA	2.6
1	A	35	PRO	2.5
1	B	750	LEU	2.4
1	A	687	LEU	2.4
1	A	752	GLU	2.4
1	A	253	GLU	2.3
1	B	746	LYS	2.3
1	A	83	TYR	2.3
1	A	43	VAL	2.3
1	B	378	ILE	2.3
1	B	151	VAL	2.2
1	A	572	PHE	2.2
1	A	53	LEU	2.2
1	A	699	PHE	2.2
1	A	92	GLU	2.2
1	A	47	ALA	2.1
1	A	257	ARG	2.1
1	B	596	GLU	2.1
1	A	76	GLY	2.1
1	A	70	LYS	2.1
1	A	376	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	146	THR	2.1
1	A	592	ASP	2.0
1	A	565	ALA	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

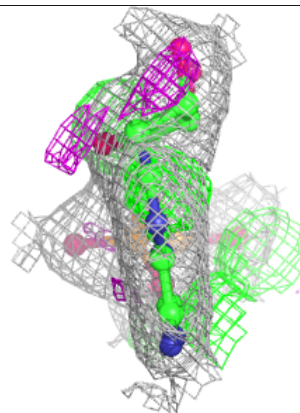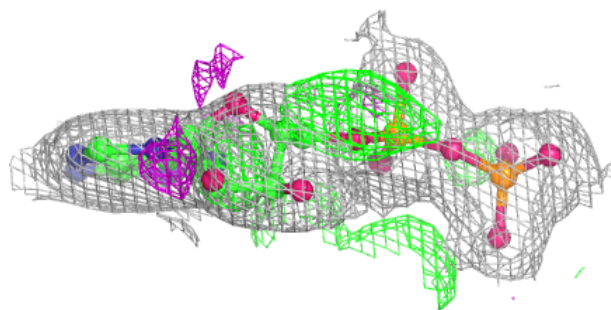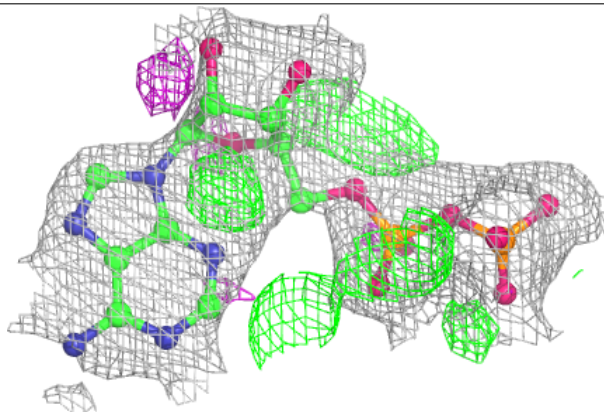| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	B	1000	27/27	0.95	0.19	23,54,71,84	0
3	ADP	A	1000	27/27	0.95	0.16	26,50,70,83	0
2	MG	B	800	1/1	0.96	0.18	32,32,32,32	0
2	MG	A	800	1/1	0.98	0.19	31,31,31,31	0

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 1000:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
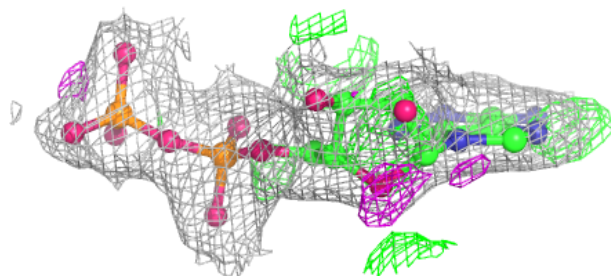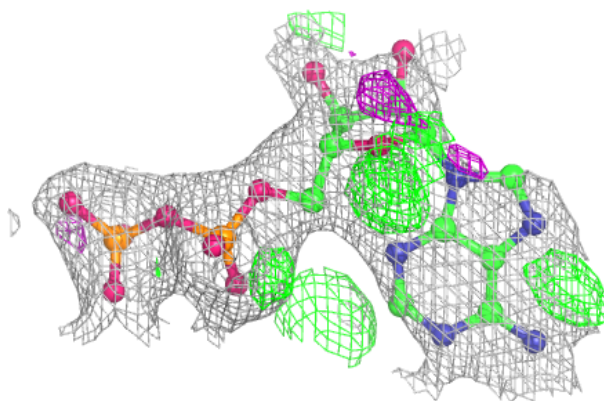
Electron density around ADP A 1000:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.