



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:37 PM UTC

PDB ID : 4FRZ / pdb_00004frz
Title : Arabidopsis KCBP motor domain dimerized via regulatory domain
Authors : Vinogradova, M.
Deposited on : 2012-06-26
Resolution : 2.40 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

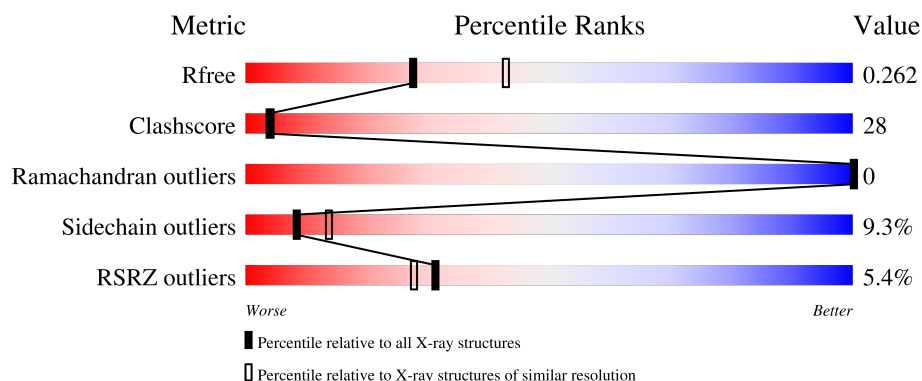
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	386	5% 50% 34% 8% 8%
1	B	386	5% 51% 31% 8% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMD	A	1304	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5831 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 calmodulin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2840	1776	501	550	13			
1	B	349	Total	C	N	O	S	0	0	0
			2805	1761	492	540	12			

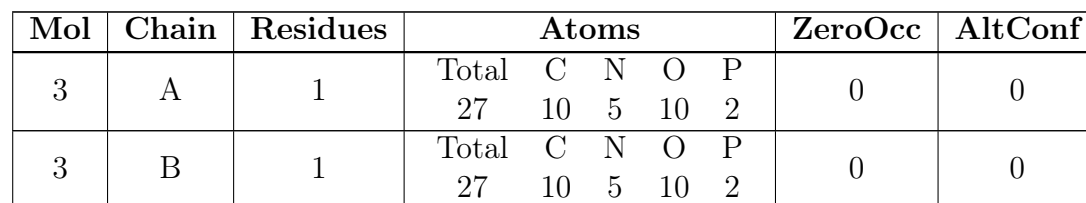
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1131	ASN	CYS	engineered mutation	UNP Q9FHN8
B	1131	ASN	CYS	engineered mutation	UNP Q9FHN8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0
4	A	1	Total C N 5 3 2	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

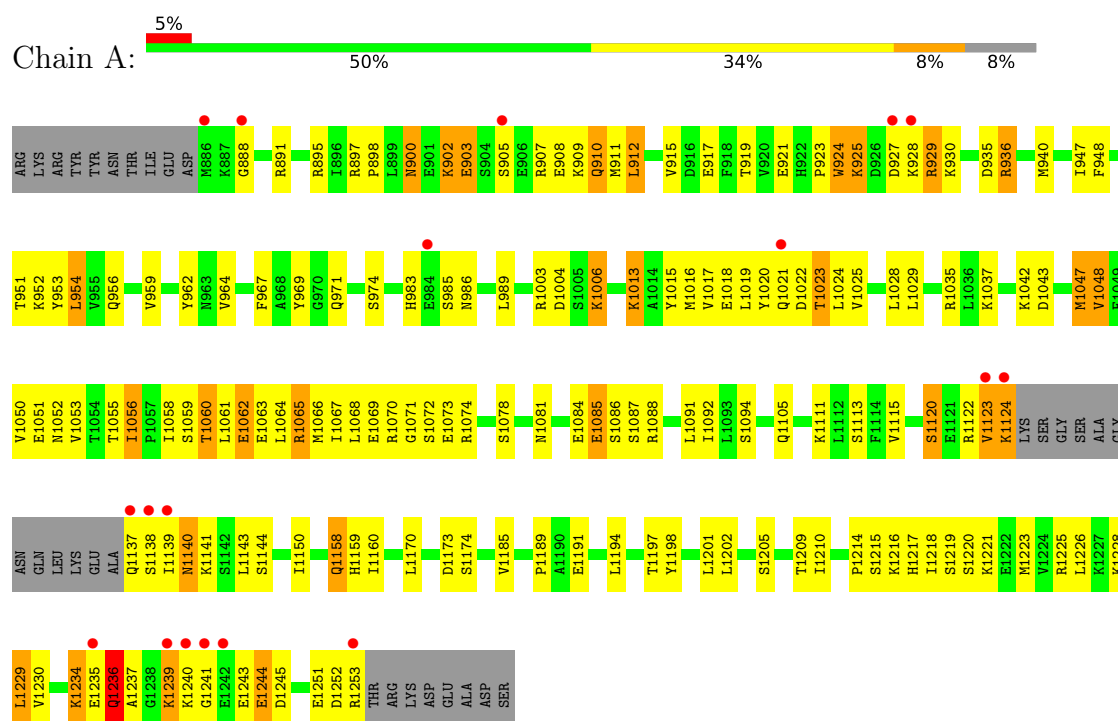
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	44	Total	O	0	0
			44	44		

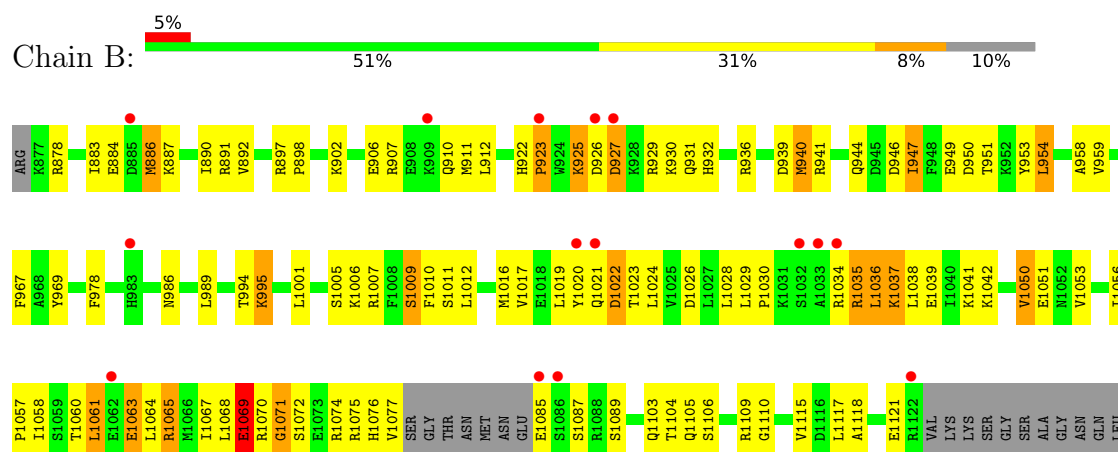
3 Residue-property plots

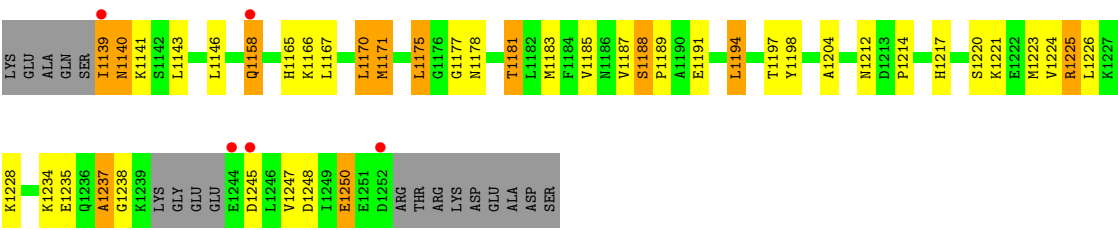
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Kinesin-like calmodulin-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.71Å 75.07Å 120.60Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 25.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.40) 91.9 (25.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , (Not available) 0.225 , 0.262	Depositor DCC
R_{free} test set	2948 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5831	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, IMD, EDO, 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	0.72	5/2881 (0.2%)	1.18	26/3869 (0.7%)
1	B	0.68	4/2846 (0.1%)	1.17	21/3822 (0.5%)
All	All	0.70	9/5727 (0.2%)	1.17	47/7691 (0.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	924	TRP	C-N	10.00	1.47	1.33
1	A	925	LYS	C-O	-7.30	1.15	1.23
1	B	883	ILE	CA-CB	-7.10	1.46	1.54
1	A	1047	MET	SD-CE	-6.48	1.63	1.79
1	B	1005	SER	CA-C	-6.27	1.44	1.52
1	B	1006	LYS	N-CA	-6.26	1.38	1.46
1	A	1229	LEU	CA-C	-5.86	1.45	1.52
1	B	1037	LYS	N-CA	-5.68	1.39	1.46
1	A	1023	THR	N-CA	-5.39	1.39	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1140	ASN	N-CA-C	-11.54	99.31	113.50
1	A	925	LYS	N-CA-C	9.66	123.86	110.24
1	A	1056	ILE	N-CA-C	9.32	118.05	107.89
1	B	1074	ARG	N-CA-C	-8.96	101.03	114.64
1	A	1138	SER	N-CA-C	-8.34	102.19	111.28
1	A	1251	GLU	N-CA-C	8.13	123.39	113.38
1	A	986	ASN	CA-C-N	8.02	128.08	119.90
1	A	986	ASN	C-N-CA	8.02	128.08	119.90
1	A	1243	GLU	N-CA-C	-7.82	98.91	110.48
1	B	940	MET	N-CA-C	7.63	122.26	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1236	GLN	N-CA-C	-7.03	104.71	113.28
1	A	928	LYS	N-CA-C	-6.85	96.03	108.02
1	B	923	PRO	N-CA-CB	6.74	110.33	103.25
1	B	1237	ALA	N-CA-C	-6.73	104.02	111.36
1	A	903	GLU	N-CA-C	-6.72	103.65	110.97
1	A	1252	ASP	N-CA-C	6.40	120.08	109.96
1	B	995	LYS	N-CA-C	-6.40	104.31	111.28
1	B	1065	ARG	N-CA-C	-6.29	104.50	111.36
1	B	1141	LYS	N-CA-C	-6.17	104.10	111.69
1	B	886	MET	N-CA-C	-6.15	105.81	113.38
1	B	1063	GLU	N-CA-C	-6.13	104.71	111.82
1	A	964	VAL	N-CA-C	6.08	116.69	108.17
1	B	878	ARG	N-CA-C	-5.92	100.25	109.72
1	B	883	ILE	CB-CA-C	-5.87	104.35	112.04
1	A	1234	LYS	N-CA-C	-5.84	104.92	111.28
1	A	923	PRO	N-CA-CB	5.80	109.34	103.25
1	A	915	VAL	CB-CA-C	-5.79	104.57	111.81
1	B	1071	GLY	N-CA-C	-5.70	105.89	112.73
1	B	1022	ASP	CB-CA-C	-5.64	102.64	111.39
1	A	1087	SER	N-CA-C	-5.61	106.21	113.16
1	B	927	ASP	CB-CA-C	-5.57	102.71	111.51
1	B	1181	THR	N-CA-C	5.54	117.93	108.90
1	A	1086	SER	N-CA-C	-5.51	102.85	110.35
1	A	989	LEU	N-CA-C	5.51	117.09	111.14
1	A	1019	LEU	CA-C-N	-5.50	114.30	122.56
1	A	1019	LEU	C-N-CA	-5.50	114.30	122.56
1	A	1218	ILE	N-CA-C	5.49	115.79	108.11
1	A	1229	LEU	CB-CA-C	-5.47	102.26	110.90
1	B	1087	SER	N-CA-C	-5.44	106.31	113.17
1	A	1022	ASP	N-CA-C	-5.37	107.09	113.38
1	B	1009	SER	N-CA-C	-5.28	100.57	109.07
1	B	1250	GLU	CB-CA-C	-5.20	101.39	112.63
1	A	936	ARG	CB-CA-C	5.16	118.03	109.72
1	B	989	LEU	N-CA-C	5.16	116.59	110.97
1	A	910	GLN	N-CA-C	-5.16	102.06	110.20
1	B	1069	GLU	N-CA-C	5.05	116.86	111.36
1	A	1084	GLU	N-CA-C	5.05	117.08	109.41

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	2840	0	2862	163	0
1	B	2805	0	2826	164	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	15	0	15	10	0
4	B	5	0	5	0	0
5	A	4	0	6	0	0
5	B	8	0	12	3	0
6	A	54	0	0	2	0
6	B	44	0	0	4	0
All	All	5831	0	5750	323	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 28.

All (323) 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:1234:LYS:HD3	1:A:1241:GLY:CA	1.38	1.48
1:A:1234:LYS:CD	1:A:1241:GLY:HA2	1.43	1.43
1:B:1024:LEU:HD22	1:B:1038:LEU:CD1	1.73	1.19
1:A:1047:MET:CE	4:A:1304:IMD:H4	1.78	1.13
1:A:1047:MET:HE3	4:A:1304:IMD:H4	1.11	1.08
1:B:1024:LEU:CD2	1:B:1038:LEU:CD1	2.32	1.06
1:B:1139:ILE:HG12	1:B:1140:ASN:H	1.25	1.02
1:A:1020:TYR:CD2	1:A:1021:GLN:HG3	1.94	1.02
1:A:1137:GLN:N	1:A:1140:ASN:HD22	1.58	1.01
1:B:1024:LEU:HD22	1:B:1038:LEU:HD12	1.38	0.99
1:A:1016:MET:HE3	1:A:1071:GLY:HA3	1.43	0.99
1:B:1158:GLN:HE21	1:B:1158:GLN:HA	1.28	0.98
1:A:1047:MET:HE3	4:A:1304:IMD:C4	1.95	0.96
1:B:1024:LEU:CD2	1:B:1038:LEU:HD13	1.94	0.95
1:B:1024:LEU:HD22	1:B:1038:LEU:HD13	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:LEU:CD2	1:B:1038:LEU:HD12	1.93	0.94
1:B:1019:LEU:HD12	1:B:1023:THR:O	1.69	0.93
1:B:1139:ILE:HG12	1:B:1140:ASN:N	1.85	0.91
1:B:1029:LEU:HD21	1:B:1035:ARG:HG2	1.52	0.88
1:B:1139:ILE:CG1	1:B:1140:ASN:H	1.86	0.88
1:A:1058:ILE:HD11	1:A:1067:ILE:HD12	1.57	0.87
1:B:1020:TYR:CE2	1:B:1021:GLN:CD	2.55	0.85
1:B:898:PRO:HA	1:B:940:MET:HE2	1.57	0.84
1:A:1140:ASN:O	1:A:1144:SER:HB2	1.78	0.83
1:A:1088:ARG:HA	1:A:1139:ILE:HG21	1.60	0.82
1:A:1234:LYS:HE2	1:A:1240:LYS:O	1.80	0.82
1:A:900:ASN:ND2	1:A:903:GLU:HG3	1.95	0.82
1:B:1034:ARG:HB3	1:B:1036:LEU:CD1	2.11	0.81
1:B:1060:THR:HG22	1:B:1063:GLU:HB2	1.62	0.81
1:B:1017:VAL:HG21	1:B:1024:LEU:HD21	1.64	0.80
1:B:1039:GLU:HG2	1:B:1041:LYS:HE3	1.62	0.80
1:B:1068:LEU:O	1:B:1072:SER:HB2	1.82	0.79
1:A:1234:LYS:HD3	1:A:1241:GLY:HA3	1.57	0.79
1:B:1072:SER:O	1:B:1075:ARG:HG3	1.83	0.79
1:A:1234:LYS:CE	1:A:1241:GLY:HA2	2.13	0.78
1:A:907:ARG:O	1:A:907:ARG:HG3	1.82	0.77
1:B:1118:ALA:HA	6:B:1409:HOH:O	1.85	0.77
1:A:1236:GLN:OE1	1:A:1236:GLN:HA	1.84	0.76
1:A:1235:GLU:HG2	1:A:1240:LYS:HA	1.67	0.76
1:B:1139:ILE:N	1:B:1139:ILE:HD13	2.00	0.76
1:B:898:PRO:HA	1:B:940:MET:CE	2.15	0.76
1:A:1020:TYR:HD2	1:A:1021:GLN:HG3	1.46	0.76
1:A:1060:THR:HG23	1:A:1063:GLU:HB2	1.69	0.75
1:B:923:PRO:HA	1:B:929:ARG:HG2	1.68	0.75
1:B:995:LYS:HE3	6:B:1412:HOH:O	1.87	0.74
1:B:1178:ASN:OD1	1:B:1214:PRO:HA	1.87	0.74
1:A:1123:VAL:HG21	1:A:1139:ILE:HD11	1.70	0.73
1:B:1017:VAL:HG21	1:B:1024:LEU:CD2	2.19	0.73
1:B:1158:GLN:HA	1:B:1158:GLN:NE2	2.04	0.73
1:A:1226:LEU:O	1:A:1229:LEU:HB2	1.89	0.73
1:A:1229:LEU:N	1:A:1229:LEU:HD12	2.04	0.72
1:A:1016:MET:CE	1:A:1071:GLY:HA3	2.17	0.72
1:B:1024:LEU:HD23	1:B:1038:LEU:CD1	2.20	0.71
1:A:1234:LYS:CD	1:A:1241:GLY:CA	2.26	0.71
1:A:1237:ALA:HB2	1:B:1237:ALA:HA	1.71	0.71
1:A:912:LEU:HD13	1:A:1189:PRO:HA	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:PRO:HA	5:B:1305:EDO:H11	1.73	0.69
1:B:1020:TYR:CE2	1:B:1021:GLN:HG3	2.28	0.68
1:B:1220:SER:O	1:B:1224:VAL:HG23	1.93	0.68
1:B:1058:ILE:HD11	1:B:1067:ILE:CD1	2.23	0.68
1:A:1137:GLN:N	1:A:1140:ASN:ND2	2.37	0.68
1:A:1236:GLN:OE1	1:A:1236:GLN:CA	2.41	0.68
1:A:912:LEU:HD12	1:A:912:LEU:N	2.08	0.68
1:A:1020:TYR:HE2	1:A:1021:GLN:NE2	1.91	0.67
1:A:1120:SER:HA	1:A:1143:LEU:HD12	1.76	0.67
1:A:1028:LEU:HD21	1:A:1067:ILE:HG23	1.75	0.67
1:A:1223:MET:HE3	1:B:1223:MET:HG2	1.77	0.66
1:B:1065:ARG:O	1:B:1069:GLU:HG2	1.95	0.66
1:A:1017:VAL:CG2	1:A:1024:LEU:HD22	2.26	0.65
1:B:1167:LEU:HD11	1:B:1171:MET:HE2	1.77	0.65
1:B:1187:VAL:HG11	1:B:1197:THR:HG23	1.77	0.65
1:B:1020:TYR:CE2	1:B:1021:GLN:NE2	2.65	0.65
1:B:1020:TYR:OH	1:B:1021:GLN:NE2	2.30	0.65
1:B:1019:LEU:HD21	1:B:1165:HIS:HE1	1.62	0.64
1:A:898:PRO:HA	1:A:940:MET:HG3	1.79	0.64
1:A:953:TYR:CE1	1:A:954:LEU:HD13	2.33	0.64
1:B:890:ILE:HG12	1:B:1181:THR:HB	1.79	0.64
1:B:1058:ILE:HD11	1:B:1067:ILE:HD11	1.79	0.63
1:A:924:TRP:CD1	1:A:930:LYS:HE2	2.34	0.63
1:B:1020:TYR:CE2	1:B:1021:GLN:CG	2.82	0.63
1:A:1017:VAL:HG21	1:A:1024:LEU:HD22	1.81	0.62
1:B:1021:GLN:O	1:B:1022:ASP:HB2	1.98	0.62
1:A:1088:ARG:HA	1:A:1139:ILE:CG2	2.28	0.62
1:A:1234:LYS:HD3	1:A:1241:GLY:HA2	0.65	0.61
1:B:1024:LEU:HD23	1:B:1038:LEU:HD12	1.81	0.61
1:A:1020:TYR:HE2	1:A:1021:GLN:HE21	1.46	0.61
1:B:1139:ILE:N	1:B:1139:ILE:CD1	2.64	0.61
1:B:912:LEU:HD11	1:B:1187:VAL:HG11	1.82	0.61
1:B:1020:TYR:CZ	1:B:1021:GLN:NE2	2.68	0.61
1:B:1028:LEU:O	1:B:1030:PRO:HD3	2.01	0.61
1:A:1150:ILE:HG23	1:A:1210:ILE:HD11	1.83	0.60
1:B:947:ILE:O	1:B:951:THR:HG23	2.02	0.59
1:A:1139:ILE:HG13	1:A:1140:ASN:N	2.17	0.59
1:A:1229:LEU:N	1:A:1229:LEU:CD1	2.65	0.59
1:A:898:PRO:HB3	1:A:940:MET:HG3	1.85	0.59
1:B:1139:ILE:CG1	1:B:1140:ASN:N	2.50	0.59
1:A:1021:GLN:C	1:A:1023:THR:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:LYS:HG3	1:B:926:ASP:HA	1.85	0.59
1:A:1234:LYS:HB3	1:A:1241:GLY:HA3	1.85	0.58
1:B:1121:GLU:OE2	1:B:1121:GLU:N	2.35	0.58
1:A:1237:ALA:HB2	1:B:1237:ALA:CA	2.32	0.58
1:B:1146:LEU:HD11	1:B:1175:LEU:HD21	1.85	0.58
1:B:953:TYR:CE2	5:B:1304:EDO:H12	2.38	0.58
1:B:1016:MET:HE3	1:B:1071:GLY:HA3	1.86	0.58
1:B:1020:TYR:HE2	1:B:1021:GLN:CD	2.11	0.58
1:B:1020:TYR:O	1:B:1023:THR:HB	2.04	0.57
1:B:1001:LEU:HD11	1:B:1012:LEU:HD21	1.86	0.57
1:A:907:ARG:O	1:A:907:ARG:CG	2.51	0.57
1:A:1062:GLU:O	1:A:1066:MET:HG2	2.04	0.57
1:A:1217:HIS:HB2	4:A:1304:IMD:C2	2.34	0.57
1:B:911:MET:HE2	1:B:1191:GLU:HG3	1.87	0.57
1:B:1029:LEU:CD2	1:B:1035:ARG:HG2	2.29	0.57
1:B:1034:ARG:HB3	1:B:1036:LEU:HD11	1.85	0.57
1:B:925:LYS:HG3	1:B:926:ASP:CA	2.35	0.57
1:A:1122:ARG:NH2	1:A:1140:ASN:OD1	2.37	0.56
1:B:1105:GLN:HB2	1:B:1221:LYS:HD2	1.87	0.56
1:A:1029:LEU:O	1:A:1074:ARG:NH1	2.34	0.56
1:A:1234:LYS:CG	1:A:1241:GLY:CA	2.82	0.56
1:B:1158:GLN:HE21	1:B:1158:GLN:CA	2.08	0.56
1:B:910:GLN:HE22	1:B:940:MET:HE3	1.70	0.56
1:A:1065:ARG:HH11	1:A:1065:ARG:CG	2.19	0.55
1:A:1143:LEU:N	1:A:1143:LEU:HD23	2.21	0.55
1:B:1146:LEU:HD11	1:B:1175:LEU:CD2	2.36	0.55
1:A:898:PRO:CA	1:A:940:MET:HG3	2.36	0.55
1:A:917:GLU:CD	1:A:917:GLU:H	2.14	0.55
1:A:924:TRP:HD1	1:A:930:LYS:HE2	1.70	0.55
1:B:967:PHE:HB3	1:B:1115:VAL:HB	1.89	0.55
1:A:1105:GLN:HG3	1:A:1221:LYS:HZ3	1.72	0.55
1:B:886:MET:O	1:B:891:ARG:NH2	2.40	0.55
1:A:1215:SER:HA	4:A:1305:IMD:C2	2.37	0.55
1:A:956:GLN:O	1:A:959:VAL:HG22	2.06	0.54
1:B:1075:ARG:NH2	1:B:1089:SER:OG	2.34	0.54
1:A:1139:ILE:HG13	1:A:1140:ASN:H	1.70	0.54
1:B:925:LYS:CG	1:B:926:ASP:HA	2.38	0.54
1:B:884:GLU:HA	1:B:887:LYS:HG2	1.89	0.54
1:A:1223:MET:HE2	1:B:1226:LEU:HD12	1.90	0.54
1:B:1104:THR:HG22	1:B:1106:SER:HB2	1.90	0.54
1:A:912:LEU:N	1:A:912:LEU:CD1	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:912:LEU:HD23	1:B:922:HIS:HB3	1.88	0.54
1:B:1042:LYS:HD3	6:B:1417:HOH:O	2.08	0.54
1:A:898:PRO:HB3	1:A:940:MET:CG	2.38	0.53
1:B:1019:LEU:HD21	1:B:1165:HIS:CE1	2.43	0.53
1:B:967:PHE:CB	1:B:1115:VAL:HB	2.38	0.53
1:B:1060:THR:CG2	1:B:1063:GLU:HB2	2.35	0.53
1:A:1064:LEU:O	1:A:1068:LEU:HG	2.07	0.53
1:B:1001:LEU:HD22	1:B:1010:PHE:CG	2.44	0.53
1:B:953:TYR:CE1	1:B:954:LEU:HD13	2.44	0.53
1:A:1078:SER:OG	1:A:1081:ASN:O	2.26	0.53
1:B:1117:LEU:HD21	1:B:1171:MET:CE	2.39	0.53
1:A:947:ILE:O	1:A:951:THR:HG23	2.09	0.53
1:A:1013:LYS:HD2	6:A:1451:HOH:O	2.08	0.53
1:A:900:ASN:HD21	1:A:903:GLU:HG3	1.72	0.53
1:B:897:ARG:NH2	1:B:1188:SER:HB2	2.23	0.53
1:A:1020:TYR:CE2	1:A:1021:GLN:HG3	2.41	0.53
1:B:1020:TYR:CD2	1:B:1021:GLN:HG3	2.44	0.52
1:B:1026:ASP:OD2	1:B:1026:ASP:C	2.52	0.52
1:A:902:LYS:HA	1:A:905:SER:OG	2.09	0.52
1:B:910:GLN:OE1	1:B:940:MET:HE1	2.09	0.52
1:A:1198:TYR:CZ	1:A:1202:LEU:HD11	2.45	0.52
1:A:911:MET:HG3	1:A:1191:GLU:HA	1.91	0.52
1:A:1185:VAL:O	1:A:1185:VAL:HG13	2.09	0.52
1:A:1244:GLU:CG	1:A:1245:ASP:N	2.72	0.52
1:B:931:GLN:NE2	6:B:1432:HOH:O	2.42	0.52
1:B:1061:LEU:HD12	1:B:1061:LEU:C	2.34	0.52
1:A:1215:SER:O	4:A:1304:IMD:H2	2.09	0.52
1:B:1058:ILE:HG13	1:B:1064:LEU:HD12	1.91	0.52
1:A:898:PRO:CB	1:A:940:MET:HG3	2.41	0.51
1:B:1103:GLN:HG3	1:B:1104:THR:N	2.26	0.51
1:A:1234:LYS:O	1:A:1239:LYS:O	2.28	0.51
1:B:1068:LEU:O	1:B:1072:SER:CB	2.57	0.51
1:A:895:ARG:CZ	1:A:947:ILE:HD12	2.41	0.51
1:B:925:LYS:CG	1:B:926:ASP:CA	2.89	0.51
1:B:930:LYS:HD3	1:B:1198:TYR:HE1	1.75	0.51
1:A:891:ARG:HA	1:A:935:ASP:OD1	2.11	0.51
1:A:1061:LEU:O	1:A:1061:LEU:HD12	2.11	0.51
1:A:1137:GLN:CB	1:A:1139:ILE:HG12	2.41	0.51
1:B:1058:ILE:HD11	1:B:1067:ILE:HD12	1.92	0.51
1:B:1165:HIS:ND1	1:B:1166:LYS:N	2.59	0.51
1:A:1015:TYR:HB3	1:A:1055:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:ARG:HA	1:B:1034:ARG:HH11	1.76	0.50
1:B:1061:LEU:HD12	1:B:1061:LEU:O	2.11	0.50
1:A:1013:LYS:HA	1:A:1056:ILE:O	2.10	0.50
1:A:1056:ILE:HG21	1:A:1067:ILE:HD11	1.94	0.50
1:A:1225:ARG:O	1:A:1229:LEU:HD13	2.11	0.50
1:A:1068:LEU:O	1:A:1072:SER:OG	2.22	0.50
1:A:897:ARG:HH22	1:A:903:GLU:CD	2.19	0.50
1:A:1105:GLN:HG3	1:A:1221:LYS:NZ	2.27	0.50
1:A:1215:SER:HA	4:A:1305:IMD:H2	1.94	0.50
1:A:891:ARG:NH2	1:A:953:TYR:OH	2.45	0.50
1:B:1063:GLU:O	1:B:1067:ILE:HG13	2.12	0.50
1:A:1048:VAL:HG13	1:A:1173:ASP:CG	2.37	0.49
1:A:1021:GLN:C	1:A:1023:THR:N	2.67	0.49
1:A:921:GLU:HB2	1:A:930:LYS:O	2.12	0.49
1:A:927:ASP:OD1	1:A:927:ASP:O	2.30	0.49
1:B:1039:GLU:CG	1:B:1041:LYS:HE3	2.38	0.49
1:A:1092:ILE:HG12	1:A:1115:VAL:HG13	1.94	0.49
1:A:1137:GLN:N	1:A:1140:ASN:HB3	2.27	0.49
1:A:1230:VAL:O	1:A:1234:LYS:HB2	2.13	0.49
1:A:1017:VAL:HG22	1:A:1024:LEU:HD22	1.95	0.48
1:B:1065:ARG:O	1:B:1069:GLU:CG	2.61	0.48
1:A:930:LYS:HD2	1:A:1198:TYR:HE1	1.78	0.48
1:B:922:HIS:HE1	1:B:932:HIS:NE2	2.12	0.48
1:B:925:LYS:CB	1:B:926:ASP:HA	2.44	0.48
1:A:948:PHE:O	1:A:952:LYS:HB2	2.14	0.48
1:A:1051:GLU:O	1:A:1052:ASN:HB2	2.13	0.48
1:B:1021:GLN:O	1:B:1022:ASP:CB	2.62	0.48
1:A:1047:MET:HE1	4:A:1304:IMD:H4	1.84	0.48
1:A:1159:HIS:C	1:A:1160:ILE:HD13	2.38	0.48
1:B:926:ASP:O	1:B:927:ASP:HB2	2.14	0.47
1:B:936:ARG:NH1	1:B:950:ASP:OD2	2.47	0.47
1:A:1105:GLN:CG	1:A:1221:LYS:HZ3	2.26	0.47
1:A:1124:LYS:HD2	1:A:1124:LYS:N	2.29	0.47
1:B:1016:MET:HE1	1:B:1068:LEU:HA	1.97	0.47
1:B:1109:ARG:HD2	1:B:1217:HIS:CE1	2.50	0.47
1:B:925:LYS:HG3	1:B:926:ASP:CB	2.44	0.47
1:B:1017:VAL:CG2	1:B:1024:LEU:HD23	2.45	0.47
1:B:1185:VAL:HG13	1:B:1185:VAL:O	2.15	0.47
1:A:927:ASP:O	1:A:927:ASP:CG	2.58	0.46
1:A:1003:ARG:NH1	1:A:1004:ASP:OD1	2.48	0.46
1:A:1021:GLN:O	1:A:1023:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:MET:O	1:A:940:MET:HG2	2.15	0.46
1:A:1065:ARG:CG	1:A:1065:ARG:NH1	2.77	0.46
1:B:1139:ILE:CD1	1:B:1140:ASN:H	2.27	0.46
1:B:902:LYS:HD2	1:B:906:GLU:OE2	2.15	0.46
1:B:1017:VAL:CG2	1:B:1024:LEU:CD2	2.93	0.46
1:B:969:TYR:HB3	1:B:1183:MET:HE2	1.97	0.46
1:A:1158:GLN:HA	1:A:1158:GLN:NE2	2.31	0.45
1:B:892:VAL:HG11	1:B:1204:ALA:HB1	1.97	0.45
1:A:897:ARG:O	1:A:1189:PRO:HD3	2.15	0.45
1:A:956:GLN:NE2	1:A:959:VAL:CG2	2.79	0.45
1:B:1020:TYR:HE1	1:B:1085:GLU:N	2.14	0.45
1:B:1109:ARG:O	1:B:1109:ARG:HG2	2.15	0.45
1:A:1052:ASN:N	1:A:1052:ASN:HD22	2.14	0.45
1:B:1247:VAL:CG1	1:B:1248:ASP:N	2.79	0.45
1:A:924:TRP:CG	1:A:925:LYS:H	2.34	0.45
1:A:1058:ILE:HD11	1:A:1067:ILE:CD1	2.35	0.45
1:A:1069:GLU:O	1:A:1073:GLU:HG3	2.17	0.45
1:A:1105:GLN:CG	1:A:1221:LYS:NZ	2.80	0.45
1:B:1077:VAL:HG12	1:B:1077:VAL:O	2.16	0.45
1:A:1235:GLU:CG	1:A:1240:LYS:HG2	2.47	0.45
1:B:1139:ILE:O	1:B:1143:LEU:HD23	2.17	0.45
1:A:1020:TYR:CE2	1:A:1021:GLN:NE2	2.76	0.45
1:B:1177:GLY:O	1:B:1212:ASN:HB3	2.17	0.45
1:A:1028:LEU:CD2	1:A:1067:ILE:HG23	2.44	0.44
1:B:1050:VAL:HG13	1:B:1053:VAL:HG11	1.99	0.44
1:B:1117:LEU:HD21	1:B:1171:MET:HE1	1.98	0.44
1:A:1235:GLU:HG2	1:A:1240:LYS:HG2	1.99	0.44
1:B:953:TYR:CD2	5:B:1304:EDO:H12	2.52	0.44
1:B:978:PHE:HZ	1:B:986:ASN:HD22	1.63	0.44
1:B:1011:SER:C	1:B:1012:LEU:HD12	2.43	0.44
1:A:967:PHE:HB3	1:A:1115:VAL:HB	2.00	0.44
1:B:1225:ARG:HE	1:B:1225:ARG:HB2	1.67	0.44
1:A:1017:VAL:HG22	1:A:1018:GLU:N	2.33	0.44
1:B:1187:VAL:HG13	1:B:1197:THR:OG1	2.17	0.44
1:B:1104:THR:O	1:B:1105:GLN:HB2	2.17	0.44
1:B:1247:VAL:HG12	1:B:1248:ASP:N	2.33	0.44
1:A:1047:MET:CE	4:A:1304:IMD:C4	2.69	0.43
1:B:897:ARG:O	1:B:1189:PRO:HD3	2.17	0.43
1:B:941:ARG:HB2	1:B:941:ARG:CZ	2.48	0.43
1:B:1029:LEU:HD12	1:B:1030:PRO:HD2	2.00	0.43
1:A:1139:ILE:O	1:A:1140:ASN:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:ILE:C	1:A:1141:LYS:N	2.74	0.43
1:B:1034:ARG:HB3	1:B:1036:LEU:HD13	1.97	0.43
1:B:1143:LEU:N	1:B:1143:LEU:HD22	2.34	0.43
1:A:1123:VAL:C	1:A:1124:LYS:HD2	2.44	0.43
1:A:969:TYR:CZ	1:A:1120:SER:HB2	2.54	0.43
1:B:910:GLN:HE21	1:B:910:GLN:HB3	1.56	0.43
1:A:1016:MET:HE2	1:A:1028:LEU:HD21	2.01	0.43
1:B:958:ALA:O	1:B:1110:GLY:HA3	2.19	0.43
1:B:1117:LEU:HD21	1:B:1171:MET:HE2	2.00	0.43
1:A:962:TYR:OH	1:A:1216:LYS:HE2	2.19	0.43
1:B:1187:VAL:CG1	1:B:1197:THR:HG23	2.47	0.42
1:A:1205:SER:O	1:A:1209:THR:HG23	2.19	0.42
4:A:1303:IMD:H2	6:A:1419:HOH:O	2.18	0.42
1:B:907:ARG:HH11	1:B:907:ARG:HG2	1.84	0.42
1:A:930:LYS:HD2	1:A:1198:TYR:CE1	2.54	0.42
1:A:1225:ARG:HG2	1:A:1225:ARG:HH11	1.84	0.42
1:A:1006:LYS:HB2	1:A:1006:LYS:NZ	2.34	0.42
1:A:1094:SER:HB3	1:A:1111:LYS:HE2	2.01	0.42
1:A:1140:ASN:OD1	1:A:1140:ASN:C	2.62	0.42
1:B:1170:LEU:HD12	1:B:1170:LEU:HA	1.90	0.42
1:B:1235:GLU:O	1:B:1238:GLY:N	2.52	0.42
1:B:944:GLN:HG2	1:B:986:ASN:HD21	1.84	0.42
1:B:946:ASP:O	1:B:949:GLU:HB3	2.19	0.42
1:B:1050:VAL:HG13	1:B:1053:VAL:CG1	2.50	0.42
1:A:888:GLY:HA2	1:A:1214:PRO:HD3	2.00	0.42
1:A:929:ARG:HB3	1:A:929:ARG:CZ	2.48	0.42
1:A:1037:LYS:H	1:A:1037:LYS:HG2	1.67	0.42
1:A:1085:GLU:CD	1:A:1085:GLU:H	2.26	0.42
1:A:1220:SER:H	1:A:1223:MET:HG3	1.84	0.42
1:B:939:ASP:C	1:B:939:ASP:OD1	2.62	0.42
1:B:1234:LYS:O	1:B:1237:ALA:HB3	2.20	0.42
1:A:903:GLU:O	1:A:908:GLU:HG3	2.20	0.42
1:A:1139:ILE:CG1	1:A:1140:ASN:N	2.82	0.42
1:A:1219:SER:HB3	1:A:1223:MET:HB2	2.02	0.42
1:B:1069:GLU:HG2	1:B:1069:GLU:H	1.56	0.42
1:A:1197:THR:O	1:A:1201:LEU:HG	2.20	0.42
1:A:1029:LEU:HD22	1:A:1035:ARG:HB3	2.02	0.41
1:A:1237:ALA:CB	1:B:1237:ALA:HA	2.46	0.41
1:B:1104:THR:CG2	1:B:1106:SER:HB2	2.50	0.41
1:A:1043:ASP:OD2	1:A:1043:ASP:C	2.64	0.41
1:A:983:HIS:HD2	1:A:985:SER:OG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:ILE:CG1	1:A:1140:ASN:H	2.32	0.41
1:B:897:ARG:CZ	1:B:1188:SER:HB2	2.50	0.41
1:B:1039:GLU:HB3	1:B:1051:GLU:HB3	2.02	0.41
1:B:1247:VAL:HG12	1:B:1248:ASP:O	2.20	0.41
1:A:1120:SER:HA	1:A:1143:LEU:CD1	2.48	0.41
1:A:1244:GLU:HG2	1:A:1245:ASP:N	2.29	0.41
1:B:1109:ARG:NH1	1:B:1109:ARG:HG3	2.36	0.41
1:A:1060:THR:HG23	1:A:1063:GLU:CB	2.43	0.41
1:A:1158:GLN:CA	1:A:1158:GLN:HE21	2.34	0.41
1:B:1034:ARG:O	1:B:1035:ARG:C	2.64	0.41
1:B:1194:LEU:HD23	1:B:1194:LEU:HA	1.94	0.40
1:A:917:GLU:CD	1:A:917:GLU:N	2.79	0.40
1:B:994:THR:HG22	1:B:1061:LEU:HD13	2.03	0.40
1:B:1056:ILE:HA	1:B:1057:PRO:HD3	1.96	0.40
1:B:1070:ARG:HG3	1:B:1071:GLY:N	2.36	0.40
1:A:936:ARG:HA	1:A:936:ARG:HD2	1.81	0.40
1:A:971:GLN:O	1:A:974:SER:OG	2.36	0.40
1:B:1035:ARG:HE	1:B:1035:ARG:HB3	1.42	0.40
1:A:1018:GLU:HB3	1:A:1025:VAL:CG2	2.52	0.40
1:B:1070:ARG:CG	1:B:1071:GLY:N	2.84	0.40
1:B:1103:GLN:HG3	1:B:1104:THR:H	1.86	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	352/386 (91%)	339 (96%)	13 (4%)	0	100	100
1	B	341/386 (88%)	330 (97%)	11 (3%)	0	100	100
All	All	693/772 (90%)	669 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	319/346 (92%)	284 (89%)	35 (11%)	6	9
1	B	315/346 (91%)	291 (92%)	24 (8%)	12	21
All	All	634/692 (92%)	575 (91%)	59 (9%)	8	14

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	900	ASN
1	A	902	LYS
1	A	909	LYS
1	A	910	GLN
1	A	912	LEU
1	A	919	THR
1	A	929	ARG
1	A	954	LEU
1	A	1006	LYS
1	A	1013	LYS
1	A	1042	LYS
1	A	1048	VAL
1	A	1050	VAL
1	A	1053	VAL
1	A	1059	SER
1	A	1060	THR
1	A	1062	GLU
1	A	1065	ARG
1	A	1070	ARG
1	A	1085	GLU
1	A	1091	LEU
1	A	1113	SER
1	A	1120	SER
1	A	1123	VAL
1	A	1124	LYS

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Mol	Chain	Res	Type
1	A	1140	ASN
1	A	1158	GLN
1	A	1170	LEU
1	A	1174	SER
1	A	1194	LEU
1	A	1228	LYS
1	A	1236	GLN
1	A	1239	LYS
1	A	1244	GLU
1	A	1253	ARG
1	B	925	LYS
1	B	947	ILE
1	B	954	LEU
1	B	959	VAL
1	B	1007	ARG
1	B	1009	SER
1	B	1035	ARG
1	B	1036	LEU
1	B	1037	LYS
1	B	1050	VAL
1	B	1061	LEU
1	B	1069	GLU
1	B	1076	HIS
1	B	1139	ILE
1	B	1158	GLN
1	B	1170	LEU
1	B	1171	MET
1	B	1175	LEU
1	B	1188	SER
1	B	1194	LEU
1	B	1225	ARG
1	B	1228	LYS
1	B	1245	ASP
1	B	1250	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	900	ASN
1	A	922	HIS
1	A	931	GLN
1	A	956	GLN

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Mol	Chain	Res	Type
1	A	971	GLN
1	A	983	HIS
1	A	1052	ASN
1	A	1076	HIS
1	A	1103	GLN
1	A	1157	ASN
1	A	1158	GLN
1	A	1186	ASN
1	B	922	HIS
1	B	931	GLN
1	B	956	GLN
1	B	986	ASN
1	B	1021	GLN
1	B	1103	GLN
1	B	1157	ASN
1	B	1158	GLN
1	B	1217	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	B	1302	2	28,29,29	1.32	3 (10%)	43,45,45	1.16	3 (6%)
4	IMD	B	1303	-	5,5,5	0.27	0	5,5,5	0.46	0
3	ADP	A	1302	2	28,29,29	1.35	2 (7%)	43,45,45	1.08	2 (4%)
4	IMD	A	1303	-	5,5,5	0.31	0	5,5,5	0.44	0
5	EDO	B	1305	-	3,3,3	0.34	0	2,2,2	0.42	0
4	IMD	A	1305	-	5,5,5	0.34	0	5,5,5	0.43	0
5	EDO	B	1304	-	3,3,3	0.41	0	2,2,2	0.15	0
5	EDO	A	1306	-	3,3,3	0.81	0	2,2,2	0.42	0
4	IMD	A	1304	-	5,5,5	0.58	0	5,5,5	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	1302	2	-	2/16/32/32	0/3/3/3
4	IMD	B	1303	-	-	-	0/1/1/1
3	ADP	A	1302	2	-	2/16/32/32	0/3/3/3
4	IMD	A	1303	-	-	-	0/1/1/1
5	EDO	B	1305	-	-	0/1/1/1	-
4	IMD	A	1305	-	-	-	0/1/1/1
5	EDO	B	1304	-	-	0/1/1/1	-
5	EDO	A	1306	-	-	0/1/1/1	-
4	IMD	A	1304	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	ADP	C2-N1	3.62	1.40	1.33
3	B	1302	ADP	C2-N1	3.54	1.40	1.33
3	A	1302	ADP	PA-O3A	-3.29	1.55	1.59
3	B	1302	ADP	PA-O3A	-2.51	1.56	1.59
3	B	1302	ADP	C1'-N9	2.41	1.53	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	ADP	N3-C2-N1	-3.49	123.31	128.58
3	A	1302	ADP	N3-C2-N1	-3.39	123.45	128.58
3	B	1302	ADP	C2-N1-C6	2.82	123.36	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	ADP	C2-N1-C6	2.67	123.11	118.73
3	B	1302	ADP	C3'-C2'-C1'	2.54	106.26	101.46

There are no chirality outliers.

All (4) torsion outliers are listed below:

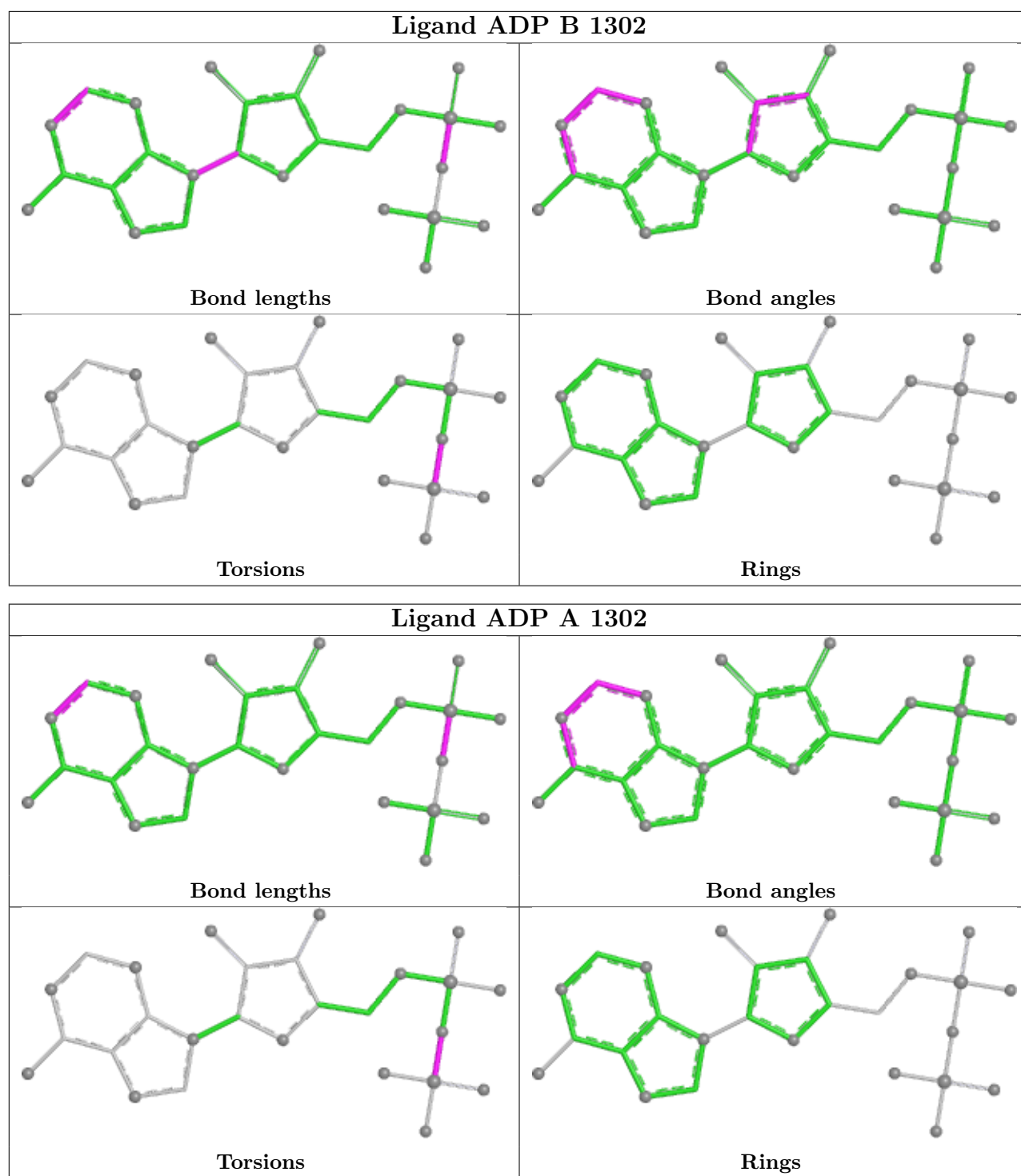
Mol	Chain	Res	Type	Atoms
3	A	1302	ADP	PA-O3A-PB-O3B
3	B	1302	ADP	PA-O3A-PB-O3B
3	A	1302	ADP	PA-O3A-PB-O2B
3	B	1302	ADP	PA-O3A-PB-O2B

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1303	IMD	1	0
5	B	1305	EDO	1	0
4	A	1305	IMD	2	0
5	B	1304	EDO	2	0
4	A	1304	IMD	7	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 ⓘ

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	356/386 (92%)	0.18	18 (5%) 33 30	9, 34, 70, 85	0
1	B	349/386 (90%)	0.19	20 (5%) 29 25	13, 33, 62, 84	0
All	All	705/772 (91%)	0.18	38 (5%) 31 28	9, 34, 67, 85	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1241	GLY	7.3
1	A	1139	ILE	4.8
1	B	1033	ALA	4.8
1	B	1139	ILE	4.7
1	B	1021	GLN	4.4
1	B	1032	SER	4.3
1	B	1085	GLU	4.3
1	A	927	ASP	3.8
1	A	886	MET	3.4
1	B	1122	ARG	3.3
1	A	1138	SER	3.1
1	A	1235	GLU	3.0
1	B	1086	SER	3.0
1	A	1123	VAL	3.0
1	A	1021	GLN	2.8
1	B	1020	TYR	2.7
1	B	923	PRO	2.7
1	A	1137	GLN	2.7
1	A	1253	ARG	2.7
1	A	1242	GLU	2.7
1	A	905	SER	2.6
1	B	1158	GLN	2.6
1	B	1245	ASP	2.6
1	B	1062	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	928	LYS	2.5
1	A	1240	LYS	2.4
1	A	1239	LYS	2.4
1	A	984	GLU	2.4
1	B	927	ASP	2.4
1	B	909	LYS	2.3
1	A	1124	LYS	2.3
1	B	885	ASP	2.2
1	B	1244	GLU	2.2
1	B	1034	ARG	2.2
1	B	983	HIS	2.1
1	B	1252	ASP	2.1
1	B	926	ASP	2.1
1	A	888	GLY	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.

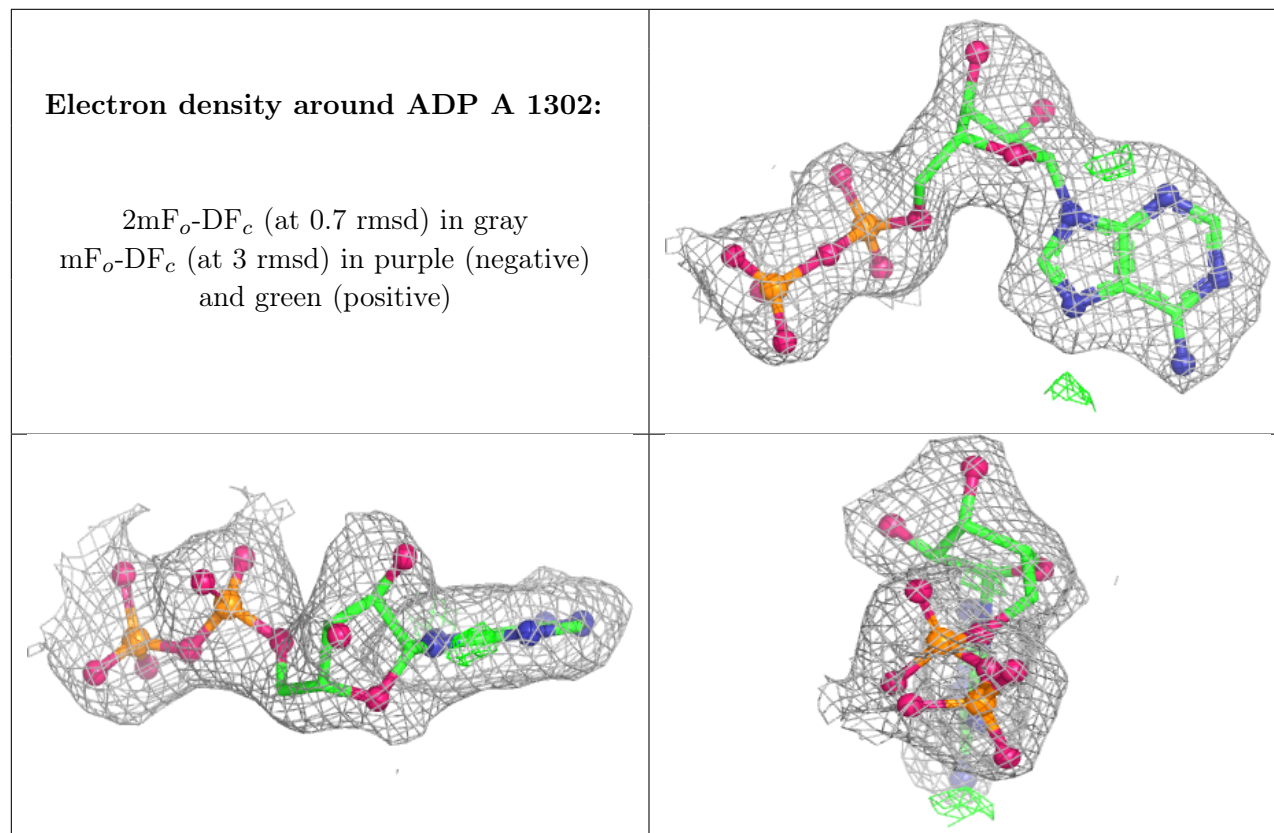
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	1304	4/4	0.74	0.15	44,47,49,52	0
4	IMD	A	1305	5/5	0.77	0.17	65,66,66,69	0
4	IMD	A	1303	5/5	0.82	0.17	53,54,57,58	0
4	IMD	A	1304	5/5	0.82	0.21	57,58,61,62	0
5	EDO	A	1306	4/4	0.83	0.21	43,47,51,53	0
5	EDO	B	1305	4/4	0.87	0.18	32,35,44,46	0
4	IMD	B	1303	5/5	0.90	0.10	35,35,38,39	0
2	MG	A	1301	1/1	0.94	0.07	25,25,25,25	0
3	ADP	A	1302	27/27	0.96	0.07	21,29,35,40	0

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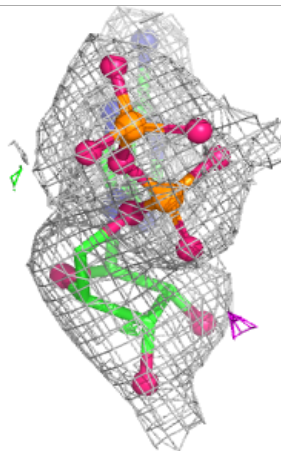
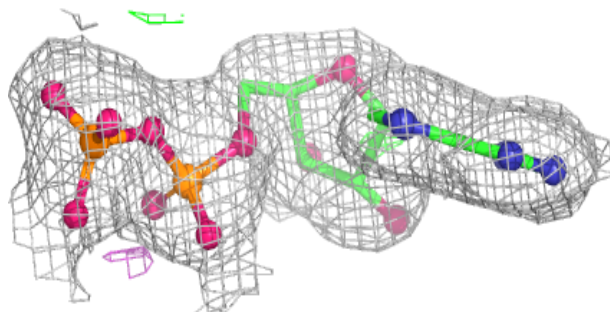
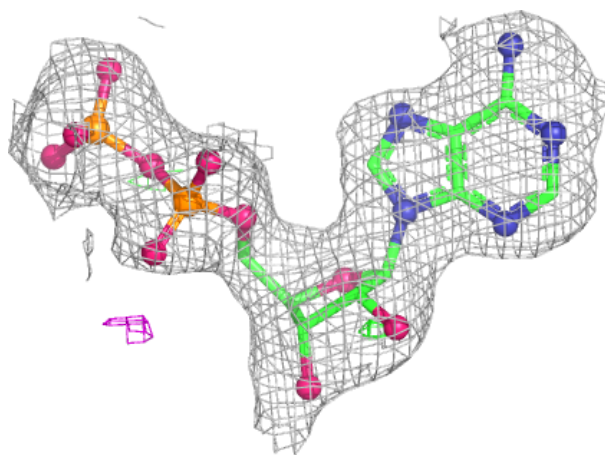
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	B	1302	27/27	0.96	0.08	21,37,46,51	0
2	MG	B	1301	1/1	0.96	0.07	30,30,30,30	0

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 1302:

$2mF_o-DF_c$ (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.