



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 04:29 AM EDT

PDB ID : 2OWM
Title : Motor domain of Neurospora crassa kinesin-3 (NcKin3)
Authors : Marx, A.; Muller, J.; Mandelkow, E.-M.; Woehlke, G.; Mandelkow, E.
Deposited on : 2007-02-16
Resolution : 3.25 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

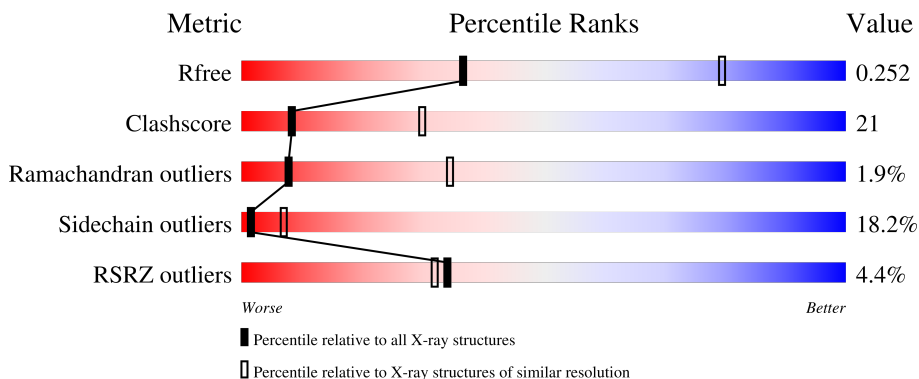
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	443	 44% 23% 6% 26%
1	B	443	 45% 22% 7% 26%
1	C	443	 43% 24% 7% 26%
1	D	443	 45% 21% 6% 27%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10338 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 Related to KINESIN-LIKE PROTEIN KIF1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2560	1609	445	495	11	0	0	0
1	B	327	2561	1609	449	492	11	0	0	0
1	C	328	2560	1609	445	495	11	0	0	0
1	D	325	2545	1600	444	490	11	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLU	LYS	conflict	UNP Q9C2M3
A	83	ASP	ASN	conflict	UNP Q9C2M3
A	252	GLY	ARG	conflict	UNP Q9C2M3
B	59	GLU	LYS	conflict	UNP Q9C2M3
B	83	ASP	ASN	conflict	UNP Q9C2M3
B	252	GLY	ARG	conflict	UNP Q9C2M3
C	59	GLU	LYS	conflict	UNP Q9C2M3
C	83	ASP	ASN	conflict	UNP Q9C2M3
C	252	GLY	ARG	conflict	UNP Q9C2M3
D	59	GLU	LYS	conflict	UNP Q9C2M3
D	83	ASP	ASN	conflict	UNP Q9C2M3
D	252	GLY	ARG	conflict	UNP Q9C2M3

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

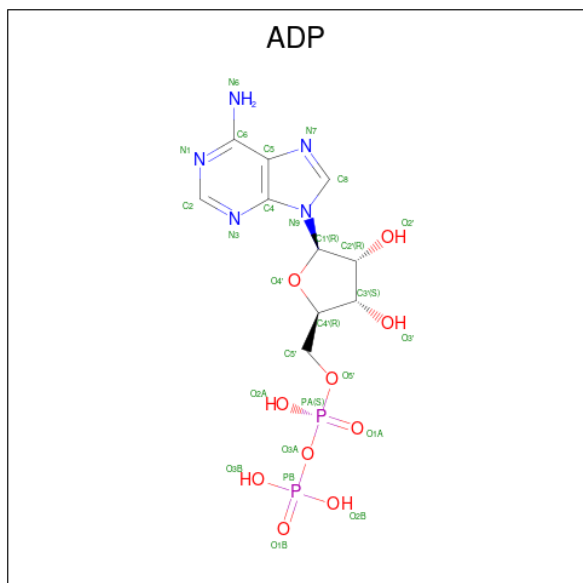
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0

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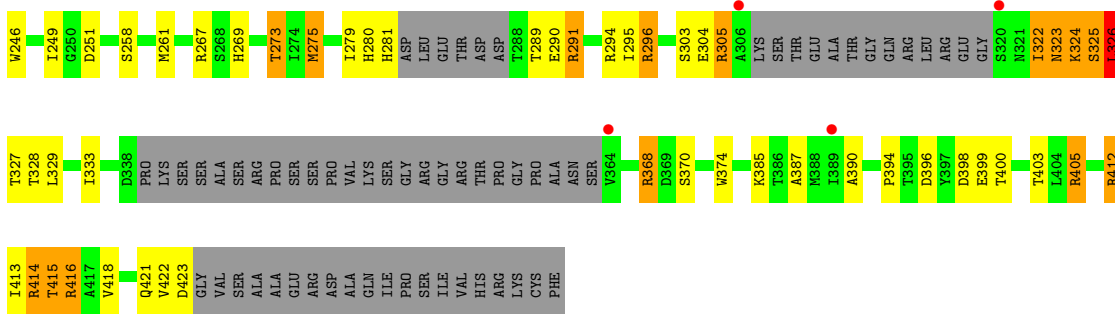
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

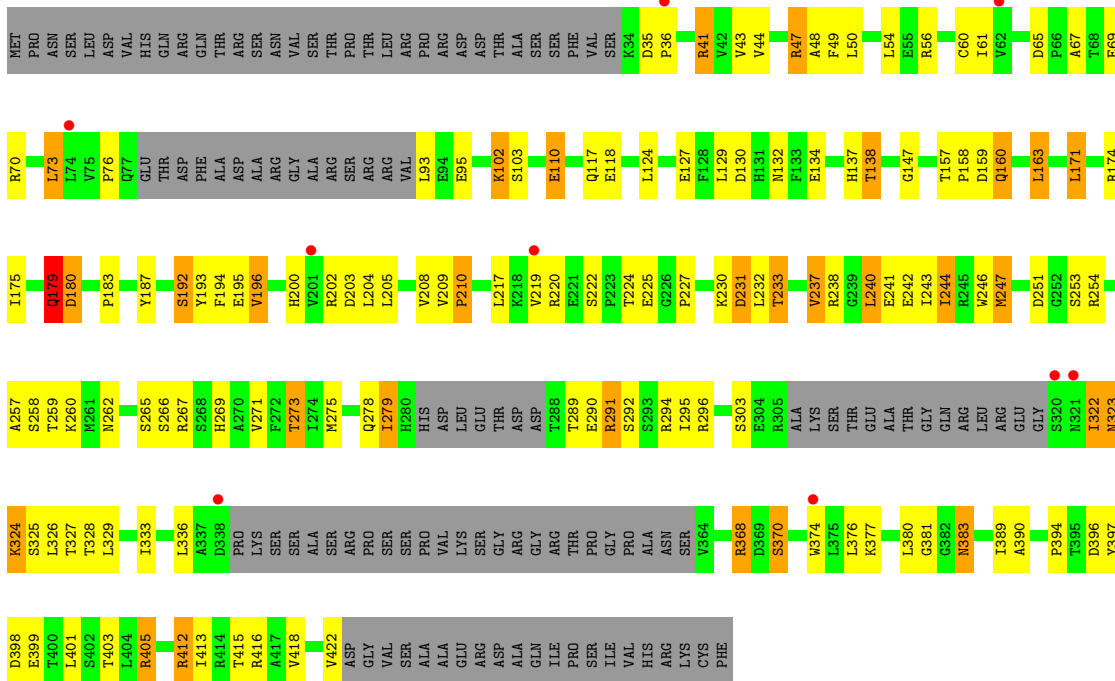
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



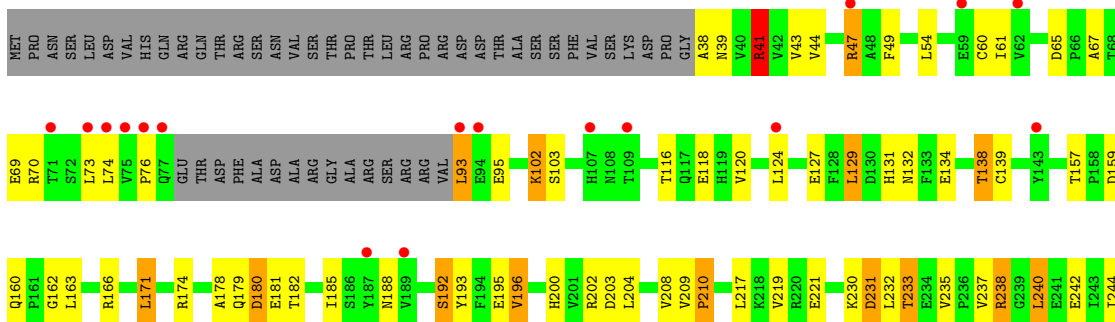
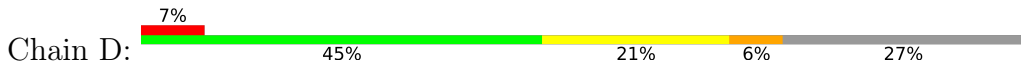
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 27 10 5 10 2	0	0
3	D	1	Total C N O P 27 10 5 10 2	0	0

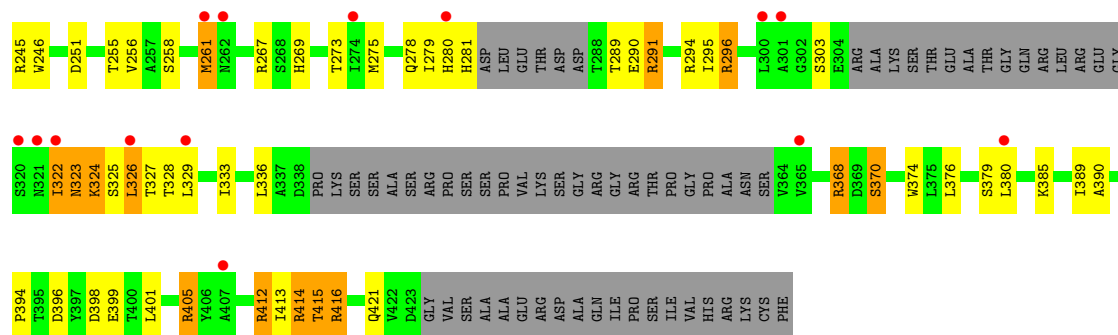


● Molecule 1: Related to KINESIN-LIKE PROTEIN KIF1C



● Molecule 1: Related to KINESIN-LIKE PROTEIN KIF1C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.94Å 98.41Å 111.76Å 90.00° 91.86° 90.00°	Depositor
Resolution (Å)	111.80 – 3.25 111.71 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (111.80-3.25) 100.0 (111.71-3.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.26Å)	Xtrriage
Refinement program	REFMAC refmac_5.2.0005	Depositor
R, R_{free}	0.210 , 0.256 0.209 , 0.252	Depositor DCC
R_{free} test set	1329 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtrriage
Anisotropy	0.329	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10338	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.92	0/2610	0.94	3/3546 (0.1%)
1	B	0.88	1/2611 (0.0%)	0.93	4/3546 (0.1%)
1	C	0.86	0/2610	0.92	2/3546 (0.1%)
1	D	0.78	1/2595 (0.0%)	0.87	3/3525 (0.1%)
All	All	0.86	2/10426 (0.0%)	0.92	12/14163 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	134	GLU	CG-CD	5.84	1.60	1.51
1	B	134	GLU	CG-CD	5.43	1.60	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	A	166	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	D	41	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	C	41	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	254	ARG	NE-CZ-NH1	-6.07	117.26	120.30
1	D	41	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	41	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	238	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	41	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	326	LEU	CA-CB-CG	5.07	126.95	115.30
1	D	93	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	326	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2560	0	2475	115	1
1	B	2561	0	2482	116	0
1	C	2560	0	2475	117	0
1	D	2545	0	2464	94	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
All	All	10338	0	9944	426	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (426) 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:157:THR:HG23	1:A:158:PRO:HD2	1.32	1.10
1:B:305:ARG:HH11	1:B:305:ARG:HG3	1.02	1.07
1:B:412:ARG:HG2	1:B:412:ARG:HH11	1.17	1.05
1:A:132:ASN:HD21	1:A:138:THR:HB	1.22	1.04
1:C:157:THR:HG23	1:C:158:PRO:HD2	1.39	1.04
1:D:132:ASN:HD21	1:D:138:THR:HB	1.23	1.04
1:D:412:ARG:HG2	1:D:412:ARG:HH11	1.23	1.03
1:A:405:ARG:HG3	1:A:405:ARG:HH11	1.20	1.01
1:B:235:VAL:HG13	1:D:210:PRO:HB3	1.40	1.01
1:B:210:PRO:HB3	1:D:235:VAL:HG13	1.45	0.99
1:C:405:ARG:HG3	1:C:405:ARG:HH11	1.28	0.97
1:D:405:ARG:HG3	1:D:405:ARG:HH11	1.29	0.97
1:C:157:THR:HB	1:C:160:GLN:HB2	1.45	0.97
1:C:69:GLU:HG2	1:C:102:LYS:HA	1.46	0.96
1:B:305:ARG:HH11	1:B:305:ARG:CG	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:HG2	1:A:412:ARG:HH11	1.30	0.95
1:A:157:THR:HB	1:A:160:GLN:HB2	1.49	0.94
1:B:303:SER:C	1:B:305:ARG:H	1.71	0.94
1:B:405:ARG:HG3	1:B:405:ARG:HH11	1.33	0.93
1:D:414:ARG:NH1	1:D:414:ARG:HB3	1.85	0.92
1:B:203:ASP:OD2	1:B:233:THR:HG23	1.71	0.91
1:B:414:ARG:NH1	1:B:414:ARG:HB3	1.84	0.91
1:B:132:ASN:HD21	1:B:138:THR:HB	1.34	0.90
1:C:132:ASN:HD21	1:C:138:THR:HB	1.35	0.89
1:D:414:ARG:HB3	1:D:414:ARG:HH11	1.37	0.88
1:B:305:ARG:HG3	1:B:305:ARG:NH1	1.83	0.88
1:A:203:ASP:OD2	1:A:233:THR:HG23	1.74	0.88
1:B:69:GLU:HG2	1:B:102:LYS:HA	1.56	0.88
1:C:412:ARG:HG2	1:C:412:ARG:HH11	1.37	0.87
1:A:132:ASN:ND2	1:A:138:THR:HB	1.89	0.86
1:D:69:GLU:HG2	1:D:102:LYS:HA	1.54	0.86
1:A:241:GLU:OE2	1:C:258:SER:HB3	1.74	0.85
1:D:203:ASP:OD2	1:D:233:THR:HG23	1.76	0.85
1:C:157:THR:HB	1:C:160:GLN:CB	2.06	0.85
1:B:238:ARG:HG3	1:B:238:ARG:HH11	1.42	0.84
1:D:132:ASN:ND2	1:D:138:THR:HB	1.93	0.84
1:D:294:ARG:O	1:D:294:ARG:HG3	1.76	0.84
1:D:333:ILE:HG23	1:D:413:ILE:HD11	1.58	0.84
1:A:222:SER:OG	1:A:225:GLU:N	2.10	0.84
1:B:280:HIS:ND1	1:C:36:PRO:HD3	1.93	0.83
1:D:414:ARG:HH11	1:D:414:ARG:CB	1.90	0.83
1:A:69:GLU:HG2	1:A:102:LYS:HA	1.59	0.83
1:A:220:ARG:HH11	1:A:220:ARG:CG	1.90	0.82
1:C:203:ASP:OD2	1:C:233:THR:HG23	1.79	0.82
1:B:412:ARG:HH11	1:B:412:ARG:CG	1.93	0.81
1:A:244:ILE:HD13	1:C:262:ASN:HA	1.62	0.81
1:D:238:ARG:HG3	1:D:238:ARG:HH11	1.46	0.80
1:D:414:ARG:HH11	1:D:414:ARG:CG	1.94	0.80
1:B:157:THR:HB	1:B:160:GLN:HB2	1.62	0.80
1:A:294:ARG:O	1:A:294:ARG:HG3	1.80	0.79
1:A:157:THR:HG23	1:A:158:PRO:CD	2.14	0.78
1:D:157:THR:HG22	1:D:159:ASP:H	1.48	0.78
1:C:405:ARG:HH11	1:C:405:ARG:CG	1.97	0.77
1:B:261:MET:O	1:D:244:ILE:HD13	1.85	0.76
1:A:157:THR:HB	1:A:160:GLN:CB	2.16	0.76
1:C:69:GLU:CG	1:C:102:LYS:HA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ARG:HB3	1:B:414:ARG:HH11	1.48	0.76
1:D:69:GLU:CG	1:D:102:LYS:HA	2.16	0.76
1:B:303:SER:O	1:B:305:ARG:N	2.18	0.76
1:A:405:ARG:HH11	1:A:405:ARG:CG	1.98	0.76
1:B:157:THR:HG22	1:B:159:ASP:H	1.51	0.76
1:B:132:ASN:ND2	1:B:138:THR:HB	2.00	0.75
1:C:333:ILE:HG23	1:C:413:ILE:HD11	1.68	0.75
1:B:294:ARG:O	1:B:294:ARG:HG3	1.84	0.75
1:B:405:ARG:HH11	1:B:405:ARG:CG	1.99	0.74
1:A:157:THR:CG2	1:A:158:PRO:HD2	2.14	0.74
1:B:303:SER:C	1:B:305:ARG:N	2.41	0.74
1:C:294:ARG:HG3	1:C:294:ARG:O	1.85	0.74
1:B:322:ILE:HG13	1:B:322:ILE:O	1.87	0.74
1:C:132:ASN:ND2	1:C:138:THR:HB	2.03	0.73
1:B:69:GLU:CG	1:B:102:LYS:HA	2.19	0.73
1:A:322:ILE:HG13	1:A:322:ILE:O	1.86	0.72
1:A:258:SER:HB3	1:C:241:GLU:OE2	1.90	0.71
1:D:412:ARG:HH11	1:D:412:ARG:CG	2.01	0.71
1:A:69:GLU:CG	1:A:102:LYS:HA	2.20	0.71
1:A:157:THR:HG22	1:A:159:ASP:H	1.53	0.71
1:A:333:ILE:HG23	1:A:413:ILE:HD11	1.71	0.70
1:C:267:ARG:HD3	1:C:322:ILE:HD11	1.73	0.70
1:C:43:VAL:HG23	1:C:102:LYS:HB2	1.72	0.70
1:C:157:THR:CG2	1:C:158:PRO:HD2	2.19	0.70
1:D:157:THR:HB	1:D:160:GLN:HB2	1.73	0.70
1:C:244:ILE:HB	1:C:247:MET:CE	2.21	0.70
1:D:405:ARG:HH11	1:D:405:ARG:CG	2.04	0.70
1:B:414:ARG:HH11	1:B:414:ARG:CB	2.03	0.70
1:B:412:ARG:HG2	1:B:412:ARG:NH1	1.98	0.70
1:A:405:ARG:HG3	1:A:405:ARG:NH1	2.01	0.69
1:C:187:TYR:CE2	1:C:278:GLN:HG3	2.27	0.69
1:B:280:HIS:CD2	1:B:281:HIS:N	2.61	0.69
1:B:333:ILE:HG23	1:B:413:ILE:HD11	1.74	0.69
1:D:291:ARG:NH1	1:D:421:GLN:OE1	2.25	0.69
1:A:244:ILE:CD1	1:C:262:ASN:HA	2.23	0.68
1:A:244:ILE:HB	1:A:247:MET:CE	2.23	0.68
1:D:44:VAL:HG12	1:D:390:ALA:HB3	1.74	0.68
1:D:240:LEU:CD2	1:D:244:ILE:HG23	2.22	0.68
1:C:160:GLN:HA	1:C:160:GLN:NE2	2.07	0.68
1:D:368:ARG:HB3	1:D:368:ARG:HH11	1.59	0.68
1:A:267:ARG:HD3	1:A:322:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:HH11	1:A:412:ARG:CG	2.05	0.67
1:A:47:ARG:HE	1:A:394:PRO:CD	2.07	0.67
1:B:414:ARG:HH11	1:B:414:ARG:CG	2.07	0.67
1:C:405:ARG:HG3	1:C:405:ARG:NH1	2.06	0.66
1:B:416:ARG:HG2	1:B:416:ARG:HH11	1.61	0.66
1:A:43:VAL:CG2	1:A:102:LYS:HB2	2.26	0.66
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.61	0.66
1:B:244:ILE:HD13	1:D:261:MET:O	1.95	0.65
1:C:157:THR:HG23	1:C:158:PRO:CD	2.19	0.65
1:B:43:VAL:CG2	1:B:102:LYS:HB2	2.27	0.64
1:C:203:ASP:HB2	1:C:217:LEU:HD21	1.80	0.64
1:C:171:LEU:HD12	1:C:171:LEU:C	2.17	0.64
1:B:305:ARG:CG	1:B:305:ARG:NH1	2.45	0.64
1:C:322:ILE:HG13	1:C:322:ILE:O	1.97	0.64
1:D:43:VAL:CG2	1:D:102:LYS:HB2	2.28	0.64
1:A:157:THR:HG22	1:A:159:ASP:N	2.13	0.64
1:B:405:ARG:HG3	1:B:405:ARG:NH1	2.11	0.64
1:C:157:THR:CB	1:C:160:GLN:HB2	2.26	0.63
1:C:324:LYS:O	1:C:328:THR:HG23	1.97	0.63
1:C:127:GLU:O	1:C:130:ASP:HB2	1.98	0.63
1:A:303:SER:HA	1:A:326:LEU:HD11	1.80	0.63
1:A:192:SER:HB2	1:A:232:LEU:HD22	1.80	0.63
1:B:192:SER:HB2	1:B:232:LEU:HD22	1.81	0.63
1:B:246:TRP:CH2	1:D:210:PRO:HD3	2.34	0.62
1:D:180:ASP:OD1	1:D:180:ASP:N	2.32	0.62
1:D:414:ARG:HH11	1:D:414:ARG:HG2	1.62	0.62
1:B:291:ARG:NH1	1:B:421:GLN:OE1	2.33	0.62
1:B:47:ARG:HE	1:B:394:PRO:CD	2.12	0.61
1:A:157:THR:CG2	1:A:158:PRO:CD	2.77	0.61
1:C:43:VAL:CG2	1:C:102:LYS:HB2	2.29	0.61
1:A:43:VAL:HG23	1:A:102:LYS:HB2	1.82	0.61
1:B:69:GLU:OE2	1:B:102:LYS:HE3	2.00	0.61
1:D:416:ARG:HG2	1:D:416:ARG:HH11	1.65	0.61
1:B:43:VAL:HG23	1:B:102:LYS:HB2	1.83	0.60
1:D:47:ARG:HE	1:D:394:PRO:CD	2.15	0.60
1:A:220:ARG:CG	1:A:220:ARG:NH1	2.59	0.60
1:D:69:GLU:HG3	1:D:103:SER:H	1.66	0.60
1:D:181:GLU:O	1:D:182:THR:HG23	2.00	0.60
1:B:280:HIS:CE1	1:C:36:PRO:HD3	2.35	0.60
1:C:44:VAL:HG12	1:C:390:ALA:HB3	1.83	0.60
1:A:269:HIS:HE1	1:A:326:LEU:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:SER:HA	1:C:326:LEU:HD11	1.84	0.60
1:A:160:GLN:HA	1:A:160:GLN:NE2	2.17	0.60
1:D:303:SER:HA	1:D:326:LEU:HD11	1.82	0.60
1:C:368:ARG:HH11	1:C:368:ARG:HB3	1.67	0.59
1:A:240:LEU:HD22	1:A:244:ILE:HG23	1.84	0.59
1:B:180:ASP:OD1	1:B:180:ASP:N	2.35	0.59
1:B:414:ARG:NH1	1:B:414:ARG:CB	2.60	0.59
1:C:65:ASP:HB2	1:C:70:ARG:NH1	2.17	0.59
1:B:61:ILE:HG21	1:B:76:PRO:HG3	1.84	0.59
1:C:157:THR:HG22	1:C:159:ASP:H	1.68	0.59
1:C:47:ARG:HE	1:C:394:PRO:CD	2.16	0.58
1:D:322:ILE:O	1:D:322:ILE:HG13	2.02	0.58
1:C:157:THR:CG2	1:C:158:PRO:CD	2.80	0.58
1:D:178:ALA:HA	1:D:181:GLU:HG2	1.86	0.58
1:D:203:ASP:HB2	1:D:217:LEU:HD21	1.86	0.57
1:B:267:ARG:HD3	1:B:322:ILE:HD11	1.86	0.57
1:D:43:VAL:HG23	1:D:102:LYS:HB2	1.86	0.57
1:D:324:LYS:O	1:D:328:THR:HG23	2.03	0.57
1:B:240:LEU:CD2	1:B:244:ILE:HG23	2.34	0.57
1:C:238:ARG:HG3	1:C:238:ARG:HH11	1.68	0.57
1:A:47:ARG:HB2	3:A:1002:ADP:C6	2.39	0.57
1:B:230:LYS:O	1:B:231:ASP:HB2	2.04	0.57
1:C:69:GLU:HG3	1:C:103:SER:H	1.69	0.57
1:B:49:PHE:HZ	1:B:60:CYS:HB2	1.70	0.56
1:D:69:GLU:OE2	1:D:102:LYS:HE3	2.04	0.56
1:A:187:TYR:CE2	1:A:278:GLN:HG3	2.41	0.56
1:B:69:GLU:HG3	1:B:103:SER:H	1.70	0.56
1:A:203:ASP:HB2	1:A:217:LEU:HD21	1.88	0.56
1:A:412:ARG:HG2	1:A:412:ARG:NH1	2.10	0.56
1:B:178:ALA:HA	1:B:181:GLU:HG2	1.88	0.56
1:C:47:ARG:HH12	1:C:50:LEU:HD11	1.70	0.56
1:C:160:GLN:NE2	1:C:160:GLN:CA	2.68	0.56
1:D:192:SER:HB2	1:D:232:LEU:HD22	1.86	0.56
1:D:267:ARG:HD3	1:D:322:ILE:HD11	1.88	0.56
1:A:368:ARG:HH11	1:A:368:ARG:HB3	1.70	0.56
1:A:220:ARG:HH11	1:A:220:ARG:HG2	1.69	0.56
1:A:171:LEU:HD12	1:A:171:LEU:C	2.27	0.55
1:C:222:SER:OG	1:C:225:GLU:N	2.26	0.55
1:D:279:ILE:HG12	1:D:290:GLU:HB2	1.88	0.55
1:B:157:THR:HG22	1:B:159:ASP:N	2.22	0.55
1:B:416:ARG:HH12	1:C:174:ARG:CZ	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:HIS:HD2	1:B:281:HIS:N	2.05	0.54
1:C:412:ARG:HH11	1:C:412:ARG:CG	2.15	0.54
1:A:399:GLU:OE1	1:A:399:GLU:HA	2.08	0.54
1:B:44:VAL:HG12	1:B:390:ALA:HB3	1.88	0.54
1:B:414:ARG:HH11	1:B:414:ARG:HG2	1.73	0.54
1:C:257:ALA:HB2	1:C:265:SER:HA	1.90	0.54
1:B:203:ASP:HB2	1:B:217:LEU:HD21	1.90	0.54
1:B:210:PRO:HD3	1:D:246:TRP:CH2	2.42	0.54
1:D:157:THR:HG22	1:D:159:ASP:N	2.20	0.54
1:A:47:ARG:HE	1:A:394:PRO:HD2	1.70	0.54
1:B:273:THR:HA	1:B:295:ILE:O	2.08	0.54
1:A:262:ASN:HA	1:C:244:ILE:HD13	1.89	0.54
1:B:41:ARG:NH2	1:B:127:GLU:OE1	2.41	0.54
1:D:49:PHE:HZ	1:D:60:CYS:HB2	1.72	0.54
1:D:61:ILE:HG21	1:D:76:PRO:HG3	1.90	0.54
1:C:230:LYS:O	1:C:231:ASP:HB2	2.08	0.53
1:A:56:ARG:HG2	1:A:56:ARG:O	2.09	0.53
1:B:47:ARG:HE	1:B:394:PRO:HD2	1.72	0.53
1:A:47:ARG:HE	1:A:394:PRO:HD3	1.73	0.53
1:A:49:PHE:CZ	1:A:60:CYS:HB2	2.43	0.53
1:A:61:ILE:HG21	1:A:76:PRO:HG3	1.90	0.53
1:B:324:LYS:O	1:B:328:THR:HG23	2.09	0.53
1:B:368:ARG:HH11	1:B:368:ARG:HB3	1.72	0.53
1:A:230:LYS:O	1:A:231:ASP:HB2	2.08	0.53
1:B:49:PHE:CZ	1:B:60:CYS:HB2	2.43	0.53
1:D:280:HIS:CD2	1:D:281:HIS:N	2.75	0.53
1:D:49:PHE:CZ	1:D:60:CYS:HB2	2.43	0.53
1:A:227:PRO:HG2	1:A:374:TRP:O	2.08	0.53
1:C:61:ILE:HG21	1:C:76:PRO:HG3	1.91	0.53
1:A:257:ALA:HB2	1:A:265:SER:HA	1.89	0.53
1:C:47:ARG:HE	1:C:394:PRO:HD3	1.74	0.52
1:C:47:ARG:NH1	1:C:147:GLY:O	2.42	0.52
1:C:323:ASN:O	1:C:325:SER:N	2.43	0.52
1:D:336:LEU:HD11	1:D:380:LEU:O	2.10	0.52
1:B:279:ILE:HG12	1:B:290:GLU:HB2	1.92	0.52
1:C:195:GLU:HB3	1:C:204:LEU:HD11	1.92	0.52
1:B:399:GLU:OE1	1:B:399:GLU:HA	2.10	0.51
1:D:238:ARG:HH11	1:D:238:ARG:CG	2.20	0.51
1:A:49:PHE:HZ	1:A:60:CYS:HB2	1.75	0.51
1:A:220:ARG:NH1	1:A:220:ARG:HG2	2.24	0.51
1:D:414:ARG:NH1	1:D:414:ARG:CB	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:HG23	1:A:290:GLU:HB3	1.92	0.51
1:B:39:ASN:ND2	1:B:414:ARG:HG3	2.24	0.51
1:B:303:SER:HA	1:B:326:LEU:HD11	1.92	0.51
1:C:328:THR:OG1	1:C:370:SER:HB3	2.10	0.51
1:C:56:ARG:O	1:C:56:ARG:HG2	2.11	0.51
1:D:171:LEU:C	1:D:171:LEU:HD12	2.31	0.51
1:D:412:ARG:HG2	1:D:412:ARG:NH1	2.04	0.51
1:B:139:CYS:HA	1:B:296:ARG:O	2.11	0.50
1:D:131:HIS:CD2	1:D:385:LYS:HD2	2.46	0.50
1:D:376:LEU:O	1:D:379:SER:N	2.40	0.50
1:C:405:ARG:CG	1:C:405:ARG:NH1	2.67	0.50
1:A:390:ALA:HB1	1:A:403:THR:HG22	1.94	0.50
1:C:69:GLU:HG3	1:C:103:SER:N	2.26	0.50
1:C:157:THR:HG22	1:C:159:ASP:N	2.25	0.50
1:D:396:ASP:OD1	1:D:399:GLU:HB2	2.12	0.50
1:D:69:GLU:HG3	1:D:103:SER:N	2.26	0.50
1:A:160:GLN:NE2	1:A:160:GLN:CA	2.73	0.50
1:A:157:THR:CG2	1:A:158:PRO:N	2.75	0.49
1:B:390:ALA:HB1	1:B:403:THR:HG22	1.93	0.49
1:C:240:LEU:HD22	1:C:244:ILE:HG23	1.93	0.49
1:C:187:TYR:CZ	1:C:278:GLN:HG3	2.46	0.49
1:A:412:ARG:CG	1:A:412:ARG:NH1	2.71	0.49
1:B:157:THR:HB	1:B:160:GLN:H	1.76	0.49
1:B:181:GLU:O	1:B:182:THR:HG23	2.12	0.49
1:B:238:ARG:HH11	1:B:238:ARG:CG	2.19	0.49
1:C:399:GLU:OE1	1:C:399:GLU:HA	2.12	0.49
1:D:412:ARG:CG	1:D:412:ARG:NH1	2.68	0.49
1:A:65:ASP:HB2	1:A:70:ARG:NH1	2.27	0.49
1:A:262:ASN:HA	1:C:244:ILE:CD1	2.43	0.49
1:D:47:ARG:HE	1:D:394:PRO:HD2	1.78	0.49
1:D:47:ARG:HE	1:D:394:PRO:HD3	1.77	0.49
1:C:227:PRO:HG2	1:C:374:TRP:O	2.13	0.48
1:D:65:ASP:HB2	1:D:70:ARG:NH1	2.28	0.48
1:C:192:SER:HB2	1:C:232:LEU:HD22	1.96	0.48
1:C:222:SER:C	1:C:224:THR:H	2.16	0.48
1:A:157:THR:CB	1:A:160:GLN:HB2	2.33	0.48
1:B:238:ARG:HG3	1:B:238:ARG:NH1	2.21	0.48
1:D:39:ASN:ND2	1:D:414:ARG:HG3	2.29	0.48
1:C:222:SER:C	1:C:224:THR:N	2.68	0.48
1:A:69:GLU:HG3	1:A:103:SER:H	1.79	0.47
1:D:278:GLN:HG3	1:D:291:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:HE	1:B:394:PRO:HD3	1.79	0.47
1:B:69:GLU:HG3	1:B:103:SER:N	2.28	0.47
1:A:195:GLU:HB3	1:A:204:LEU:HD11	1.97	0.47
1:B:127:GLU:O	1:B:130:ASP:HB2	2.14	0.47
1:B:143:TYR:CD1	1:B:144:GLY:N	2.82	0.47
1:C:179:GLN:HE21	1:C:179:GLN:HA	1.79	0.47
1:C:269:HIS:HE1	1:C:326:LEU:HB2	1.80	0.47
1:D:157:THR:HB	1:D:160:GLN:H	1.79	0.47
1:A:240:LEU:HD22	1:A:244:ILE:CG2	2.44	0.47
1:A:405:ARG:CG	1:A:405:ARG:NH1	2.67	0.47
1:B:416:ARG:HG2	1:B:416:ARG:NH1	2.27	0.47
1:C:240:LEU:O	1:C:243:ILE:HG22	2.14	0.47
1:A:238:ARG:HG3	1:A:238:ARG:HH11	1.79	0.47
1:C:180:ASP:HA	1:C:183:PRO:HG3	1.96	0.47
1:C:205:LEU:HD22	1:C:246:TRP:HE3	1.80	0.47
1:B:412:ARG:CG	1:B:412:ARG:NH1	2.61	0.47
1:D:195:GLU:HB3	1:D:204:LEU:HD11	1.97	0.47
1:D:368:ARG:NH1	1:D:374:TRP:NE1	2.63	0.47
1:A:46:VAL:HG13	1:A:46:VAL:O	2.15	0.47
1:C:73:LEU:HD13	1:C:397:TYR:CE1	2.50	0.47
1:D:240:LEU:CD2	1:D:244:ILE:CG2	2.92	0.47
1:D:269:HIS:HE1	1:D:326:LEU:HB2	1.80	0.47
1:C:251:ASP:C	1:C:253:SER:H	2.18	0.46
1:B:47:ARG:HH12	1:B:50:LEU:HD11	1.80	0.46
1:D:132:ASN:HD21	1:D:138:THR:CB	2.12	0.46
1:A:138:THR:HG22	1:A:295:ILE:HA	1.97	0.46
1:A:240:LEU:O	1:A:243:ILE:HG22	2.14	0.46
1:C:137:HIS:HD2	1:C:383:ASN:ND2	2.13	0.46
1:A:117:GLN:HG3	1:A:160:GLN:NE2	2.30	0.46
1:B:195:GLU:HB3	1:B:204:LEU:HD11	1.97	0.46
1:D:368:ARG:HH12	1:D:374:TRP:HE1	1.64	0.46
1:C:110:GLU:H	1:C:110:GLU:HG3	1.53	0.46
1:C:196:VAL:HA	1:C:200:HIS:O	2.15	0.46
1:B:323:ASN:O	1:B:325:SER:N	2.49	0.46
1:C:157:THR:CG2	1:C:158:PRO:N	2.78	0.46
1:A:108:ASN:OD1	1:A:110:GLU:HG3	2.16	0.46
1:B:190:LYS:HB2	1:B:275:MET:HG2	1.99	0.45
1:D:139:CYS:HA	1:D:296:ARG:O	2.15	0.45
1:B:396:ASP:O	1:B:400:THR:HB	2.17	0.45
1:D:74:LEU:HA	1:D:95:GLU:HG3	1.97	0.45
1:B:240:LEU:O	1:B:243:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TRP:HA	1:B:249:ILE:HG12	1.99	0.45
1:C:49:PHE:HZ	1:C:60:CYS:HB2	1.81	0.45
1:C:138:THR:HG22	1:C:295:ILE:HA	1.99	0.45
1:C:44:VAL:HA	1:C:390:ALA:O	2.17	0.45
1:A:132:ASN:OD1	1:A:295:ILE:HG12	2.17	0.45
1:D:368:ARG:NH1	1:D:374:TRP:HE1	2.14	0.45
1:A:117:GLN:HG3	1:A:160:GLN:HE21	1.81	0.45
1:A:237:VAL:HG11	1:A:243:ILE:HA	1.99	0.45
1:A:323:ASN:O	1:A:325:SER:N	2.50	0.45
1:B:138:THR:CG2	1:B:295:ILE:HG23	2.46	0.45
1:A:273:THR:HA	1:A:295:ILE:O	2.17	0.45
1:D:230:LYS:O	1:D:231:ASP:HB2	2.17	0.45
1:B:41:ARG:O	1:B:387:ALA:HA	2.17	0.45
1:D:38:ALA:O	1:D:415:THR:N	2.49	0.45
1:D:116:THR:O	1:D:120:VAL:HG23	2.17	0.45
1:D:328:THR:OG1	1:D:370:SER:HB3	2.17	0.45
1:A:47:ARG:NH1	1:A:147:GLY:O	2.50	0.44
1:A:401:LEU:O	1:A:405:ARG:HG2	2.17	0.44
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.74	0.44
1:C:390:ALA:HB1	1:C:403:THR:HG22	1.98	0.44
1:A:324:LYS:O	1:A:328:THR:HG23	2.17	0.44
1:B:418:VAL:HG11	1:C:134:GLU:HG2	1.98	0.44
1:A:69:GLU:HG3	1:A:103:SER:N	2.33	0.44
1:C:273:THR:HA	1:C:295:ILE:O	2.18	0.44
1:A:277:LYS:HB2	1:A:292:SER:HB3	2.00	0.44
1:B:47:ARG:NH1	1:B:147:GLY:O	2.51	0.44
1:C:368:ARG:NH1	1:C:374:TRP:HE1	2.16	0.44
1:C:69:GLU:OE2	1:C:102:LYS:HE3	2.18	0.44
1:C:117:GLN:HG3	1:C:160:GLN:HE21	1.83	0.44
1:C:237:VAL:HG12	1:C:242:GLU:HB3	1.99	0.44
1:D:195:GLU:OE2	1:D:255:THR:OG1	2.24	0.44
1:D:240:LEU:HD23	1:D:244:ILE:HG23	1.98	0.44
1:A:209:VAL:HA	1:A:210:PRO:HD2	1.72	0.44
1:B:368:ARG:NH1	1:B:374:TRP:HE1	2.16	0.44
1:C:396:ASP:OD1	1:C:399:GLU:HB2	2.18	0.44
1:D:217:LEU:HD12	1:D:230:LYS:O	2.18	0.44
1:A:238:ARG:HB2	1:A:242:GLU:OE2	2.18	0.44
1:C:47:ARG:HB2	3:C:1002:ADP:C6	2.53	0.44
1:C:117:GLN:HG3	1:C:160:GLN:NE2	2.33	0.44
1:C:209:VAL:HA	1:C:210:PRO:HD2	1.70	0.44
1:C:368:ARG:NH1	1:C:374:TRP:NE1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLN:NE2	1:A:160:GLN:O	2.43	0.43
1:B:240:LEU:CD2	1:B:240:LEU:C	2.86	0.43
1:C:171:LEU:HD11	1:C:175:ILE:HD11	2.00	0.43
1:D:235:VAL:HG11	1:D:246:TRP:CE2	2.53	0.43
1:D:129:LEU:HD13	1:D:174:ARG:CZ	2.47	0.43
1:D:196:VAL:HA	1:D:200:HIS:O	2.18	0.43
1:A:179:GLN:HE21	1:A:179:GLN:HA	1.84	0.43
1:B:171:LEU:C	1:B:171:LEU:HD12	2.39	0.43
1:B:65:ASP:HB2	1:B:70:ARG:NH1	2.34	0.43
1:B:196:VAL:HA	1:B:200:HIS:O	2.18	0.43
1:B:242:GLU:O	1:B:246:TRP:HD1	2.00	0.43
1:D:41:ARG:NH2	1:D:127:GLU:OE1	2.51	0.43
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.71	0.43
1:A:389:ILE:HG21	1:A:389:ILE:HD13	1.74	0.43
1:C:49:PHE:CZ	1:C:60:CYS:HB2	2.54	0.43
1:A:267:ARG:CZ	1:A:322:ILE:HG12	2.48	0.43
1:B:38:ALA:O	1:B:415:THR:N	2.50	0.43
1:D:323:ASN:O	1:D:325:SER:N	2.52	0.43
1:B:56:ARG:O	1:B:56:ARG:HG2	2.19	0.43
1:B:368:ARG:NH1	1:B:374:TRP:NE1	2.67	0.43
1:A:267:ARG:HA	1:A:301:ALA:HB1	2.01	0.42
1:A:147:GLY:H	3:A:1002:ADP:PB	2.42	0.42
1:A:157:THR:HG22	1:A:158:PRO:N	2.33	0.42
1:D:132:ASN:CG	1:D:295:ILE:HG12	2.40	0.42
1:A:279:ILE:HG23	1:A:290:GLU:CB	2.50	0.42
1:D:162:GLY:O	1:D:166:ARG:CG	2.67	0.42
1:B:145:GLN:O	1:B:150:LYS:NZ	2.52	0.42
1:C:47:ARG:HE	1:C:394:PRO:HD2	1.83	0.42
1:B:164:ILE:O	1:B:165:PRO:C	2.58	0.42
1:C:244:ILE:HA	1:C:247:MET:HE2	2.02	0.42
1:A:175:ILE:HD13	1:A:187:TYR:HB2	2.02	0.42
1:B:422:VAL:CG1	1:B:423:ASP:N	2.83	0.42
1:C:219:VAL:O	1:C:220:ARG:NH1	2.47	0.42
1:A:141:PHE:CE1	1:A:388:MET:HG3	2.55	0.42
1:A:328:THR:OG1	1:A:370:SER:HB3	2.19	0.42
1:C:194:PHE:CE2	1:C:271:VAL:HB	2.54	0.42
1:A:41:ARG:HH11	1:A:41:ARG:HB2	1.85	0.42
1:B:162:GLY:O	1:B:163:LEU:C	2.58	0.42
1:B:131:HIS:HA	1:B:134:GLU:HB2	2.02	0.42
1:C:279:ILE:HG23	1:C:290:GLU:HB3	2.01	0.42
1:C:291:ARG:O	1:C:291:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:THR:HG22	1:C:158:PRO:N	2.35	0.42
1:A:47:ARG:HH12	1:A:50:LEU:HD11	1.85	0.41
1:A:164:ILE:O	1:A:165:PRO:C	2.59	0.41
1:A:222:SER:C	1:A:224:THR:H	2.23	0.41
1:A:240:LEU:O	1:A:241:GLU:C	2.59	0.41
1:A:173:GLN:HE21	1:A:173:GLN:HB2	1.65	0.41
1:C:389:ILE:HD13	1:C:389:ILE:HG21	1.79	0.41
1:C:132:ASN:CG	1:C:295:ILE:HG12	2.41	0.41
1:D:209:VAL:HA	1:D:210:PRO:HD2	1.83	0.41
1:D:401:LEU:O	1:D:405:ARG:HG2	2.20	0.41
1:A:47:ARG:HB2	3:A:1002:ADP:C5	2.55	0.41
1:D:138:THR:HG22	1:D:295:ILE:HA	2.03	0.41
1:A:41:ARG:O	1:A:387:ALA:HA	2.21	0.41
1:B:157:THR:CB	1:B:160:GLN:HB2	2.42	0.41
1:B:178:ALA:O	1:B:180:ASP:N	2.54	0.41
1:B:221:GLU:HG3	1:B:374:TRP:HH2	1.86	0.41
1:A:269:HIS:CE1	1:A:326:LEU:HB2	2.52	0.41
1:B:47:ARG:HB2	3:B:1002:ADP:C6	2.56	0.41
1:B:138:THR:HG22	1:B:295:ILE:HA	2.02	0.41
1:C:203:ASP:HB2	1:C:217:LEU:CD2	2.49	0.41
1:C:412:ARG:CG	1:C:412:ARG:NH1	2.80	0.41
1:D:43:VAL:HG13	1:D:389:ILE:HG23	2.02	0.41
1:C:267:ARG:CZ	1:C:322:ILE:HG12	2.51	0.41
1:C:336:LEU:HD11	1:C:380:LEU:O	2.21	0.41
1:A:69:GLU:OE2	1:A:102:LYS:HE3	2.21	0.40
1:B:131:HIS:CD2	1:B:385:LYS:HD2	2.56	0.40
1:C:43:VAL:HG23	1:C:102:LYS:CB	2.46	0.40
1:C:47:ARG:HG2	1:C:48:ALA:N	2.36	0.40
1:C:401:LEU:O	1:C:405:ARG:HG2	2.20	0.40
1:A:44:VAL:HG12	1:A:390:ALA:HB3	2.02	0.40
1:B:43:VAL:HG21	1:B:102:LYS:HB2	2.02	0.40
1:C:376:LEU:O	1:C:377:LYS:C	2.59	0.40
1:A:101:ASP:O	1:A:102:LYS:HG2	2.21	0.40
1:A:141:PHE:CZ	1:A:388:MET:HB2	2.56	0.40
1:A:222:SER:HA	1:A:223:PRO:HD3	1.92	0.40
1:C:171:LEU:HD12	1:C:171:LEU:O	2.20	0.40
1:C:368:ARG:HH12	1:C:374:TRP:HE1	1.69	0.40
1:D:399:GLU:OE1	1:D:399:GLU:HA	2.19	0.40
1:B:54:LEU:HD22	1:B:54:LEU:HA	1.97	0.40
1:C:381:GLY:CA	1:C:415:THR:HG22	2.52	0.40
1:A:73:LEU:HD13	1:A:397:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:HIS:HE1	1:B:326:LEU:HB2	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:OE2	1:A:220:ARG:NH1[2_646]	1.97	0.23

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	318/443 (72%)	286 (90%)	26 (8%)	6 (2%)	8	34
1	B	317/443 (72%)	282 (89%)	29 (9%)	6 (2%)	8	34
1	C	318/443 (72%)	288 (91%)	24 (8%)	6 (2%)	8	34
1	D	315/443 (71%)	284 (90%)	25 (8%)	6 (2%)	8	34
All	All	1268/1772 (72%)	1140 (90%)	104 (8%)	24 (2%)	8	34

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ALA
1	A	210	PRO
1	A	324	LYS
1	B	304	GLU
1	B	324	LYS
1	C	324	LYS
1	D	324	LYS
1	A	179	GLN
1	A	231	ASP

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Mol	Chain	Res	Type
1	A	259	THR
1	B	67	ALA
1	B	231	ASP
1	C	179	GLN
1	C	231	ASP
1	D	67	ALA
1	B	188	ASN
1	B	210	PRO
1	C	67	ALA
1	C	210	PRO
1	D	210	PRO
1	D	231	ASP
1	D	261	MET
1	C	163	LEU
1	D	188	ASN

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	278/389 (72%)	225 (81%)	53 (19%)	1 6
1	B	278/389 (72%)	229 (82%)	49 (18%)	2 8
1	C	278/389 (72%)	227 (82%)	51 (18%)	1 7
1	D	277/389 (71%)	228 (82%)	49 (18%)	2 8
All	All	1111/1556 (71%)	909 (82%)	202 (18%)	1 7

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	41	ARG
1	A	47	ARG
1	A	54	LEU
1	A	73	LEU
1	A	93	LEU

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Mol	Chain	Res	Type
1	A	95	GLU
1	A	97	SER
1	A	102	LYS
1	A	118	GLU
1	A	124	LEU
1	A	129	LEU
1	A	138	THR
1	A	160	GLN
1	A	163	LEU
1	A	171	LEU
1	A	179	GLN
1	A	180	ASP
1	A	193	TYR
1	A	196	VAL
1	A	202	ARG
1	A	208	VAL
1	A	219	VAL
1	A	220	ARG
1	A	233	THR
1	A	237	VAL
1	A	240	LEU
1	A	244	ILE
1	A	245	ARG
1	A	259	THR
1	A	260	LYS
1	A	266	SER
1	A	273	THR
1	A	275	MET
1	A	279	ILE
1	A	289	THR
1	A	291	ARG
1	A	292	SER
1	A	322	ILE
1	A	323	ASN
1	A	325	SER
1	A	327	THR
1	A	329	LEU
1	A	368	ARG
1	A	370	SER
1	A	383	ASN
1	A	398	ASP
1	A	405	ARG

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Mol	Chain	Res	Type
1	A	411	LYS
1	A	412	ARG
1	A	416	ARG
1	A	418	VAL
1	A	422	VAL
1	B	41	ARG
1	B	47	ARG
1	B	54	LEU
1	B	73	LEU
1	B	93	LEU
1	B	97	SER
1	B	102	LYS
1	B	118	GLU
1	B	124	LEU
1	B	129	LEU
1	B	138	THR
1	B	163	LEU
1	B	171	LEU
1	B	179	GLN
1	B	180	ASP
1	B	185	ILE
1	B	193	TYR
1	B	196	VAL
1	B	202	ARG
1	B	208	VAL
1	B	221	GLU
1	B	233	THR
1	B	237	VAL
1	B	238	ARG
1	B	240	LEU
1	B	242	GLU
1	B	245	ARG
1	B	251	ASP
1	B	258	SER
1	B	273	THR
1	B	275	MET
1	B	289	THR
1	B	291	ARG
1	B	296	ARG
1	B	305	ARG
1	B	322	ILE
1	B	323	ASN

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Mol	Chain	Res	Type
1	B	325	SER
1	B	326	LEU
1	B	327	THR
1	B	329	LEU
1	B	368	ARG
1	B	370	SER
1	B	398	ASP
1	B	405	ARG
1	B	412	ARG
1	B	414	ARG
1	B	415	THR
1	B	416	ARG
1	C	35	ASP
1	C	41	ARG
1	C	47	ARG
1	C	54	LEU
1	C	73	LEU
1	C	93	LEU
1	C	95	GLU
1	C	102	LYS
1	C	110	GLU
1	C	118	GLU
1	C	124	LEU
1	C	129	LEU
1	C	138	THR
1	C	160	GLN
1	C	163	LEU
1	C	171	LEU
1	C	179	GLN
1	C	180	ASP
1	C	192	SER
1	C	193	TYR
1	C	196	VAL
1	C	202	ARG
1	C	208	VAL
1	C	233	THR
1	C	237	VAL
1	C	240	LEU
1	C	244	ILE
1	C	247	MET
1	C	259	THR
1	C	260	LYS

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Mol	Chain	Res	Type
1	C	266	SER
1	C	273	THR
1	C	275	MET
1	C	279	ILE
1	C	289	THR
1	C	291	ARG
1	C	292	SER
1	C	296	ARG
1	C	322	ILE
1	C	323	ASN
1	C	327	THR
1	C	329	LEU
1	C	368	ARG
1	C	370	SER
1	C	383	ASN
1	C	398	ASP
1	C	405	ARG
1	C	412	ARG
1	C	416	ARG
1	C	418	VAL
1	C	422	VAL
1	D	41	ARG
1	D	47	ARG
1	D	54	LEU
1	D	73	LEU
1	D	93	LEU
1	D	102	LYS
1	D	118	GLU
1	D	124	LEU
1	D	129	LEU
1	D	138	THR
1	D	163	LEU
1	D	171	LEU
1	D	179	GLN
1	D	180	ASP
1	D	185	ILE
1	D	192	SER
1	D	193	TYR
1	D	196	VAL
1	D	202	ARG
1	D	208	VAL
1	D	219	VAL

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Mol	Chain	Res	Type
1	D	221	GLU
1	D	233	THR
1	D	237	VAL
1	D	238	ARG
1	D	240	LEU
1	D	242	GLU
1	D	245	ARG
1	D	251	ASP
1	D	256	VAL
1	D	258	SER
1	D	273	THR
1	D	275	MET
1	D	289	THR
1	D	291	ARG
1	D	296	ARG
1	D	322	ILE
1	D	323	ASN
1	D	326	LEU
1	D	327	THR
1	D	329	LEU
1	D	368	ARG
1	D	370	SER
1	D	398	ASP
1	D	405	ARG
1	D	412	ARG
1	D	414	ARG
1	D	415	THR
1	D	416	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	160	GLN
1	A	173	GLN
1	A	179	GLN
1	B	173	GLN
1	B	280	HIS
1	C	160	GLN
1	C	173	GLN
1	C	179	GLN
1	D	173	GLN

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Mol	Chain	Res	Type
1	D	280	HIS
1	D	323	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	1002	-	24,29,29	1.13	3 (12%)	29,45,45	1.67	5 (17%)
3	ADP	B	1002	2	24,29,29	1.10	1 (4%)	29,45,45	1.66	6 (20%)
3	ADP	D	1002	2	24,29,29	1.26	2 (8%)	29,45,45	1.54	6 (20%)
3	ADP	C	1002	2	24,29,29	1.11	2 (8%)	29,45,45	1.71	5 (17%)

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	1002	-	-	0/12/32/32	0/3/3/3
3	ADP	B	1002	2	-	0/12/32/32	0/3/3/3
3	ADP	D	1002	2	-	0/12/32/32	0/3/3/3
3	ADP	C	1002	2	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	ADP	C2-N3	3.38	1.37	1.32
3	C	1002	ADP	C2-N3	2.85	1.36	1.32
3	B	1002	ADP	O4'-C1'	2.81	1.45	1.41
3	A	1002	ADP	C2-N3	2.42	1.36	1.32
3	D	1002	ADP	C5-C4	2.34	1.47	1.40
3	A	1002	ADP	C5-N7	-2.24	1.31	1.39
3	A	1002	ADP	C2'-C1'	-2.09	1.50	1.53
3	C	1002	ADP	C5-C4	2.05	1.46	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	ADP	C5-C6-N6	-4.22	113.94	120.35
3	B	1002	ADP	PA-O3A-PB	-4.11	118.71	132.83
3	C	1002	ADP	N6-C6-N1	4.05	126.97	118.57
3	C	1002	ADP	N3-C2-N1	-3.88	122.61	128.68
3	A	1002	ADP	N6-C6-N1	3.79	126.45	118.57
3	D	1002	ADP	PA-O3A-PB	-3.69	120.16	132.83
3	A	1002	ADP	PA-O3A-PB	-3.61	120.44	132.83
3	C	1002	ADP	PA-O3A-PB	-3.48	120.89	132.83
3	D	1002	ADP	N3-C2-N1	-3.34	123.45	128.68
3	B	1002	ADP	N3-C2-N1	-3.29	123.53	128.68
3	C	1002	ADP	C5-C6-N6	-3.12	115.61	120.35
3	B	1002	ADP	O2B-PB-O1B	2.89	121.99	110.68
3	A	1002	ADP	N3-C2-N1	-2.83	124.25	128.68
3	B	1002	ADP	N6-C6-N1	2.64	124.05	118.57
3	D	1002	ADP	C5-C6-N6	-2.41	116.69	120.35
3	A	1002	ADP	O2B-PB-O1B	2.37	119.98	110.68
3	D	1002	ADP	N6-C6-N1	2.37	123.49	118.57
3	D	1002	ADP	O2B-PB-O1B	2.34	119.85	110.68
3	C	1002	ADP	O2B-PB-O1B	2.34	119.85	110.68
3	B	1002	ADP	O2B-PB-O3A	-2.04	97.78	104.64
3	B	1002	ADP	O3'-C3'-C2'	-2.02	105.30	111.82
3	D	1002	ADP	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

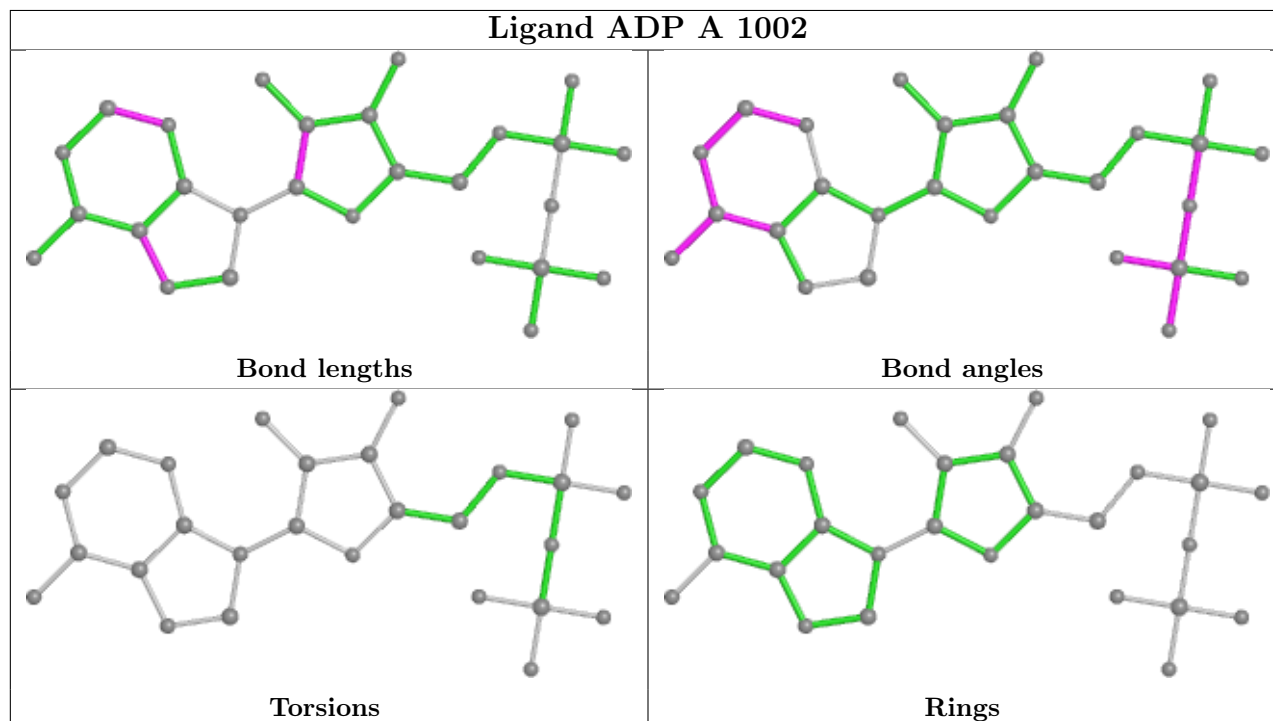
There are no torsion outliers.

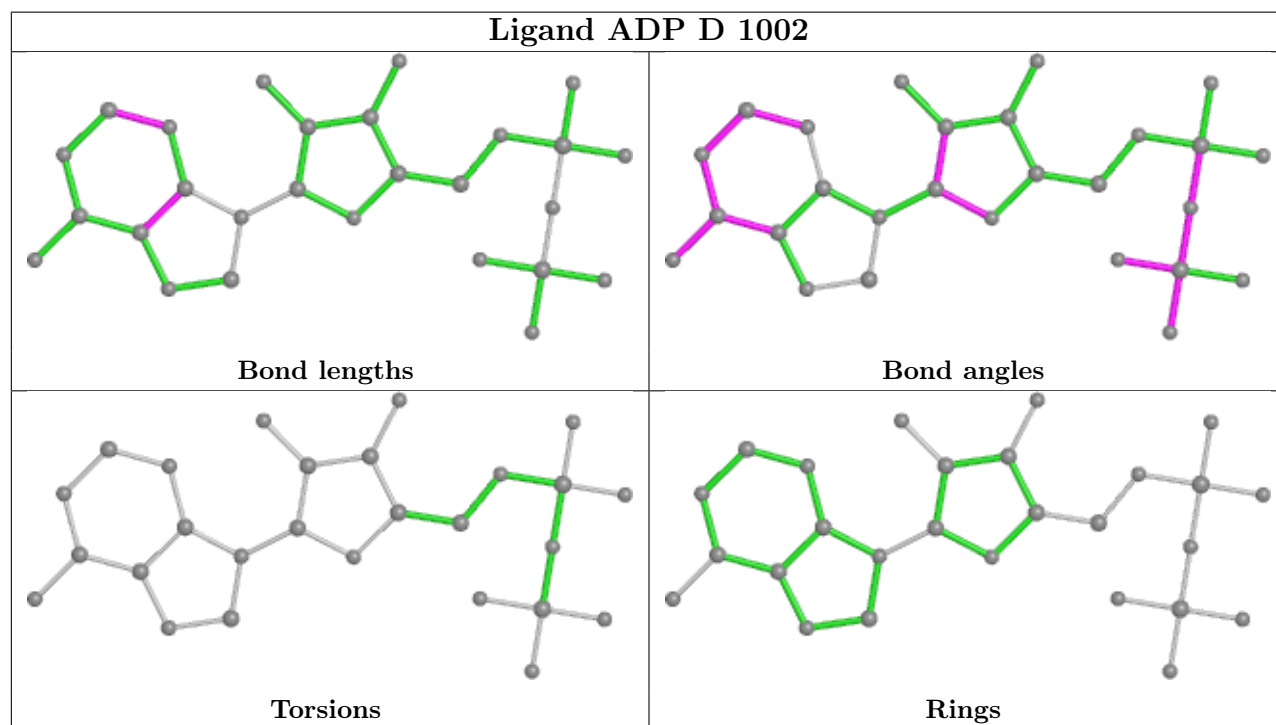
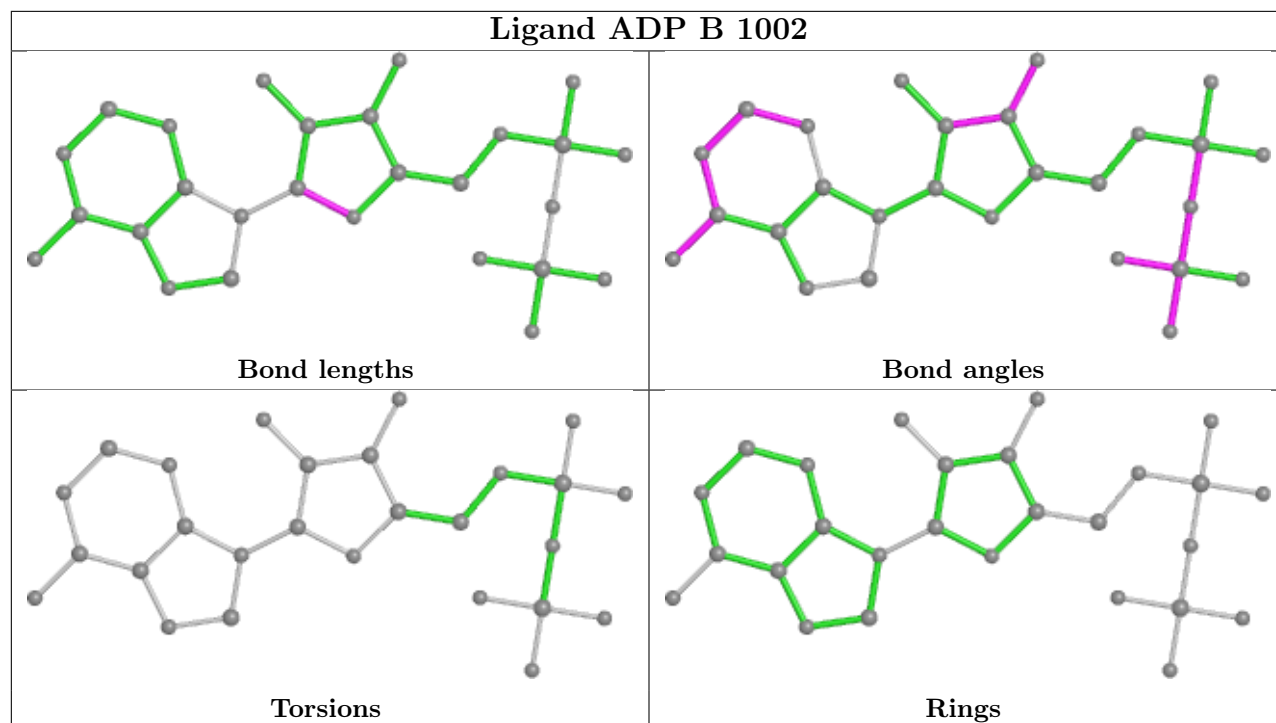
There are no ring outliers.

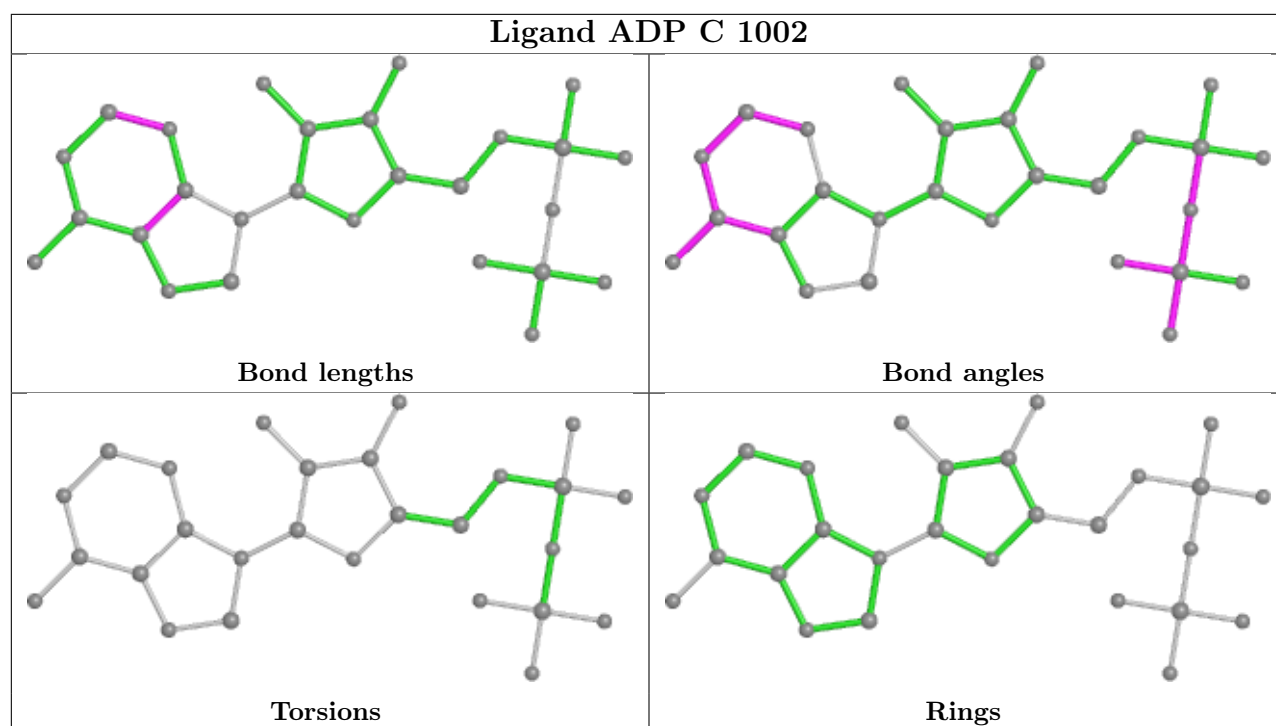
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	ADP	3	0
3	B	1002	ADP	1	0
3	C	1002	ADP	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/443 (74%)	0.22	6 (1%) 68 65	70, 76, 79, 83	0
1	B	327/443 (73%)	0.34	11 (3%) 45 42	68, 76, 79, 90	0
1	C	328/443 (74%)	0.32	9 (2%) 54 51	70, 76, 79, 83	0
1	D	325/443 (73%)	0.57	31 (9%) 8 9	67, 76, 79, 82	0
All	All	1308/1772 (73%)	0.36	57 (4%) 34 32	67, 76, 79, 90	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	SER	7.3
1	D	320	SER	5.4
1	D	77	GLN	5.3
1	D	73	LEU	5.2
1	D	93	LEU	4.5
1	C	36	PRO	4.3
1	D	75	VAL	4.2
1	B	320	SER	4.1
1	D	74	LEU	3.8
1	D	261	MET	3.7
1	B	306	ALA	3.4
1	D	94	GLU	3.4
1	D	274	ILE	3.3
1	B	141	PHE	3.2
1	A	320	SER	3.1
1	C	321	ASN	3.0
1	A	278	GLN	3.0
1	D	326	LEU	2.9
1	B	124	LEU	2.9
1	D	76	PRO	2.9
1	C	338	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	143	TYR	2.8
1	A	280	HIS	2.8
1	D	62	VAL	2.8
1	D	407	ALA	2.7
1	D	321	ASN	2.7
1	A	380	LEU	2.7
1	D	262	ASN	2.6
1	C	219	VAL	2.6
1	B	212	LYS	2.5
1	B	73	LEU	2.5
1	B	364	VAL	2.5
1	A	290	GLU	2.4
1	A	321	ASN	2.4
1	D	365	VAL	2.3
1	C	374	TRP	2.3
1	D	322	ILE	2.3
1	B	389	ILE	2.3
1	D	109	THR	2.3
1	D	380	LEU	2.2
1	D	189	VAL	2.2
1	C	62	VAL	2.2
1	B	94	GLU	2.2
1	D	280	HIS	2.2
1	D	124	LEU	2.1
1	D	300	LEU	2.1
1	C	201	VAL	2.1
1	D	59	GLU	2.1
1	B	142	ALA	2.1
1	D	329	LEU	2.1
1	D	47	ARG	2.0
1	D	187	TYR	2.0
1	D	301	ALA	2.0
1	B	213	PRO	2.0
1	C	74	LEU	2.0
1	D	71	THR	2.0
1	D	107	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

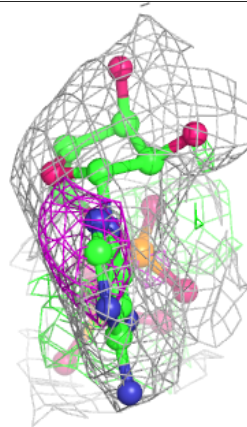
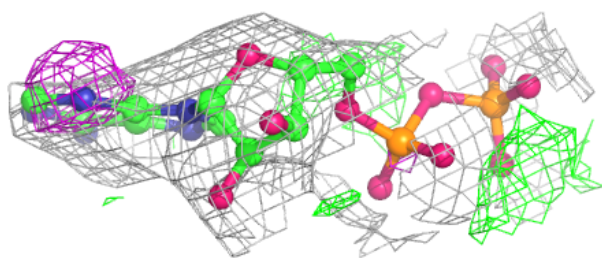
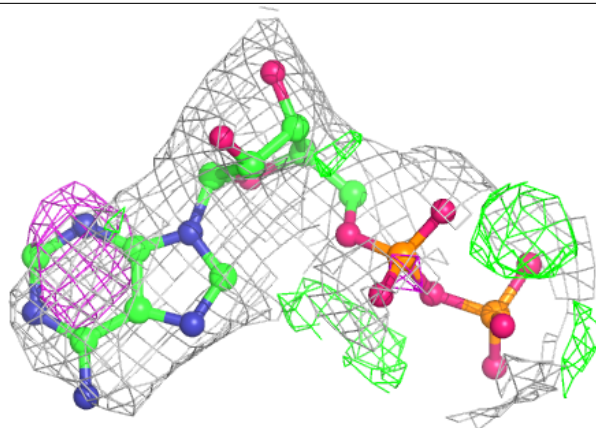
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	D	1002	27/27	0.89	0.20	72,75,76,77	0
2	MG	D	1001	1/1	0.91	0.22	61,61,61,61	0
3	ADP	C	1002	27/27	0.92	0.22	72,75,77,77	0
2	MG	C	1001	1/1	0.92	0.29	60,60,60,60	0
2	MG	A	1001	1/1	0.93	0.29	61,61,61,61	0
3	ADP	B	1002	27/27	0.94	0.21	72,75,77,77	0
3	ADP	A	1002	27/27	0.95	0.17	72,75,77,77	0
2	MG	B	1001	1/1	0.97	0.19	61,61,61,61	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.

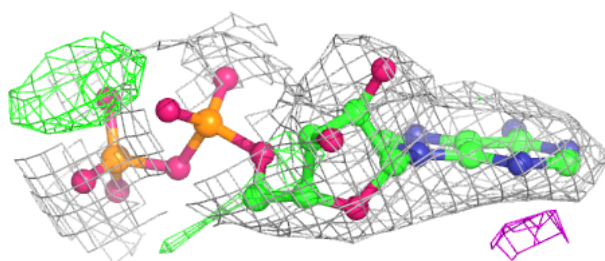
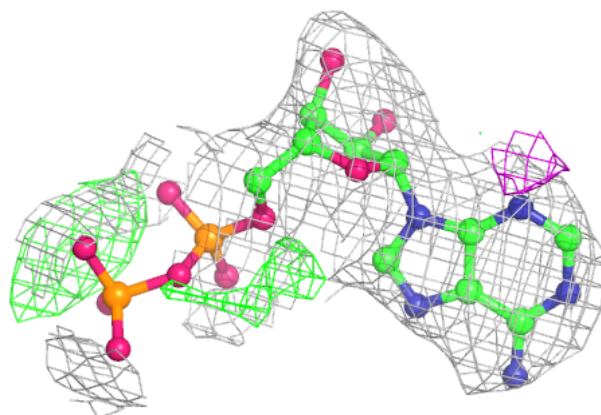
Electron density around ADP D 1002:

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

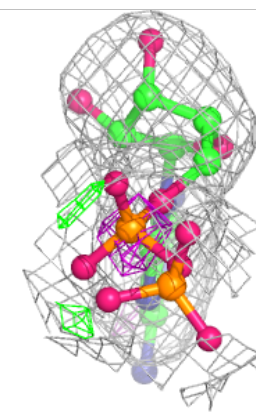
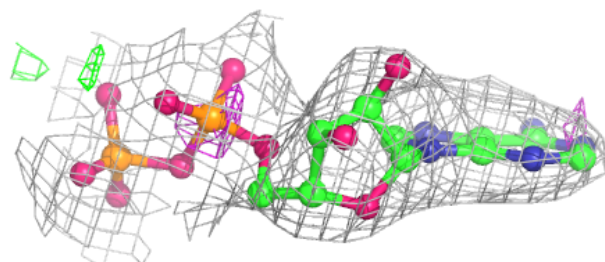
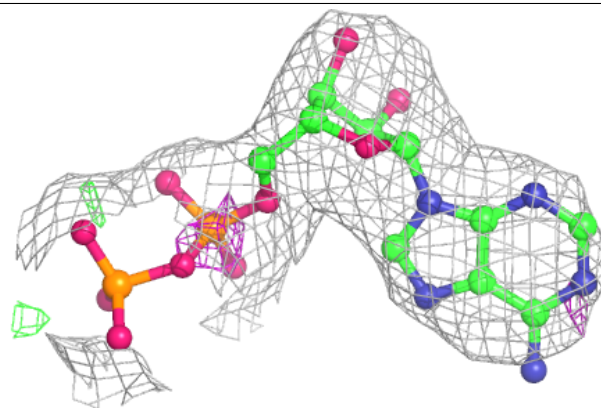


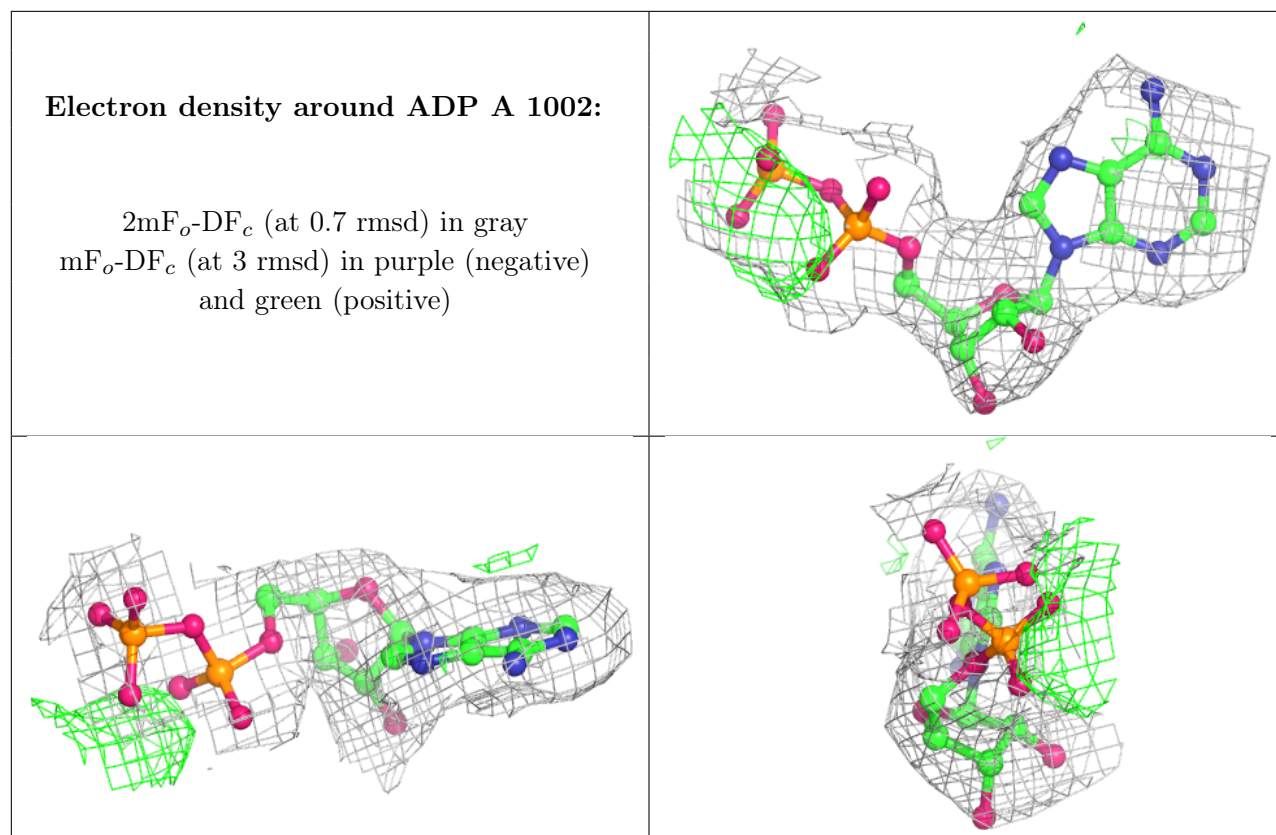
Electron density around ADP C 1002:

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

**Electron density around ADP B 1002:**

$2mF_o-DF_c$ (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.