Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 03:16 am GMT

PDB ID	:	3ZZN
Title	:	5-Mutant (R79W, R151A, E279A, E299A,E313A) Lactate-Dehydrogenase from Thermus thermophillus
Authors	:	Colletier, J.P.; Mraihi, S.; Madern, D.
Deposited on	:	2011-09-02
Resolution	:	2.90 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:

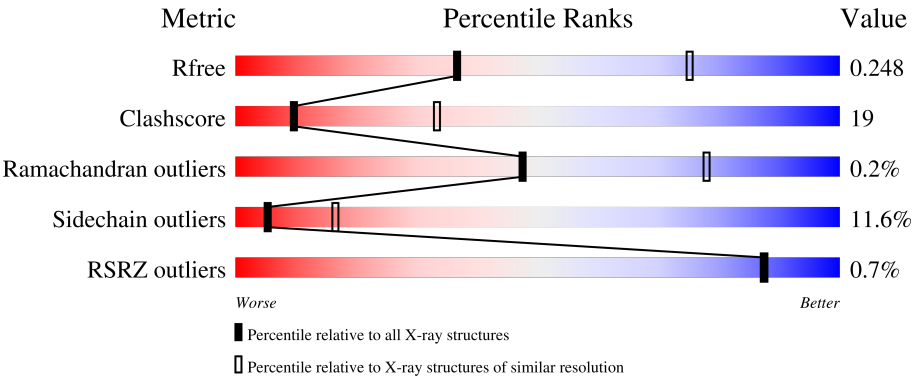
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	310	71% 24% 6%
1	B	310	69% 24% 7%
1	C	310	69% 25% 5%
1	D	310	71% 23% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9876 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.

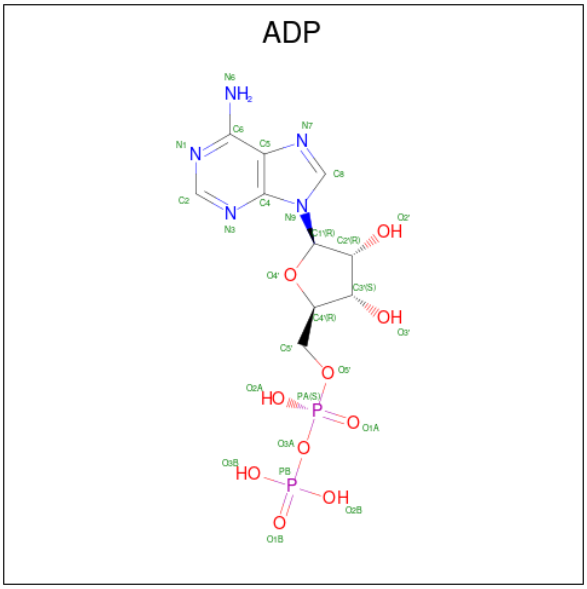
- Molecule 1 is a protein called LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	6	0
			2342	1490	422	427	3			
1	B	310	Total	C	N	O	S	0	10	0
			2386	1512	438	432	4			
1	C	310	Total	C	N	O	S	0	4	0
			2343	1488	425	427	3			
1	D	310	Total	C	N	O	S	0	6	0
			2335	1479	427	426	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	TRP	ARG	engineered mutation	UNP Q5SJA1
A	151	ALA	ARG	engineered mutation	UNP Q5SJA1
A	279	ALA	GLU	engineered mutation	UNP Q5SJA1
A	299	ALA	GLU	engineered mutation	UNP Q5SJA1
A	313	ALA	GLU	engineered mutation	UNP Q5SJA1
B	79	TRP	ARG	engineered mutation	UNP Q5SJA1
B	151	ALA	ARG	engineered mutation	UNP Q5SJA1
B	279	ALA	GLU	engineered mutation	UNP Q5SJA1
B	299	ALA	GLU	engineered mutation	UNP Q5SJA1
B	313	ALA	GLU	engineered mutation	UNP Q5SJA1
C	79	TRP	ARG	engineered mutation	UNP Q5SJA1
C	151	ALA	ARG	engineered mutation	UNP Q5SJA1
C	279	ALA	GLU	engineered mutation	UNP Q5SJA1
C	299	ALA	GLU	engineered mutation	UNP Q5SJA1
C	313	ALA	GLU	engineered mutation	UNP Q5SJA1
D	79	TRP	ARG	engineered mutation	UNP Q5SJA1
D	151	ALA	ARG	engineered mutation	UNP Q5SJA1
D	279	ALA	GLU	engineered mutation	UNP Q5SJA1
D	299	ALA	GLU	engineered mutation	UNP Q5SJA1
D	313	ALA	GLU	engineered mutation	UNP Q5SJA1

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



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

- Molecule 3 is water.

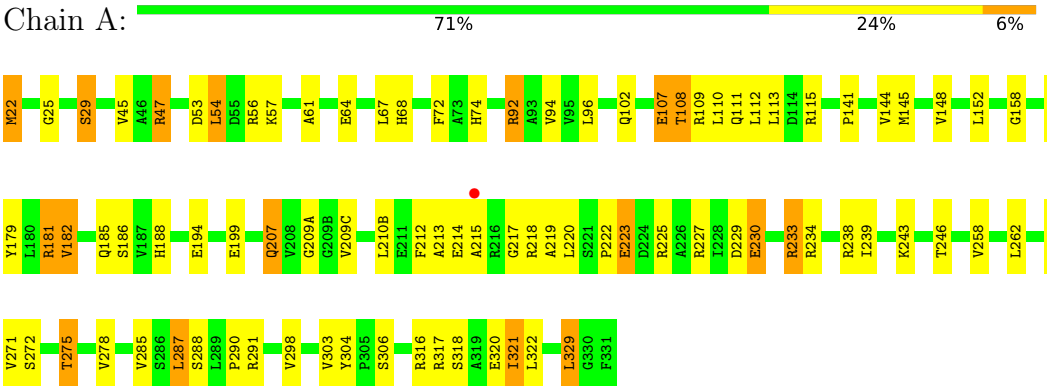
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	113	Total	O	0	0
			113	113		
3	C	105	Total	O	0	0
			105	105		
3	D	78	Total	O	0	0
			78	78		

3 Residue-property plots (i)

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

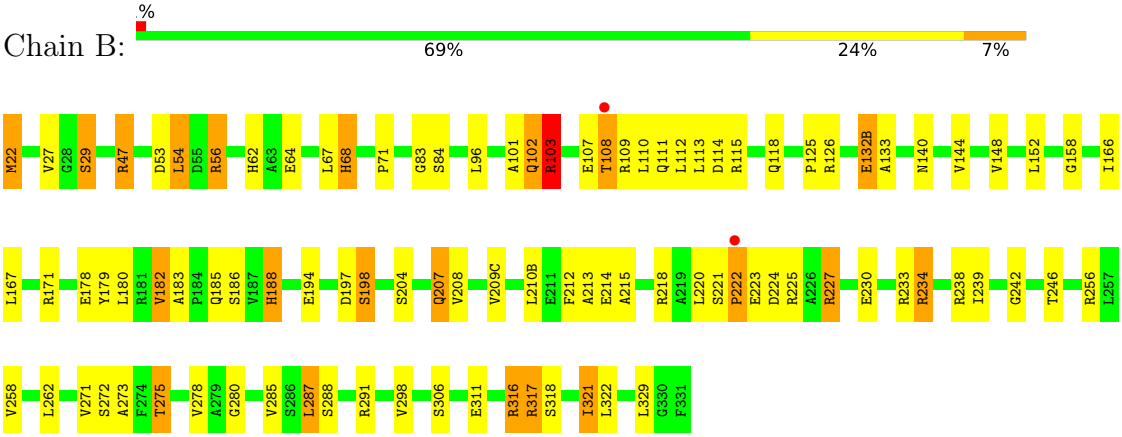
• Molecule 1: LACTATE DEHYDROGENASE

Chain A:



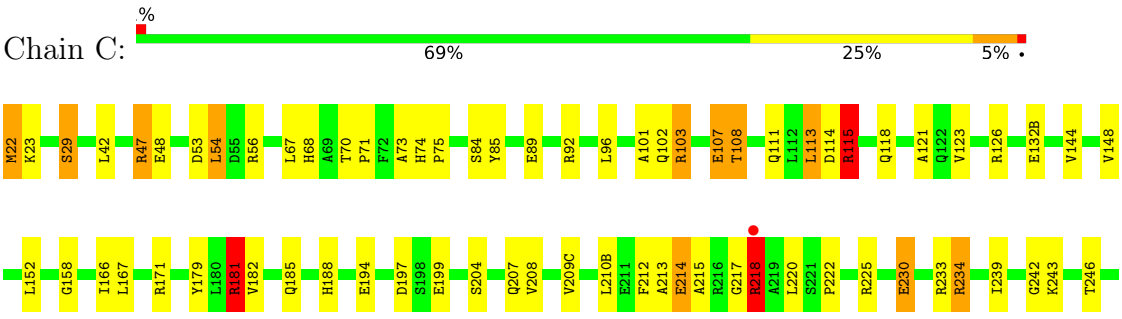
• Molecule 1: LACTATE DEHYDROGENASE

Chain B:



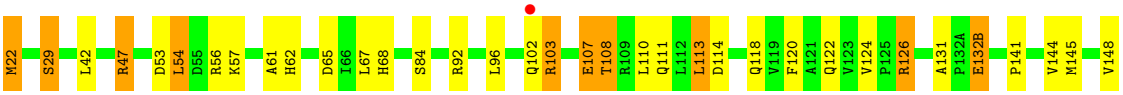
• Molecule 1: LACTATE DEHYDROGENASE

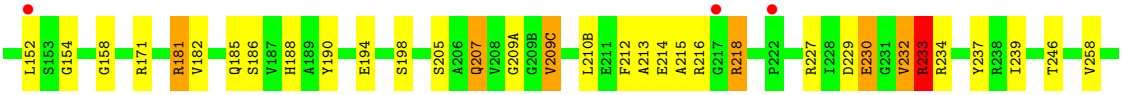
Chain C:

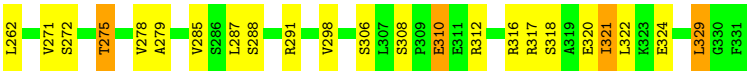


• Molecule 1: LACTATE DEHYDROGENASE

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.12Å 59.60Å 153.08Å 90.00° 93.37° 90.00°	Depositor
Resolution (Å)	45.47 – 2.90 44.57 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.47-2.90) 96.3 (44.57-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.251 0.185 , 0.248	Depositor DCC
R_{free} test set	2040 reflections (5.93%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9876	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.55	0/2385	0.71	0/3247
1	B	0.57	0/2429	0.75	1/3303 (0.0%)
1	C	0.52	0/2386	0.75	4/3247 (0.1%)
1	D	0.81	2/2376 (0.1%)	0.91	9/3233 (0.3%)
All	All	0.62	2/9576 (0.0%)	0.78	14/13030 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	3
1	D	0	3
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	VAL	C-N	-21.91	0.83	1.34
1	D	233	ARG	C-N	-20.11	0.87	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	233	ARG	O-C-N	-13.08	101.77	122.70
1	D	233	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	D	233	ARG	NE-CZ-NH1	11.42	126.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	218	ARG	N-CA-C	10.29	138.78	111.00
1	D	233	ARG	CA-C-N	9.13	137.29	117.20
1	D	232	VAL	C-N-CA	9.00	144.20	121.70
1	D	232	VAL	O-C-N	-7.26	111.09	122.70
1	D	233	ARG	CD-NE-CZ	6.30	132.43	123.60
1	C	181	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	D	181	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	218	ARG	N-CA-C	5.80	126.67	111.00
1	B	27	VAL	C-N-CA	5.55	133.97	122.30
1	C	181	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	214	GLU	CB-CA-C	-5.33	99.74	110.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	ALA	Mainchain
1	B	133	ALA	Mainchain
1	B	188[A]	HIS	Mainchain
1	C	103	ARG	Sidechain
1	C	115	ARG	Mainchain
1	C	218	ARG	Mainchain
1	D	126	ARG	Sidechain
1	D	218	ARG	Peptide
1	D	233	ARG	Sidechain

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	2342	0	2378	96	0
1	B	2386	0	2428	92	0
1	C	2343	0	2392	103	0
1	D	2335	0	2373	97	0
2	A	27	0	12	1	0
2	D	27	0	12	2	0
3	A	120	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	113	0	0	17	0
3	C	105	0	0	17	0
3	D	78	0	0	6	0
All	All	9876	0	9595	370	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 19.

All (370) 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:D:232:VAL:O	1:D:233:ARG:N	1.72	1.21
1:A:22:MET:HG3	1:A:92:ARG:NE	1.62	1.14
1:D:232:VAL:CA	1:D:233:ARG:N	2.11	1.11
1:D:232:VAL:C	1:D:233:ARG:CA	2.19	1.11
1:C:47[A]:ARG:HG3	1:C:47[A]:ARG:HH11	1.05	1.09
1:A:22:MET:HG3	1:A:92:ARG:HE	0.98	1.06
1:B:103[A]:ARG:NH1	3:B:2036:HOH:O	1.89	1.04
1:B:234:ARG:HG3	1:B:234:ARG:HH11	1.22	1.02
1:B:234:ARG:HH11	1:B:234:ARG:CG	1.73	1.00
1:D:22:MET:HG3	1:D:92:ARG:HE	1.22	0.98
1:B:132(B)[B]:GLU:OE2	3:B:2047:HOH:O	1.79	0.97
1:A:22:MET:CG	1:A:92:ARG:HE	1.77	0.96
1:C:47[A]:ARG:HH11	1:C:47[A]:ARG:CG	1.78	0.96
1:C:56[B]:ARG:CG	1:C:56[B]:ARG:HH11	1.80	0.92
1:A:145:MET:HG2	3:A:2057:HOH:O	1.69	0.91
1:C:56[B]:ARG:HH11	1:C:56[B]:ARG:HG2	1.31	0.91
1:C:47[A]:ARG:HG3	1:C:47[A]:ARG:NH1	1.70	0.90
1:D:232:VAL:C	1:D:233:ARG:N	0.83	0.88
1:C:194:GLU:HG3	1:C:322:LEU:HD21	1.54	0.87
1:D:194:GLU:HG3	1:D:322:LEU:HD21	1.56	0.87
1:B:234:ARG:HG3	1:B:234:ARG:NH1	1.82	0.86
3:C:2023:HOH:O	1:D:171[A]:ARG:HD3	1.75	0.84
1:C:56[B]:ARG:HG2	1:C:56[B]:ARG:NH1	1.88	0.84
1:D:237:TYR:CG	3:D:2062:HOH:O	2.32	0.82
1:B:84:SER:HB2	3:B:2017:HOH:O	1.81	0.81
1:B:29:SER:HB2	1:B:53:ASP:HB2	1.61	0.80
1:D:29:SER:HB2	1:D:53:ASP:HB2	1.63	0.79
1:D:154:GLY:HA2	3:D:2037:HOH:O	1.81	0.79
1:C:29:SER:HB2	1:C:53:ASP:HB2	1.64	0.79
1:C:47[A]:ARG:HD2	1:C:47[A]:ARG:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG23	1:A:111:GLN:HG3	1.63	0.78
1:D:103:ARG:O	1:D:107:GLU:HB3	1.84	0.78
1:D:230:GLU:OE1	1:D:234[A]:ARG:HG3	1.85	0.77
1:A:304:TYR:HD1	3:A:2110:HOH:O	1.67	0.76
1:D:131:ALA:C	1:D:132(B)[A]:GLU:H	1.87	0.76
1:D:234[B]:ARG:HH11	1:D:234[B]:ARG:CG	1.98	0.76
1:B:108:THR:HG21	3:B:2038:HOH:O	1.87	0.75
1:C:217:GLY:O	1:C:218:ARG:HG3	1.87	0.74
1:D:22:MET:HG2	1:D:262:LEU:CD2	2.15	0.74
1:D:108:THR:HG23	1:D:111:GLN:HG3	1.69	0.74
1:A:22:MET:HG2	1:A:262:LEU:CD2	2.18	0.74
1:C:181:ARG:HH21	1:C:218:ARG:HH22	1.35	0.74
1:D:122:GLN:O	1:D:126:ARG:HG3	1.88	0.73
1:A:144:VAL:HG12	3:A:2057:HOH:O	1.89	0.73
1:C:225:ARG:HD3	3:C:2081:HOH:O	1.88	0.72
1:A:179:TYR:CE1	1:A:218:ARG:HB3	2.24	0.72
1:C:22:MET:HG2	1:C:262:LEU:CD2	2.19	0.72
1:A:179:TYR:HE1	1:A:218:ARG:HB3	1.54	0.72
1:B:194:GLU:HG3	1:B:322:LEU:HD21	1.68	0.72
1:A:57:LYS:HE2	3:A:2017:HOH:O	1.88	0.72
1:C:68:HIS:CD2	1:D:171[B]:ARG:NH2	2.58	0.72
1:C:217:GLY:C	1:C:218:ARG:HG3	2.09	0.71
1:D:279:ALA:O	1:D:316[B]:ARG:HG3	1.90	0.71
1:C:108:THR:HG23	1:C:111:GLN:HG3	1.72	0.71
1:D:113:LEU:HG	1:D:329:LEU:HD12	1.72	0.71
1:D:234[B]:ARG:HH11	1:D:234[B]:ARG:HG3	1.55	0.71
1:C:113:LEU:HG	1:C:329:LEU:HD12	1.72	0.70
1:A:29:SER:HB2	1:A:53:ASP:HB2	1.74	0.70
1:A:181:ARG:HD3	1:A:218:ARG:NH2	2.05	0.70
1:C:210(B):LEU:O	1:C:213:ALA:HB3	1.92	0.70
3:C:2023:HOH:O	1:D:171[A]:ARG:CD	2.37	0.70
1:D:22:MET:HG2	1:D:262:LEU:HD23	1.74	0.69
1:C:256:ARG:NH1	1:C:256:ARG:HG3	2.08	0.68
1:D:214:GLU:CA	3:D:2055:HOH:O	2.42	0.68
1:B:22[B]:MET:N	1:B:47[B]:ARG:HE	1.90	0.68
1:C:171[B]:ARG:HD2	3:C:2064:HOH:O	1.92	0.68
1:A:113:LEU:HG	1:A:329:LEU:HD12	1.76	0.68
1:B:22[A]:MET:N	3:B:2001:HOH:O	2.26	0.68
1:B:194:GLU:OE1	1:B:198:SER:OG	2.10	0.68
1:D:212:PHE:HA	1:D:215:ALA:HB3	1.76	0.68
1:A:22:MET:HG2	1:A:262:LEU:HD23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:HG23	1:B:111:GLN:HG3	1.77	0.67
1:C:230:GLU:OE1	1:C:234:ARG:HG3	1.94	0.66
1:C:103:ARG:O	1:C:107:GLU:HB3	1.95	0.66
1:B:114:ASP:O	1:B:118:GLN:HG3	1.96	0.66
1:A:64:GLU:HG2	1:B:171[C]:ARG:HH22	1.61	0.66
1:A:317:ARG:O	1:A:321:ILE:HG22	1.95	0.66
1:C:256:ARG:HG3	1:C:256:ARG:HH11	1.61	0.65
1:B:113:LEU:HG	1:B:329:LEU:HD12	1.78	0.65
1:D:317:ARG:O	1:D:321:ILE:HG22	1.97	0.65
1:B:113:LEU:HD11	1:B:144:VAL:HG11	1.78	0.65
1:B:221:SER:O	1:B:224:ASP:N	2.30	0.65
1:C:323:LYS:HA	3:C:2101:HOH:O	1.96	0.64
1:B:321:ILE:HD11	3:B:2080:HOH:O	1.97	0.64
1:C:179:TYR:CZ	1:C:220:LEU:HD23	2.33	0.64
1:C:113:LEU:HG	1:C:329:LEU:CD1	2.28	0.64
1:D:108:THR:CG2	1:D:111:GLN:HG3	2.27	0.64
1:B:210(B):LEU:O	1:B:213:ALA:HB3	1.97	0.64
1:C:181:ARG:HE	1:C:218:ARG:NH2	1.94	0.64
1:B:212:PHE:HA	1:B:215:ALA:HB3	1.80	0.63
1:C:22:MET:HG2	1:C:262:LEU:HD23	1.79	0.63
1:D:113:LEU:HG	1:D:329:LEU:CD1	2.29	0.63
1:A:212:PHE:HA	1:A:215:ALA:HB3	1.79	0.63
1:B:221:SER:O	1:B:223:GLU:N	2.30	0.63
1:A:72:PHE:HB3	3:A:2025:HOH:O	1.97	0.63
1:C:212:PHE:HA	1:C:215:ALA:HB3	1.81	0.62
1:C:108:THR:CG2	1:C:111:GLN:HG3	2.28	0.62
1:D:56:ARG:NH2	1:D:84:SER:HB3	2.15	0.62
1:D:148:VAL:O	1:D:152:LEU:HG	2.00	0.61
1:D:210(B):LEU:O	1:D:213:ALA:HB3	2.00	0.61
1:A:113:LEU:HG	1:A:329:LEU:CD1	2.30	0.61
1:A:22:MET:HG3	1:A:92:ARG:CD	2.29	0.61
1:C:113:LEU:HD11	1:C:144:VAL:HG11	1.82	0.61
1:A:210(B):LEU:O	1:A:213:ALA:HB3	2.01	0.61
1:D:56:ARG:HH21	1:D:84:SER:HB3	1.65	0.61
1:C:291:ARG:NH1	3:C:2102:HOH:O	2.21	0.60
1:D:113:LEU:HD11	1:D:144:VAL:HG11	1.82	0.60
1:B:207:GLN:NE2	1:C:207:GLN:NE2	2.49	0.60
1:D:22:MET:CG	1:D:262:LEU:HD23	2.31	0.60
1:A:56[A]:ARG:HD3	3:A:2016:HOH:O	2.00	0.60
1:B:214:GLU:CA	3:B:2087:HOH:O	2.49	0.60
1:C:102:GLN:HB2	3:C:2036:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HD2	1:A:223[B]:GLU:OE1	2.02	0.60
1:B:113:LEU:HG	1:B:329:LEU:CD1	2.32	0.60
1:A:179:TYR:CZ	1:A:220:LEU:HD23	2.36	0.59
1:B:108:THR:CG2	1:B:111:GLN:HG3	2.32	0.59
1:C:84:SER:HB2	3:C:2015:HOH:O	2.02	0.59
1:D:230:GLU:OE1	1:D:234[B]:ARG:HG3	2.02	0.59
1:C:256:ARG:NH1	1:C:256:ARG:O	2.36	0.59
1:A:47:ARG:HG3	3:A:2026:HOH:O	2.02	0.59
1:A:304:TYR:CD1	3:A:2110:HOH:O	2.48	0.58
1:C:108:THR:HG22	1:C:111:GLN:OE1	2.03	0.58
1:D:234[B]:ARG:CG	1:D:234[B]:ARG:NH1	2.66	0.58
1:B:316:ARG:HG3	1:B:317:ARG:N	2.18	0.58
1:D:103:ARG:NH1	3:D:2023:HOH:O	2.37	0.58
1:A:217:GLY:C	1:A:218:ARG:HG3	2.24	0.58
1:D:310:GLU:CD	1:D:310:GLU:H	2.07	0.58
1:A:22:MET:CG	1:A:262:LEU:HD23	2.34	0.58
1:A:182:VAL:HG13	1:A:186:SER:OG	2.04	0.57
1:B:317:ARG:O	1:B:321:ILE:HG22	2.03	0.57
1:A:113:LEU:HD11	1:A:144:VAL:HG11	1.87	0.57
1:B:148:VAL:O	1:B:152:LEU:HG	2.04	0.57
1:C:179:TYR:HE1	1:C:218:ARG:HB2	1.69	0.57
1:D:102:GLN:HB2	3:D:2021:HOH:O	2.04	0.57
1:A:148:VAL:O	1:A:152:LEU:HG	2.05	0.57
1:C:179:TYR:CE1	1:C:218:ARG:HB3	2.40	0.57
1:D:229:ASP:OD1	1:D:233:ARG:NE	2.38	0.57
1:A:45:VAL:HA	3:A:2011:HOH:O	2.05	0.57
1:C:179:TYR:HE1	1:C:218:ARG:CB	2.17	0.57
1:D:22:MET:HB2	3:D:2002:HOH:O	2.04	0.57
1:A:320:GLU:HG2	3:A:2115:HOH:O	2.04	0.56
1:C:22:MET:CG	1:C:262:LEU:HD23	2.35	0.56
1:B:188[A]:HIS:CD2	3:B:2068:HOH:O	2.58	0.56
1:C:115:ARG:HG2	1:C:115:ARG:HH11	1.70	0.56
1:C:217:GLY:N	3:C:2077:HOH:O	2.32	0.56
1:A:230:GLU:OE1	1:A:234:ARG:HG2	2.04	0.56
1:A:181:ARG:HD3	1:A:218:ARG:CZ	2.36	0.56
1:D:329:LEU:HD23	1:D:329:LEU:O	2.06	0.56
1:D:22:MET:CG	1:D:92:ARG:HE	2.08	0.56
1:C:222:PRO:HG3	3:C:2082:HOH:O	2.06	0.56
1:C:304:TYR:HE1	3:C:2098:HOH:O	1.88	0.55
1:A:209(A):GLY:HA2	1:D:188[B]:HIS:HE1	1.71	0.55
1:A:229:ASP:CG	1:A:233:ARG:HH21	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56[B]:ARG:CG	1:C:56[B]:ARG:NH1	2.48	0.55
1:A:275:THR:CG2	1:A:291:ARG:HH22	2.20	0.54
1:C:148:VAL:O	1:C:152:LEU:HG	2.07	0.54
1:D:108:THR:HG22	1:D:111:GLN:OE1	2.07	0.54
1:A:209(A):GLY:C	1:D:188[B]:HIS:CE1	2.81	0.54
1:C:275:THR:CG2	1:C:291:ARG:HH22	2.20	0.54
1:D:317:ARG:O	1:D:321:ILE:CG2	2.55	0.54
1:A:258:VAL:O	1:A:262:LEU:HD12	2.08	0.54
1:B:108:THR:HG22	1:B:111:GLN:OE1	2.08	0.54
1:C:179:TYR:CE1	1:C:218:ARG:CB	2.91	0.54
1:C:115:ARG:HG2	1:C:115:ARG:NH1	2.23	0.53
1:A:329:LEU:HD23	1:A:329:LEU:O	2.08	0.53
1:D:278:VAL:HG11	1:D:287:LEU:HD21	1.89	0.53
1:A:22:MET:CG	1:A:92:ARG:NE	2.50	0.53
1:B:221:SER:C	1:B:223:GLU:N	2.62	0.53
1:B:101:ALA:O	1:B:115:ARG:NH2	2.42	0.53
1:B:329:LEU:HD23	1:B:329:LEU:O	2.09	0.52
1:B:275:THR:HG23	1:B:285:VAL:O	2.09	0.52
1:C:273:ALA:O	1:C:275:THR:HG22	2.09	0.52
1:A:74:HIS:HE1	3:A:2009:HOH:O	1.92	0.52
1:D:114:ASP:O	1:D:118:GLN:HG3	2.09	0.52
1:B:113:LEU:HD11	1:B:144:VAL:CG1	2.39	0.52
1:B:188[A]:HIS:CE1	3:B:2077:HOH:O	2.63	0.52
1:D:275:THR:HG23	1:D:285:VAL:O	2.10	0.52
1:A:141:PRO:HG2	3:A:2057:HOH:O	2.09	0.52
1:B:140:ASN:OD1	3:B:2050:HOH:O	2.19	0.52
1:B:188[A]:HIS:CD2	3:B:2075:HOH:O	2.62	0.52
1:D:239:ILE:CG2	1:D:246:THR:HG22	2.40	0.52
1:B:178:GLU:HB2	3:B:2072:HOH:O	2.10	0.52
1:A:239:ILE:CG2	1:A:246:THR:HG22	2.40	0.51
1:D:258:VAL:O	1:D:262:LEU:HD12	2.10	0.51
1:C:181:ARG:NH2	1:C:218:ARG:HH22	2.06	0.51
1:D:120:PHE:O	1:D:124:VAL:HG23	2.10	0.51
1:B:239:ILE:HG21	1:B:246:THR:HG22	1.93	0.51
1:A:207:GLN:NE2	1:D:207:GLN:NE2	2.59	0.51
1:A:266:LYS:HE2	3:A:2100:HOH:O	2.09	0.51
1:B:239:ILE:CG2	1:B:246:THR:HG22	2.41	0.51
1:D:53:ASP:OD2	2:D:1332:ADP:H1'	2.11	0.51
1:A:194:GLU:HG3	1:A:322:LEU:HD21	1.93	0.51
1:C:275:THR:HG21	1:C:291:ARG:HH22	1.75	0.51
1:D:239:ILE:HG21	1:D:246:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:O	1:A:288:SER:HA	2.11	0.50
1:A:278:VAL:HG11	1:A:287:LEU:HD21	1.93	0.50
1:B:102[B]:GLN:O	1:B:103[B]:ARG:O	2.28	0.50
1:B:179:TYR:CZ	1:B:220:LEU:HD23	2.46	0.50
1:A:213:ALA:HB1	1:A:218:ARG:O	2.12	0.50
1:A:275:THR:HG23	1:A:285:VAL:O	2.11	0.50
1:D:271:VAL:O	1:D:288:SER:HA	2.11	0.50
1:A:217:GLY:C	1:A:218:ARG:CG	2.79	0.50
1:B:132(B)[B]:GLU:HG3	3:B:2047:HOH:O	2.11	0.50
1:A:182:VAL:CG1	1:A:186:SER:OG	2.59	0.50
1:A:145:MET:CG	3:A:2057:HOH:O	2.44	0.50
1:B:258:VAL:O	1:B:262:LEU:HD12	2.12	0.50
1:C:114:ASP:O	1:C:118:GLN:HG3	2.12	0.50
1:A:188[A]:HIS:CE1	1:D:209(A):GLY:C	2.85	0.50
1:D:22:MET:HG3	1:D:92:ARG:NE	2.07	0.50
1:C:89:GLU:HB3	3:C:2002:HOH:O	2.11	0.49
1:A:275:THR:HG21	1:A:291:ARG:HH22	1.76	0.49
1:A:107:GLU:OE2	1:A:115:ARG:NH1	2.44	0.49
1:A:185:GLN:N	1:A:185:GLN:OE1	2.44	0.49
1:D:185:GLN:OE1	1:D:185:GLN:N	2.45	0.49
1:C:113:LEU:HD11	1:C:144:VAL:CG1	2.42	0.49
1:C:220:LEU:O	1:C:225:ARG:NH2	2.45	0.49
1:B:317:ARG:O	1:B:321:ILE:CG2	2.60	0.49
1:C:271:VAL:O	1:C:288:SER:HA	2.13	0.49
1:C:217:GLY:O	1:C:218:ARG:CG	2.60	0.49
1:A:167:LEU:HB2	3:A:2065:HOH:O	2.11	0.49
1:B:271:VAL:O	1:B:288:SER:HA	2.13	0.49
1:C:68:HIS:CD2	1:D:171[B]:ARG:CZ	2.96	0.49
1:D:232:VAL:O	1:D:233:ARG:CA	2.51	0.49
1:B:185:GLN:OE1	1:B:185:GLN:N	2.47	0.48
1:C:199:GLU:O	1:C:233:ARG:NH1	2.44	0.48
1:C:329:LEU:HD23	1:C:329:LEU:O	2.12	0.48
1:D:272:SER:HA	1:D:287:LEU:O	2.13	0.48
1:A:217:GLY:O	1:A:218:ARG:CG	2.62	0.48
1:B:102[B]:GLN:O	1:B:107:GLU:OE1	2.31	0.48
3:C:2020:HOH:O	1:D:171[B]:ARG:NH1	2.46	0.48
1:C:56[B]:ARG:HH11	1:C:56[B]:ARG:HG3	1.75	0.48
1:A:234:ARG:HD2	1:A:234:ARG:HA	1.50	0.48
1:C:56[B]:ARG:NH2	3:C:2015:HOH:O	2.46	0.48
1:C:181:ARG:HE	1:C:218:ARG:CZ	2.27	0.48
1:A:234:ARG:CB	1:A:238:ARG:NH1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:CD1	1:B:208:VAL:HG21	2.44	0.48
1:B:234:ARG:HB3	1:B:238:ARG:NH1	2.29	0.48
1:C:278:VAL:HG11	1:C:287:LEU:HD21	1.96	0.47
1:A:234:ARG:HB2	1:A:238:ARG:HH12	1.79	0.47
1:B:158:GLY:HA2	1:B:298:VAL:CG2	2.44	0.47
1:C:317:ARG:O	1:C:321:ILE:CG2	2.63	0.47
1:B:204:SER:HB3	1:B:311:GLU:OE1	2.14	0.47
1:B:278:VAL:HG11	1:B:287:LEU:HD21	1.96	0.47
1:B:103[B]:ARG:HG3	1:B:115:ARG:NH2	2.29	0.47
1:A:171[B]:ARG:HH22	1:B:64:GLU:HG2	1.80	0.47
1:B:234:ARG:HH11	1:B:234:ARG:HG2	1.69	0.47
1:C:108:THR:HG21	3:C:2042:HOH:O	2.14	0.47
1:D:212:PHE:O	1:D:212:PHE:CG	2.68	0.46
1:A:239:ILE:HG21	1:A:246:THR:HG22	1.96	0.46
1:C:101:ALA:O	1:C:115:ARG:NH2	2.49	0.46
1:D:207:GLN:HB2	1:D:209(C):VAL:O	2.15	0.46
1:A:64:GLU:HG2	1:B:171[C]:ARG:NH2	2.30	0.46
1:D:232:VAL:CB	1:D:233:ARG:N	2.77	0.46
1:A:53:ASP:OD1	2:A:1332:ADP:O2'	2.33	0.46
1:C:256:ARG:HH11	1:C:256:ARG:CG	2.25	0.46
1:A:317:ARG:O	1:A:321:ILE:CG2	2.60	0.46
1:D:22:MET:HG2	1:D:262:LEU:HD22	1.97	0.46
1:A:199:GLU:O	1:A:233:ARG:NH1	2.46	0.46
1:B:56[A]:ARG:HH22	1:B:83:GLY:HA2	1.81	0.46
1:B:221:SER:O	1:B:222:PRO:C	2.54	0.46
1:A:102:GLN:OE1	1:A:112:LEU:HD22	2.15	0.46
1:A:234:ARG:O	1:A:238:ARG:HG3	2.16	0.46
1:B:227[A]:ARG:HB2	1:B:227[A]:ARG:CZ	2.40	0.46
1:D:229:ASP:O	1:D:233:ARG:HB3	2.15	0.46
1:A:61:ALA:HB2	1:B:242:GLY:HA3	1.98	0.46
1:C:121:ALA:HA	1:C:152:LEU:HD13	1.98	0.46
1:A:272:SER:HA	1:A:287:LEU:O	2.16	0.46
1:B:47[A]:ARG:O	1:B:47[A]:ARG:HG3	2.14	0.45
1:B:102[B]:GLN:O	1:B:102[B]:GLN:NE2	2.49	0.45
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.81	0.45
1:A:243:LYS:HZ2	1:B:62:HIS:CE1	2.34	0.45
1:B:272:SER:HA	1:B:287:LEU:O	2.15	0.45
1:C:208:VAL:HG11	1:C:212:PHE:CE2	2.50	0.45
1:A:107:GLU:HG3	1:A:111:GLN:HB2	1.98	0.45
1:B:102[B]:GLN:HG2	1:B:112:LEU:HD22	1.99	0.45
1:C:73:ALA:HA	3:C:2030:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:O	1:C:262:LEU:HD12	2.16	0.45
1:D:67:LEU:HA	1:D:67:LEU:HD12	1.67	0.45
1:C:317:ARG:O	1:C:321:ILE:HG22	2.15	0.45
1:A:316:ARG:HG3	1:A:316:ARG:HH11	1.80	0.45
1:C:70:THR:OG1	1:C:71:PRO:HD3	2.17	0.45
1:B:280:GLY:HA3	1:B:316:ARG:HH21	1.82	0.45
1:D:53:ASP:OD1	2:D:1332:ADP:O2'	2.35	0.45
1:C:132(B):GLU:OE1	1:C:132(B):GLU:HA	2.17	0.45
1:D:132(B)[A]:GLU:O	1:D:132(B)[A]:GLU:HG3	2.17	0.45
1:C:243:LYS:HD2	1:D:62:HIS:CE1	2.52	0.45
1:A:179:TYR:HD2	1:A:227:ARG:HH22	1.63	0.44
1:C:92:ARG:HG3	1:C:92:ARG:NH1	2.32	0.44
1:C:166:ILE:HG13	1:C:167:LEU:N	2.32	0.44
1:C:188[A]:HIS:HE1	3:C:2073:HOH:O	2.00	0.44
1:B:197:ASP:O	1:B:233:ARG:NH1	2.49	0.44
1:B:212:PHE:O	1:B:212:PHE:CG	2.70	0.44
1:D:275:THR:CG2	1:D:291:ARG:HH22	2.30	0.44
1:D:308:SER:OG	1:D:310:GLU:HG2	2.17	0.44
1:A:108:THR:C	1:A:110:LEU:N	2.71	0.44
1:B:103[A]:ARG:O	1:B:107:GLU:HB3	2.17	0.44
1:C:47[A]:ARG:CG	1:C:47[A]:ARG:NH1	2.47	0.44
1:C:67:LEU:HA	1:C:67:LEU:HD12	1.73	0.44
1:D:131:ALA:C	1:D:132(B)[A]:GLU:N	2.60	0.44
1:A:269:TYR:HA	3:A:2104:HOH:O	2.16	0.44
1:B:275:THR:CG2	1:B:291:ARG:HH22	2.30	0.44
1:D:54:LEU:HA	1:D:54:LEU:HD23	1.60	0.44
1:D:287:LEU:C	1:D:287:LEU:HD12	2.37	0.44
1:C:181:ARG:HE	1:C:218:ARG:HH22	1.64	0.44
1:A:68:HIS:CD2	1:B:171[C]:ARG:HE	2.35	0.44
1:B:109:ARG:NH2	3:B:2041:HOH:O	2.47	0.44
1:B:221:SER:C	1:B:223:GLU:H	2.22	0.44
1:A:25:GLY:O	1:A:94:VAL:HA	2.18	0.43
1:D:188[B]:HIS:NE2	1:D:190:TYR:CZ	2.77	0.43
1:B:210(B):LEU:HD22	1:B:225:ARG:HH21	1.83	0.43
1:D:132(B)[A]:GLU:O	1:D:132(B)[A]:GLU:CG	2.66	0.43
1:D:230:GLU:OE1	1:D:230:GLU:HA	2.19	0.43
1:C:179:TYR:CE1	1:C:220:LEU:HD23	2.53	0.43
1:C:275:THR:HG23	1:C:285:VAL:O	2.18	0.43
1:B:182:VAL:HG13	1:B:186:SER:OG	2.18	0.43
1:D:113:LEU:HD11	1:D:144:VAL:CG1	2.49	0.43
1:D:141:PRO:O	1:D:145:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLY:HA2	1:A:298:VAL:CG2	2.48	0.43
1:B:67:LEU:HA	1:B:67:LEU:HD12	1.72	0.43
1:D:122:GLN:OE1	1:D:126:ARG:NH1	2.51	0.43
1:C:272:SER:HA	1:C:287:LEU:O	2.19	0.43
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.60	0.43
1:C:85:TYR:OH	1:C:123:VAL:HG22	2.19	0.43
1:D:158:GLY:HA2	1:D:298:VAL:CG2	2.49	0.43
1:A:217:GLY:O	1:A:218:ARG:HG2	2.18	0.42
1:C:212:PHE:O	1:C:212:PHE:CG	2.71	0.42
1:C:256:ARG:NH2	1:C:265:GLU:OE1	2.39	0.42
1:D:320:GLU:O	1:D:324:GLU:HG3	2.19	0.42
1:A:113:LEU:HA	3:A:2039:HOH:O	2.19	0.42
1:C:158:GLY:HA2	1:C:298:VAL:CG2	2.49	0.42
1:D:103:ARG:HG3	1:D:107:GLU:CD	2.39	0.42
1:C:239:ILE:CG2	1:C:246:THR:HG22	2.49	0.42
1:D:47:ARG:HD2	1:D:47:ARG:HA	1.61	0.42
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.79	0.42
1:B:109:ARG:NH2	3:B:2042:HOH:O	2.53	0.42
1:B:22[B]:MET:N	1:B:47[B]:ARG:HH21	2.18	0.42
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.63	0.42
1:A:290:PRO:HB2	1:A:303:VAL:HB	2.02	0.42
1:C:213:ALA:HB1	1:C:218:ARG:O	2.19	0.42
1:C:74:HIS:HA	1:C:75:PRO:HD3	1.87	0.42
1:C:204:SER:HB3	1:C:311:GLU:OE1	2.20	0.42
1:C:239:ILE:HD13	1:D:65:ASP:HA	2.02	0.41
1:A:179:TYR:CE1	1:A:220:LEU:HD23	2.55	0.41
3:A:2103:HOH:O	1:D:186:SER:HB3	2.20	0.41
1:B:54:LEU:HA	1:B:54:LEU:HD23	1.63	0.41
1:C:23:LYS:HG3	1:C:48:GLU:HB3	2.02	0.41
1:B:166:ILE:HG13	1:B:167:LEU:N	2.36	0.41
1:B:233:ARG:NH2	3:B:2084:HOH:O	2.51	0.41
1:C:316:ARG:HG3	1:C:316:ARG:HH11	1.86	0.41
1:A:188[A]:HIS:HE1	1:D:209(A):GLY:HA2	1.85	0.41
1:B:183:ALA:O	1:B:186:SER:OG	2.38	0.41
1:B:256[A]:ARG:HA	1:B:256[A]:ARG:HD2	1.75	0.41
1:D:108:THR:HG23	1:D:111:GLN:H	1.86	0.41
1:A:108:THR:O	1:A:109:ARG:C	2.59	0.41
1:A:67:LEU:HD12	1:A:67:LEU:HA	1.72	0.41
1:A:234:ARG:CB	1:A:238:ARG:HH12	2.34	0.41
1:B:208:VAL:HG11	1:B:212:PHE:CE2	2.55	0.41
1:C:102:GLN:HG3	1:C:103:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLY:HA3	1:D:61:ALA:HB2	2.02	0.41
1:B:68:HIS:O	1:B:71:PRO:HD2	2.21	0.41
1:D:144:VAL:HG12	1:D:145:MET:N	2.36	0.41
1:D:110:LEU:HA	1:D:110:LEU:HD12	1.78	0.40
1:B:273:ALA:O	1:B:275:THR:HG22	2.20	0.40
1:D:212:PHE:HA	1:D:215:ALA:CB	2.48	0.40
1:B:188[A]:HIS:CE1	3:B:2076:HOH:O	2.74	0.40
1:B:316:ARG:HE	1:B:316:ARG:HB2	1.44	0.40
1:A:210(B):LEU:HD22	1:A:225[B]:ARG:HH21	1.87	0.40
1:A:212:PHE:O	1:A:212:PHE:CG	2.74	0.40
1:B:258:VAL:HG12	1:B:262:LEU:HD12	2.03	0.40
1:C:42:LEU:HD12	1:D:42:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/310 (101%)	302 (96%)	12 (4%)	0	100	100
1	B	317/310 (102%)	304 (96%)	9 (3%)	4 (1%)	12	37
1	C	312/310 (101%)	303 (97%)	9 (3%)	0	100	100
1	D	314/310 (101%)	302 (96%)	12 (4%)	0	100	100
All	All	1257/1240 (101%)	1211 (96%)	42 (3%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103[A]	ARG
1	B	103[B]	ARG
1	B	218	ARG

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Mol	Chain	Res	Type
1	B	222	PRO

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	229/228 (100%)	204 (89%)	25 (11%)	6 19
1	B	235/228 (103%)	200 (85%)	35 (15%)	3 9
1	C	232/228 (102%)	206 (89%)	26 (11%)	6 18
1	D	229/228 (100%)	200 (87%)	29 (13%)	4 13
All	All	925/912 (101%)	810 (88%)	115 (12%)	5 14

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	29	SER
1	A	47	ARG
1	A	54	LEU
1	A	92	ARG
1	A	96	LEU
1	A	107	GLU
1	A	108	THR
1	A	171[A]	ARG
1	A	171[B]	ARG
1	A	181	ARG
1	A	182	VAL
1	A	207	GLN
1	A	209(C)	VAL
1	A	214	GLU
1	A	223[A]	GLU
1	A	223[B]	GLU
1	A	230	GLU
1	A	233	ARG
1	A	275	THR

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	306	SER
1	A	318	SER
1	A	321	ILE
1	A	329	LEU
1	B	22[A]	MET
1	B	22[B]	MET
1	B	29	SER
1	B	47[A]	ARG
1	B	47[B]	ARG
1	B	54	LEU
1	B	56[A]	ARG
1	B	56[B]	ARG
1	B	68	HIS
1	B	96	LEU
1	B	102[A]	GLN
1	B	102[B]	GLN
1	B	103[A]	ARG
1	B	103[B]	ARG
1	B	108	THR
1	B	110	LEU
1	B	125	PRO
1	B	126	ARG
1	B	132(B)[A]	GLU
1	B	132(B)[B]	GLU
1	B	182	VAL
1	B	198	SER
1	B	207	GLN
1	B	209(C)	VAL
1	B	227[A]	ARG
1	B	227[B]	ARG
1	B	230	GLU
1	B	234	ARG
1	B	275	THR
1	B	287	LEU
1	B	306	SER
1	B	316	ARG
1	B	317	ARG
1	B	318	SER
1	B	321	ILE
1	C	22	MET
1	C	29	SER

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Mol	Chain	Res	Type
1	C	47[A]	ARG
1	C	47[B]	ARG
1	C	54	LEU
1	C	96	LEU
1	C	107	GLU
1	C	108	THR
1	C	113	LEU
1	C	115	ARG
1	C	126	ARG
1	C	181	ARG
1	C	182	VAL
1	C	185	GLN
1	C	197	ASP
1	C	209(C)	VAL
1	C	214	GLU
1	C	218	ARG
1	C	230	GLU
1	C	234	ARG
1	C	275	THR
1	C	287	LEU
1	C	306	SER
1	C	318	SER
1	C	321	ILE
1	C	324	GLU
1	D	22	MET
1	D	29	SER
1	D	47	ARG
1	D	54	LEU
1	D	57	LYS
1	D	68	HIS
1	D	96	LEU
1	D	103	ARG
1	D	107	GLU
1	D	108	THR
1	D	113	LEU
1	D	132(B)[A]	GLU
1	D	132(B)[B]	GLU
1	D	181	ARG
1	D	182	VAL
1	D	198	SER
1	D	205	SER
1	D	207	GLN

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Mol	Chain	Res	Type
1	D	209(C)	VAL
1	D	216	ARG
1	D	227	ARG
1	D	230	GLU
1	D	275	THR
1	D	306	SER
1	D	310	GLU
1	D	312	ARG
1	D	318	SER
1	D	321	ILE
1	D	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	74	HIS
1	A	207	GLN
1	B	207	GLN
1	C	68	HIS
1	C	140	ASN
1	C	185	GLN
1	C	207	GLN
1	D	207	GLN

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	1332	-	24,29,29	0.92	1 (4%)	29,45,45	1.35	3 (10%)
2	ADP	D	1332	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1332	-	-	1/12/32/32	0/3/3/3
2	ADP	D	1332	-	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1332	ADP	C5-C4	2.31	1.47	1.40
2	A	1332	ADP	C5-C4	2.25	1.46	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1332	ADP	PA-O3A-PB	-3.54	120.66	132.83
2	A	1332	ADP	N3-C2-N1	-3.26	123.58	128.68
2	D	1332	ADP	N3-C2-N1	-3.24	123.61	128.68
2	D	1332	ADP	C3'-C2'-C1'	2.76	105.14	100.98
2	A	1332	ADP	PA-O3A-PB	-2.75	123.40	132.83
2	A	1332	ADP	C4-C5-N7	-2.69	106.60	109.40
2	D	1332	ADP	C4-C5-N7	-2.63	106.66	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1332	ADP	C5'-O5'-PA-O2A
2	D	1332	ADP	C5'-O5'-PA-O3A
2	D	1332	ADP	O4'-C4'-C5'-O5'
2	D	1332	ADP	C3'-C4'-C5'-O5'
2	D	1332	ADP	PB-O3A-PA-O5'
2	A	1332	ADP	O4'-C4'-C5'-O5'

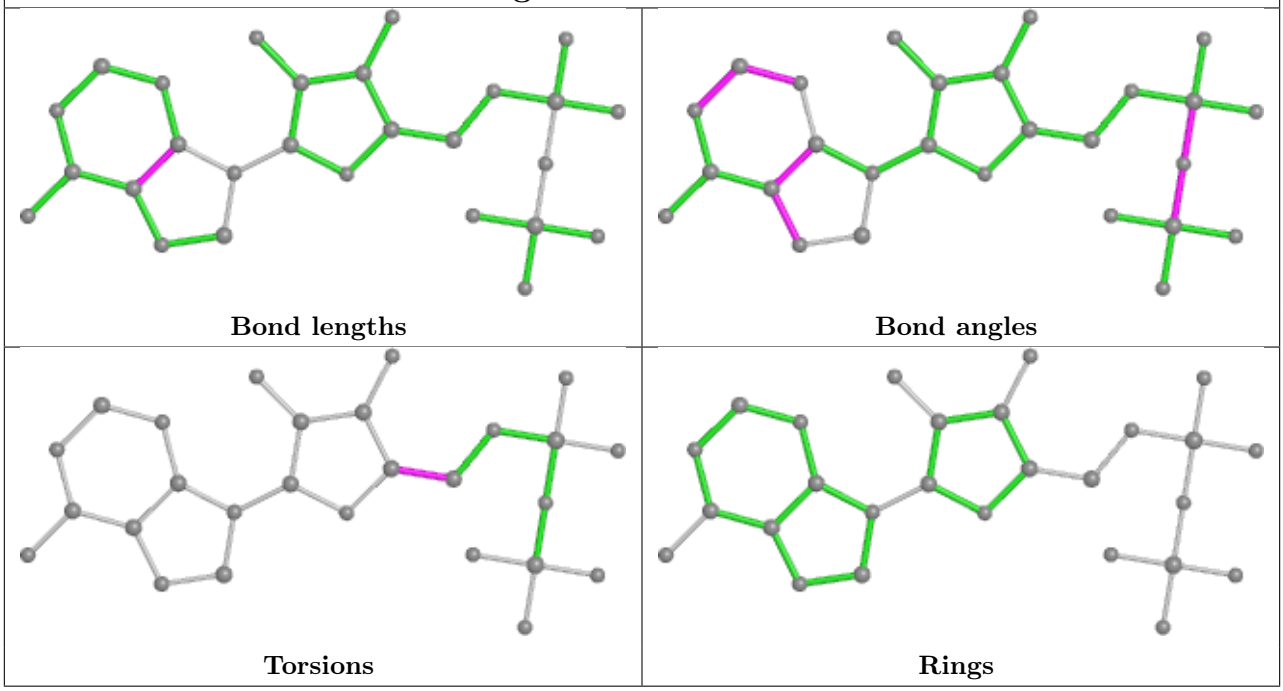
There are no ring outliers.

2 monomers are involved in 3 short contacts:

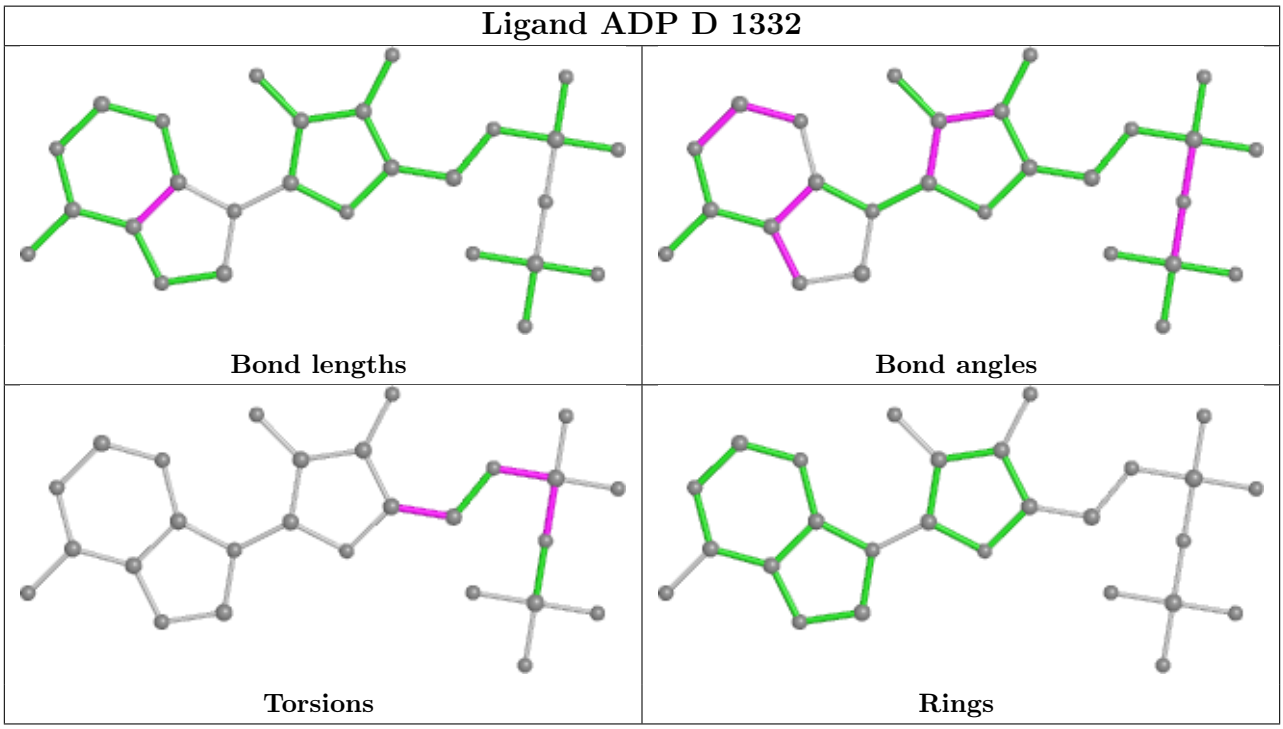
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1332	ADP	1	0
2	D	1332	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 1332



Ligand ADP D 1332



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	188[B]:HIS	C	189:ALA	N	1.14
1	D	233:ARG	C	234[B]:ARG	N	0.87
1	D	233:ARG	C	234[A]:ARG	N	0.87
1	D	232:VAL	C	233:ARG	N	0.83

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, 95^{th} 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	310/310 (100%)	-0.32	1 (0%)	94	94	14, 36, 75, 120	0
1	B	310/310 (100%)	-0.32	2 (0%)	89	89	14, 34, 71, 108	0
1	C	310/310 (100%)	-0.22	2 (0%)	89	89	18, 37, 76, 114	0
1	D	310/310 (100%)	-0.21	4 (1%)	77	77	17, 38, 77, 120	0
All	All	1240/1240 (100%)	-0.27	9 (0%)	87	87	14, 36, 76, 120	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	PRO	4.2
1	D	217	GLY	3.0
1	C	218	ARG	2.7
1	A	215	ALA	2.7
1	D	152	LEU	2.3
1	D	102	GLN	2.2
1	B	222	PRO	2.1
1	B	108	THR	2.0
1	C	308	SER	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

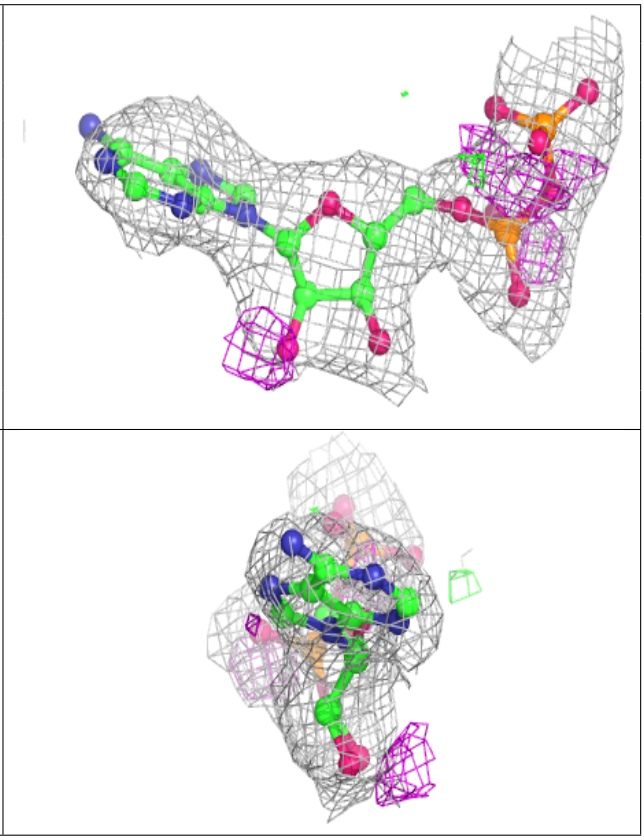
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ADP	D	1332	27/27	0.93	0.20	40,54,67,89	0
2	ADP	A	1332	27/27	0.97	0.14	12,27,45,58	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.

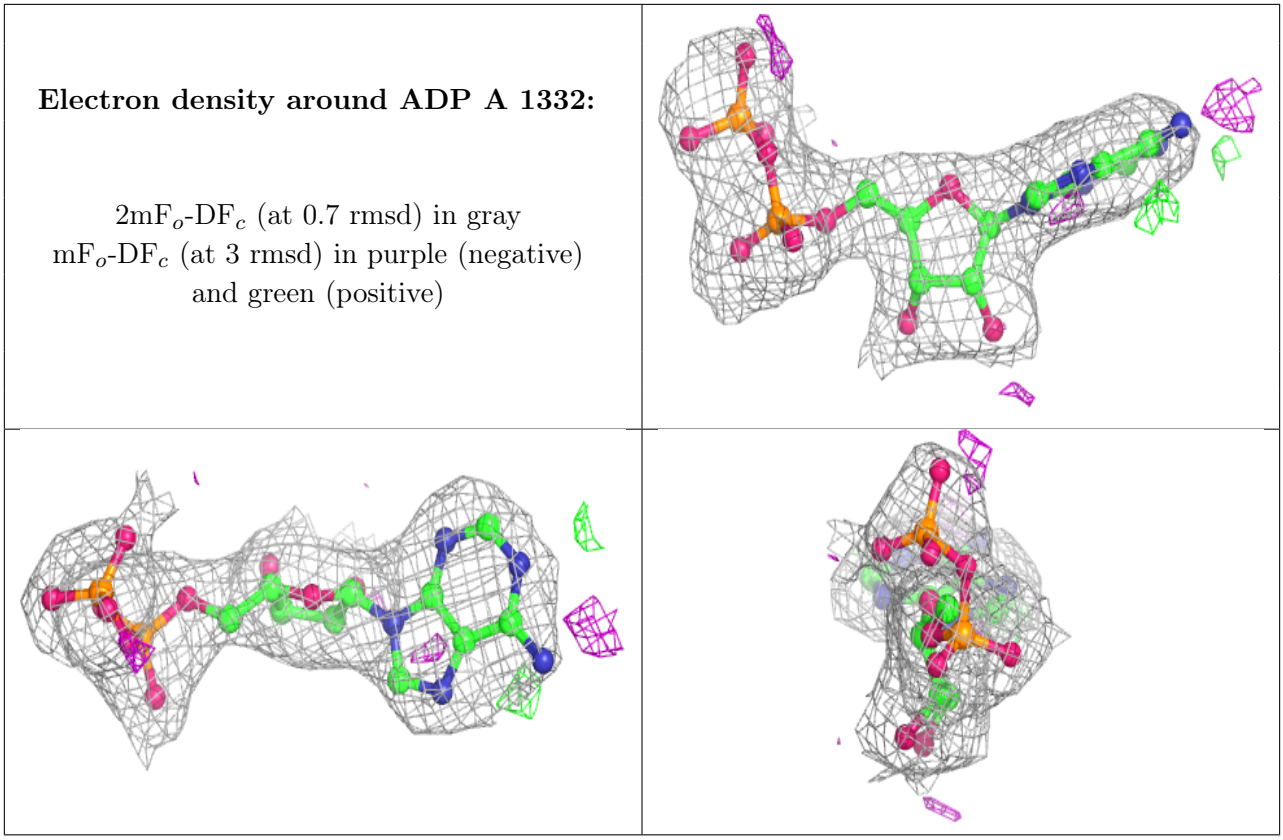
Electron density around ADP D 1332:

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



Electron density around ADP A 1332:

$2mF_o$-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.