Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2024 – 12:06 PM EST

PDB ID	:	3K5I
Title	:	Crystal structure of N5-carboxyaminoimidazole synthase from aspergillus clavatus in complex with ADP and 5-aminoimadazole ribonucleotide
Authors	:	Thoden, J.B.; Holden, H.M.; Paritala, H.; Firestine, S.M.
Deposited on	:	2009-10-07
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

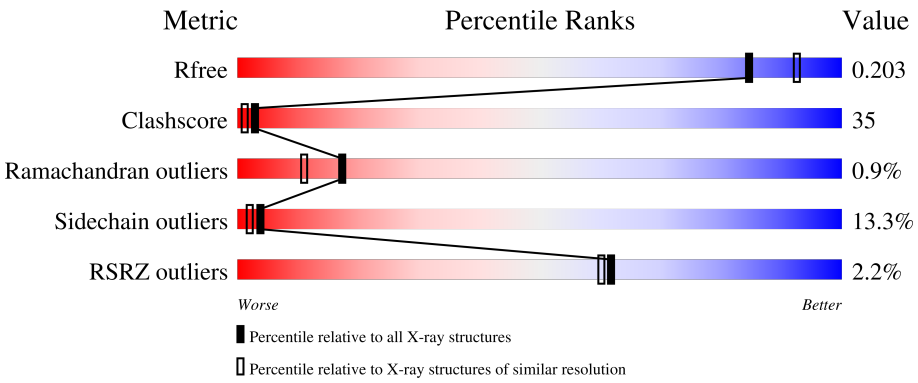
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	403	47% 39% 7% 5%
1	B	403	4% 37% 40% 13% • 7%
1	C	403	% 41% 42% 10% • 5%
1	D	403	3% 35% 43% 12% • 7%

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
6	AIR	A	402	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13147 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 Phosphoribosyl-aminoimidazole carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2975	1870	523	566	16	0	5	0
1	B	376	2944	1850	516	563	15	0	6	0
1	C	382	2995	1881	529	569	16	0	6	0
1	D	373	2888	1816	506	550	16	0	1	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	HIS	-	expression tag	UNP A1CII2
A	-18	GLY	-	expression tag	UNP A1CII2
A	-17	SER	-	expression tag	UNP A1CII2
A	-16	SER	-	expression tag	UNP A1CII2
A	-15	HIS	-	expression tag	UNP A1CII2
A	-14	HIS	-	expression tag	UNP A1CII2
A	-13	HIS	-	expression tag	UNP A1CII2
A	-12	HIS	-	expression tag	UNP A1CII2
A	-11	HIS	-	expression tag	UNP A1CII2
A	-10	HIS	-	expression tag	UNP A1CII2
A	-9	SER	-	expression tag	UNP A1CII2
A	-8	SER	-	expression tag	UNP A1CII2
A	-7	GLU	-	expression tag	UNP A1CII2
A	-6	ASN	-	expression tag	UNP A1CII2
A	-5	LEU	-	expression tag	UNP A1CII2
A	-4	TYR	-	expression tag	UNP A1CII2
A	-3	PHE	-	expression tag	UNP A1CII2
A	-2	GLN	-	expression tag	UNP A1CII2
A	-1	GLY	-	expression tag	UNP A1CII2
A	0	HIS	-	expression tag	UNP A1CII2
B	-19	HIS	-	expression tag	UNP A1CII2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A1CII2
B	-17	SER	-	expression tag	UNP A1CII2
B	-16	SER	-	expression tag	UNP A1CII2
B	-15	HIS	-	expression tag	UNP A1CII2
B	-14	HIS	-	expression tag	UNP A1CII2
B	-13	HIS	-	expression tag	UNP A1CII2
B	-12	HIS	-	expression tag	UNP A1CII2
B	-11	HIS	-	expression tag	UNP A1CII2
B	-10	HIS	-	expression tag	UNP A1CII2
B	-9	SER	-	expression tag	UNP A1CII2
B	-8	SER	-	expression tag	UNP A1CII2
B	-7	GLU	-	expression tag	UNP A1CII2
B	-6	ASN	-	expression tag	UNP A1CII2
B	-5	LEU	-	expression tag	UNP A1CII2
B	-4	TYR	-	expression tag	UNP A1CII2
B	-3	PHE	-	expression tag	UNP A1CII2
B	-2	GLN	-	expression tag	UNP A1CII2
B	-1	GLY	-	expression tag	UNP A1CII2
B	0	HIS	-	expression tag	UNP A1CII2
C	-19	HIS	-	expression tag	UNP A1CII2
C	-18	GLY	-	expression tag	UNP A1CII2
C	-17	SER	-	expression tag	UNP A1CII2
C	-16	SER	-	expression tag	UNP A1CII2
C	-15	HIS	-	expression tag	UNP A1CII2
C	-14	HIS	-	expression tag	UNP A1CII2
C	-13	HIS	-	expression tag	UNP A1CII2
C	-12	HIS	-	expression tag	UNP A1CII2
C	-11	HIS	-	expression tag	UNP A1CII2
C	-10	HIS	-	expression tag	UNP A1CII2
C	-9	SER	-	expression tag	UNP A1CII2
C	-8	SER	-	expression tag	UNP A1CII2
C	-7	GLU	-	expression tag	UNP A1CII2
C	-6	ASN	-	expression tag	UNP A1CII2
C	-5	LEU	-	expression tag	UNP A1CII2
C	-4	TYR	-	expression tag	UNP A1CII2
C	-3	PHE	-	expression tag	UNP A1CII2
C	-2	GLN	-	expression tag	UNP A1CII2
C	-1	GLY	-	expression tag	UNP A1CII2
C	0	HIS	-	expression tag	UNP A1CII2
D	-19	HIS	-	expression tag	UNP A1CII2
D	-18	GLY	-	expression tag	UNP A1CII2
D	-17	SER	-	expression tag	UNP A1CII2

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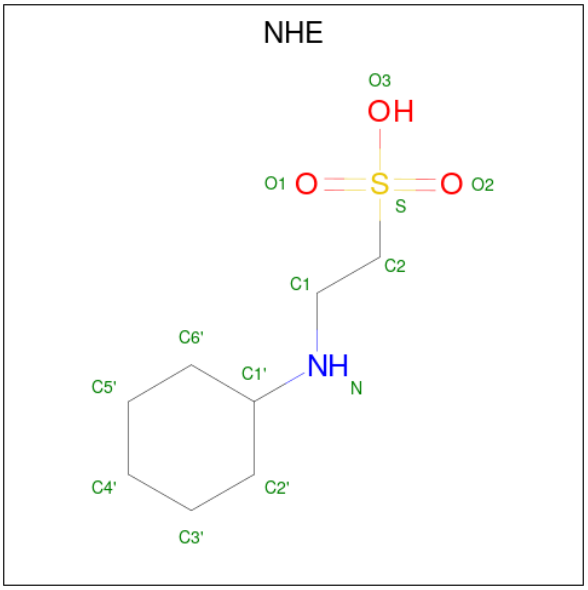
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A1CII2
D	-15	HIS	-	expression tag	UNP A1CII2
D	-14	HIS	-	expression tag	UNP A1CII2
D	-13	HIS	-	expression tag	UNP A1CII2
D	-12	HIS	-	expression tag	UNP A1CII2
D	-11	HIS	-	expression tag	UNP A1CII2
D	-10	HIS	-	expression tag	UNP A1CII2
D	-9	SER	-	expression tag	UNP A1CII2
D	-8	SER	-	expression tag	UNP A1CII2
D	-7	GLU	-	expression tag	UNP A1CII2
D	-6	ASN	-	expression tag	UNP A1CII2
D	-5	LEU	-	expression tag	UNP A1CII2
D	-4	TYR	-	expression tag	UNP A1CII2
D	-3	PHE	-	expression tag	UNP A1CII2
D	-2	GLN	-	expression tag	UNP A1CII2
D	-1	GLY	-	expression tag	UNP A1CII2
D	0	HIS	-	expression tag	UNP A1CII2

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

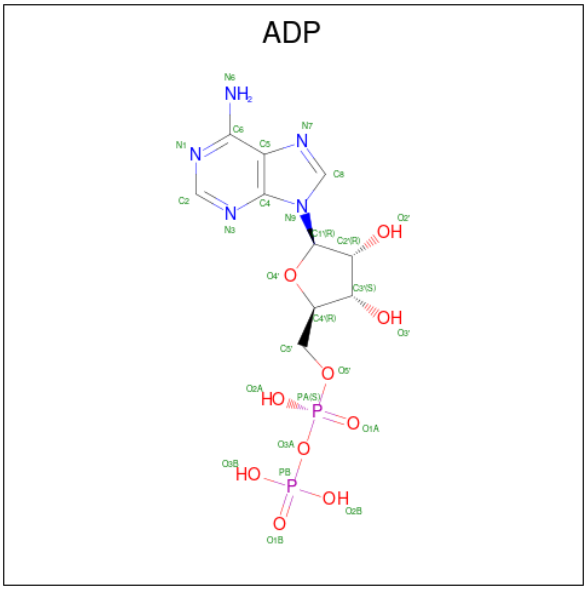
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	13	8	1	3	1	0	0
3	C	1	13	8	1	3	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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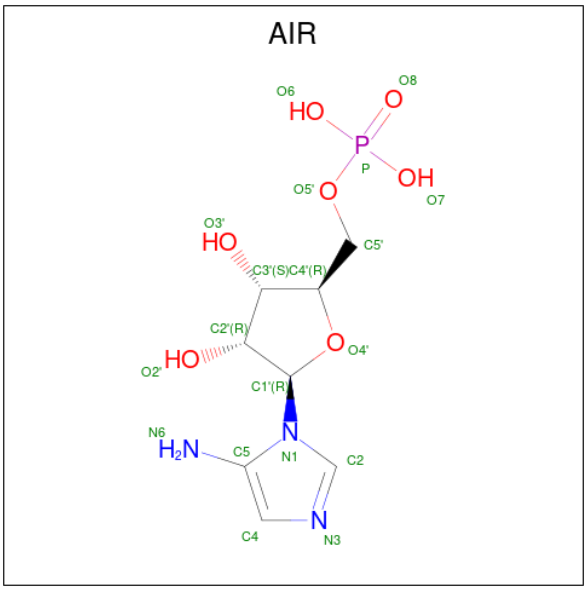
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	D	1	1	1	0	0

- Molecule 6 is 5-AMINOIMIDAZOLE RIBONUCLEOTIDE (three-letter code: AIR) (formula: $C_8H_{14}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	19	8	3	7	1	0	0
6	B	1	19	8	3	7	1	0	0
6	C	1	19	8	3	7	1	0	0
6	D	1	19	8	3	7	1	0	0

- Molecule 7 is water.

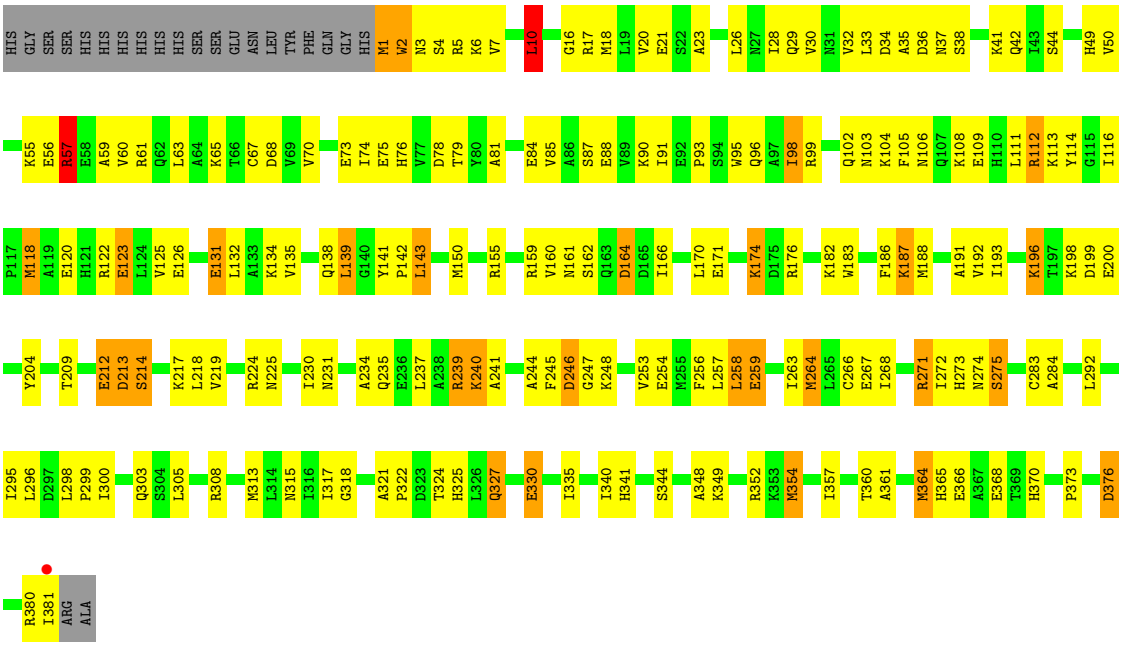
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	322	322	322	0	0
7	B	266	266	266	0	0
7	C	299	299	299	0	0
7	D	243	243	243	0	0

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.

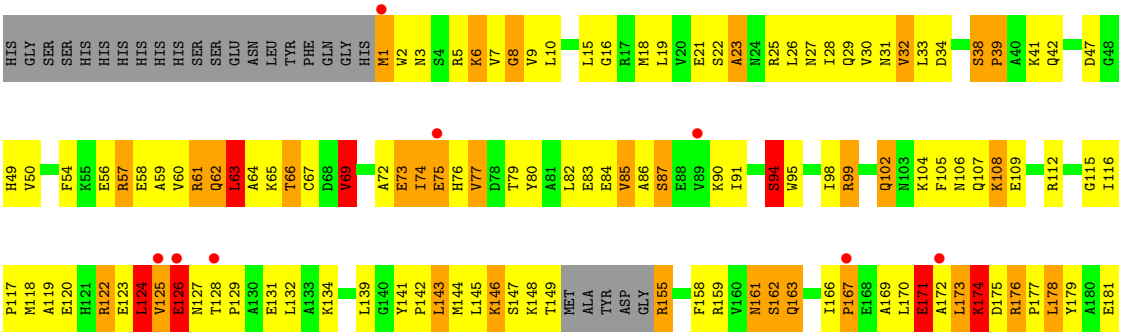
• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

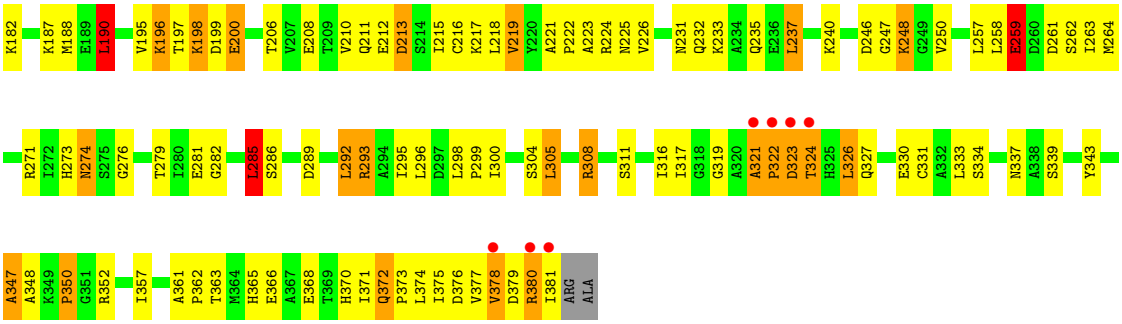
Chain A: 47% 39% 7% 5%



• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

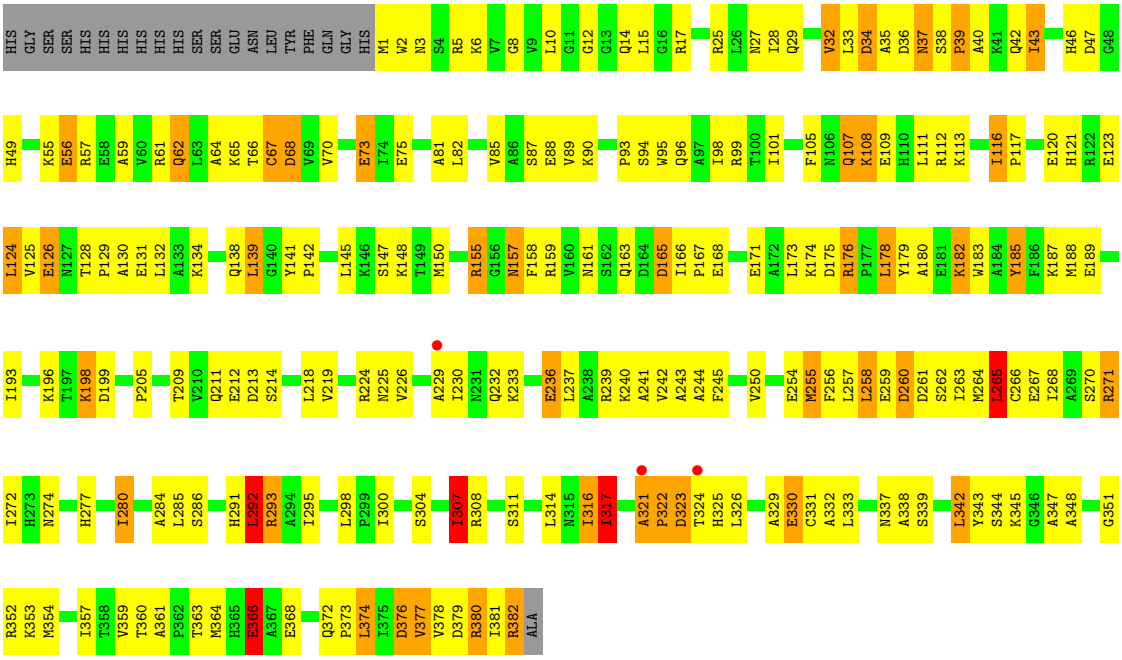
Chain B: 4% 37% 40% 13% • 7%





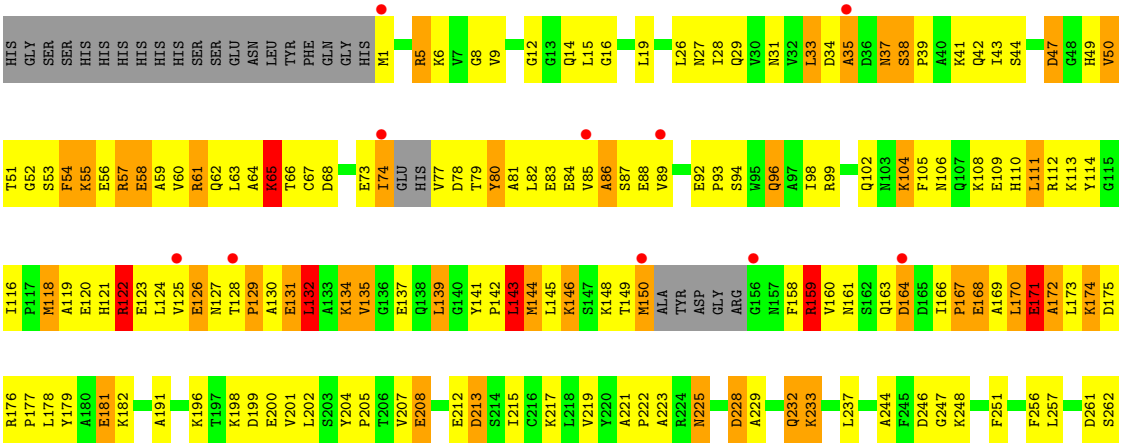
- Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

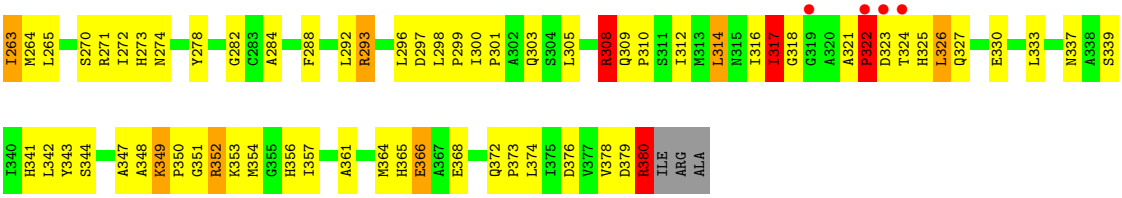
Chain C:



- Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

Chain D:




I263
M264
L265
S270
R271
I272
H273
N274
Y278
G282
C283
A284
F288
L292
R293
L296
D297
L298
P299
I300
P301
A302
Q303
S304
L305
R308
Q309
P310
S311
I312
M313
L314
N315
I316
I317
G318
G319
A320
A321
P322
D323
T324
H325
L326
Q327
E330
L333
N337
A338
S339
I340
H341
L342
Y343
S344
A347
A348
K349
P350
G351
R352
K353
M354
G355
H356
I357
A361
M364
H365
E366
A367
E368
Q372
P373
L374
I375
D376
V377
V378
D379
R380
ILE
ARG
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.50Å 134.20Å 98.50Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 44.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.00) 91.9 (44.73-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.62 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.203 , 0.269 0.207 , 0.203	Depositor DCC
R_{free} test set	11671 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å^2)	14.5	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 135.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13147	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.75% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, AIR, MG, ADP, NA

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	0.85	2/3049 (0.1%)	1.67	38/4128 (0.9%)
1	B	0.80	0/3019	1.68	58/4086 (1.4%)
1	C	0.83	0/3072	1.69	47/4157 (1.1%)
1	D	0.81	0/2941	1.68	48/3980 (1.2%)
All	All	0.83	2/12081 (0.0%)	1.68	191/16351 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ALA	CA-CB	6.50	1.66	1.52
1	A	192	VAL	CB-CG1	5.80	1.65	1.52

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	308	ARG	NE-CZ-NH1	-22.98	108.81	120.30
1	A	57	ARG	NE-CZ-NH2	-18.40	111.10	120.30
1	C	308	ARG	NE-CZ-NH2	14.93	127.77	120.30
1	A	57	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	B	352	ARG	NE-CZ-NH1	12.95	126.77	120.30
1	B	352	ARG	NE-CZ-NH2	-12.39	114.11	120.30
1	B	271	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	D	293	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	D	374	LEU	CB-CG-CD2	-10.38	93.35	111.00
1	A	68	ASP	CB-CG-OD2	-10.31	109.02	118.30
1	C	67	CYS	CA-CB-SG	-10.25	95.56	114.00
1	A	271	ARG	NE-CZ-NH1	10.13	125.37	120.30
1	A	155	ARG	NE-CZ-NH1	10.11	125.35	120.30
1	A	26	LEU	CB-CG-CD1	-10.09	93.85	111.00
1	C	307	ILE	CG1-CB-CG2	-9.95	89.51	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	176	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	C	155	ARG	NE-CZ-NH2	9.86	125.23	120.30
1	D	263	ILE	CG1-CB-CG2	-9.66	90.14	111.40
1	B	69	VAL	CB-CA-C	-9.64	93.09	111.40
1	D	50	VAL	CB-CA-C	-9.62	93.11	111.40
1	B	321	ALA	C-N-CD	-9.22	100.32	120.60
1	A	36	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	C	43	ILE	CG1-CB-CG2	-8.73	92.20	111.40
1	B	333	LEU	CB-CG-CD1	-8.62	96.34	111.00
1	D	317	ILE	CB-CA-C	-8.56	94.48	111.60
1	A	257	LEU	CB-CG-CD1	8.35	125.19	111.00
1	B	34	ASP	CB-CG-OD2	8.32	125.79	118.30
1	B	108	LYS	CD-CE-NZ	8.19	130.55	111.70
1	D	139	LEU	CB-CG-CD1	-8.10	97.23	111.00
1	D	228	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	C	265	LEU	CA-CB-CG	-7.96	96.99	115.30
1	D	271	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	32	VAL	CB-CA-C	-7.72	96.72	111.40
1	C	116	ILE	CB-CA-C	-7.68	96.23	111.60
1	D	308	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	B	122	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	A	10	LEU	CB-CG-CD2	-7.58	98.11	111.00
1	D	366	GLU	OE1-CD-OE2	7.51	132.32	123.30
1	C	292	LEU	CB-CG-CD2	-7.41	98.41	111.00
1	C	175	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	132	LEU	CB-CG-CD1	7.37	123.52	111.00
1	B	248	LYS	CD-CE-NZ	-7.22	95.09	111.70
1	B	176	ARG	C-N-CD	-7.21	104.75	120.60
1	A	10	LEU	CB-CG-CD1	7.19	123.23	111.00
1	B	190	LEU	CB-CG-CD1	-7.18	98.79	111.00
1	A	218	LEU	CB-CG-CD2	-7.18	98.80	111.00
1	C	1	MET	CG-SD-CE	7.17	111.66	100.20
1	B	77	VAL	CB-CA-C	-7.14	97.83	111.40
1	C	376	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	A	98	ILE	CG1-CB-CG2	-7.04	95.92	111.40
1	A	239	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	68	ASP	CB-CG-OD1	6.94	124.55	118.30
1	A	258	LEU	CA-CB-CG	-6.92	99.39	115.30
1	C	99	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	B	143	LEU	CB-CG-CD2	6.88	122.69	111.00
1	D	111	LEU	CA-CB-CG	-6.87	99.50	115.30
1	D	159	ARG	NE-CZ-NH1	-6.86	116.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	THR	N-CA-C	6.85	129.50	111.00
1	A	79	THR	CA-CB-CG2	-6.83	102.83	112.40
1	B	271	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	63	LEU	CA-CB-CG	6.78	130.90	115.30
1	D	273	HIS	N-CA-CB	-6.78	98.39	110.60
1	B	124	LEU	CB-CG-CD1	-6.76	99.51	111.00
1	D	326	LEU	CA-CB-CG	-6.73	99.82	115.30
1	A	354	MET	CG-SD-CE	6.68	110.89	100.20
1	C	292	LEU	CB-CG-CD1	-6.68	99.64	111.00
1	A	143	LEU	CB-CG-CD1	-6.65	99.70	111.00
1	B	259[A]	GLU	N-CA-CB	6.63	122.54	110.60
1	B	259[B]	GLU	N-CA-CB	6.63	122.54	110.60
1	B	257	LEU	CB-CG-CD1	6.60	122.22	111.00
1	D	199	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	B	122	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	C	256	PHE	CB-CA-C	-6.47	97.45	110.40
1	A	60	VAL	CA-CB-CG2	6.45	120.58	110.90
1	D	349	LYS	N-CA-C	-6.43	93.62	111.00
1	A	357	ILE	CB-CA-C	-6.43	98.75	111.60
1	D	215	ILE	CB-CA-C	-6.42	98.77	111.60
1	A	78	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	B	273	HIS	N-CA-CB	-6.40	99.08	110.60
1	B	67	CYS	CA-CB-SG	-6.38	102.51	114.00
1	B	171	GLU	N-CA-C	-6.38	93.76	111.00
1	C	32	VAL	CB-CA-C	-6.34	99.34	111.40
1	C	366	GLU	N-CA-CB	-6.33	99.20	110.60
1	A	18	MET	CA-CB-CG	-6.30	102.59	113.30
1	C	374	LEU	CA-CB-CG	-6.27	100.87	115.30
1	C	342	LEU	CA-CB-CG	-6.25	100.92	115.30
1	B	23	ALA	N-CA-CB	6.24	118.83	110.10
1	D	5	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	D	366	GLU	CG-CD-OE2	-6.23	105.83	118.30
1	A	2	TRP	N-CA-C	-6.22	94.19	111.00
1	B	173	LEU	CB-CG-CD1	-6.15	100.54	111.00
1	A	218	LEU	CB-CA-C	-6.08	98.64	110.20
1	B	305	LEU	CB-CG-CD1	-6.07	100.67	111.00
1	D	256	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	D	33	LEU	CB-CG-CD2	-6.03	100.74	111.00
1	C	189	GLU	OE1-CD-OE2	6.01	130.52	123.30
1	D	380	ARG	N-CA-C	5.98	127.16	111.00
1	A	330	GLU	CG-CD-OE1	-5.98	106.34	118.30
1	D	232	GLN	CA-CB-CG	-5.97	100.27	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MET	CB-CA-C	5.89	122.18	110.40
1	D	171	GLU	N-CA-C	-5.89	95.09	111.00
1	A	113	LYS	CB-CA-C	-5.89	98.62	110.40
1	A	376	ASP	CB-CG-OD1	-5.86	113.02	118.30
1	B	219	VAL	CB-CA-C	-5.81	100.36	111.40
1	C	178	LEU	CB-CA-C	-5.77	99.24	110.20
1	A	188	MET	CA-CB-CG	5.77	123.10	113.30
1	D	314	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	C	258	LEU	CA-CB-CG	-5.67	102.25	115.30
1	C	125	VAL	CB-CA-C	5.66	122.16	111.40
1	B	370	HIS	CB-CA-C	-5.66	99.08	110.40
1	C	271	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	C	354	MET	N-CA-CB	-5.62	100.47	110.60
1	B	343	TYR	N-CA-C	5.62	126.17	111.00
1	A	76	HIS	N-CA-CB	-5.60	100.52	110.60
1	C	68	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	300	ILE	CG1-CB-CG2	5.59	123.71	111.40
1	B	99	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	188	MET	N-CA-CB	5.59	120.66	110.60
1	C	380	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	308	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	199	ASP	CB-CA-C	-5.58	99.24	110.40
1	D	202	LEU	CB-CG-CD2	-5.57	101.52	111.00
1	C	155	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	68	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	B	94	SER	N-CA-C	5.54	125.95	111.00
1	B	261	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	322	PRO	N-CA-C	5.51	126.44	112.10
1	D	68	ASP	N-CA-C	5.51	125.89	111.00
1	D	264	MET	CG-SD-CE	-5.51	91.39	100.20
1	D	118	MET	CB-CA-C	-5.50	99.40	110.40
1	B	261	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	B	199	ASP	N-CA-C	5.48	125.79	111.00
1	B	182	LYS	CD-CE-NZ	5.48	124.30	111.70
1	B	85	VAL	CB-CA-C	-5.47	101.00	111.40
1	B	8	GLY	N-CA-C	-5.47	99.43	113.10
1	D	170	LEU	CB-CG-CD1	5.47	120.30	111.00
1	D	135	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	327[A]	GLN	CB-CA-C	-5.44	99.52	110.40
1	A	327[B]	GLN	CB-CA-C	-5.44	99.52	110.40
1	D	257	LEU	CB-CG-CD1	5.43	120.24	111.00
1	D	333	LEU	CB-CG-CD1	-5.41	101.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	293	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	C	43	ILE	CB-CA-C	-5.38	100.85	111.60
1	A	111	LEU	CB-CG-CD1	5.34	120.09	111.00
1	C	317	ILE	N-CA-CB	-5.34	98.51	110.80
1	B	258	LEU	CB-CG-CD2	-5.33	101.93	111.00
1	B	285	LEU	CB-CG-CD1	5.33	120.06	111.00
1	B	292	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	C	321	ALA	C-N-CD	-5.32	108.91	120.60
1	D	233	LYS	CA-CB-CG	5.32	125.09	113.40
1	A	213	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	182	LYS	CD-CE-NZ	-5.27	99.57	111.70
1	D	80	TYR	CA-CB-CG	-5.26	103.40	113.40
1	C	165	ASP	CB-CA-C	-5.26	99.88	110.40
1	B	60	VAL	CB-CA-C	-5.26	101.41	111.40
1	B	161	ASN	N-CA-C	5.26	125.20	111.00
1	B	126	GLU	N-CA-C	5.25	125.19	111.00
1	C	255	MET	N-CA-CB	-5.25	101.14	110.60
1	D	143	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	A	112	ARG	CG-CD-NE	-5.25	100.78	111.80
1	A	271	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
1	B	50	VAL	CB-CA-C	-5.22	101.49	111.40
1	C	62	GLN	CB-CA-C	-5.21	99.97	110.40
1	A	271	ARG	CB-CA-C	-5.20	100.01	110.40
1	A	164	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	D	199	ASP	N-CA-C	5.18	124.98	111.00
1	B	376	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	B	248	LYS	CG-CD-CE	-5.16	96.41	111.90
1	B	347	ALA	N-CA-C	5.16	124.94	111.00
1	C	377	VAL	CB-CA-C	-5.15	101.61	111.40
1	B	257	LEU	N-CA-C	-5.15	97.09	111.00
1	D	323	ASP	N-CA-CB	-5.14	101.35	110.60
1	D	305	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	C	293	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	217	LYS	CB-CA-C	-5.12	100.17	110.40
1	D	8	GLY	N-CA-C	-5.10	100.34	113.10
1	C	292	LEU	N-CA-CB	-5.10	100.21	110.40
1	D	65	LYS	N-CA-CB	-5.09	101.43	110.60
1	C	157	ASN	CB-CA-C	-5.09	100.22	110.40
1	C	1	MET	CA-CB-CG	5.09	121.95	113.30
1	C	286	SER	CA-CB-OG	-5.06	97.53	111.20
1	A	292	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	D	200	GLU	CB-CA-C	-5.06	100.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ILE	N-CA-C	-5.05	97.37	111.00
1	B	162	SER	CB-CA-C	-5.04	100.52	110.10
1	B	246[A]	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	246[B]	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	382	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	181	GLU	OE1-CD-OE2	5.03	129.34	123.30
1	C	185	TYR	OH-CZ-CE2	5.03	133.68	120.10
1	D	122	ARG	N-CA-C	-5.02	97.44	111.00

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	2975	0	2984	162	0
1	B	2944	0	2953	200	0
1	C	2995	0	3008	208	0
1	D	2888	0	2908	278	0
2	A	1	0	0	0	0
3	A	13	0	17	1	0
3	C	13	0	17	5	0
4	A	27	0	10	1	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	19	0	11	0	0
6	B	19	0	11	2	0
6	C	19	0	12	2	0
6	D	19	0	12	2	0
7	A	322	0	0	18	0
7	B	266	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	299	0	0	18	0
7	D	243	0	0	26	0
All	All	13147	0	11979	841	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 35.

All (841) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:THR:HG23	1:C:381:ILE:HG21	1.25	1.17
1:D:53:SER:HB3	1:D:56:GLU:HG3	1.20	1.16
1:C:62:GLN:HE22	1:C:65[A]:LYS:HE3	1.09	1.12
1:A:116:ILE:HD11	1:A:240:LYS:HD3	1.28	1.12
1:A:187:LYS:HE2	1:A:259:GLU:HA	1.35	1.08
1:D:322:PRO:HA	1:D:348:ALA:HB3	1.11	1.06
1:C:361:ALA:HB1	1:C:366:GLU:HG2	1.08	1.04
1:D:128:THR:HG23	1:D:131:GLU:H	1.19	1.03
1:B:33:LEU:HB2	1:B:63:LEU:HD13	1.38	1.03
1:D:112:ARG:HG2	1:D:118:MET:HE1	1.40	1.03
1:B:126:GLU:HB2	1:B:128:THR:HG23	1.35	1.02
1:D:316:ILE:HD11	1:D:357:ILE:HD11	1.38	1.02
1:B:57:ARG:HG3	1:B:57:ARG:HH11	1.20	1.02
1:D:316:ILE:HG13	7:D:769:HOH:O	1.63	0.97
1:A:324:THR:HG23	1:A:381:ILE:HD12	1.49	0.94
1:D:105:PHE:HB3	1:D:148:LYS:HD3	1.48	0.94
1:A:55:LYS:HE2	1:A:150:MET:HE1	1.51	0.92
1:A:325:HIS:CE1	1:A:348:ALA:HB2	2.05	0.92
1:B:371:ILE:HG23	1:B:375:ILE:HD11	1.50	0.91
1:C:62:GLN:NE2	1:C:65[A]:LYS:HE3	1.83	0.91
1:B:33:LEU:CB	1:B:63:LEU:HD13	1.99	0.91
1:C:212:GLU:HG2	7:C:480:HOH:O	1.69	0.90
1:C:361:ALA:HB1	1:C:366:GLU:CG	2.00	0.88
1:D:108:LYS:HD3	1:D:121:HIS:ND1	1.88	0.88
1:B:1:MET:HG3	1:B:2:TRP:H	1.37	0.87
1:D:322:PRO:CA	1:D:348:ALA:HB3	2.02	0.86
1:C:361:ALA:CB	1:C:366:GLU:HG2	2.02	0.86
1:D:126:GLU:HB2	1:D:128:THR:HG22	1.58	0.86
1:D:128:THR:CG2	1:D:131:GLU:HB3	2.06	0.86
1:A:1:MET:H2	1:A:4:SER:CB	1.88	0.85
1:A:61:ARG:HH22	1:A:84:GLU:HG2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:THR:HG23	1:D:131:GLU:N	1.91	0.85
1:A:32:VAL:HG23	1:A:49:HIS:CE1	2.12	0.85
1:D:110:HIS:O	1:D:113:LYS:HD3	1.77	0.85
1:B:371:ILE:HG23	1:B:375:ILE:CD1	2.07	0.84
1:B:233[A]:LYS:HD2	1:B:263:ILE:HD12	1.59	0.84
1:C:324:THR:CG2	1:C:381:ILE:HG21	2.06	0.84
1:C:381:ILE:O	1:C:382:ARG:C	2.13	0.83
1:D:324:THR:HA	1:D:327:GLN:OE1	1.77	0.83
1:C:265:LEU:HG	1:C:266:CYS:N	1.92	0.83
1:D:356:HIS:HA	7:D:769:HOH:O	1.77	0.83
1:D:174:LYS:O	1:D:176:ARG:HG2	1.78	0.83
1:A:116:ILE:CD1	1:A:240:LYS:HD3	2.08	0.83
1:C:120:GLU:HG2	1:C:139:LEU:HD23	1.60	0.83
1:C:120:GLU:HG2	1:C:139:LEU:CD2	2.08	0.82
1:D:112:ARG:HG2	1:D:118:MET:CE	2.09	0.82
1:D:318:GLY:HA3	1:D:349:LYS:O	1.80	0.82
1:A:61:ARG:HH22	1:A:84:GLU:CG	1.92	0.82
1:B:187:LYS:HD3	1:B:259[A]:GLU:HG2	1.62	0.81
1:B:69:VAL:HG22	7:B:517:HOH:O	1.79	0.81
1:C:17:ARG:HD3	7:C:618:HOH:O	1.79	0.81
1:D:80:TYR:O	1:D:83:GLU:HB3	1.81	0.81
1:C:116:ILE:HD13	1:C:240:LYS:HE2	1.61	0.80
1:D:233:LYS:HD2	1:D:263:ILE:HD12	1.61	0.80
1:D:110:HIS:HA	1:D:113:LYS:HD3	1.62	0.80
1:D:129:PRO:HD3	1:D:170:LEU:HD13	1.64	0.80
1:C:236[B]:GLU:HG2	1:C:237:LEU:N	1.97	0.79
1:D:105:PHE:CB	1:D:148:LYS:HD3	2.11	0.79
1:D:39:PRO:HA	1:D:42:GLN:NE2	1.96	0.79
1:A:187:LYS:HE3	1:A:258:LEU:O	1.83	0.79
1:B:94:SER:O	1:B:98:ILE:HG13	1.83	0.79
1:D:357:ILE:HD12	7:D:769:HOH:O	1.83	0.78
1:B:83:GLU:HG3	1:B:95:TRP:CE2	2.18	0.78
1:D:110:HIS:HA	1:D:113:LYS:CD	2.12	0.78
1:B:282:GLY:O	1:B:308:ARG:HG3	1.84	0.78
1:B:145:LEU:CD2	1:B:173:LEU:HD12	2.14	0.78
1:B:316:ILE:HD11	1:B:357:ILE:HD11	1.65	0.78
1:B:57:ARG:O	1:B:61:ARG:HG3	1.84	0.77
1:D:39:PRO:HA	1:D:42:GLN:HE21	1.49	0.77
1:B:125:VAL:HG23	1:B:131:GLU:OE2	1.84	0.77
1:A:196:LYS:NZ	1:A:245:PHE:O	2.17	0.77
1:B:83:GLU:HG3	1:B:95:TRP:CZ2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HE2	1:A:259:GLU:CA	2.14	0.77
7:C:420:HOH:O	1:D:339:SER:HB2	1.84	0.77
1:B:372:GLN:HB3	1:B:373:PRO:HD3	1.66	0.76
1:D:316:ILE:CD1	1:D:357:ILE:HD11	2.14	0.76
1:C:363:THR:O	1:C:366:GLU:HB3	1.86	0.76
1:B:162:SER:HB2	7:B:425:HOH:O	1.85	0.76
1:B:57:ARG:HG3	1:B:57:ARG:NH1	1.96	0.75
1:B:188:MET:HE2	1:B:190:LEU:HD21	1.69	0.75
1:C:89:VAL:HG12	1:C:90:LYS:H	1.52	0.75
1:C:205:PRO:HG2	1:C:307:ILE:HD12	1.67	0.75
1:A:321:ALA:HB3	1:A:324:THR:OG1	1.86	0.75
1:C:150:MET:HE3	1:C:150:MET:HA	1.69	0.74
1:D:308:ARG:HD3	7:D:391:HOH:O	1.87	0.74
1:C:317:ILE:HD11	1:C:353:LYS:HG2	1.70	0.74
1:D:164:ASP:O	1:D:167:PRO:HD2	1.87	0.74
1:C:317:ILE:HG23	1:C:351:GLY:HA2	1.69	0.74
1:C:147:SER:HA	1:C:178:LEU:HD23	1.68	0.74
1:D:132:LEU:HD13	1:D:166:ILE:HG12	1.69	0.74
1:D:376:ASP:O	1:D:380:ARG:HG2	1.88	0.74
1:A:103:ASN:HB3	1:A:106:ASN:HB2	1.69	0.73
1:D:128:THR:CG2	1:D:131:GLU:H	1.97	0.73
1:A:246:ASP:HB3	7:A:455:HOH:O	1.88	0.73
1:B:380:ARG:N	7:B:568:HOH:O	2.22	0.73
1:D:57:ARG:HH11	1:D:61:ARG:HD2	1.53	0.72
1:B:145:LEU:HD23	1:B:173:LEU:HD12	1.72	0.72
1:C:196:LYS:NZ	1:C:245:PHE:O	2.23	0.72
7:B:524:HOH:O	1:D:225:ASN:HB3	1.90	0.72
1:C:205:PRO:HG2	1:C:307:ILE:CD1	2.19	0.72
1:D:122:ARG:HG3	1:D:135:VAL:HG22	1.72	0.72
1:D:228:ASP:O	1:D:232:GLN:HG3	1.91	0.71
1:D:33:LEU:HD13	1:D:50:VAL:HG11	1.72	0.70
1:D:272:ILE:HD12	1:D:288:PHE:HE2	1.56	0.70
1:D:31:ASN:ND2	1:D:66:THR:HG22	2.06	0.70
1:D:12:GLY:O	1:D:39:PRO:HD2	1.90	0.70
1:C:347:ALA:N	7:C:614:HOH:O	2.25	0.69
1:D:108:LYS:NZ	1:D:119:ALA:O	2.25	0.69
1:A:37:ASN:ND2	7:A:644:HOH:O	2.25	0.69
1:D:159:ARG:NH1	1:D:161:ASN:OD1	2.25	0.69
1:A:108:LYS:CE	1:A:118:MET:HE2	2.23	0.69
1:B:126:GLU:HB2	1:B:128:THR:CG2	2.17	0.69
1:B:316:ILE:HD11	1:B:357:ILE:CD1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ILE:C	1:C:317:ILE:HD13	2.12	0.69
1:B:116:ILE:O	1:B:118:MET:HG3	1.92	0.69
1:D:352:ARG:HG2	1:D:354:MET:SD	2.33	0.69
1:B:38:SER:O	1:B:42:GLN:HG3	1.93	0.68
1:C:8:GLY:HA3	1:C:67:CYS:SG	2.33	0.68
1:D:171:GLU:OE1	1:D:172:ALA:HA	1.93	0.68
1:B:74:ILE:HD12	1:B:77:VAL:HG13	1.76	0.68
1:C:254:GLU:OE2	1:C:267:GLU:HG2	1.93	0.68
4:A:400:ADP:H5'2	7:A:392:HOH:O	1.92	0.68
1:D:6:LYS:HD3	1:D:29:GLN:OE1	1.94	0.68
1:D:174:LYS:H	1:D:174:LYS:HD2	1.58	0.68
1:C:157:ASN:O	3:C:384:NHE:HC22	1.93	0.68
1:D:174:LYS:NZ	1:D:176:ARG:HH11	1.92	0.68
1:A:186:PHE:HB3	1:A:256:PHE:HB3	1.75	0.68
1:B:141:TYR:HB3	1:B:161:ASN:O	1.92	0.68
1:B:321:ALA:HB3	1:B:324:THR:HG23	1.76	0.68
1:A:61:ARG:NH2	7:A:540:HOH:O	2.26	0.67
1:D:316:ILE:HD11	1:D:357:ILE:CD1	2.21	0.67
1:D:167:PRO:HB2	7:D:515:HOH:O	1.93	0.67
1:B:177:PRO:C	1:B:178:LEU:HG	2.12	0.67
1:C:271:ARG:HG3	1:C:272:ILE:O	1.93	0.67
1:C:258:LEU:HD12	1:C:262:SER:OG	1.94	0.67
1:D:143:LEU:CD2	1:D:160:VAL:HB	2.24	0.67
1:A:108:LYS:HE3	1:A:118:MET:HE2	1.77	0.67
1:B:104:LYS:O	1:B:108:LYS:HD2	1.95	0.67
1:C:324:THR:HG22	1:C:325:HIS:N	2.08	0.67
1:D:322:PRO:HA	1:D:348:ALA:CB	2.06	0.67
1:D:248:LYS:HE2	1:D:297:ASP:OD1	1.95	0.67
1:C:317:ILE:HD13	1:C:317:ILE:N	2.09	0.66
1:D:14:GLN:HG3	1:D:343:TYR:CE1	2.30	0.66
1:D:78:ASP:OD1	1:D:80:TYR:HB2	1.95	0.66
1:D:173:LEU:HB2	1:D:178:LEU:HD11	1.77	0.66
1:D:57:ARG:O	1:D:61:ARG:HG3	1.94	0.66
1:D:27:ASN:C	7:D:587:HOH:O	2.33	0.66
1:B:80:TYR:O	1:B:84:GLU:HG3	1.94	0.66
1:D:262:SER:HA	7:D:525:HOH:O	1.94	0.66
1:C:285:LEU:HG	1:C:304:SER:HB3	1.77	0.66
1:A:90:LYS:HB3	7:A:629:HOH:O	1.96	0.66
1:B:233[B]:LYS:HD2	7:B:657:HOH:O	1.96	0.65
1:D:322:PRO:HD3	7:D:606:HOH:O	1.95	0.65
1:D:143:LEU:HD21	1:D:160:VAL:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LYS:HD3	1:B:247:GLY:O	1.97	0.65
1:A:109:GLU:OE2	1:A:112:ARG:NH1	2.30	0.65
1:B:109:GLU:CD	1:B:112:ARG:HH21	1.99	0.65
1:C:150:MET:HE3	1:C:150:MET:CA	2.24	0.65
1:B:61:ARG:HH22	1:B:84:GLU:HB3	1.60	0.65
1:B:319:GLY:O	1:B:350:PRO:HG3	1.97	0.65
1:D:62:GLN:O	1:D:65:LYS:HB3	1.96	0.65
1:B:10:LEU:HD11	1:B:82:LEU:HD21	1.78	0.65
1:D:120:GLU:CD	1:D:182:LYS:HD3	2.17	0.65
1:D:321:ALA:O	1:D:324:THR:HG23	1.97	0.65
1:D:130:ALA:O	7:D:663:HOH:O	2.15	0.65
1:D:217:LYS:NZ	1:D:379:ASP:OD1	2.27	0.65
1:A:108:LYS:HE3	1:A:118:MET:CE	2.26	0.64
1:A:187:LYS:CE	1:A:259:GLU:HA	2.22	0.64
1:C:277:HIS:O	1:C:280:ILE:HG13	1.98	0.64
1:A:122:ARG:NE	1:A:138:GLN:OE1	2.30	0.64
1:B:322:PRO:HA	1:B:348:ALA:HB3	1.78	0.64
1:D:196:LYS:HG3	1:D:201:VAL:HG22	1.80	0.64
1:A:120:GLU:HG2	1:A:139:LEU:HD23	1.79	0.64
1:B:377:VAL:HG12	1:B:378:VAL:N	2.12	0.64
1:C:193:ILE:HG23	1:C:250:VAL:HG13	1.79	0.64
1:B:368:GLU:O	7:B:582:HOH:O	2.14	0.64
1:A:10:LEU:HD13	1:A:63:LEU:CD2	2.28	0.64
1:C:89:VAL:HG12	1:C:90:LYS:N	2.13	0.64
1:C:258:LEU:HB2	1:C:260:ASP:OD1	1.98	0.64
1:C:330:GLU:O	1:C:333:LEU:HB2	1.98	0.64
1:A:171:GLU:OE2	1:A:174:LYS:HE2	1.98	0.64
1:B:371:ILE:CG2	1:B:375:ILE:HD11	2.27	0.64
1:D:110:HIS:O	1:D:113:LYS:HB2	1.99	0.63
1:B:85:VAL:HG12	1:B:85:VAL:O	1.97	0.63
1:B:188:MET:SD	1:B:208:GLU:HG3	2.38	0.63
1:D:120:GLU:HG3	7:D:482:HOH:O	1.98	0.63
1:D:110:HIS:HE1	1:D:244:ALA:O	1.80	0.63
1:D:73:GLU:C	1:D:74:ILE:HG13	2.14	0.63
1:B:324:THR:HA	1:B:327:GLN:HG2	1.80	0.63
1:C:159:ARG:NE	1:C:161:ASN:OD1	2.29	0.63
1:D:144:MET:HB3	1:D:146:LYS:HD3	1.81	0.63
1:A:191:ALA:HA	1:A:253:VAL:O	1.99	0.63
1:D:158:PHE:CE2	1:D:169:ALA:HB2	2.33	0.63
1:D:204:TYR:HB3	1:D:205:PRO:CD	2.28	0.63
1:C:332:ALA:HB1	1:C:357:ILE:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ASN:HD22	1:D:66:THR:HG22	1.64	0.63
1:D:146:LYS:O	1:D:178:LEU:HD23	1.99	0.63
1:D:15:LEU:HG	6:D:402:AIR:HC1'	1.81	0.62
1:C:284:ALA:HB1	1:D:337:ASN:HA	1.81	0.62
1:B:375:ILE:O	1:B:378:VAL:HG12	1.99	0.62
1:D:131:GLU:O	1:D:134:LYS:HB2	1.98	0.62
1:B:129:PRO:HD3	1:B:170:LEU:HD13	1.79	0.62
1:D:53:SER:OG	1:D:55:LYS:HB2	1.99	0.62
1:C:34:ASP:OD1	1:C:35:ALA:N	2.30	0.62
1:D:174:LYS:HZ2	1:D:176:ARG:HH11	1.47	0.62
1:B:232:GLN:HG2	7:B:540:HOH:O	1.99	0.62
1:D:39:PRO:CA	1:D:42:GLN:HE21	2.13	0.62
1:B:15:LEU:HD12	6:B:402:AIR:HC2	1.82	0.62
1:B:363:THR:OG1	1:B:366:GLU:HB2	2.00	0.62
1:B:59:ALA:O	1:B:62[B]:GLN:HB2	2.00	0.62
1:C:109:GLU:OE1	1:C:109:GLU:HA	1.99	0.62
1:D:74:ILE:HD12	1:D:77:VAL:CG1	2.30	0.62
1:D:94:SER:O	1:D:98:ILE:HG13	2.00	0.62
1:B:223:ALA:HB1	1:B:226:VAL:HG21	1.81	0.61
1:D:128:THR:HG23	1:D:131:GLU:HB3	1.82	0.61
1:A:114:TYR:O	1:A:240:LYS:HE2	2.00	0.61
1:C:316:ILE:HA	7:C:822:HOH:O	1.99	0.61
1:A:380:ARG:O	1:A:381:ILE:HG23	2.00	0.61
1:C:32:VAL:HG23	1:C:49:HIS:CE1	2.35	0.61
1:A:322:PRO:HB2	7:A:651:HOH:O	1.99	0.61
1:B:177:PRO:HA	7:B:714:HOH:O	1.99	0.61
1:C:174:LYS:O	1:C:176:ARG:HG3	2.01	0.61
1:D:324:THR:O	1:D:327:GLN:N	2.30	0.61
1:A:131:GLU:O	1:A:135:VAL:HG23	2.01	0.61
1:B:147:SER:HA	1:B:178:LEU:HD23	1.82	0.61
1:D:365:HIS:O	1:D:368:GLU:HB2	1.99	0.61
1:B:105:PHE:HB3	1:B:148:LYS:HE2	1.82	0.61
1:D:102:GLN:O	1:D:149:THR:HG22	1.99	0.61
1:A:17:ARG:O	1:A:21:GLU:HG3	2.00	0.61
1:A:33:LEU:O	1:A:34:ASP:HB2	2.00	0.61
1:B:163:GLN:O	1:B:166:ILE:HG13	2.01	0.61
1:C:142:PRO:HB3	1:C:161:ASN:HA	1.83	0.61
1:C:332:ALA:CB	1:C:357:ILE:HD12	2.31	0.60
1:C:141:TYR:HB3	1:C:161:ASN:O	2.01	0.60
1:B:120[A]:GLU:HG3	1:B:139:LEU:HD22	1.82	0.60
1:C:159:ARG:HD2	1:C:183:TRP:CH2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:GLN:HB3	1:C:373:PRO:HD3	1.82	0.60
1:C:376:ASP:O	1:C:380:ARG:HG3	2.01	0.60
1:D:54:PHE:CD2	1:D:55:LYS:HD3	2.36	0.60
1:A:38:SER:O	1:A:42:GLN:HG3	2.01	0.60
1:A:325:HIS:CE1	1:A:348:ALA:CB	2.82	0.60
1:D:110:HIS:HD2	1:D:113:LYS:NZ	1.99	0.60
1:D:364:MET:O	1:D:368:GLU:HG3	2.02	0.60
1:B:372:GLN:HA	1:B:375:ILE:HD12	1.83	0.60
1:C:124:LEU:HD13	1:C:179:TYR:HA	1.82	0.60
1:D:158:PHE:CD2	1:D:169:ALA:CB	2.85	0.60
1:D:108:LYS:HD3	1:D:121:HIS:CE1	2.37	0.59
1:D:282:GLY:O	1:D:308:ARG:HG3	2.02	0.59
1:A:120:GLU:HG2	1:A:139:LEU:CD2	2.32	0.59
1:A:317:ILE:HG13	7:A:412:HOH:O	2.03	0.59
1:B:171:GLU:O	1:B:173:LEU:N	2.35	0.59
1:A:324:THR:CG2	1:A:381:ILE:HD12	2.28	0.59
1:C:316:ILE:O	1:C:317:ILE:HD13	2.03	0.59
1:A:104:LYS:O	1:A:108:LYS:HG3	2.02	0.59
1:B:61:ARG:NH1	1:B:84:GLU:OE1	2.35	0.59
1:A:55:LYS:HE2	1:A:150:MET:CE	2.26	0.59
1:B:1:MET:HG3	1:B:2:TRP:N	2.12	0.59
1:D:33:LEU:HD13	1:D:50:VAL:CG1	2.32	0.59
1:D:116:ILE:O	1:D:118:MET:HG3	2.03	0.59
1:D:212:GLU:O	1:D:213:ASP:HB2	2.03	0.59
1:D:143:LEU:O	1:D:143:LEU:HD23	2.03	0.59
1:D:96:GLN:HA	1:D:96:GLN:HE21	1.67	0.58
1:A:352:ARG:O	1:A:354:MET:HG2	2.02	0.58
1:A:88:GLU:HG2	7:A:693:HOH:O	2.03	0.58
1:A:196:LYS:HD2	1:A:247:GLY:O	2.02	0.58
1:B:33:LEU:HB2	1:B:63:LEU:CD1	2.23	0.58
1:A:20:VAL:O	1:A:21:GLU:C	2.37	0.58
1:A:32:VAL:HG23	1:A:49:HIS:ND1	2.18	0.58
1:B:32:VAL:H	1:B:49:HIS:HD1	1.51	0.58
1:B:224:ARG:O	1:B:226:VAL:HG23	2.04	0.58
1:B:8:GLY:HA2	1:B:31:ASN:O	2.03	0.58
1:B:10:LEU:HD12	1:B:72:ALA:HB2	1.86	0.58
1:C:321:ALA:O	1:C:323:ASP:N	2.36	0.58
1:A:1:MET:N	1:A:4:SER:CB	2.63	0.58
1:B:158:PHE:CE2	1:B:169:ALA:HB2	2.38	0.58
1:B:158:PHE:CD2	1:B:169:ALA:HB2	2.39	0.58
1:D:149:THR:HB	1:D:150:MET:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ILE:HG13	1:D:357:ILE:HD12	1.85	0.58
1:A:104:LYS:HE3	1:A:267:GLU:OE1	2.03	0.58
1:C:338:ALA:HB2	1:C:359:VAL:HG22	1.86	0.58
1:C:171:GLU:OE1	1:C:171:GLU:HA	2.04	0.57
1:D:12:GLY:O	1:D:38:SER:HB2	2.04	0.57
1:D:143:LEU:HD23	1:D:143:LEU:C	2.24	0.57
1:D:204:TYR:HB3	1:D:205:PRO:HD2	1.86	0.57
1:D:126:GLU:HB2	1:D:128:THR:CG2	2.32	0.57
1:A:174:LYS:O	1:A:176:ARG:HG3	2.05	0.57
1:A:253:VAL:HG22	1:A:268:ILE:HG13	1.86	0.57
3:A:385:NHE:HC21	7:A:615:HOH:O	2.03	0.57
1:D:41:LYS:HE2	1:D:49:HIS:HB3	1.86	0.57
1:D:38:SER:O	1:D:39:PRO:C	2.41	0.57
1:D:105:PHE:CE1	1:D:123:GLU:HB2	2.39	0.57
1:B:286:SER:O	1:B:289:ASP:HB2	2.05	0.57
1:C:157:ASN:O	3:C:384:NHE:H2'1	2.04	0.57
1:D:37:ASN:HA	7:D:542:HOH:O	2.05	0.57
1:B:80:TYR:CE1	1:B:99:ARG:NH1	2.73	0.57
1:C:101:ILE:HA	1:C:107:GLN:HB2	1.85	0.57
1:D:110:HIS:CA	1:D:113:LYS:HD3	2.35	0.56
1:B:237:LEU:C	1:B:237:LEU:HD12	2.25	0.56
1:A:61:ARG:NH1	7:A:386:HOH:O	2.38	0.56
1:C:62:GLN:HE21	1:C:62:GLN:HA	1.71	0.56
1:B:56:GLU:HB3	1:B:58:GLU:OE2	2.06	0.56
1:B:171:GLU:O	1:B:174:LYS:N	2.39	0.56
1:B:372:GLN:CB	1:B:373:PRO:HD3	2.34	0.56
1:A:132:LEU:HD23	1:A:166:ILE:HG23	1.88	0.56
1:B:2:TRP:CE3	1:B:3:ASN:HB3	2.40	0.56
1:B:75:GLU:HG3	1:B:102:GLN:HB2	1.87	0.56
1:D:145:LEU:CD1	1:D:178:LEU:HD22	2.35	0.56
1:C:8:GLY:CA	1:C:67:CYS:SG	2.93	0.56
1:C:165:ASP:HA	7:C:605:HOH:O	2.06	0.56
1:D:134:LYS:N	7:D:663:HOH:O	2.38	0.56
1:A:248:LYS:HD2	7:A:604:HOH:O	2.06	0.56
1:A:324:THR:O	1:A:325:HIS:C	2.43	0.56
1:B:233[A]:LYS:NZ	1:B:262:SER:HA	2.21	0.56
1:A:143:LEU:C	1:A:143:LEU:HD12	2.26	0.55
1:C:116:ILE:HG22	1:C:117:PRO:N	2.18	0.55
1:C:321:ALA:O	1:C:324:THR:HB	2.05	0.55
1:C:196:LYS:HE3	1:C:242:VAL:CG1	2.36	0.55
1:D:6:LYS:HD3	1:D:29:GLN:CD	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ASP:OD1	1:D:47:ASP:C	2.44	0.55
1:C:187:LYS:HE3	1:C:258:LEU:O	2.06	0.55
1:B:237:LEU:HD12	1:B:237:LEU:O	2.06	0.55
1:D:145:LEU:HD12	1:D:178:LEU:HD22	1.88	0.55
1:C:145:LEU:HG	1:C:173:LEU:HD12	1.88	0.55
1:C:81:ALA:O	1:C:85:VAL:HG22	2.07	0.55
1:B:174:LYS:H	1:B:174:LYS:HD2	1.71	0.55
1:C:284:ALA:CB	1:D:337:ASN:HA	2.36	0.55
1:B:23:ALA:HB1	1:B:28:ILE:HB	1.89	0.55
1:B:381:ILE:HG22	1:B:381:ILE:O	2.07	0.55
1:B:188:MET:CE	1:B:190:LEU:HD21	2.36	0.55
1:D:128:THR:HG23	1:D:131:GLU:CB	2.37	0.55
1:D:56:GLU:O	1:D:60:VAL:HG23	2.07	0.54
1:D:317:ILE:HG22	1:D:351:GLY:C	2.27	0.54
1:C:329:ALA:O	1:C:332:ALA:HB3	2.07	0.54
1:C:17:ARG:NH1	1:C:39:PRO:O	2.41	0.54
1:B:293:ARG:HD3	1:B:299:PRO:O	2.06	0.54
1:C:317:ILE:CD1	1:C:353:LYS:HA	2.37	0.54
1:B:373:PRO:O	1:B:377:VAL:HG23	2.07	0.54
1:C:89:VAL:CG1	1:C:90:LYS:H	2.18	0.54
1:B:79:THR:HA	1:B:82:LEU:HB2	1.89	0.54
1:B:166:ILE:HB	1:B:167:PRO:HD3	1.90	0.54
1:D:150:MET:HE2	7:D:485:HOH:O	2.07	0.54
1:C:2:TRP:HB3	1:D:330:GLU:OE2	2.06	0.54
1:C:27:ASN:N	1:C:27:ASN:HD22	2.05	0.54
1:A:10:LEU:HD12	1:A:33:LEU:HD23	1.90	0.54
1:C:129:PRO:O	1:C:130:ALA:C	2.45	0.54
1:D:82:LEU:O	1:D:83:GLU:C	2.46	0.54
1:A:95:TRP:CZ3	1:A:96:GLN:HG3	2.42	0.54
1:B:212:GLU:O	1:B:213:ASP:HB2	2.07	0.54
1:D:126:GLU:O	1:D:127:ASN:HB2	2.06	0.54
1:D:322:PRO:HB3	1:D:347:ALA:HB1	1.89	0.54
1:B:33:LEU:HD11	1:B:59:ALA:HB1	1.90	0.53
1:B:119:ALA:HB3	1:B:181:GLU:OE2	2.08	0.53
1:B:2:TRP:CZ3	1:B:3:ASN:HB3	2.43	0.53
1:B:124:LEU:HD23	1:B:127:ASN:HA	1.89	0.53
1:C:187:LYS:HE2	1:C:259:GLU:HA	1.90	0.53
1:A:170:LEU:O	1:A:171:GLU:C	2.45	0.53
1:B:167:PRO:HB2	7:B:710:HOH:O	2.08	0.53
1:A:61:ARG:NH2	1:A:84:GLU:HG2	2.17	0.53
1:C:62:GLN:HE21	1:C:62:GLN:CA	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:GLN:HB2	7:D:508:HOH:O	2.08	0.53
1:A:120:GLU:HB3	1:A:182:LYS:HB3	1.90	0.53
1:B:66:THR:O	1:B:66:THR:OG1	2.25	0.53
1:B:132:LEU:HD23	1:B:166:ILE:HG23	1.91	0.53
1:B:323:ASP:O	1:B:326:LEU:N	2.37	0.53
1:D:110:HIS:C	1:D:113:LYS:HD3	2.27	0.53
1:A:6:LYS:HG2	1:A:29:GLN:HB3	1.91	0.53
1:B:7:VAL:O	1:B:30:VAL:HA	2.09	0.53
1:C:333:LEU:HD13	1:D:299:PRO:HD2	1.91	0.53
1:D:28:ILE:N	7:D:587:HOH:O	2.42	0.53
1:A:318:GLY:N	1:A:352:ARG:O	2.39	0.53
1:D:300:ILE:O	1:D:300:ILE:HG22	2.09	0.53
1:D:316:ILE:CG1	1:D:357:ILE:HD11	2.39	0.53
1:B:276:GLY:O	1:B:279:THR:HG23	2.09	0.53
1:A:75:GLU:OE1	1:A:271:ARG:HG2	2.09	0.53
1:D:81:ALA:O	1:D:84:GLU:HB2	2.08	0.53
1:D:237:LEU:O	1:D:237:LEU:HD12	2.08	0.53
1:A:10:LEU:HD13	1:A:63:LEU:HD22	1.91	0.52
1:A:141:TYR:HA	1:A:142:PRO:C	2.28	0.52
1:D:96:GLN:HA	1:D:96:GLN:NE2	2.24	0.52
1:A:335:ILE:HG23	1:A:370:HIS:O	2.09	0.52
1:B:123:GLU:HA	1:B:179:TYR:CB	2.39	0.52
1:B:174:LYS:H	1:B:174:LYS:CD	2.21	0.52
1:C:321:ALA:HB1	1:C:322:PRO:HD2	1.90	0.52
1:A:131:GLU:O	1:A:134:LYS:HB3	2.08	0.52
1:B:198:LYS:CA	1:B:248:LYS:HD3	2.39	0.52
1:D:50:VAL:CG1	1:D:51:THR:N	2.68	0.52
1:D:50:VAL:HG12	1:D:51:THR:N	2.15	0.52
1:D:176:ARG:HB2	1:D:177:PRO:HD2	1.91	0.52
1:B:126:GLU:HG2	1:B:131:GLU:CD	2.30	0.52
1:C:291:HIS:O	1:C:295:ILE:HG12	2.09	0.52
1:D:59:ALA:O	1:D:62:GLN:N	2.42	0.52
1:B:231:ASN:OD1	1:B:235:GLN:NE2	2.41	0.52
1:B:285:LEU:HD22	1:B:304:SER:HB2	1.92	0.52
1:A:81:ALA:O	1:A:85:VAL:HG22	2.09	0.52
1:B:274:ASN:C	1:B:274:ASN:HD22	2.10	0.52
1:B:155:ARG:NH1	7:B:553:HOH:O	2.43	0.52
1:A:95:TRP:CH2	1:A:96:GLN:HG3	2.45	0.52
1:B:197:THR:O	1:B:198:LYS:C	2.49	0.52
1:A:254:GLU:OE1	1:A:273:HIS:NE2	2.43	0.51
1:B:106:ASN:O	1:B:107:GLN:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LYS:O	1:C:236[B]:GLU:OE1	2.28	0.51
1:A:159:ARG:HD2	1:A:183:TRP:CH2	2.45	0.51
1:B:281:GLU:OE2	1:B:339:SER:OG	2.27	0.51
1:D:74:ILE:HD12	1:D:77:VAL:HG13	1.93	0.51
1:C:3:ASN:OD1	1:C:3:ASN:N	2.43	0.51
1:B:56:GLU:OE2	1:B:58:GLU:OE2	2.28	0.51
1:D:64:ALA:HB1	1:D:89:VAL:HG11	1.92	0.51
1:D:158:PHE:CZ	1:D:168:GLU:HG2	2.45	0.51
1:B:6:LYS:HE2	7:B:478:HOH:O	2.10	0.51
1:C:62:GLN:NE2	1:C:62:GLN:HA	2.25	0.51
1:D:141:TYR:HB3	1:D:161:ASN:O	2.11	0.51
1:B:74:ILE:HD12	1:B:77:VAL:CG1	2.40	0.51
4:D:400:ADP:H5'2	7:D:393:HOH:O	2.11	0.51
1:D:114:TYR:CD2	1:D:114:TYR:N	2.78	0.51
1:D:143:LEU:HB2	1:D:181:GLU:O	2.11	0.51
1:A:116:ILE:HD11	1:A:240:LYS:CD	2.20	0.51
1:C:230:ILE:HA	1:C:233:LYS:HE2	1.93	0.51
1:C:317:ILE:HD12	1:C:353:LYS:HA	1.93	0.51
1:C:257:LEU:HD11	1:C:261:ASP:HA	1.93	0.51
1:D:53:SER:C	1:D:55:LYS:H	2.14	0.51
1:D:119:ALA:O	7:D:545:HOH:O	2.19	0.51
1:A:299:PRO:C	1:A:300:ILE:HG13	2.32	0.50
1:C:61:ARG:NH2	1:C:65[B]:LYS:HE3	2.27	0.50
1:C:95:TRP:CZ3	1:C:96[B]:GLN:HG3	2.47	0.50
1:D:122:ARG:CG	1:D:135:VAL:HG22	2.41	0.50
1:A:99:ARG:O	1:A:102:GLN:HG2	2.11	0.50
1:C:377:VAL:HG12	1:C:378:VAL:N	2.25	0.50
1:D:54:PHE:HD2	1:D:55:LYS:HD3	1.73	0.50
1:A:122:ARG:HB2	1:A:135:VAL:HG13	1.93	0.50
1:D:14:GLN:CB	1:D:343:TYR:CD1	2.93	0.50
1:D:128:THR:CG2	1:D:131:GLU:CB	2.86	0.50
1:C:134:LYS:O	1:C:138:GLN:HG3	2.11	0.50
1:D:92:GLU:HA	1:D:93:PRO:C	2.31	0.50
1:D:316:ILE:HG21	1:D:325:HIS:HB2	1.94	0.50
1:A:61:ARG:HG3	1:A:85:VAL:HG11	1.94	0.50
1:B:371:ILE:HG23	1:B:375:ILE:HD12	1.91	0.50
1:C:10:LEU:HD11	1:C:82:LEU:HD21	1.93	0.50
1:A:224:ARG:O	1:A:225:ASN:HB2	2.12	0.50
1:B:85:VAL:C	1:B:87:SER:H	2.14	0.50
1:D:372:GLN:HB3	1:D:373:PRO:HD3	1.92	0.50
1:C:2:TRP:CD1	1:D:330:GLU:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327[B]:GLN:NE2	1:A:330:GLU:OE2	2.44	0.50
1:B:146:LYS:NZ	4:B:400:ADP:C8	2.79	0.50
1:B:212:GLU:HB3	7:B:572:HOH:O	2.11	0.50
1:C:38:SER:O	1:C:42:GLN:HG3	2.12	0.50
1:C:62:GLN:NE2	1:C:62:GLN:CA	2.74	0.50
1:D:57:ARG:HH11	1:D:61:ARG:CD	2.24	0.50
1:B:233[B]:LYS:NZ	7:B:657:HOH:O	2.34	0.49
1:C:258:LEU:O	1:C:261:ASP:N	2.45	0.49
1:B:109:GLU:OE2	1:B:112:ARG:NH2	2.45	0.49
1:B:122:ARG:HG2	1:B:122:ARG:HH11	1.77	0.49
1:B:28:ILE:HD13	1:B:296:LEU:HD11	1.94	0.49
1:B:80:TYR:HA	1:B:99:ARG:NH2	2.27	0.49
1:C:176:ARG:HD2	7:C:586:HOH:O	2.11	0.49
1:D:233:LYS:NZ	1:D:261:ASP:O	2.45	0.49
1:B:85:VAL:C	1:B:87:SER:N	2.64	0.49
1:B:233[A]:LYS:HB3	1:B:263:ILE:HD12	1.94	0.49
1:B:293:ARG:HG2	1:B:298:LEU:HB2	1.93	0.49
1:B:331:CYS:SG	1:B:377:VAL:HG21	2.52	0.49
1:B:379:ASP:O	1:B:380:ARG:C	2.50	0.49
1:C:380:ARG:HG2	7:C:617:HOH:O	2.11	0.49
1:D:316:ILE:CG1	1:D:357:ILE:CD1	2.91	0.49
1:C:93:PRO:HG2	1:C:98:ILE:HD11	1.94	0.49
1:C:348:ALA:HB3	7:C:536:HOH:O	2.12	0.49
1:A:159:ARG:HD2	1:A:183:TRP:HH2	1.78	0.49
1:A:212:GLU:CD	1:A:217:LYS:HD2	2.33	0.49
1:D:325:HIS:CD2	1:D:326:LEU:HD21	2.47	0.49
1:A:56:GLU:HB3	1:A:59:ALA:HB3	1.95	0.49
1:B:64:ALA:CB	1:B:85:VAL:HG11	2.42	0.49
1:B:197:THR:HG21	7:B:409:HOH:O	2.12	0.49
1:D:39:PRO:O	1:D:42:GLN:HB2	2.13	0.49
1:D:174:LYS:C	1:D:176:ARG:H	2.16	0.49
1:D:14:GLN:HB3	1:D:343:TYR:CD1	2.48	0.49
1:D:66:THR:HG22	1:D:66:THR:O	2.12	0.49
1:B:126:GLU:HG2	1:B:131:GLU:OE2	2.13	0.48
1:C:29[A]:GLN:HE21	1:C:46:HIS:CE1	2.31	0.48
1:C:233:LYS:HB2	1:C:263:ILE:CD1	2.43	0.48
1:D:92:GLU:OE1	1:D:93:PRO:HA	2.13	0.48
1:D:96:GLN:HE21	1:D:96:GLN:CA	2.26	0.48
1:D:105:PHE:O	1:D:108:LYS:HB2	2.12	0.48
1:D:372:GLN:N	1:D:373:PRO:CD	2.76	0.48
1:B:145:LEU:HB3	1:B:158:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLN:NE2	7:D:485:HOH:O	2.45	0.48
1:A:143:LEU:CD1	1:A:160:VAL:HB	2.42	0.48
1:A:380:ARG:O	1:A:381:ILE:CG2	2.62	0.48
1:C:317:ILE:HA	1:C:352:ARG:O	2.14	0.48
1:D:79:THR:HA	1:D:82:LEU:HD12	1.95	0.48
1:D:62:GLN:HG2	7:D:398:HOH:O	2.12	0.48
1:B:105:PHE:O	1:B:109:GLU:HG2	2.13	0.48
1:B:240:LYS:HB2	7:B:570:HOH:O	2.13	0.48
1:A:75:GLU:OE1	1:A:271:ARG:HD3	2.13	0.48
1:C:213:ASP:O	1:C:214:SER:HB2	2.13	0.48
1:C:363:THR:OG1	1:C:366:GLU:HB2	2.14	0.48
1:D:52:GLY:HA2	7:D:726:HOH:O	2.13	0.48
7:A:572:HOH:O	1:B:27:ASN:HB3	2.14	0.48
1:D:29:GLN:NE2	1:D:31:ASN:OD1	2.43	0.48
1:D:57:ARG:HD3	1:D:84:GLU:OE1	2.13	0.48
1:D:110:HIS:HA	1:D:113:LYS:HD2	1.94	0.48
1:D:146:LYS:C	1:D:178:LEU:HD23	2.34	0.48
1:D:171:GLU:O	1:D:174:LYS:HG3	2.13	0.48
1:D:316:ILE:O	1:D:354:MET:HB2	2.13	0.48
1:A:108:LYS:HE2	1:A:118:MET:HE2	1.96	0.48
1:A:125:VAL:N	1:A:131:GLU:OE1	2.47	0.48
1:D:174:LYS:O	1:D:176:ARG:N	2.43	0.48
1:D:125:VAL:HG13	1:D:126:GLU:OE1	2.14	0.48
1:D:158:PHE:CE2	1:D:169:ALA:CB	2.97	0.48
1:A:199:ASP:OD2	1:A:199:ASP:N	2.47	0.48
1:B:145:LEU:HB3	1:B:158:PHE:HB3	1.95	0.48
1:C:62:GLN:O	1:C:62:GLN:HG3	2.12	0.48
1:C:205:PRO:CG	1:C:307:ILE:HD12	2.40	0.48
1:D:9:VAL:HG13	1:D:9:VAL:O	2.14	0.48
1:D:41:LYS:HZ1	1:D:51:THR:HA	1.79	0.47
1:D:237:LEU:HD12	1:D:237:LEU:C	2.34	0.47
1:A:5:ARG:NH2	1:A:296:LEU:O	2.47	0.47
1:B:174:LYS:N	1:B:174:LYS:CD	2.77	0.47
1:C:15:LEU:HB2	6:C:402:AIR:O2'	2.13	0.47
1:C:126:GLU:O	1:C:131:GLU:OE1	2.32	0.47
1:C:158:PHE:CZ	1:C:168:GLU:HG2	2.48	0.47
1:D:316:ILE:HG13	1:D:357:ILE:CD1	2.44	0.47
1:D:73:GLU:OE1	6:D:402:AIR:O3'	2.21	0.47
1:D:143:LEU:CD2	1:D:143:LEU:N	2.78	0.47
1:A:235:GLN:O	1:A:239:ARG:HG3	2.13	0.47
1:A:284:ALA:CB	1:B:337:ASN:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:HB2	1:B:292:LEU:HD11	1.96	0.47
1:C:94:SER:O	1:C:98:ILE:HD12	2.14	0.47
1:C:105:PHE:HE1	1:C:121:HIS:CD2	2.32	0.47
1:A:230:ILE:O	1:A:231:ASN:C	2.53	0.47
1:A:368:GLU:HG2	7:A:633:HOH:O	2.15	0.47
1:C:293:ARG:HA	1:C:298:LEU:HB2	1.96	0.47
1:B:198:LYS:HA	1:B:248:LYS:HD3	1.95	0.47
1:D:6:LYS:O	1:D:67:CYS:HB2	2.15	0.47
1:D:16:GLY:N	1:D:73:GLU:HG3	2.30	0.47
1:D:63:LEU:O	1:D:66:THR:HB	2.14	0.47
1:D:94:SER:H	1:D:247:GLY:HA3	1.79	0.47
1:D:317:ILE:H	1:D:317:ILE:HG12	1.43	0.47
1:A:104:LYS:HE2	7:A:478:HOH:O	2.13	0.47
1:A:213:ASP:O	1:A:214:SER:HB2	2.15	0.47
1:B:29:GLN:HA	7:B:756:HOH:O	2.15	0.47
1:C:17:ARG:N	1:C:40:ALA:HB2	2.30	0.47
1:C:229:ALA:O	1:C:233:LYS:HG3	2.15	0.47
1:D:26:LEU:O	1:D:27:ASN:HB2	2.14	0.47
1:D:229:ALA:O	1:D:233:LYS:HB2	2.15	0.47
1:A:263:ILE:HG22	1:A:264:MET:N	2.30	0.47
1:B:174:LYS:HD3	1:B:175:ASP:H	1.80	0.47
1:C:33:LEU:O	1:C:34:ASP:HB2	2.14	0.47
1:D:219:VAL:O	1:D:312:ILE:HA	2.15	0.47
1:C:90:LYS:HA	7:C:874:HOH:O	2.14	0.47
1:C:139:LEU:HB3	1:C:182:LYS:HB2	1.97	0.47
1:D:322:PRO:C	1:D:348:ALA:HB3	2.35	0.47
1:C:2:TRP:CE3	1:C:3:ASN:HB3	2.49	0.47
1:C:324:THR:O	1:C:325:HIS:C	2.53	0.47
1:D:28:ILE:C	7:D:587:HOH:O	2.51	0.47
1:C:43:ILE:HG21	1:C:43:ILE:HD13	1.75	0.46
1:D:41:LYS:NZ	1:D:51:THR:HA	2.30	0.46
1:D:96:GLN:HB3	7:D:497:HOH:O	2.15	0.46
1:A:116:ILE:CD1	1:A:240:LYS:CD	2.89	0.46
1:B:38:SER:O	1:B:39:PRO:C	2.51	0.46
1:B:105:PHE:CB	1:B:148:LYS:HE2	2.45	0.46
1:B:123:GLU:HA	1:B:179:TYR:HB3	1.97	0.46
1:C:381:ILE:O	1:C:381:ILE:HG22	2.13	0.46
1:A:61:ARG:NH2	1:A:84:GLU:OE2	2.49	0.46
1:C:132:LEU:HD23	1:C:166:ILE:HG12	1.97	0.46
1:A:34:ASP:OD1	1:A:35:ALA:N	2.38	0.46
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:THR:HG23	1:C:381:ILE:CG2	2.19	0.46
1:D:325:HIS:CD2	1:D:326:LEU:CD2	2.99	0.46
1:A:231:ASN:O	1:A:234:ALA:HB3	2.16	0.46
1:A:340:ILE:O	7:A:459:HOH:O	2.21	0.46
1:B:223:ALA:CB	1:B:226:VAL:HG21	2.46	0.46
1:C:25:ARG:HD2	7:D:589:HOH:O	2.15	0.46
1:D:116:ILE:HG21	1:D:265:LEU:HD22	1.96	0.46
1:D:361:ALA:CB	1:D:366:GLU:HB3	2.45	0.46
1:C:239:ARG:HG2	1:C:239:ARG:HH11	1.80	0.46
1:C:345:LYS:O	7:C:614:HOH:O	2.21	0.46
1:D:44:SER:HB3	1:D:49:HIS:HE2	1.80	0.46
1:D:126:GLU:HG2	1:D:131:GLU:CD	2.36	0.46
1:C:64:ALA:C	1:C:66:THR:H	2.19	0.46
1:C:105:PHE:CE1	1:C:121:HIS:CD2	3.04	0.46
1:C:105:PHE:HB3	1:C:148:LYS:HG2	1.98	0.46
1:D:272:ILE:HD12	1:D:288:PHE:CE2	2.44	0.46
1:A:50:VAL:HG13	7:A:422:HOH:O	2.15	0.46
1:A:67:CYS:SG	1:A:70:VAL:HG22	2.55	0.46
1:A:209:THR:HG22	1:A:219:VAL:HG22	1.98	0.46
1:C:57:ARG:HD3	1:C:81:ALA:HB2	1.98	0.46
1:C:183:TRP:HB3	1:C:185:TYR:CE2	2.51	0.46
1:B:115:GLY:O	1:B:117:PRO:HD3	2.16	0.46
1:B:158:PHE:CD2	1:B:169:ALA:CB	2.99	0.46
1:A:67:CYS:SG	1:A:70:VAL:CG2	3.04	0.45
1:D:66:THR:O	1:D:66:THR:CG2	2.64	0.45
1:D:144:MET:O	1:D:181:GLU:N	2.35	0.45
1:A:360:THR:O	1:A:361:ALA:HB2	2.16	0.45
1:D:131:GLU:CG	1:D:132:LEU:N	2.78	0.45
1:A:1:MET:N	1:A:4:SER:OG	2.27	0.45
1:A:55:LYS:CE	1:A:150:MET:HE1	2.34	0.45
1:B:86:ALA:HB2	1:B:91:ILE:HD12	1.98	0.45
1:B:233[A]:LYS:HD2	1:B:263:ILE:CD1	2.40	0.45
1:D:158:PHE:CD2	1:D:169:ALA:HA	2.51	0.45
1:B:5:ARG:NH1	7:B:648:HOH:O	2.50	0.45
1:B:59:ALA:O	1:B:62[A]:GLN:HB3	2.15	0.45
1:C:257:LEU:HD12	1:C:258:LEU:N	2.32	0.45
1:D:158:PHE:CD2	1:D:169:ALA:HB2	2.52	0.45
1:B:38:SER:H	1:B:41:LYS:HD2	1.82	0.45
1:C:142:PRO:CB	1:C:161:ASN:HA	2.47	0.45
1:C:233:LYS:HB2	1:C:263:ILE:HD11	1.98	0.45
1:C:311:SER:HB3	1:C:360:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LYS:O	1:D:137:GLU:HB2	2.16	0.45
1:D:309:GLN:HB3	1:D:310:PRO:HD2	1.99	0.45
1:B:372:GLN:N	1:B:373:PRO:CD	2.79	0.45
1:C:372:GLN:N	1:C:373:PRO:CD	2.79	0.45
1:D:208:GLU:HB3	1:D:223:ALA:HA	1.97	0.45
1:A:283:CYS:HA	1:A:308:ARG:HG3	1.97	0.45
1:B:16:GLY:N	1:B:73:GLU:OE2	2.38	0.45
1:C:150:MET:HA	1:C:150:MET:CE	2.43	0.45
1:D:92:GLU:OE1	1:D:248:LYS:N	2.43	0.45
1:D:83:GLU:O	1:D:86:ALA:HB3	2.17	0.45
1:D:85:VAL:C	1:D:87:SER:H	2.20	0.45
1:B:33:LEU:HB3	1:B:63:LEU:HD13	1.89	0.45
1:C:101:ILE:HD13	1:C:268:ILE:HG23	1.99	0.45
1:C:116:ILE:HG23	1:C:117:PRO:HD2	1.98	0.45
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.66	0.45
1:C:2:TRP:CZ3	1:C:3:ASN:HB3	2.52	0.45
1:C:124:LEU:N	1:C:124:LEU:CD1	2.80	0.45
1:C:317:ILE:HD12	1:C:317:ILE:HA	1.62	0.45
4:C:400:ADP:O5'	4:C:400:ADP:H8	2.00	0.45
1:C:187:LYS:HE2	1:C:259:GLU:CA	2.46	0.44
1:C:187:LYS:O	1:C:188:MET:HB2	2.18	0.44
1:D:104:LYS:NZ	4:D:400:ADP:O2B	2.50	0.44
1:D:296:LEU:O	1:D:297:ASP:HB2	2.16	0.44
1:A:7:VAL:HB	1:A:30:VAL:HG22	2.00	0.44
1:A:135:VAL:O	1:A:138:GLN:HB2	2.17	0.44
1:C:89:VAL:CG1	1:C:90:LYS:N	2.79	0.44
1:D:317:ILE:HG22	1:D:351:GLY:CA	2.47	0.44
1:A:61:ARG:HH22	1:A:84:GLU:CD	2.19	0.44
1:A:204:TYR:CZ	1:A:305:LEU:HD22	2.53	0.44
1:D:316:ILE:CD1	1:D:357:ILE:CD1	2.89	0.44
1:D:317:ILE:HG12	7:D:725:HOH:O	2.16	0.44
1:A:1:MET:HB3	1:A:2:TRP:H	1.48	0.44
1:A:298:LEU:N	1:A:298:LEU:HD23	2.32	0.44
1:B:122:ARG:O	1:B:179:TYR:HB2	2.18	0.44
1:C:3:ASN:HB2	1:C:28:ILE:HG12	2.00	0.44
1:D:59:ALA:HB3	1:D:60:VAL:H	1.61	0.44
1:D:111:LEU:HD23	1:D:111:LEU:HA	1.68	0.44
1:D:159:ARG:HH11	1:D:159:ARG:CG	2.29	0.44
1:C:14:GLN:HB3	1:C:343:TYR:CD1	2.53	0.44
1:C:56:GLU:HG2	1:C:59:ALA:CB	2.48	0.44
1:B:141:TYR:HA	1:B:142:PRO:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLU:CG	1:C:139:LEU:HD23	2.41	0.44
1:C:323:ASP:O	1:C:326:LEU:HB2	2.17	0.44
1:D:80:TYR:CE1	1:D:99:ARG:CZ	3.01	0.44
1:A:20:VAL:HG11	1:A:44:SER:HB2	2.00	0.44
1:B:132:LEU:HG	1:B:166:ILE:HD13	1.99	0.44
1:B:365:HIS:HB2	7:B:566:HOH:O	2.17	0.44
1:C:14:GLN:HG3	1:C:343:TYR:CE1	2.53	0.44
1:C:260:ASP:OD2	1:C:262:SER:HB3	2.17	0.44
1:D:106:ASN:HD22	1:D:106:ASN:HA	1.58	0.44
1:D:317:ILE:HG22	1:D:351:GLY:HA2	2.00	0.44
1:A:1:MET:N	1:A:4:SER:HB3	2.33	0.44
1:A:254:GLU:OE1	1:A:273:HIS:CE1	2.71	0.44
1:B:47:ASP:C	7:B:579:HOH:O	2.56	0.44
1:B:75:GLU:N	7:B:422:HOH:O	2.39	0.44
1:D:93:PRO:CB	1:D:247:GLY:HA3	2.48	0.44
1:D:278:TYR:CD2	1:D:278:TYR:C	2.91	0.44
1:C:68:ASP:O	1:C:89:VAL:CG1	2.66	0.43
1:C:292:LEU:HA	1:C:292:LEU:HD23	1.29	0.43
1:C:344:SER:HB2	1:D:27:ASN:ND2	2.33	0.43
1:D:57:ARG:HD2	1:D:61:ARG:HD2	1.99	0.43
1:D:58:GLU:O	1:D:59:ALA:C	2.56	0.43
1:D:126:GLU:CB	1:D:128:THR:HG22	2.39	0.43
1:B:105:PHE:CB	1:B:148:LYS:CE	2.96	0.43
1:B:73:GLU:OE1	6:B:402:AIR:O3'	2.16	0.43
1:C:2:TRP:NE1	1:D:330:GLU:HB2	2.33	0.43
1:A:108:LYS:HE3	1:A:118:MET:HE1	2.00	0.43
1:D:120:GLU:CG	1:D:182:LYS:HD3	2.47	0.43
1:D:128:THR:HG23	1:D:131:GLU:CA	2.48	0.43
1:A:61:ARG:HG3	1:A:85:VAL:CG1	2.48	0.43
1:A:295:ILE:HG21	1:A:295:ILE:HD13	1.77	0.43
1:B:58:GLU:HG2	1:B:59:ALA:N	2.33	0.43
1:C:56:GLU:HG2	1:C:59:ALA:H	1.83	0.43
1:C:116:ILE:CD1	1:C:240:LYS:HE2	2.41	0.43
1:B:75:GLU:O	1:B:77:VAL:N	2.50	0.43
1:D:111:LEU:HB3	1:D:116:ILE:CG1	2.48	0.43
1:D:145:LEU:HD23	1:D:169:ALA:HB1	2.00	0.43
1:A:32:VAL:CG2	1:A:49:HIS:CE1	2.94	0.43
1:A:327[A]:GLN:HE21	1:A:327[A]:GLN:HB3	1.44	0.43
1:B:206:THR:HB	1:B:231:ASN:ND2	2.34	0.43
1:B:300:ILE:HG21	1:B:300:ILE:HD13	1.78	0.43
1:B:317:ILE:HD12	7:B:483:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASP:O	1:C:37:ASN:CB	2.65	0.43
1:C:321:ALA:HB3	1:C:324:THR:OG1	2.19	0.43
1:D:171:GLU:OE1	1:D:172:ALA:CA	2.63	0.43
1:D:171:GLU:CD	1:D:172:ALA:N	2.71	0.43
1:D:361:ALA:HB1	1:D:366:GLU:HB3	2.01	0.43
1:A:75:GLU:OE1	1:A:271:ARG:CD	2.67	0.43
1:B:188:MET:HE1	1:B:226:VAL:HG22	1.99	0.43
1:C:116:ILE:CG2	1:C:117:PRO:N	2.81	0.43
1:C:241:ALA:O	1:C:244:ALA:HB3	2.19	0.43
1:A:263:ILE:CG2	1:A:264:MET:N	2.82	0.43
1:C:101:ILE:HD12	1:C:270:SER:HB3	2.00	0.43
1:C:121:HIS:HB2	1:C:180:ALA:O	2.18	0.43
1:C:232:GLN:HG3	7:C:495:HOH:O	2.18	0.43
1:D:233:LYS:HD2	1:D:263:ILE:CD1	2.40	0.43
1:D:316:ILE:N	7:D:769:HOH:O	2.51	0.43
1:D:324:THR:O	1:D:325:HIS:C	2.57	0.43
1:B:197:THR:OG1	1:B:200:GLU:N	2.36	0.43
1:B:215:ILE:O	1:B:216:CYS:C	2.57	0.43
1:C:166:ILE:N	1:C:167:PRO:CD	2.82	0.43
1:C:218:LEU:HD21	1:C:314:LEU:HD13	2.00	0.43
1:D:158:PHE:CE2	1:D:169:ALA:HA	2.53	0.43
1:C:55:LYS:NZ	7:C:580:HOH:O	2.52	0.42
1:C:211:GLN:HG2	4:C:400:ADP:O3'	2.18	0.42
1:C:265:LEU:HG	1:C:266:CYS:H	1.78	0.42
1:B:170:LEU:O	1:B:171:GLU:C	2.56	0.42
1:C:12:GLY:O	1:C:38:SER:HB3	2.19	0.42
1:C:43:ILE:HA	1:D:43:ILE:O	2.19	0.42
1:C:324:THR:CG2	1:C:381:ILE:CG2	2.88	0.42
1:D:31:ASN:ND2	1:D:66:THR:CG2	2.78	0.42
1:A:74:ILE:CG1	1:A:75:GLU:N	2.81	0.42
1:A:162:SER:OG	1:A:164:ASP:HB2	2.19	0.42
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.40	0.42
1:B:166:ILE:CB	1:B:167:PRO:HD3	2.48	0.42
1:C:61:ARG:HH22	1:C:65[B]:LYS:CE	2.32	0.42
1:C:187:LYS:HE2	1:C:259:GLU:O	2.20	0.42
1:C:331:CYS:SG	1:C:374:LEU:HD12	2.59	0.42
1:A:318:GLY:HA3	1:A:349:LYS:O	2.19	0.42
1:B:316:ILE:HD13	1:B:316:ILE:HG21	1.70	0.42
1:C:285:LEU:HD23	1:C:285:LEU:HA	1.63	0.42
1:C:337:ASN:HA	1:D:284:ALA:HB1	2.01	0.42
1:C:379:ASP:O	1:C:382:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:PHE:CZ	1:D:123:GLU:HB2	2.54	0.42
1:A:143:LEU:HD12	1:A:143:LEU:O	2.20	0.42
1:B:57:ARG:NH1	1:B:57:ARG:CG	2.73	0.42
1:C:14:GLN:HB3	1:C:343:TYR:CG	2.55	0.42
3:C:384:NHE:C1	7:C:535:HOH:O	2.66	0.42
3:C:384:NHE:HC12	7:C:535:HOH:O	2.19	0.42
1:D:33:LEU:HD11	1:D:52:GLY:HA3	2.02	0.42
1:D:174:LYS:NZ	1:D:176:ARG:NH1	2.65	0.42
1:C:33:LEU:HD11	1:C:59:ALA:HB1	2.01	0.42
7:C:922:HOH:O	1:D:284:ALA:HA	2.19	0.42
1:B:210:VAL:N	1:B:218:LEU:O	2.38	0.42
1:C:73:GLU:OE1	6:C:402:AIR:O3'	2.29	0.42
1:C:108:LYS:O	1:C:109:GLU:C	2.57	0.42
1:C:242:VAL:HG12	1:C:243:ALA:N	2.29	0.42
1:A:16:GLY:O	1:A:20:VAL:HG23	2.19	0.42
1:A:116:ILE:N	1:A:116:ILE:HD13	2.34	0.42
1:A:142:PRO:HG2	1:A:183:TRP:CE3	2.54	0.42
1:C:257:LEU:HD12	1:C:258:LEU:H	1.84	0.42
1:C:364:MET:O	1:C:368:GLU:HG3	2.19	0.42
1:D:110:HIS:CD2	1:D:113:LYS:NZ	2.85	0.42
1:A:142:PRO:HB3	1:A:161:ASN:HA	2.02	0.42
1:A:315:ASN:HB3	1:A:317:ILE:HD11	2.02	0.42
1:D:143:LEU:N	1:D:143:LEU:HD22	2.35	0.42
1:A:134:LYS:O	1:A:138:GLN:HG3	2.20	0.42
1:B:18:MET:O	1:B:21:GLU:HB2	2.20	0.42
1:B:195:VAL:HG22	1:B:250:VAL:HG22	2.01	0.42
1:C:337:ASN:HA	1:D:284:ALA:CB	2.50	0.42
1:D:292:LEU:HD23	1:D:292:LEU:HA	1.76	0.42
1:D:293:ARG:HA	1:D:298:LEU:HD12	2.01	0.42
1:A:341:HIS:CE1	1:B:25:ARG:CZ	3.03	0.41
1:B:365:HIS:HA	1:B:368:GLU:OE2	2.20	0.41
1:D:109:GLU:H	1:D:109:GLU:HG2	1.52	0.41
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.84	0.41
1:D:221:ALA:HA	1:D:222:PRO:HA	1.73	0.41
1:A:325:HIS:ND1	1:A:348:ALA:CB	2.83	0.41
1:B:9:VAL:HG13	1:B:9:VAL:O	2.19	0.41
1:C:324:THR:O	1:C:326:LEU:N	2.53	0.41
1:D:110:HIS:HD2	1:D:113:LYS:CE	2.33	0.41
1:A:273:HIS:ND1	1:A:275:SER:HB3	2.35	0.41
1:C:205:PRO:CG	1:C:307:ILE:CD1	2.95	0.41
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASP:O	1:A:41:LYS:NZ	2.53	0.41
1:A:198:LYS:HG2	7:A:604:HOH:O	2.21	0.41
1:A:241:ALA:O	1:A:244:ALA:HB3	2.19	0.41
1:A:256:PHE:CZ	1:A:266:CYS:SG	3.13	0.41
1:C:15:LEU:HD13	1:C:272:ILE:HG13	2.01	0.41
1:C:233:LYS:HA	1:C:236[B]:GLU:CD	2.41	0.41
1:D:59:ALA:O	1:D:62:GLN:CB	2.69	0.41
1:D:141:TYR:HA	1:D:142:PRO:C	2.41	0.41
1:D:314:LEU:HD21	1:D:378:VAL:HG21	2.02	0.41
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.84	0.41
1:B:126:GLU:O	1:B:127:ASN:C	2.57	0.41
1:C:128:THR:HA	1:C:129:PRO:HD3	1.70	0.41
1:D:34:ASP:C	1:D:35:ALA:O	2.59	0.41
1:A:33:LEU:HD11	1:A:59:ALA:HB1	2.03	0.41
1:A:61:ARG:HD2	7:A:540:HOH:O	2.21	0.41
1:A:61:ARG:O	1:A:65[A]:LYS:HG2	2.20	0.41
1:B:361:ALA:HB1	1:B:362:PRO:CD	2.50	0.41
1:C:155:ARG:O	3:C:384:NHE:H3'2	2.19	0.41
1:D:74:ILE:CD1	1:D:77:VAL:CG1	2.96	0.41
1:B:378:VAL:CG1	1:B:379:ASP:N	2.83	0.41
1:D:16:GLY:O	1:D:19:LEU:HB3	2.21	0.41
1:D:47:ASP:HB2	7:D:788:HOH:O	2.21	0.41
1:D:135:VAL:CG1	1:D:139:LEU:HD12	2.51	0.41
1:A:237:LEU:HD12	1:A:237:LEU:O	2.20	0.41
1:A:324:THR:HA	1:A:327[A]:GLN:HG3	2.02	0.41
1:C:10:LEU:HD23	1:C:33:LEU:HD23	2.03	0.41
1:C:198:LYS:HE3	1:C:198:LYS:HB3	1.85	0.41
1:C:205:PRO:HG2	1:C:307:ILE:HD13	2.02	0.41
1:C:226:VAL:HG13	1:C:230:ILE:HB	2.02	0.41
1:C:342:LEU:HB2	1:D:27:ASN:OD1	2.21	0.41
1:D:85:VAL:O	1:D:87:SER:N	2.54	0.41
1:D:316:ILE:CG2	1:D:325:HIS:HB2	2.50	0.41
1:D:341:HIS:O	1:D:356:HIS:N	2.49	0.41
1:A:3:ASN:HB2	1:A:28:ILE:HG13	2.02	0.41
1:A:91:ILE:HG22	1:A:93:PRO:O	2.20	0.41
1:A:105:PHE:CZ	1:A:123:GLU:HB3	2.55	0.41
1:A:365[B]:HIS:HB2	1:A:366:GLU:H	1.66	0.41
1:B:19:LEU:HD12	1:B:19:LEU:HA	1.86	0.41
1:B:85:VAL:O	1:B:85:VAL:CG1	2.67	0.41
1:B:188:MET:HE3	1:B:226:VAL:HG21	2.03	0.41
1:B:221:ALA:HA	1:B:222:PRO:HA	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLN:CB	1:B:373:PRO:CD	2.97	0.41
1:D:135:VAL:HG13	1:D:139:LEU:HD12	2.03	0.41
1:D:146:LYS:HB2	1:D:179:TYR:CE1	2.56	0.41
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.78	0.40
1:B:65:LYS:O	1:B:65:LYS:HD3	2.22	0.40
1:D:191:ALA:O	1:D:207:VAL:HG22	2.20	0.40
1:C:55:LYS:HE2	7:C:521:HOH:O	2.21	0.40
1:C:209:THR:HG22	1:C:219:VAL:HG22	2.04	0.40
1:C:224:ARG:O	1:C:225:ASN:HB2	2.20	0.40
7:C:922:HOH:O	1:D:308:ARG:HD2	2.19	0.40
1:A:141:TYR:HB3	1:A:161:ASN:O	2.21	0.40
1:A:373:PRO:O	1:A:376:ASP:HB2	2.22	0.40
1:B:49:HIS:N	7:B:579:HOH:O	2.26	0.40
1:C:88:GLU:O	1:C:89:VAL:HG22	2.20	0.40
1:D:33:LEU:HD11	1:D:52:GLY:CA	2.52	0.40
1:B:144:MET:HG3	1:B:146:LYS:HG2	2.03	0.40
1:B:208:GLU:O	1:B:219:VAL:HA	2.22	0.40
1:A:98:ILE:HD13	1:A:98:ILE:HG21	1.76	0.40
1:A:272:ILE:H	1:A:272:ILE:HG12	1.67	0.40
1:A:381:ILE:HG21	1:A:381:ILE:HD13	1.64	0.40
1:B:86:ALA:CB	1:B:91:ILE:HD12	2.51	0.40
1:B:166:ILE:HB	1:B:167:PRO:CD	2.52	0.40
1:B:374:LEU:O	1:B:377:VAL:HB	2.21	0.40
1:C:321:ALA:HA	1:C:322:PRO:HD3	1.78	0.40
1:C:379:ASP:O	1:C:382:ARG:CG	2.70	0.40
1:D:251:PHE:CD2	1:D:270:SER:HA	2.56	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	384/403 (95%)	365 (95%)	18 (5%)	1 (0%)	41	37
1	B	378/403 (94%)	346 (92%)	28 (7%)	4 (1%)	14	8
1	C	386/403 (96%)	368 (95%)	16 (4%)	2 (0%)	29	23
1	D	368/403 (91%)	344 (94%)	18 (5%)	6 (2%)	9	4
All	All	1516/1612 (94%)	1423 (94%)	80 (5%)	13 (1%)	17	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ALA
1	B	174	LYS
1	C	322	PRO
1	D	171	GLU
1	D	172	ALA
1	D	322	PRO
1	B	324	THR
1	B	347	ALA
1	D	35	ALA
1	A	57	ARG
1	D	86	ALA
1	C	34	ASP
1	D	175	ASP

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	322/336 (96%)	295 (92%)	27 (8%)	11	7
1	B	320/336 (95%)	260 (81%)	60 (19%)	1	0
1	C	324/336 (96%)	286 (88%)	38 (12%)	5	3
1	D	312/336 (93%)	265 (85%)	47 (15%)	3	1
All	All	1278/1344 (95%)	1106 (86%)	172 (14%)	4	2

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	LEU
1	A	57	ARG
1	A	73	GLU
1	A	87	SER
1	A	118	MET
1	A	123	GLU
1	A	126	GLU
1	A	131	GLU
1	A	139	LEU
1	A	174	LYS
1	A	187	LYS
1	A	193	ILE
1	A	196	LYS
1	A	200	GLU
1	A	212	GLU
1	A	214	SER
1	A	240	LYS
1	A	246	ASP
1	A	259	GLU
1	A	264	MET
1	A	274	ASN
1	A	275	SER
1	A	303	GLN
1	A	313	MET
1	A	344	SER
1	A	364	MET
1	B	6	LYS
1	B	22	SER
1	B	38	SER
1	B	39	PRO
1	B	54	PHE
1	B	57	ARG
1	B	61	ARG
1	B	62[A]	GLN
1	B	62[B]	GLN
1	B	63	LEU
1	B	66	THR
1	B	69	VAL
1	B	73	GLU
1	B	74	ILE
1	B	75	GLU
1	B	76	HIS

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Mol	Chain	Res	Type
1	B	87	SER
1	B	90	LYS
1	B	94	SER
1	B	102	GLN
1	B	124	LEU
1	B	125	VAL
1	B	126	GLU
1	B	134	LYS
1	B	143	LEU
1	B	146	LYS
1	B	155	ARG
1	B	159	ARG
1	B	163	GLN
1	B	167	PRO
1	B	171	GLU
1	B	174	LYS
1	B	176	ARG
1	B	178	LEU
1	B	190	LEU
1	B	196	LYS
1	B	198	LYS
1	B	200	GLU
1	B	211	GLN
1	B	213	ASP
1	B	225	ASN
1	B	237	LEU
1	B	259[A]	GLU
1	B	259[B]	GLU
1	B	264	MET
1	B	274	ASN
1	B	285	LEU
1	B	295	ILE
1	B	305	LEU
1	B	308	ARG
1	B	311	SER
1	B	322	PRO
1	B	323	ASP
1	B	326	LEU
1	B	330	GLU
1	B	334	SER
1	B	350	PRO
1	B	372	GLN

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Mol	Chain	Res	Type
1	B	378	VAL
1	B	380	ARG
1	C	5	ARG
1	C	6	LYS
1	C	37	ASN
1	C	39	PRO
1	C	47[A]	ASP
1	C	47[B]	ASP
1	C	56	GLU
1	C	70	VAL
1	C	73	GLU
1	C	75	GLU
1	C	87	SER
1	C	107	GLN
1	C	108	LYS
1	C	112[A]	ARG
1	C	112[B]	ARG
1	C	113	LYS
1	C	123	GLU
1	C	124	LEU
1	C	126	GLU
1	C	139	LEU
1	C	163	GLN
1	C	198	LYS
1	C	199	ASP
1	C	236[A]	GLU
1	C	236[B]	GLU
1	C	255	MET
1	C	260	ASP
1	C	264	MET
1	C	265	LEU
1	C	274	ASN
1	C	280	ILE
1	C	292	LEU
1	C	307	ILE
1	C	317	ILE
1	C	323	ASP
1	C	330	GLU
1	C	339	SER
1	C	366	GLU
1	D	1	MET
1	D	5	ARG

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Mol	Chain	Res	Type
1	D	37	ASN
1	D	38	SER
1	D	47	ASP
1	D	54	PHE
1	D	55	LYS
1	D	57	ARG
1	D	58	GLU
1	D	61	ARG
1	D	65	LYS
1	D	74	ILE
1	D	88	GLU
1	D	96	GLN
1	D	104	LYS
1	D	122	ARG
1	D	124	LEU
1	D	126	GLU
1	D	129	PRO
1	D	131	GLU
1	D	132	LEU
1	D	134	LYS
1	D	143	LEU
1	D	144	MET
1	D	146	LYS
1	D	150	MET
1	D	159	ARG
1	D	163	GLN
1	D	164	ASP
1	D	167	PRO
1	D	168	GLU
1	D	171	GLU
1	D	174	LYS
1	D	198	LYS
1	D	208	GLU
1	D	213	ASP
1	D	225	ASN
1	D	246	ASP
1	D	274	ASN
1	D	301	PRO
1	D	308	ARG
1	D	317	ILE
1	D	344	SER
1	D	350	PRO

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Mol	Chain	Res	Type
1	D	352	ARG
1	D	353	LYS
1	D	380	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	225	ASN
1	B	96	GLN
1	B	127	ASN
1	C	37	ASN
1	C	62	GLN
1	C	225	ASN
1	C	232	GLN
1	C	327	GLN
1	D	42	GLN
1	D	96	GLN
1	D	102	GLN
1	D	106	ASN
1	D	110	HIS
1	D	211	GLN
1	D	325	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	ADP	B	400	5	24,29,29	1.05	2 (8%)	29,45,45	1.86	8 (27%)
4	ADP	D	400	5	24,29,29	1.05	2 (8%)	29,45,45	2.41	8 (27%)
6	AIR	C	402	-	16,20,20	0.80	0	20,30,30	1.77	6 (30%)
6	AIR	D	402	-	16,20,20	0.83	0	20,30,30	1.66	4 (20%)
6	AIR	A	402	-	16,20,20	0.85	1 (6%)	20,30,30	2.29	8 (40%)
4	ADP	A	400	5	24,29,29	1.12	2 (8%)	29,45,45	3.21	13 (44%)
3	NHE	C	384	-	13,13,13	1.07	1 (7%)	16,17,17	3.48	5 (31%)
3	NHE	A	385	-	13,13,13	1.16	1 (7%)	16,17,17	2.41	6 (37%)
4	ADP	C	400	5	24,29,29	0.92	2 (8%)	29,45,45	1.97	6 (20%)
6	AIR	B	402	-	16,20,20	0.64	0	20,30,30	2.08	7 (35%)

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
4	ADP	B	400	5	-	0/12/32/32	0/3/3/3
4	ADP	D	400	5	-	0/12/32/32	0/3/3/3
6	AIR	C	402	-	-	0/6/26/26	0/2/2/2
6	AIR	D	402	-	-	0/6/26/26	0/2/2/2
6	AIR	A	402	-	1/1/5/5	5/6/26/26	0/2/2/2
4	ADP	A	400	5	-	2/12/32/32	0/3/3/3
3	NHE	C	384	-	-	5/7/15/15	0/1/1/1
3	NHE	A	385	-	-	2/7/15/15	0/1/1/1
4	ADP	C	400	5	-	2/12/32/32	0/3/3/3
6	AIR	B	402	-	-	5/6/26/26	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	ADP	C6-N6	-3.43	1.21	1.34
3	A	385	NHE	C2-S	3.30	1.82	1.77
4	B	400	ADP	C2-N1	3.11	1.39	1.33
4	D	400	ADP	C2-N1	2.78	1.39	1.33
4	A	400	ADP	C2-N1	2.74	1.39	1.33
3	C	384	NHE	C2-S	2.64	1.81	1.77
4	D	400	ADP	C6-N6	-2.43	1.25	1.34
4	B	400	ADP	C6-N6	-2.39	1.25	1.34
4	C	400	ADP	C2-N1	2.23	1.38	1.33
6	A	402	AIR	P-O6	2.07	1.62	1.54
4	C	400	ADP	C6-N6	-2.05	1.26	1.34

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	384	NHE	O1-S-C2	11.27	120.48	106.92
4	A	400	ADP	C5-C6-N6	10.17	135.81	120.35
4	D	400	ADP	C5-C6-N1	-6.94	104.61	120.35
6	A	402	AIR	C5'-C4'-C3'	6.01	137.71	115.18
4	A	400	ADP	O3B-PB-O1B	5.96	134.00	110.68
4	D	400	ADP	C2-N1-C6	5.76	128.61	118.75
4	C	400	ADP	C5-C6-N6	5.63	128.91	120.35
4	A	400	ADP	N3-C2-N1	-5.54	120.02	128.68
3	A	385	NHE	O3-S-O2	-5.46	97.92	111.27
4	C	400	ADP	N3-C2-N1	-5.17	120.60	128.68
3	C	384	NHE	C1-N-C1'	-4.95	104.42	114.14
4	A	400	ADP	N6-C6-N1	-4.77	108.68	118.57
4	D	400	ADP	C5-C6-N6	4.66	127.44	120.35
4	B	400	ADP	N3-C2-N1	-4.62	121.45	128.68
4	D	400	ADP	N6-C6-N1	4.52	127.95	118.57
4	A	400	ADP	C4-C5-N7	4.30	113.88	109.40
4	B	400	ADP	O2'-C2'-C1'	-4.24	95.20	110.85
6	B	402	AIR	C4-N3-C2	-4.20	99.23	105.78
6	A	402	AIR	C3'-C2'-C1'	-4.05	94.87	100.98
6	B	402	AIR	O4'-C4'-C3'	-3.94	97.32	105.11
3	C	384	NHE	O3-S-O1	-3.87	101.81	111.27
3	A	385	NHE	O2-S-O1	3.84	127.22	113.95
4	A	400	ADP	C3'-C2'-C1'	-3.76	95.32	100.98
4	B	400	ADP	O3'-C3'-C2'	3.52	123.21	111.82
4	A	400	ADP	O2B-PB-O1B	-3.52	96.91	110.68
3	A	385	NHE	O2-S-C2	-3.50	102.70	106.92
6	C	402	AIR	C5'-C4'-C3'	3.32	127.61	115.18
6	B	402	AIR	N3-C2-N1	3.31	117.17	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	385	NHE	O3-S-C2	3.29	111.09	105.77
3	A	385	NHE	C1-N-C1'	-3.24	107.78	114.14
6	D	402	AIR	O2'-C2'-C1'	-3.21	98.99	110.85
4	A	400	ADP	C2-N1-C6	3.18	124.19	118.75
6	C	402	AIR	O6-P-O5'	-3.17	98.31	106.73
4	C	400	ADP	C2-N1-C6	3.15	124.14	118.75
4	A	400	ADP	O2'-C2'-C1'	-3.14	99.26	110.85
6	A	402	AIR	O4'-C4'-C5'	3.10	119.58	109.37
3	C	384	NHE	O3-S-C2	-3.10	100.76	105.77
4	C	400	ADP	O4'-C1'-C2'	3.06	111.40	106.93
6	D	402	AIR	O5'-P-O8	3.05	115.02	106.47
3	C	384	NHE	O3-S-O2	-2.86	104.28	111.27
6	D	402	AIR	O3'-C3'-C2'	2.80	120.88	111.82
6	D	402	AIR	C4-N3-C2	-2.71	101.55	105.78
4	D	400	ADP	O2'-C2'-C1'	-2.69	100.92	110.85
6	B	402	AIR	O6-P-O5'	2.68	113.87	106.73
6	C	402	AIR	O2'-C2'-C3'	2.65	120.40	111.82
6	A	402	AIR	O3'-C3'-C4'	2.65	118.71	111.05
4	D	400	ADP	O3'-C3'-C4'	2.63	118.65	111.05
4	B	400	ADP	O4'-C4'-C3'	-2.62	99.93	105.11
6	B	402	AIR	O5'-P-O8	2.56	113.67	106.47
6	B	402	AIR	O4'-C4'-C5'	2.56	117.80	109.37
6	A	402	AIR	O2'-C2'-C1'	2.42	119.79	110.85
4	B	400	ADP	C5'-C4'-C3'	-2.40	106.20	115.18
4	D	400	ADP	O5'-PA-O1A	2.39	118.40	109.07
6	C	402	AIR	O7-P-O6	2.38	116.71	107.64
4	D	400	ADP	O3'-C3'-C2'	2.37	119.50	111.82
3	A	385	NHE	C2-C1-N	-2.33	104.64	111.25
6	B	402	AIR	O2'-C2'-C1'	-2.29	102.39	110.85
4	B	400	ADP	C2-N1-C6	2.26	122.62	118.75
6	C	402	AIR	O5'-P-O8	2.26	112.81	106.47
4	A	400	ADP	C5-C6-N1	-2.24	115.27	120.35
4	A	400	ADP	O4'-C4'-C3'	-2.23	100.70	105.11
4	A	400	ADP	O3'-C3'-C4'	-2.22	104.64	111.05
6	C	402	AIR	C2'-C3'-C4'	-2.20	98.37	102.64
6	A	402	AIR	C4-N3-C2	-2.15	102.43	105.78
6	A	402	AIR	O4'-C4'-C3'	-2.14	100.88	105.11
4	B	400	ADP	N6-C6-N1	2.10	122.93	118.57
4	B	400	ADP	O2B-PB-O3A	2.10	111.67	104.64
4	C	400	ADP	O2B-PB-O1B	2.08	118.81	110.68
6	A	402	AIR	N3-C2-N1	2.04	115.29	112.26
4	A	400	ADP	O3B-PB-O3A	-2.03	97.83	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	400	ADP	O3B-PB-O2B	-2.02	99.91	107.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	402	AIR	C4'

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	385	NHE	C6'-C1'-N-C1
3	C	384	NHE	N-C1-C2-S
3	C	384	NHE	C1-C2-S-O2
4	A	400	ADP	PA-O3A-PB-O3B
6	A	402	AIR	C3'-C4'-C5'-O5'
6	A	402	AIR	C5'-O5'-P-O6
6	A	402	AIR	C5'-O5'-P-O7
6	A	402	AIR	C5'-O5'-P-O8
6	B	402	AIR	C5'-O5'-P-O7
6	B	402	AIR	C5'-O5'-P-O8
6	A	402	AIR	O4'-C4'-C5'-O5'
6	B	402	AIR	C3'-C4'-C5'-O5'
6	B	402	AIR	O4'-C4'-C5'-O5'
3	C	384	NHE	C1-C2-S-O3
3	C	384	NHE	C2-C1-N-C1'
4	C	400	ADP	C3'-C4'-C5'-O5'
3	C	384	NHE	C1-C2-S-O1
4	A	400	ADP	PA-O3A-PB-O1B
4	C	400	ADP	O4'-C4'-C5'-O5'
3	A	385	NHE	C2'-C1'-N-C1
6	B	402	AIR	C5'-O5'-P-O6

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	400	ADP	1	0
4	D	400	ADP	2	0
6	C	402	AIR	2	0
6	D	402	AIR	2	0
4	A	400	ADP	1	0

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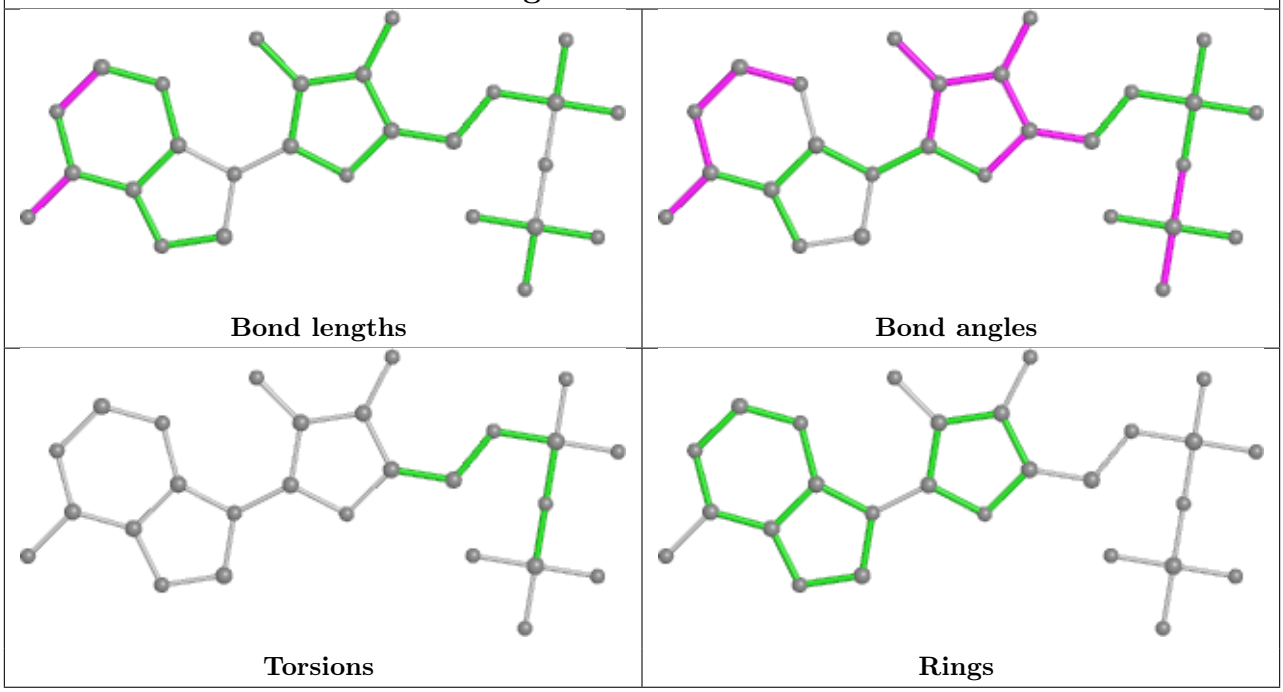
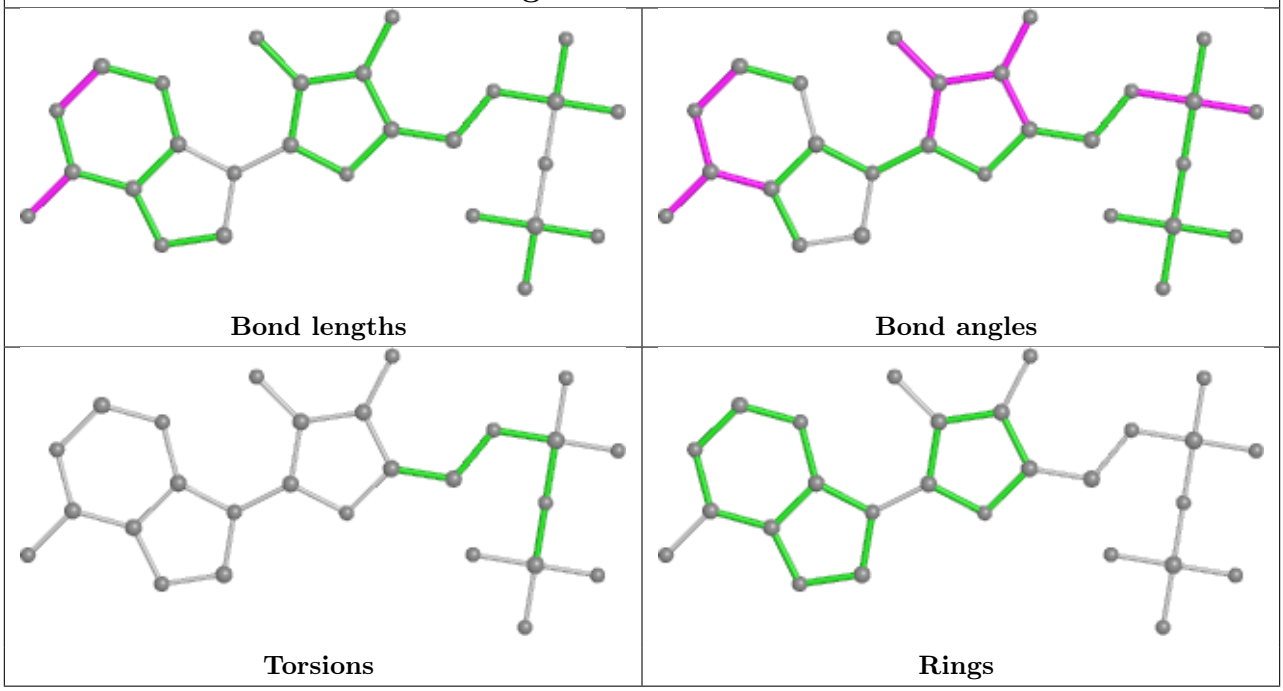
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	384	NHE	5	0
3	A	385	NHE	1	0
4	C	400	ADP	2	0
6	B	402	AIR	2	0

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.

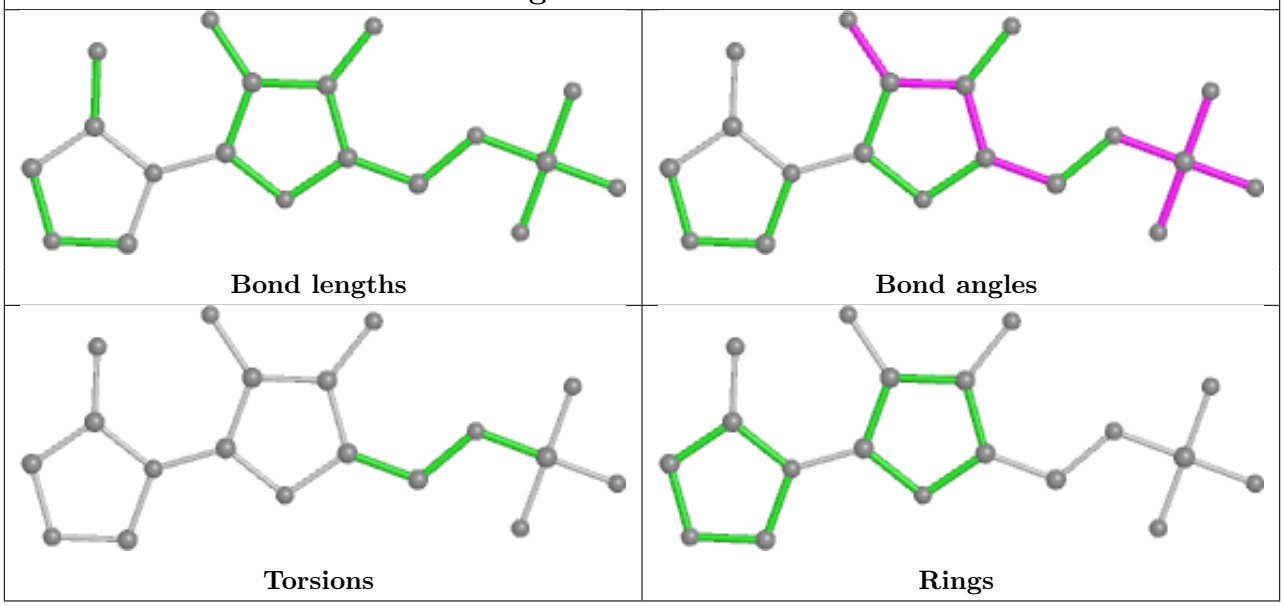
Ligand ADP B 400

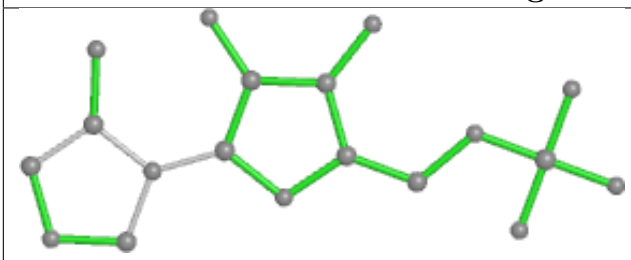
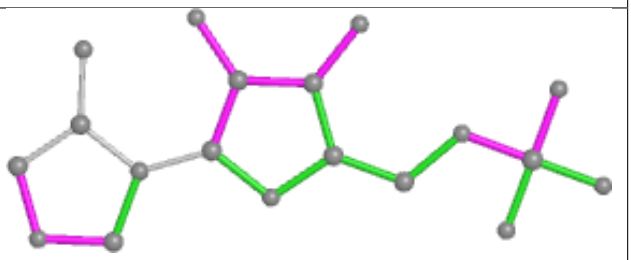
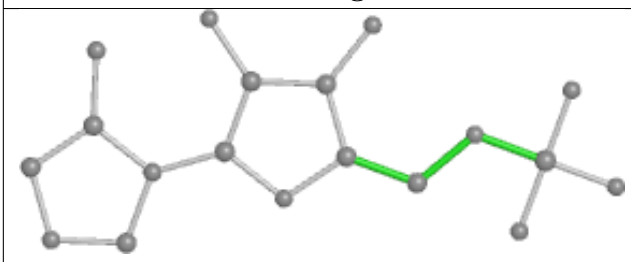
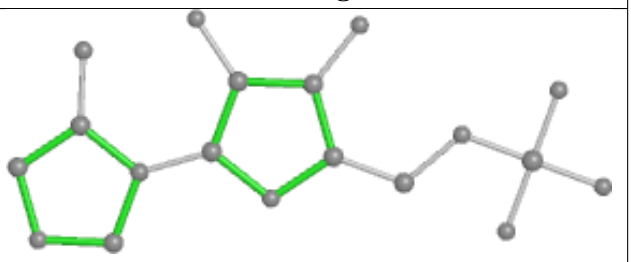


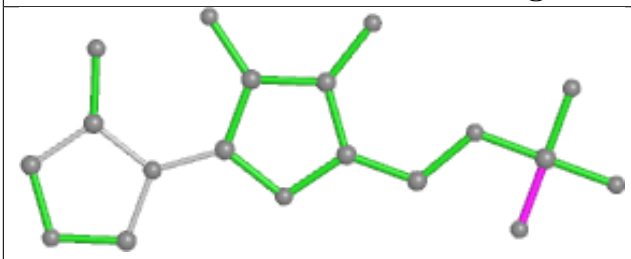
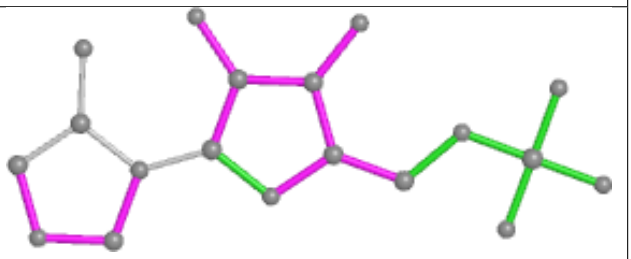
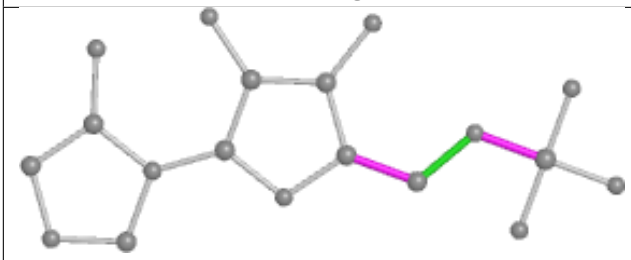
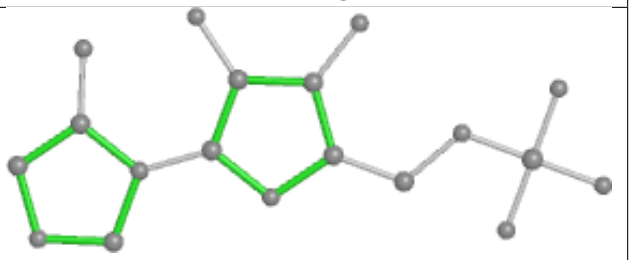
Ligand ADP D 400



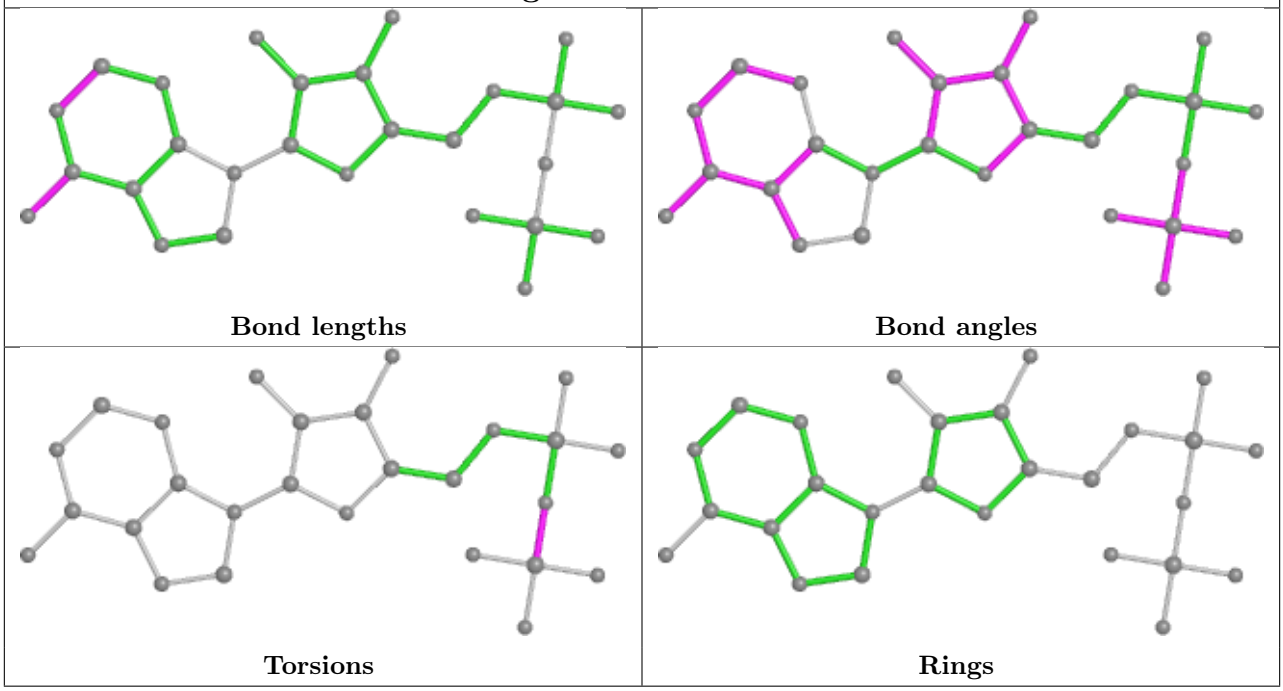
Ligand AIR C 402



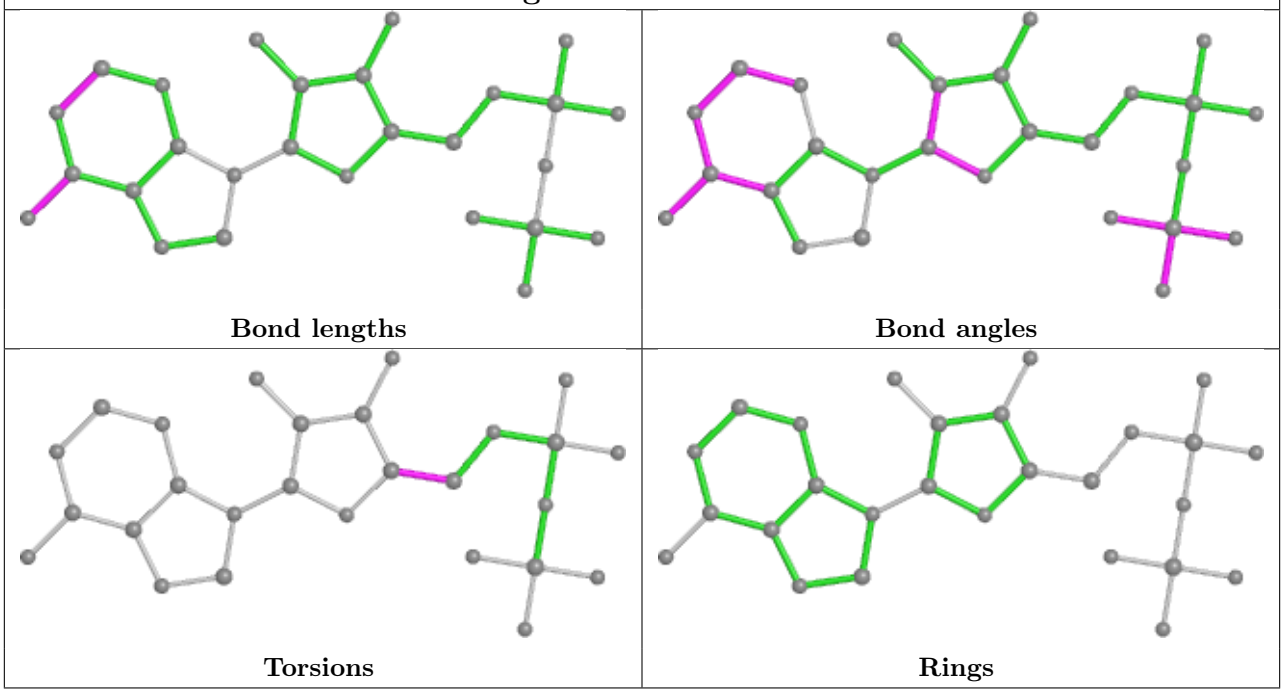
Ligand AIR D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

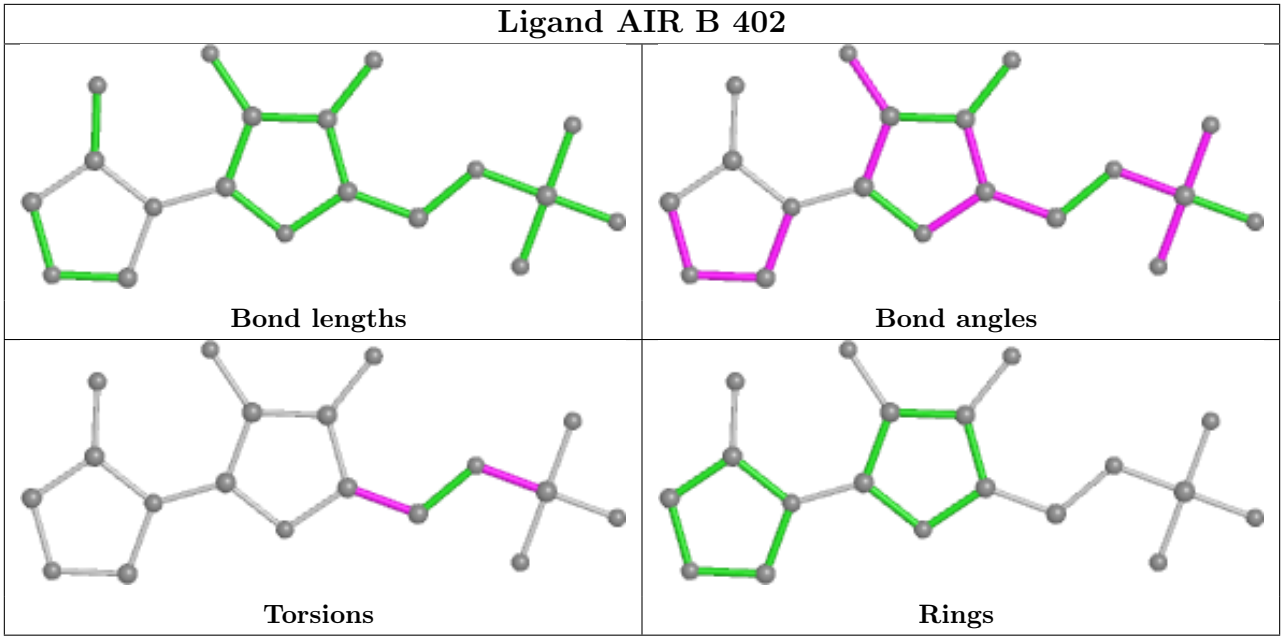
Ligand AIR A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 400



Ligand ADP C 400





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 (i)

6.1 Protein, DNA and RNA chains (i)

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	381/403 (94%)	-0.24	1 (0%)	94	93	7, 25, 59, 79	0
1	B	376/403 (93%)	0.03	15 (3%)	38	37	8, 28, 72, 93	0
1	C	382/403 (94%)	-0.24	3 (0%)	86	85	10, 27, 61, 84	0
1	D	373/403 (92%)	0.04	14 (3%)	40	39	10, 29, 71, 90	0
All	All	1512/1612 (93%)	-0.11	33 (2%)	62	60	7, 27, 67, 93	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.4
1	D	322	PRO	5.3
1	B	323	ASP	3.8
1	B	172	ALA	3.6
1	D	324	THR	3.6
1	B	125	VAL	3.5
1	D	323	ASP	3.4
1	C	321	ALA	3.2
1	B	128	THR	3.1
1	D	128	THR	3.1
1	B	321	ALA	2.7
1	B	378	VAL	2.7
1	D	319	GLY	2.6
1	B	1	MET	2.5
1	B	322	PRO	2.4
1	B	167	PRO	2.4
1	D	89	VAL	2.4
1	D	85	VAL	2.3
1	D	156	GLY	2.3
1	B	380	ARG	2.3
1	B	89	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	75	GLU	2.3
1	D	74	ILE	2.3
1	B	126	GLU	2.2
1	D	35	ALA	2.2
1	B	324	THR	2.2
1	D	164	ASP	2.1
1	C	229	ALA	2.1
1	B	381	ILE	2.1
1	A	381	ILE	2.1
1	D	150	MET	2.0
1	C	324	THR	2.0
1	D	125	VAL	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 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(Å^2)	Q<0.9
5	MG	D	401	1/1	0.84	0.10	31,31,31,31	0
2	NA	A	384	1/1	0.88	0.13	37,37,37,37	0
6	AIR	D	402	19/19	0.88	0.17	14,45,99,99	0
5	MG	B	401	1/1	0.93	0.05	27,27,27,27	0
4	ADP	D	400	27/27	0.94	0.10	8,29,56,98	0
4	ADP	B	400	27/27	0.94	0.10	4,35,63,99	0
6	AIR	B	402	19/19	0.95	0.11	2,34,99,99	0
6	AIR	A	402	19/19	0.95	0.10	1,15,23,23	0
6	AIR	C	402	19/19	0.96	0.10	4,13,32,38	0
3	NHE	C	384	13/13	0.96	0.13	17,37,56,77	0
4	ADP	C	400	27/27	0.97	0.09	4,21,41,47	0

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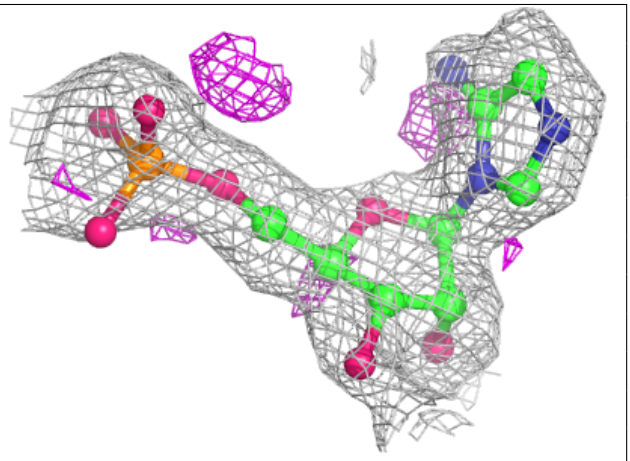
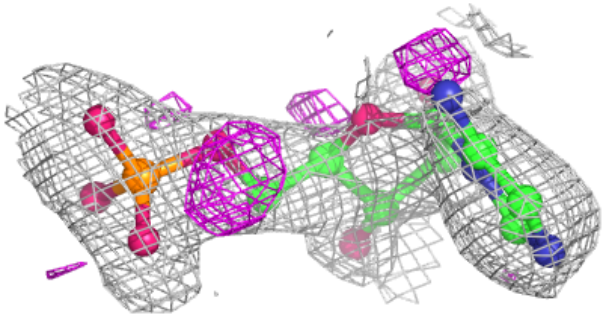
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ADP	A	400	27/27	0.97	0.08	6,19,31,99	0
5	MG	A	401	1/1	0.97	0.04	14,14,14,14	0
3	NHE	A	385	13/13	0.97	0.12	15,30,99,99	0
5	MG	C	401	1/1	0.97	0.03	18,18,18,18	0

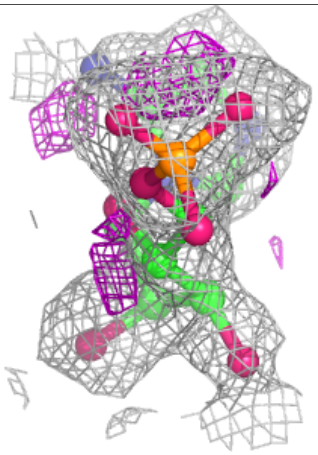
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AIR D 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

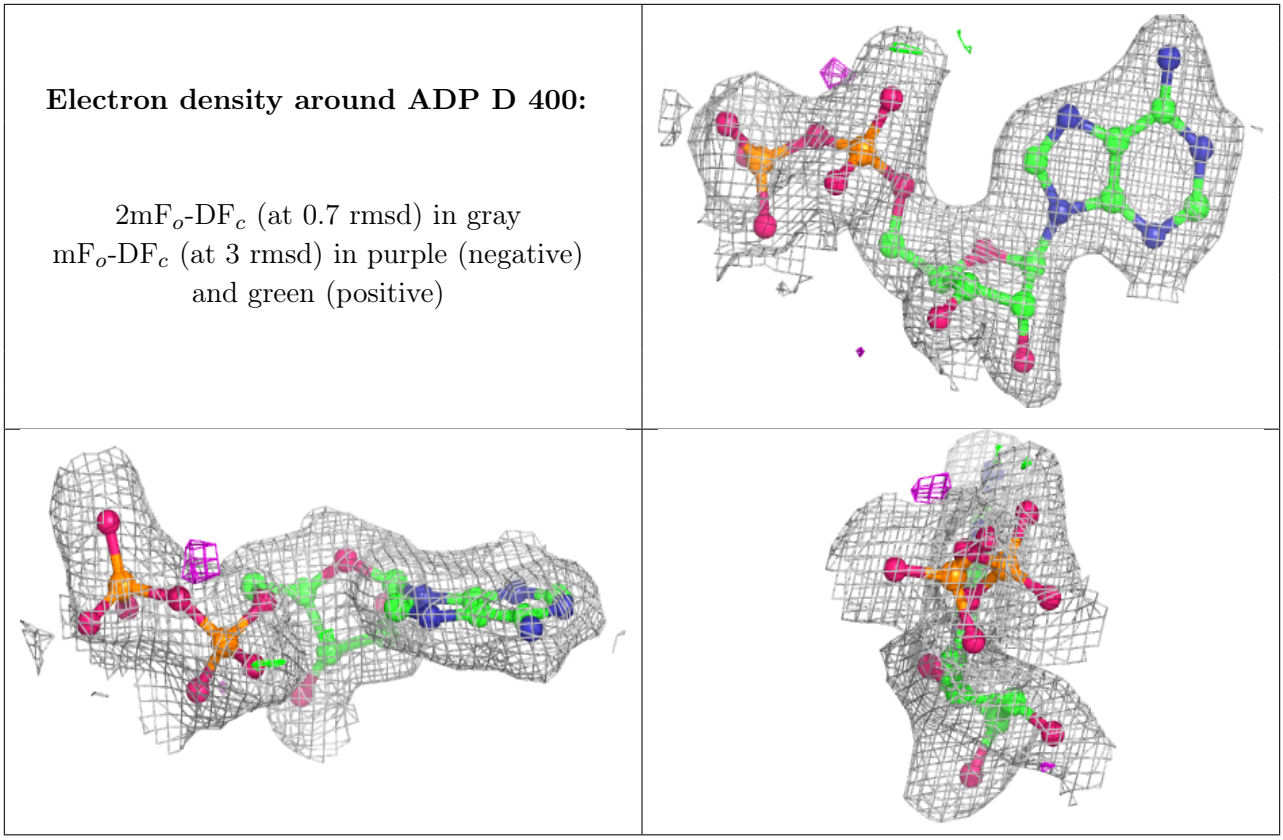






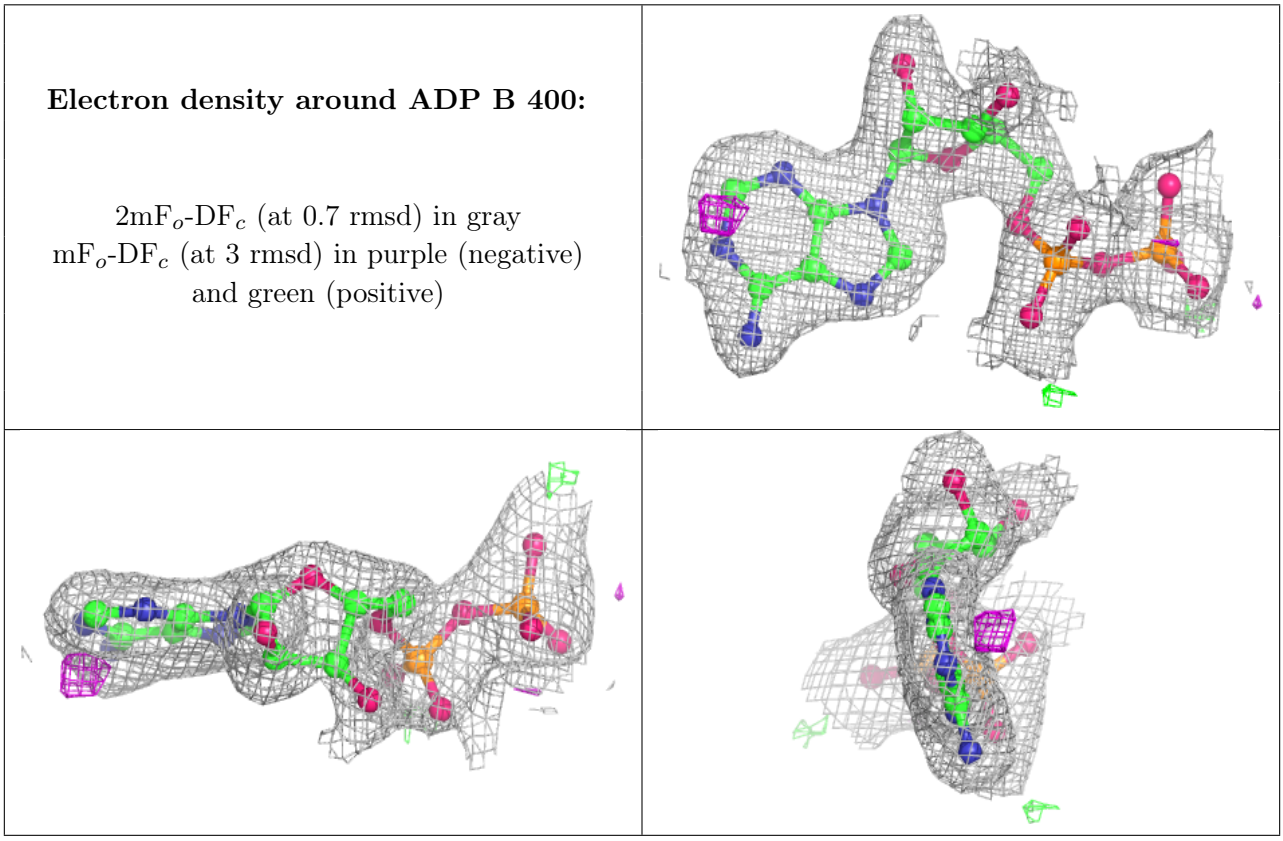
Electron density around ADP D 400:

$2mF_o$-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 400:

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



Electron density around AIR B 402:

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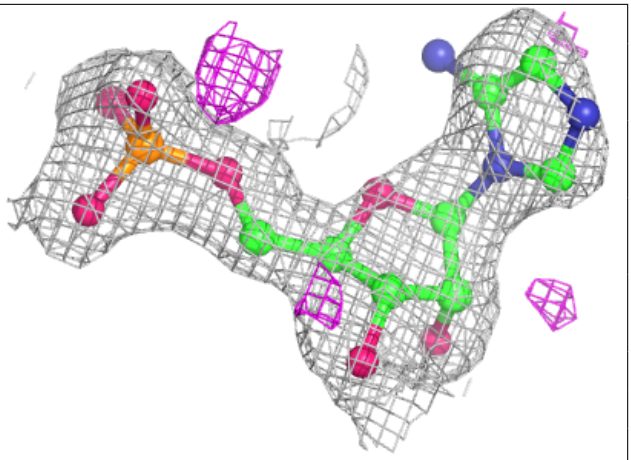
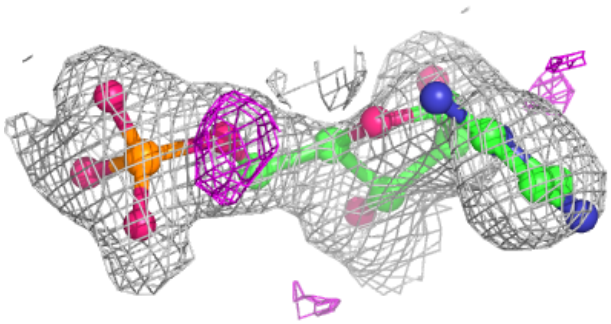
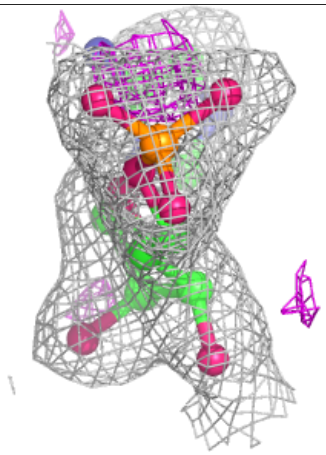
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around AIR A 402:

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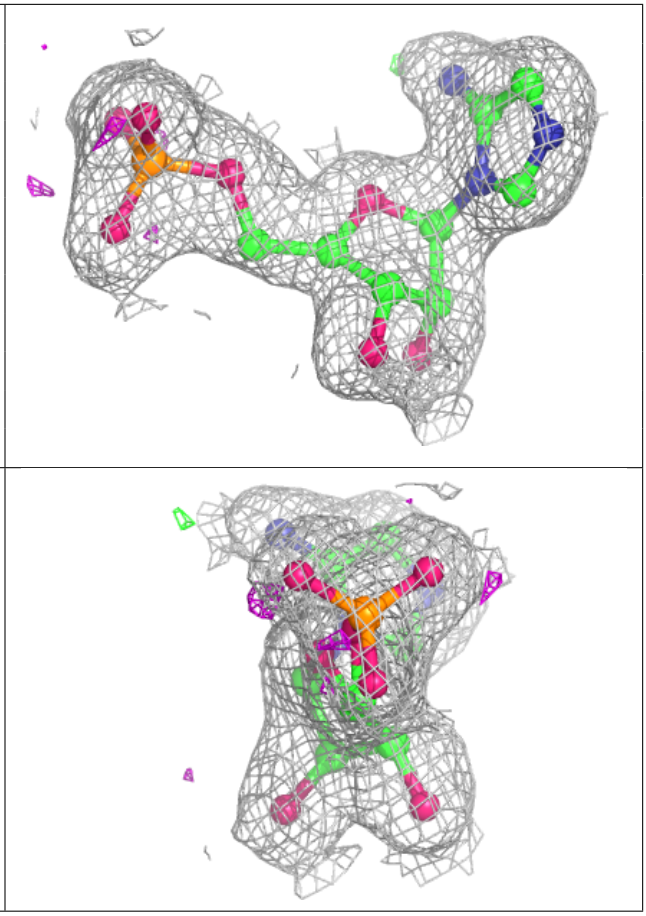
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AIR C 402:

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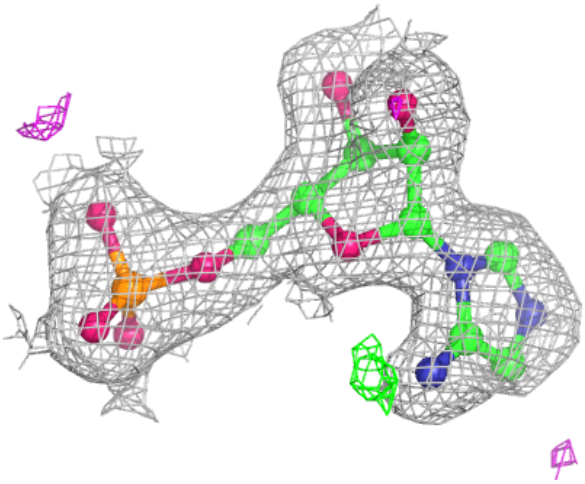
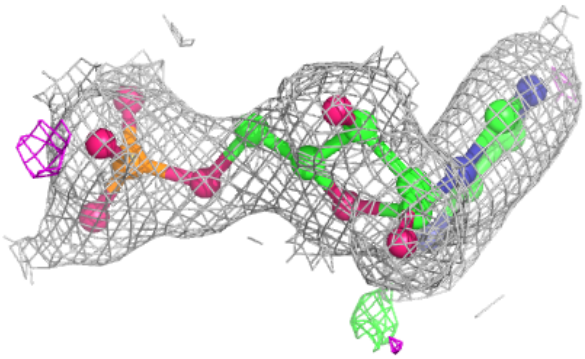
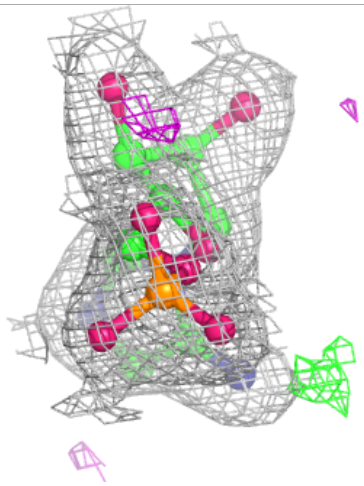
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

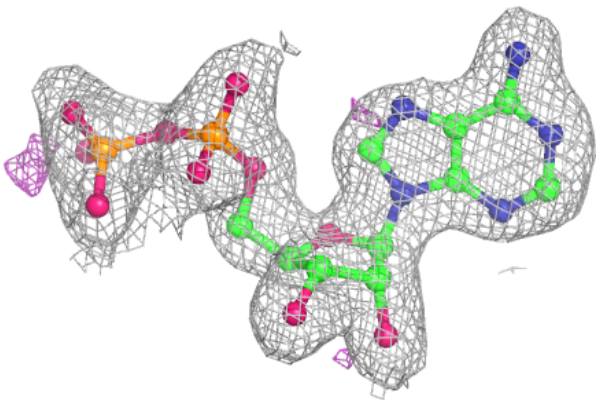


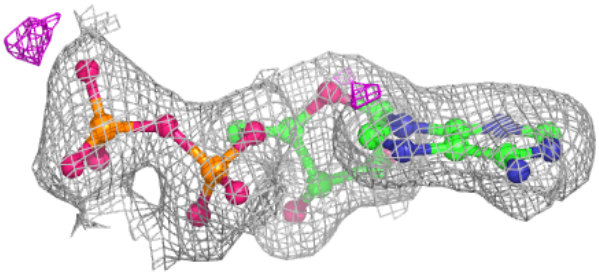


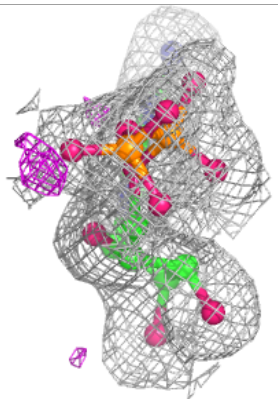


Electron density around ADP C 400:

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

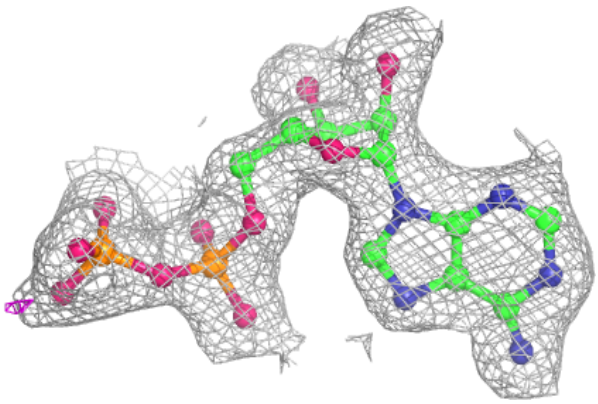


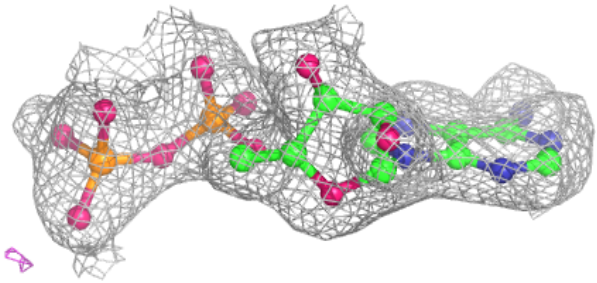


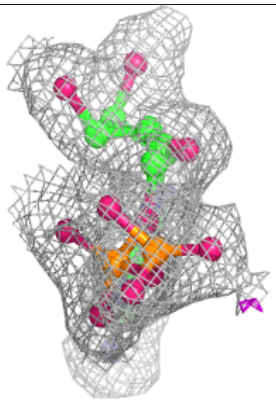


Electron density around ADP A 400:

$2mF_o$-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.