



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:34 PM UTC

PDB ID : 3K5I / pdb_00003k5i
Title : Crystal structure of N5-carboxyaminoimidazole synthase from aspergillus clavatus in complex with ADP and 5-aminoimidazole 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

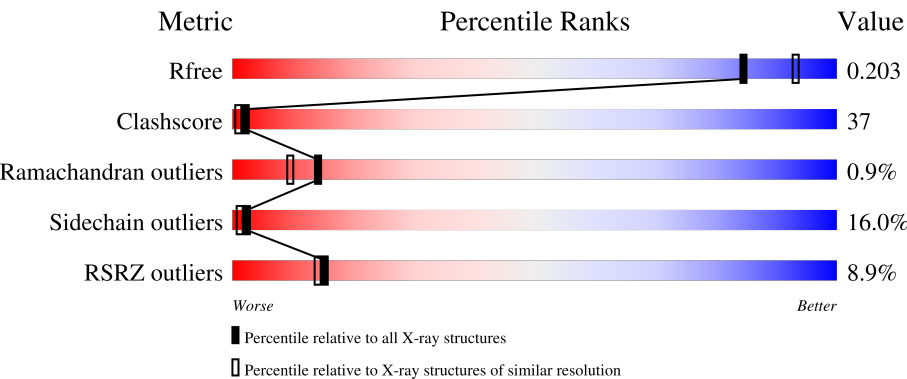
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	403	6% 38%40%14%• 5%
1	B	403	10% 29%39%20%5%7%
1	C	403	6% 35%40%17%• 5%
1	D	403	11% 27%41%20%• 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

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

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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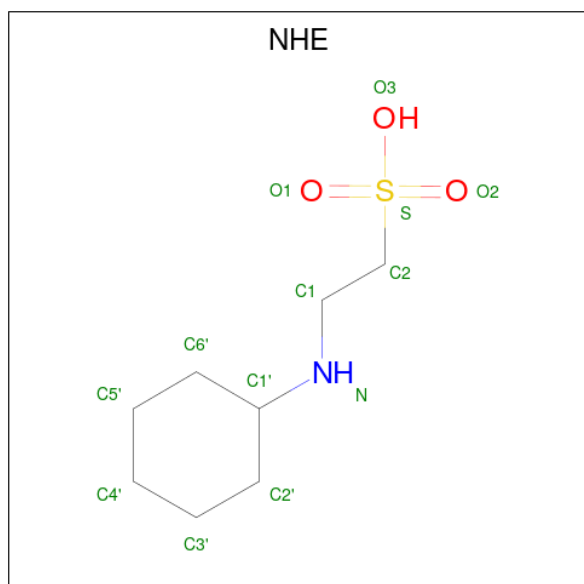
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A1CII2
D	-15	HIS	-	expression tag	UNP A1CII2
D	-14	HIS	-	expression tag	UNP A1CII2
D	-13	HIS	-	expression tag	UNP A1CII2
D	-12	HIS	-	expression tag	UNP A1CII2
D	-11	HIS	-	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 (CCD ID: NA) (formula: Na).

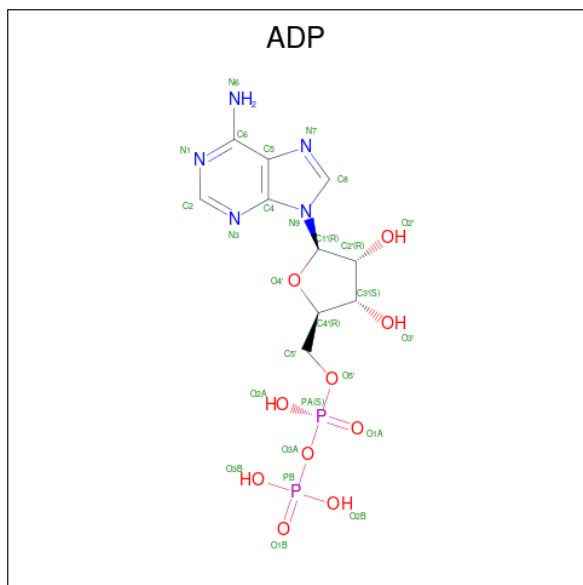
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).



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

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

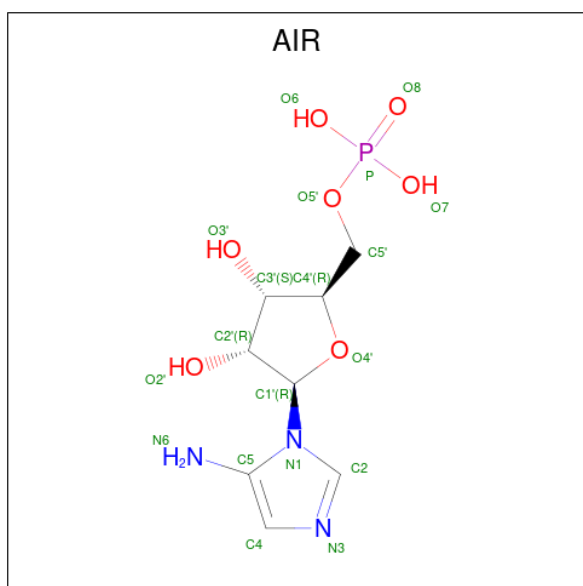


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

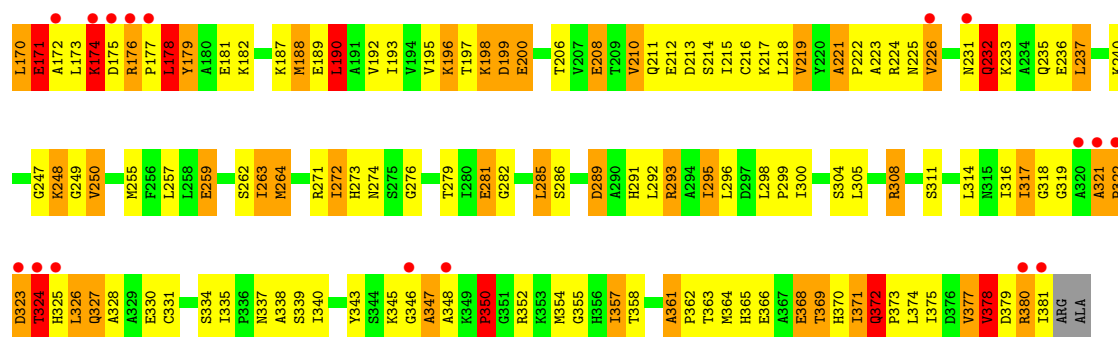
- Molecule 6 is 5-AMINOIMIDAZOLE RIBONUCLEOTIDE (CCD ID: AIR) (formula: $C_8H_{14}N_3O_7P$).



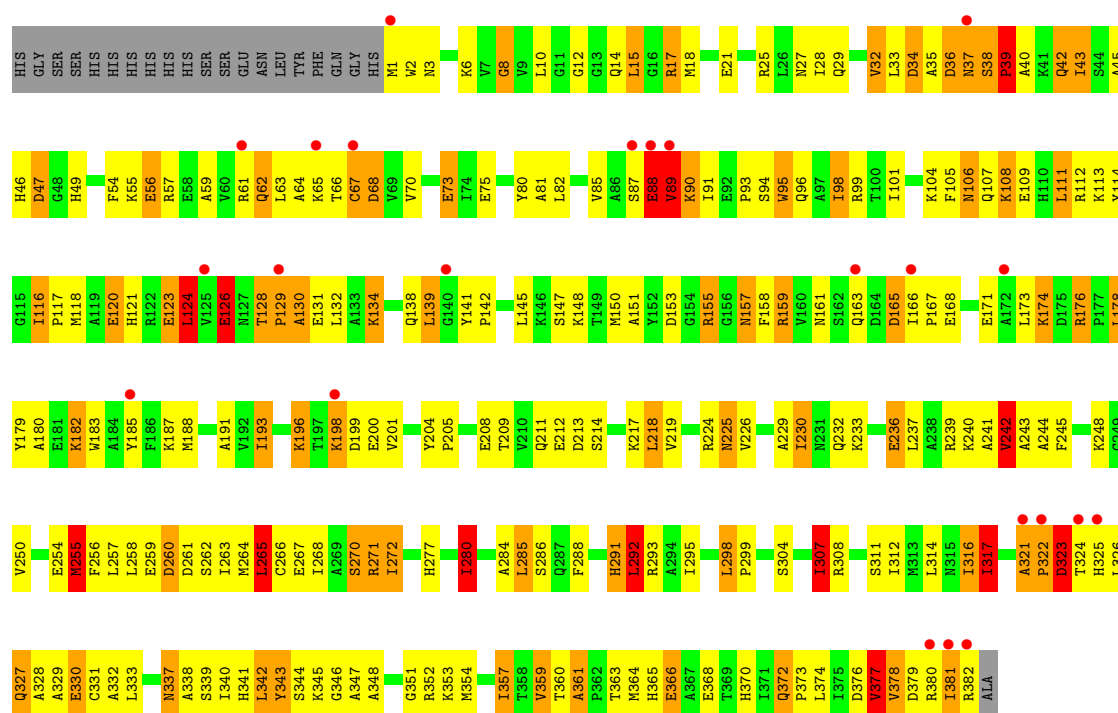
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			19	8	3	7	1		
6	B	1	Total	C	N	O	P	0	0
			19	8	3	7	1		
6	C	1	Total	C	N	O	P	0	0
			19	8	3	7	1		
6	D	1	Total	C	N	O	P	0	0
			19	8	3	7	1		

- Molecule 7 is water.

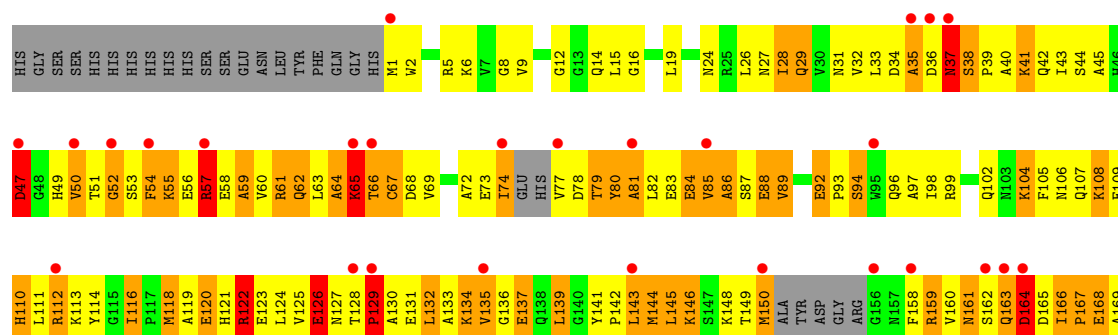
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	322	Total	O	0	0
			322	322		
7	B	266	Total	O	0	0
			266	266		
7	C	299	Total	O	0	0
			299	299		
7	D	243	Total	O	0	0
			243	243		

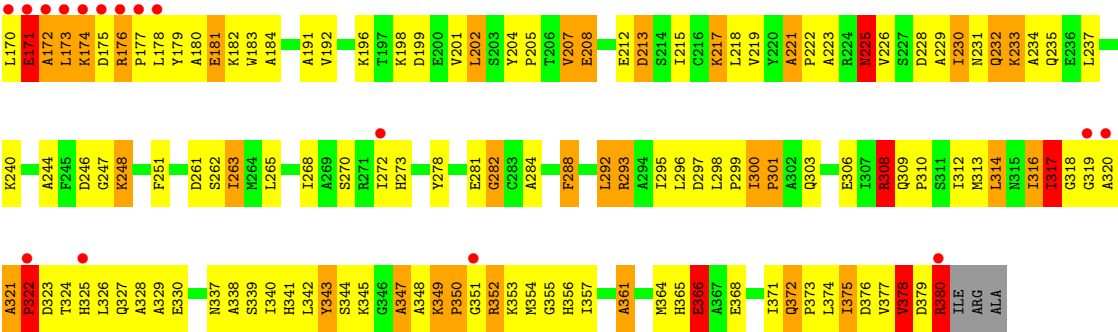


• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase



• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase





4 Data and refinement statistics

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 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.00) 91.9 (30.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.39 , 131.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.08	10/3049 (0.3%)	2.03	102/4128 (2.5%)
1	B	1.04	9/3019 (0.3%)	2.14	134/4086 (3.3%)
1	C	1.03	4/3072 (0.1%)	2.06	113/4157 (2.7%)
1	D	1.02	3/2941 (0.1%)	2.14	130/3980 (3.3%)
All	All	1.04	26/12081 (0.2%)	2.09	479/16351 (2.9%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	MET	SD-CE	-8.93	1.57	1.79
1	D	313	MET	SD-CE	8.22	2.00	1.79
1	A	23	ALA	CA-CB	8.07	1.66	1.53
1	A	60	VAL	CA-CB	7.52	1.62	1.54
1	A	1	MET	SD-CE	7.28	1.97	1.79
1	B	118	MET	SD-CE	-7.18	1.61	1.79
1	B	18	MET	SD-CE	7.12	1.97	1.79
1	B	103	ASN	C-O	-6.94	1.16	1.24
1	C	1	MET	SD-CE	6.82	1.96	1.79
1	C	18	MET	SD-CE	-6.38	1.63	1.79
1	C	307	ILE	CA-CB	6.31	1.61	1.54
1	A	144	MET	SD-CE	-6.18	1.64	1.79
1	C	43	ILE	CA-CB	6.11	1.62	1.54
1	D	166	ILE	CA-CB	6.10	1.57	1.54
1	A	18	MET	SD-CE	-5.89	1.64	1.79
1	D	221	ALA	CA-CB	5.77	1.60	1.53
1	B	101	ILE	C-O	-5.76	1.17	1.24
1	B	221	ALA	CA-CB	5.57	1.61	1.53
1	A	192	VAL	CA-CB	5.46	1.61	1.54
1	A	16	GLY	CA-C	-5.30	1.46	1.52
1	A	354	MET	SD-CE	5.19	1.92	1.79
1	A	312	ILE	CA-CB	5.16	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	ILE	CA-CB	5.14	1.59	1.54
1	B	264	MET	SD-CE	-5.06	1.67	1.79
1	B	291	HIS	CA-CB	-5.05	1.45	1.53
1	B	361	ALA	CA-CB	-5.02	1.45	1.53

All (479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	GLU	N-CA-C	-15.56	93.76	111.03
1	A	2	TRP	N-CA-C	-14.28	94.19	112.90
1	D	68	ASP	N-CA-C	13.32	125.89	111.36
1	B	161	ASN	N-CA-C	12.70	125.20	111.36
1	C	308	ARG	NE-CZ-NH1	-12.69	108.81	121.50
1	D	50	VAL	CB-CA-C	-11.79	93.11	110.33
1	D	112	ARG	N-CA-C	-11.78	98.17	112.54
1	D	317	ILE	CB-CA-C	-11.70	94.48	110.98
1	B	176	ARG	N-CA-C	11.55	124.50	109.83
1	B	32	VAL	CB-CA-C	-11.44	96.72	110.91
1	B	94	SER	N-CA-C	11.14	125.95	110.35
1	B	69	VAL	CB-CA-C	-11.00	93.09	110.69
1	B	59	ALA	N-CA-C	-10.88	99.11	110.97
1	B	343	TYR	N-CA-C	10.72	126.17	113.20
1	B	199	ASP	N-CA-C	10.15	125.79	113.41
1	B	80	TYR	N-CA-C	-9.93	99.47	111.69
1	B	126	GLU	N-CA-C	9.76	125.19	113.28
1	C	308	ARG	NE-CZ-NH2	9.52	127.77	119.20
1	C	130	ALA	N-CA-C	-9.50	100.62	110.97
1	D	129	PRO	N-CA-C	-9.42	100.78	113.40
1	C	317	ILE	N-CA-CB	-9.37	98.51	111.25
1	D	94	SER	N-CA-C	9.33	123.04	110.35
1	A	16	GLY	N-CA-C	-9.25	101.63	112.73
1	C	88	GLU	N-CA-C	9.21	121.32	111.28
1	A	345	LYS	N-CA-C	9.09	124.17	113.18
1	D	199	ASP	N-CA-C	9.02	124.98	112.45
1	A	57	ARG	NE-CZ-NH2	-9.00	111.10	119.20
1	D	161	ASN	N-CA-C	8.96	121.04	111.28
1	C	68	ASP	N-CA-C	-8.82	101.35	112.90
1	D	120	GLU	N-CA-C	-8.81	98.90	110.53
1	B	178	LEU	N-CA-C	8.76	121.20	108.86
1	B	164	ASP	N-CA-C	8.66	123.60	112.34
1	D	347	ALA	N-CA-C	8.62	123.47	109.76
1	D	317	ILE	N-CA-C	8.57	121.48	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LEU	CA-C-O	-8.52	111.45	120.40
1	D	135	VAL	CB-CA-C	-8.48	101.02	111.88
1	A	94	SER	N-CA-C	8.48	122.52	110.23
1	D	40	ALA	N-CA-C	8.37	121.53	111.82
1	C	116	ILE	CB-CA-C	-8.31	96.23	111.36
1	B	60	VAL	N-CA-C	8.23	119.00	110.36
1	B	249	GLY	CA-C-O	-8.23	115.67	122.33
1	C	67	CYS	CA-CB-SG	-8.19	95.56	114.40
1	B	60	VAL	CB-CA-C	-8.18	101.41	111.88
1	B	139	LEU	N-CA-C	8.18	122.54	112.23
1	B	77	VAL	CB-CA-C	-8.15	97.83	110.95
1	D	374	LEU	N-CA-C	-8.13	102.39	111.82
1	A	288	PHE	CA-C-O	-8.12	112.33	120.70
1	A	375	ILE	N-CA-C	-8.11	102.53	110.72
1	B	340	ILE	N-CA-C	8.05	119.52	108.89
1	D	29	GLN	N-CA-C	8.03	121.54	109.25
1	C	114	TYR	N-CA-C	-8.03	101.97	112.41
1	D	57	ARG	N-CA-C	7.93	120.70	111.02
1	D	320	ALA	N-CA-C	7.90	119.80	111.03
1	A	76	HIS	N-CA-CB	-7.88	100.52	110.45
1	C	377	VAL	CB-CA-C	-7.80	101.61	112.14
1	D	97	ALA	N-CA-C	-7.79	102.73	111.07
1	D	45	ALA	N-CA-C	7.76	121.73	109.39
1	D	183	TRP	N-CA-C	7.76	121.48	110.23
1	A	232	GLN	N-CA-C	7.72	119.47	111.14
1	A	357	ILE	CB-CA-C	-7.63	98.75	110.50
1	D	215	ILE	CB-CA-C	-7.62	98.77	110.50
1	C	42	GLN	N-CA-C	7.61	121.66	112.38
1	A	20	VAL	CA-C-N	-7.58	110.30	120.54
1	A	20	VAL	C-N-CA	-7.58	110.30	120.54
1	C	32	VAL	CB-CA-C	-7.57	99.34	110.62
1	C	372	GLN	CA-C-O	7.50	125.49	118.44
1	A	284	ALA	CA-C-O	-7.49	112.48	120.42
1	A	263	ILE	N-CA-C	7.48	120.37	108.85
1	C	151	ALA	N-CA-C	7.47	120.69	108.52
1	C	366	GLU	N-CA-CB	-7.46	99.20	110.01
1	C	47[A]	ASP	N-CA-C	7.45	121.68	112.59
1	C	47[B]	ASP	N-CA-C	7.45	121.68	112.59
1	B	112	ARG	N-CA-C	-7.42	102.89	112.23
1	D	171	GLU	N-CA-C	-7.37	95.09	110.80
1	D	116	ILE	N-CA-C	-7.32	102.33	108.63
1	C	361	ALA	N-CA-C	-7.31	101.55	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	LYS	N-CA-C	-7.31	103.83	112.89
1	D	164	ASP	N-CA-C	7.27	121.25	112.38
1	C	38	SER	N-CA-C	-7.26	99.48	110.01
1	B	146	LYS	N-CA-C	7.26	121.37	109.24
1	B	97	ALA	N-CA-C	-7.25	103.31	111.07
1	D	340	ILE	N-CA-C	7.22	118.98	108.58
1	C	21	GLU	N-CA-C	-7.19	103.44	111.28
1	B	272	ILE	N-CA-C	-7.18	99.28	109.63
1	B	345	LYS	N-CA-C	-7.18	104.50	113.18
1	B	208	GLU	CA-C-N	-7.17	111.55	122.81
1	B	208	GLU	C-N-CA	-7.17	111.55	122.81
1	B	257	LEU	N-CA-C	-7.14	97.09	108.73
1	A	55	LYS	N-CA-C	-7.14	104.58	112.72
1	D	273	HIS	N-CA-CB	-7.13	98.39	111.37
1	C	90	LYS	N-CA-C	-7.09	99.00	110.20
1	C	307	ILE	CG1-CB-CG2	-7.07	89.51	110.70
1	B	370	HIS	CB-CA-C	-7.05	99.08	110.79
1	D	32	VAL	N-CA-C	7.00	118.91	108.54
1	A	32	VAL	N-CA-C	7.00	119.14	108.71
1	A	47[A]	ASP	N-CA-C	7.00	121.53	112.92
1	A	47[B]	ASP	N-CA-C	7.00	121.53	112.92
1	D	230	ILE	N-CA-C	-6.99	103.96	110.53
1	B	120[A]	GLU	CA-C-N	-6.97	111.02	122.11
1	B	120[A]	GLU	C-N-CA	-6.97	111.02	122.11
1	B	120[B]	GLU	CA-C-N	-6.97	111.02	122.11
1	B	120[B]	GLU	C-N-CA	-6.97	111.02	122.11
1	A	81	ALA	N-CA-C	-6.97	103.69	111.28
1	D	173	LEU	CB-CA-C	-6.96	101.40	111.70
1	B	85	VAL	N-CA-C	6.96	120.80	112.80
1	D	328	ALA	N-CA-C	-6.95	103.64	111.07
1	D	232	GLN	CA-CB-CG	-6.92	100.27	114.10
1	B	28	ILE	N-CA-C	-6.90	98.50	108.36
1	D	343	TYR	N-CA-C	6.88	121.52	113.20
1	B	377	VAL	CB-CA-C	-6.87	103.09	111.88
1	B	378	VAL	N-CA-C	-6.86	103.62	110.62
1	A	266	CYS	N-CA-C	-6.86	104.91	113.55
1	D	263	ILE	CG1-CB-CG2	-6.85	90.14	110.70
1	D	176	ARG	N-CA-C	6.83	119.28	110.39
1	C	372	GLN	N-CA-C	6.83	122.78	113.77
1	C	323	ASP	N-CA-C	-6.81	104.51	114.39
1	C	286	SER	CA-CB-OG	-6.79	97.53	111.10
1	D	322	PRO	N-CA-C	6.78	126.44	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	GLN	N-CA-C	-6.78	103.03	112.45
1	B	189	GLU	CA-C-N	-6.77	111.95	122.59
1	B	189	GLU	C-N-CA	-6.77	111.95	122.59
1	D	281	GLU	N-CA-C	-6.77	104.03	112.90
1	C	292	LEU	N-CA-CB	-6.76	100.21	110.01
1	C	354	MET	N-CA-CB	-6.75	100.47	110.53
1	C	201	VAL	N-CA-C	-6.74	98.76	108.53
1	A	317	ILE	N-CA-CB	-6.73	100.09	110.86
1	C	155	ARG	NE-CZ-NH2	6.70	125.23	119.20
1	A	248	LYS	N-CA-C	-6.70	99.30	109.95
1	B	273	HIS	N-CA-CB	-6.70	99.08	111.53
1	C	124	LEU	N-CA-C	-6.70	98.33	109.24
1	D	349	LYS	N-CA-C	-6.69	93.62	107.95
1	A	126	GLU	N-CA-C	-6.67	99.21	109.14
1	A	272	ILE	N-CA-C	-6.66	100.04	109.63
1	D	319	GLY	N-CA-C	-6.64	102.98	112.55
1	B	347	ALA	N-CA-C	6.64	124.94	110.80
1	A	59	ALA	N-CA-C	-6.63	103.31	111.40
1	B	354	MET	N-CA-C	6.63	121.45	113.23
1	D	372	GLN	CA-C-O	6.61	124.65	118.44
1	D	293	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	B	149	THR	N-CA-C	6.61	129.50	111.00
1	B	368	GLU	N-CA-C	-6.60	104.17	111.36
1	D	66	THR	N-CA-C	6.57	121.45	113.17
1	B	128	THR	CB-CA-C	-6.54	98.59	108.61
1	B	328	ALA	N-CA-C	-6.54	103.84	110.97
1	C	62	GLN	CB-CA-C	-6.52	99.97	110.79
1	D	377	VAL	CA-C-N	-6.50	112.24	120.56
1	D	377	VAL	C-N-CA	-6.50	112.24	120.56
1	C	104	LYS	N-CA-C	6.48	120.05	111.75
1	B	40	ALA	N-CA-C	6.48	118.42	111.36
1	B	314	LEU	CA-C-O	6.48	127.23	120.30
1	B	248	LYS	CG-CD-CE	-6.47	96.41	111.30
1	C	255	MET	N-CA-CB	-6.47	101.14	111.62
1	A	62	GLN	N-CA-C	-6.46	103.93	110.97
1	D	316	ILE	CB-CA-C	-6.46	103.14	111.53
1	C	91	ILE	N-CA-C	-6.45	98.17	107.78
1	C	129	PRO	N-CA-C	-6.45	104.57	113.53
1	A	180	ALA	CA-C-N	-6.45	113.27	122.94
1	A	180	ALA	C-N-CA	-6.45	113.27	122.94
1	A	343	TYR	N-CA-C	6.39	120.93	113.20
1	C	242	VAL	CB-CA-C	-6.38	103.52	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	GLN	CA-C-N	-6.38	112.14	120.44
1	B	232	GLN	C-N-CA	-6.38	112.14	120.44
1	A	117	PRO	N-CA-C	-6.37	101.18	111.19
1	C	43	ILE	CB-CA-C	-6.37	100.85	111.29
1	D	37	ASN	CB-CA-C	6.36	120.39	111.86
1	B	1	MET	CB-CA-C	6.36	122.18	110.10
1	B	263	ILE	N-CA-C	6.35	117.44	108.36
1	A	253	VAL	N-CA-C	6.35	117.00	107.80
1	B	8	GLY	N-CA-C	-6.34	99.43	110.71
1	D	116	ILE	CB-CA-C	-6.33	105.06	110.94
1	B	217	LYS	CB-CA-C	-6.31	100.17	110.08
1	B	335	ILE	CB-CA-C	-6.31	105.08	110.94
1	C	343	TYR	N-CA-C	6.30	120.97	113.28
1	C	225	ASN	CB-CA-C	-6.30	102.94	111.89
1	D	338	ALA	CA-C-N	-6.30	114.39	122.77
1	D	338	ALA	C-N-CA	-6.30	114.39	122.77
1	C	120	GLU	N-CA-C	-6.29	101.62	110.50
1	B	219	VAL	CB-CA-C	-6.28	100.36	110.28
1	B	350	PRO	N-CA-C	6.28	120.36	110.50
1	C	217	LYS	N-CA-C	-6.27	104.69	112.72
1	C	381	ILE	CB-CA-C	-6.27	103.67	112.14
1	A	337	ASN	N-CA-C	6.26	120.50	112.86
1	C	256	PHE	CB-CA-C	-6.24	97.45	109.37
1	C	316	ILE	N-CA-C	-6.23	97.37	107.28
1	D	110	HIS	N-CA-C	6.22	117.73	111.07
1	B	190	LEU	N-CA-C	6.22	119.16	109.52
1	D	321	ALA	CA-C-N	6.22	127.61	119.84
1	D	321	ALA	C-N-CA	6.22	127.61	119.84
1	C	321	ALA	N-CA-C	6.21	117.88	109.24
1	D	375	ILE	CB-CA-C	-6.20	103.66	112.22
1	A	302	ALA	CA-C-O	6.18	127.09	120.10
1	A	152	TYR	N-CA-C	-6.17	99.35	108.79
1	B	317	ILE	N-CA-C	6.17	117.18	108.36
1	C	43	ILE	CG1-CB-CG2	-6.17	92.20	110.70
1	D	355	GLY	N-CA-C	-6.16	101.54	111.59
1	D	163	GLN	N-CA-C	6.16	123.92	110.80
1	D	323	ASP	N-CA-CB	-6.16	101.35	110.53
1	C	176	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	D	122	ARG	N-CA-C	-6.13	97.44	108.48
1	B	50	VAL	CB-CA-C	-6.13	101.49	110.62
1	A	309	GLN	CB-CA-C	-6.13	102.13	110.22
1	A	101	ILE	N-CA-C	6.12	117.60	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	MET	N-CA-CB	-6.12	101.65	110.65
1	C	225	ASN	N-CA-C	6.12	119.83	111.39
1	C	342	LEU	N-CA-C	-6.11	99.74	109.76
1	B	44	SER	CB-CA-C	-6.10	103.71	111.70
1	D	8	GLY	N-CA-C	-6.10	100.34	110.95
1	C	292	LEU	CB-CA-C	-6.09	101.32	110.88
1	C	8	GLY	CA-C-N	-6.08	115.21	123.12
1	C	8	GLY	C-N-CA	-6.08	115.21	123.12
1	C	280	ILE	CB-CA-C	-6.07	103.84	112.22
1	B	371	ILE	N-CA-C	6.07	120.94	112.50
1	C	321	ALA	CA-C-O	6.07	123.81	119.32
1	A	193	ILE	CB-CA-C	-6.06	103.55	111.25
1	D	234	ALA	N-CA-C	-6.05	104.77	111.36
1	B	193	ILE	CB-CG1-CD1	6.03	126.46	113.80
1	B	321	ALA	C-N-CD	-6.02	100.32	125.00
1	D	47	ASP	N-CA-C	6.01	120.22	113.01
1	D	118	MET	CB-CA-C	-6.00	99.40	111.17
1	A	225	ASN	CB-CA-C	-5.99	103.83	111.86
1	A	60	VAL	CA-CB-CG2	5.99	120.58	110.40
1	B	125	VAL	N-CA-C	-5.99	105.23	111.58
1	A	282	GLY	N-CA-C	5.98	122.08	114.66
1	D	225	ASN	N-CA-C	5.97	119.43	111.30
1	B	248	LYS	N-CA-CB	-5.97	101.80	110.70
1	D	268	ILE	CA-C-N	5.97	131.42	123.00
1	D	268	ILE	C-N-CA	5.97	131.42	123.00
1	D	207	VAL	CA-C-N	-5.96	114.58	122.99
1	D	207	VAL	C-N-CA	-5.96	114.58	122.99
1	A	271	ARG	CB-CA-C	-5.95	100.01	111.78
1	C	123	GLU	N-CA-CB	-5.95	101.61	110.17
1	C	299	PRO	CB-CA-C	-5.93	103.20	110.98
1	D	181	GLU	CB-CG-CD	-5.91	102.56	112.60
1	D	28	ILE	N-CA-C	-5.91	99.91	108.71
1	B	170	LEU	N-CA-C	5.86	118.90	111.69
1	A	177	PRO	N-CA-C	-5.85	101.02	110.55
1	D	80	TYR	CA-CB-CG	-5.83	103.40	113.90
1	A	155	ARG	N-CA-C	5.83	119.49	112.38
1	C	45	ALA	N-CA-C	5.83	119.19	108.58
1	B	108	LYS	CD-CE-NZ	5.83	130.55	111.90
1	A	327[A]	GLN	CB-CA-C	5.83	120.46	110.79
1	A	327[B]	GLN	CB-CA-C	5.83	120.46	110.79
1	A	271	ARG	CA-C-N	5.82	128.30	120.50
1	A	271	ARG	C-N-CA	5.82	128.30	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	ALA	N-CA-C	-5.82	100.56	109.64
1	A	74	ILE	O-C-N	-5.82	116.48	122.82
1	B	369	THR	N-CA-CB	5.82	118.45	110.01
1	C	54	PHE	N-CA-C	-5.82	106.03	113.01
1	A	324	THR	CA-C-N	-5.81	111.90	120.38
1	A	324	THR	C-N-CA	-5.81	111.90	120.38
1	C	159	ARG	CB-CA-C	-5.81	101.54	110.26
1	B	295	ILE	N-CA-C	5.81	118.31	111.05
1	D	350	PRO	CB-CA-C	5.81	118.96	111.64
1	D	139	LEU	N-CA-C	5.80	119.55	112.23
1	B	103	ASN	CA-C-N	5.80	128.63	120.28
1	B	103	ASN	C-N-CA	5.80	128.63	120.28
1	B	199	ASP	N-CA-CB	-5.80	102.00	110.47
1	B	338	ALA	N-CA-C	5.80	118.11	108.20
1	A	335	ILE	CA-C-N	-5.79	114.00	119.85
1	A	335	ILE	C-N-CA	-5.79	114.00	119.85
1	C	204	TYR	N-CA-C	-5.79	102.81	110.40
1	C	225	ASN	O-C-N	5.79	129.73	122.55
1	B	214	SER	N-CA-C	5.79	121.61	113.56
1	B	97	ALA	O-C-N	-5.79	116.11	122.07
1	C	327	GLN	N-CA-C	-5.78	104.58	111.69
1	D	374	LEU	CB-CG-CD2	-5.78	93.35	110.70
1	C	95	TRP	N-CA-C	-5.78	105.49	112.54
1	A	17	ARG	N-CA-C	5.77	117.65	111.36
1	D	380	ARG	N-CA-C	5.77	127.16	111.00
1	B	210	VAL	N-CA-C	5.76	116.30	107.77
1	A	377	VAL	CB-CA-C	-5.76	104.27	112.22
1	A	372	GLN	N-CA-C	5.75	122.53	109.81
1	A	18	MET	CA-CB-CG	-5.75	102.59	114.10
1	C	126	GLU	N-CA-C	-5.74	99.98	108.99
1	B	179	TYR	N-CA-C	-5.72	99.72	108.76
1	B	199	ASP	CB-CA-C	-5.71	99.24	109.24
1	D	136	GLY	N-CA-C	-5.71	105.67	113.27
1	C	17	ARG	N-CA-CB	-5.70	101.75	110.12
1	A	299	PRO	CB-CA-C	-5.69	103.94	111.23
1	D	292	LEU	N-CA-C	5.69	117.94	111.11
1	B	236	GLU	CA-CB-CG	-5.68	102.75	114.10
1	C	341	HIS	CB-CA-C	-5.67	102.05	110.62
1	B	346	GLY	CA-C-N	5.67	132.37	121.54
1	B	346	GLY	C-N-CA	5.67	132.37	121.54
1	C	291	HIS	CA-C-O	5.67	126.56	120.55
1	B	355	GLY	N-CA-C	-5.66	103.16	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	A	84	GLU	CB-CA-C	-5.66	101.39	110.79
1	A	112	ARG	CA-C-N	5.66	131.04	121.14
1	A	112	ARG	C-N-CA	5.66	131.04	121.14
1	D	24	ASN	N-CA-C	-5.65	105.21	111.36
1	B	208	GLU	O-C-N	-5.63	116.90	123.27
1	D	88	GLU	N-CA-C	5.63	120.88	112.94
1	D	180	ALA	CA-C-N	-5.62	114.78	122.93
1	D	180	ALA	C-N-CA	-5.62	114.78	122.93
1	A	367	ALA	N-CA-C	-5.62	105.23	111.36
1	A	26	LEU	CB-CG-CD1	-5.62	93.85	110.70
1	C	123	GLU	N-CA-C	-5.61	102.59	110.50
1	A	166	ILE	N-CA-C	5.61	121.00	108.88
1	D	36	ASP	N-CA-C	5.60	119.05	110.20
1	C	307	ILE	CA-C-N	5.60	128.05	120.44
1	C	307	ILE	C-N-CA	5.60	128.05	120.44
1	B	107	GLN	N-CA-C	-5.59	104.40	111.11
1	C	80	TYR	N-CA-C	-5.59	104.81	111.69
1	D	72	ALA	N-CA-C	5.59	118.59	109.59
1	B	327	GLN	CA-C-O	5.59	126.34	120.42
1	C	153	ASP	N-CA-C	5.59	119.14	111.54
1	A	66	THR	CA-C-N	-5.59	111.96	121.85
1	A	66	THR	C-N-CA	-5.59	111.96	121.85
1	B	226	VAL	N-CA-C	-5.57	99.53	107.77
1	C	337	ASN	N-CA-C	5.57	119.90	113.38
1	C	174	LYS	N-CA-C	5.55	117.46	110.24
1	D	79	THR	N-CA-C	-5.55	106.48	113.20
1	C	196	LYS	CB-CA-C	-5.55	100.59	109.75
1	B	131	GLU	N-CA-C	-5.55	105.15	111.14
1	A	32	VAL	CB-CA-C	-5.55	103.16	110.98
1	D	306	GLU	N-CA-CB	-5.55	102.43	110.36
1	B	68	ASP	N-CA-C	-5.55	105.30	112.68
1	A	10	LEU	CD1-CG-CD2	5.54	123.00	110.80
1	C	165	ASP	CB-CA-C	-5.54	99.88	110.57
1	B	23	ALA	N-CA-CB	5.54	118.83	110.30
1	C	111	LEU	N-CA-C	-5.54	106.66	113.41
1	B	162	SER	CB-CA-C	-5.53	100.52	111.91
1	C	265	LEU	CA-CB-CG	-5.52	96.99	116.30
1	D	345	LYS	CA-C-N	-5.52	116.12	121.31
1	D	345	LYS	C-N-CA	-5.52	116.12	121.31
1	D	301	PRO	CB-CA-C	5.51	118.59	111.64
1	D	67	CYS	CA-C-N	5.51	128.11	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	CYS	C-N-CA	5.51	128.11	120.29
1	A	357	ILE	CA-C-N	-5.50	115.24	122.99
1	A	357	ILE	C-N-CA	-5.50	115.24	122.99
1	D	233	LYS	CA-CB-CG	5.50	125.09	114.10
1	C	63	LEU	N-CA-C	-5.49	105.37	111.36
1	B	72	ALA	N-CA-C	5.49	118.17	109.50
1	B	6	LYS	N-CA-C	5.48	118.56	109.46
1	D	28	ILE	CB-CA-C	-5.48	103.25	110.98
1	B	368	GLU	CA-C-N	-5.48	113.32	120.44
1	B	368	GLU	C-N-CA	-5.48	113.32	120.44
1	A	334	SER	CB-CA-C	-5.48	100.94	110.09
1	A	235	GLN	N-CA-C	5.47	117.25	111.28
1	D	282	GLY	N-CA-C	5.47	118.85	112.50
1	A	213	ASP	N-CA-C	-5.47	104.35	111.74
1	D	366	GLU	CG-CD-OE2	-5.46	105.83	118.40
1	B	5	ARG	CB-CG-CD	-5.45	98.78	111.30
1	D	378	VAL	N-CA-C	-5.44	105.41	110.53
1	A	277	HIS	N-CA-C	5.44	117.97	111.71
1	A	113	LYS	CB-CA-C	-5.44	98.62	109.99
1	A	218	LEU	CB-CA-C	-5.44	98.64	109.79
1	D	84	GLU	N-CA-C	5.44	117.63	111.11
1	D	199	ASP	N-CA-CB	-5.44	102.16	110.26
1	A	57	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	B	64	ALA	O-C-N	5.43	128.95	122.27
1	C	157	ASN	CB-CA-C	-5.43	100.22	109.51
1	C	271	ARG	CA-C-N	5.43	127.89	120.35
1	C	271	ARG	C-N-CA	5.43	127.89	120.35
1	D	126	GLU	CA-C-N	-5.42	115.17	123.47
1	D	126	GLU	C-N-CA	-5.42	115.17	123.47
1	D	300	ILE	CA-C-N	-5.42	113.97	119.83
1	D	300	ILE	C-N-CA	-5.42	113.97	119.83
1	B	281	GLU	N-CA-C	-5.42	106.84	113.50
1	B	358	THR	OG1-CB-CG2	5.42	120.13	109.30
1	A	188	MET	N-CA-CB	5.41	120.66	111.57
1	A	187	LYS	N-CA-C	-5.40	106.53	113.23
1	A	306	GLU	N-CA-C	-5.40	101.73	110.32
1	B	314	LEU	CA-C-N	-5.40	112.46	120.94
1	B	314	LEU	C-N-CA	-5.40	112.46	120.94
1	B	61	ARG	CA-C-N	5.39	127.78	120.44
1	B	61	ARG	C-N-CA	5.39	127.78	120.44
1	C	200	GLU	CA-C-N	-5.39	116.15	123.10
1	C	200	GLU	C-N-CA	-5.39	116.15	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	ASN	N-CA-C	5.38	119.05	111.52
1	D	235	GLN	N-CA-C	5.38	116.82	111.07
1	B	5	ARG	CA-C-N	-5.38	114.61	122.19
1	B	5	ARG	C-N-CA	-5.38	114.61	122.19
1	B	289	ASP	CB-CA-C	-5.38	101.87	110.79
1	C	178	LEU	CB-CA-C	-5.37	99.24	109.66
1	C	218	LEU	O-C-N	5.37	129.67	123.17
1	D	329	ALA	N-CA-C	5.37	117.21	111.36
1	D	165	ASP	N-CA-C	-5.36	106.69	113.18
1	C	182	LYS	N-CA-C	-5.36	102.35	110.28
1	A	18	MET	N-CA-C	-5.35	105.61	111.82
1	D	217	LYS	N-CA-C	-5.35	105.88	112.72
1	A	179	TYR	N-CA-C	-5.34	100.61	108.79
1	D	288	PHE	CA-CB-CG	-5.34	108.46	113.80
1	C	89	VAL	CB-CA-C	5.31	118.62	110.55
1	C	106	ASN	N-CA-C	-5.31	105.58	111.36
1	B	47	ASP	N-CA-C	5.30	119.85	113.17
1	A	321	ALA	CA-C-N	-5.29	114.49	120.89
1	A	321	ALA	C-N-CA	-5.29	114.49	120.89
1	D	62	GLN	CA-C-O	5.29	126.55	121.00
1	D	361	ALA	N-CA-C	5.28	112.88	108.13
1	B	352	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	B	126	GLU	CA-C-N	-5.26	114.34	122.08
1	B	126	GLU	C-N-CA	-5.26	114.34	122.08
1	C	36	ASP	CA-C-N	-5.26	115.52	124.31
1	C	36	ASP	C-N-CA	-5.26	115.52	124.31
1	B	368	GLU	CB-CG-CD	-5.26	103.66	112.60
1	B	248	LYS	CD-CE-NZ	-5.25	95.09	111.90
1	D	107	GLN	N-CA-C	-5.25	104.81	111.11
1	D	52	GLY	N-CA-C	5.25	118.20	110.80
1	A	330	GLU	CG-CD-OE1	-5.24	106.34	118.40
1	B	372	GLN	N-CA-C	5.24	121.39	109.81
1	C	272	ILE	CB-CA-C	5.23	118.77	111.08
1	D	184	ALA	CA-C-O	-5.23	114.86	120.46
1	D	371	ILE	N-CA-C	5.23	118.45	111.44
1	B	109	GLU	CA-C-N	-5.23	113.27	120.28
1	B	109	GLU	C-N-CA	-5.23	113.27	120.28
1	D	65	LYS	N-CA-CB	-5.23	101.43	110.32
1	A	3	ASN	N-CA-C	5.22	119.20	112.41
1	A	197	THR	N-CA-CB	5.22	118.88	111.05
1	D	64	ALA	CA-C-O	5.22	126.09	120.55
1	A	233	LYS	N-CA-C	-5.22	105.59	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	HIS	CB-CA-C	-5.21	101.99	110.85
1	B	55	LYS	CB-CA-C	5.19	118.11	109.38
1	A	201	VAL	N-CA-CB	5.19	118.74	112.10
1	D	192	VAL	N-CA-CB	5.18	119.95	111.45
1	C	128	THR	CA-C-O	5.18	126.01	120.05
1	D	92	GLU	N-CA-C	5.18	118.55	109.48
1	A	309	GLN	N-CA-C	-5.18	103.56	108.22
1	B	324	THR	CA-C-N	-5.18	112.82	120.28
1	B	324	THR	C-N-CA	-5.18	112.82	120.28
1	D	32	VAL	N-CA-CB	-5.18	105.15	110.95
1	C	193	ILE	CB-CA-C	-5.17	103.89	110.98
1	B	67	CYS	CA-CB-SG	-5.17	102.51	114.40
1	C	191	ALA	CA-C-N	-5.16	114.48	122.69
1	C	191	ALA	C-N-CA	-5.16	114.48	122.69
1	A	113	LYS	N-CA-C	-5.16	106.49	112.89
1	A	304	SER	N-CA-C	5.15	119.19	113.01
1	C	359	VAL	O-C-N	-5.15	117.74	123.20
1	C	312	ILE	CB-CA-C	-5.14	103.13	110.12
1	C	370	HIS	CB-CA-C	-5.14	102.59	110.81
1	A	32	VAL	N-CA-CB	-5.13	102.65	110.86
1	B	39	PRO	CA-C-N	-5.13	113.01	120.29
1	B	39	PRO	C-N-CA	-5.13	113.01	120.29
1	C	288	PHE	N-CA-CB	5.13	117.75	110.16
1	C	298	LEU	N-CA-C	-5.13	104.23	110.13
1	C	63	LEU	CA-C-N	-5.12	113.01	120.29
1	C	63	LEU	C-N-CA	-5.12	113.01	120.29
1	B	4	SER	CA-CB-OG	-5.12	100.85	111.10
1	D	59	ALA	N-CA-C	-5.12	99.89	110.80
1	C	225	ASN	CA-C-N	5.12	130.52	122.33
1	C	225	ASN	C-N-CA	5.12	130.52	122.33
1	D	166	ILE	N-CA-CB	5.12	113.95	110.52
1	B	106	ASN	CB-CA-C	-5.11	102.30	110.79
1	C	230	ILE	CB-CA-C	-5.11	105.16	112.22
1	C	39	PRO	CA-C-N	5.11	127.55	120.29
1	C	39	PRO	C-N-CA	5.11	127.55	120.29
1	D	81	ALA	N-CA-C	-5.11	105.60	111.07
1	D	248	LYS	N-CA-C	-5.11	101.78	109.85
1	C	365	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	112	ARG	CG-CD-NE	-5.10	100.78	112.00
1	A	123	GLU	CB-CA-C	5.10	119.90	109.76
1	A	232	GLN	CB-CA-C	5.09	118.95	110.90
1	C	340	ILE	N-CA-C	5.09	116.30	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	372	GLN	N-CA-C	5.09	120.49	113.77
1	B	121	HIS	N-CA-C	-5.08	101.72	108.74
1	A	140	GLY	N-CA-C	5.07	121.50	112.22
1	B	137	GLU	N-CA-CB	-5.07	102.42	110.22
1	D	268	ILE	CB-CA-C	-5.07	103.02	110.82
1	D	226	VAL	N-CA-C	-5.07	100.35	107.75
1	D	54	PHE	N-CA-C	-5.06	107.13	113.15
1	B	38	SER	CB-CA-C	5.06	118.87	109.51
1	A	340	ILE	CB-CG1-CD1	5.06	124.42	113.80
1	C	270	SER	N-CA-C	-5.06	104.62	111.55
1	B	293	ARG	CA-CB-CG	-5.05	103.99	114.10
1	B	193	ILE	N-CA-CB	5.05	117.12	111.21
1	D	162	SER	CB-CA-C	-5.04	101.87	110.95
1	D	240	LYS	N-CA-C	-5.04	105.67	111.07
1	A	226	VAL	N-CA-C	-5.04	100.81	108.17
1	C	99	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	83	GLU	N-CA-C	-5.04	105.79	111.28
1	D	202	LEU	N-CA-C	-5.03	102.11	109.81
1	D	308	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	B	122	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	B	364	MET	CA-C-O	5.03	125.88	120.55
1	B	271	ARG	CA-C-N	5.02	127.23	120.50
1	B	271	ARG	C-N-CA	5.02	127.23	120.50
1	A	63	LEU	CB-CA-C	-5.02	102.41	110.74
1	D	2	TRP	N-CA-C	-5.00	105.95	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2975	0	2984	173	0
1	B	2944	0	2953	215	0
1	C	2995	0	3008	218	0
1	D	2888	0	2908	285	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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
7	C	299	0	0	18	0
7	D	243	0	0	26	0
All	All	13147	0	11979	884	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 37.

All (884) 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:A:108:LYS:HE3	1:A:118:MET:HE2	1.38	1.05
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:108:LYS:CE	1:A:118:MET:HE2	2.01	0.90
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:C:381:ILE:O	1:C:382:ARG:C	2.13	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:112:ARG:HG2	1:D:118:MET:HE1	1.56	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
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:A:55:LYS:HE2	1:A:150:MET:HE1	1.59	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: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:B:188:MET:HE3	1:B:190:LEU:HD21	1.59	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:188:MET:HE3	1:B:190:LEU:CD2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:188:MET:HE1	1:B:226:VAL:CG2	2.12	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
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:D:174:LYS:HZ2	1:D:176:ARG:HH11	1.33	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

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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	0.73
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:B:177:PRO:C	1:B:178:LEU:HG	2.12	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:27:ASN:C	7:D:587:HOH:O	2.33	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:B:109:GLU:CD	1:B:112:ARG:HH21	1.99	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:120:GLU:CD	1:D:182:LYS:HD3	2.17	0.69
1:D:159:ARG:NH1	1:D:161:ASN:OD1	2.25	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:73:GLU:C	1:D:74:ILE:HG13	2.14	0.67
1:D:143:LEU:CD2	1:D:160:VAL:HB	2.24	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: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:B:80:TYR:O	1:B:84:GLU:HG3	1.94	0.66
1:D:174:LYS:NZ	1:D:176:ARG:HH11	1.92	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
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: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: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:C:317:ILE:HD13	1:C:317:ILE:N	2.09	0.64
1:A:187:LYS:CE	1:A:259:GLU:HA	2.22	0.64
1:C:150:MET:HE3	1:C:150:MET:CA	2.24	0.64
1:C:277:HIS:O	1:C:280:ILE:HG13	1.98	0.64
1:A:55:LYS:HE2	1:A:150:MET:CE	2.26	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:C:193:ILE:HG23	1:C:250:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:324:THR:HA	1:B:327:GLN:HG2	1.80	0.63
1:A:20:VAL:O	1:A:21:GLU:C	2.37	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
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:143:LEU:C	1:D:143:LEU:HD23	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:SER:O	1:D:39:PRO:C	2.41	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:B:237:LEU:C	1:B:237:LEU:HD12	2.25	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:D:6:LYS:HD3	1:D:29:GLN:CD	2.26	0.61
1:C:332:ALA:CB	1:C:357:ILE:HD12	2.31	0.60
1:A:324:THR:O	1:A:325:HIS:C	2.43	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
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:143:LEU:C	1:A:143:LEU:HD12	2.26	0.60
1:D:47:ASP:OD1	1:D:47:ASP:C	2.44	0.60
1:A:38:SER:O	1:A:42:GLN:HG3	2.01	0.60
1:B:377:VAL:HG12	1:B:378:VAL:N	2.12	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:D:317:ILE:HG22	1:D:351:GLY:C	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:192:VAL:HG23	1:B:255:MET:HE1	1.85	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:C:188:MET:HE2	1:C:208:GLU:OE2	2.03	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:HD23	1:D:143:LEU:O	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:D:82:LEU:O	1:D:83:GLU:C	2.46	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:C:129:PRO:O	1:C:130:ALA:C	2.45	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:A:170:LEU:O	1:A:171:GLU:C	2.45	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
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:D:110:HIS:C	1:D:113:LYS:HD3	2.27	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: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:141:TYR:HA	1:A:142:PRO:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:385:NHE:HC21	7:A:615:HOH:O	2.03	0.57
1:B:274:ASN:C	1:B:274:ASN:HD22	2.10	0.57
1:D:41:LYS:HE2	1:D:49:HIS:HB3	1.86	0.57
1:B:126:GLU:HG2	1:B:131:GLU:CD	2.30	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:197:THR:O	1:B:198:LYS:C	2.49	0.56
1:A:61:ARG:NH1	7:A:386:HOH:O	2.38	0.56
1:B:106:ASN:O	1:B:107:GLN:C	2.48	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:B:85:VAL:C	1:B:87:SER:H	2.14	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:B:233[A]:LYS:NZ	1:B:262:SER:HA	2.21	0.56
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:A:299:PRO:C	1:A:300:ILE:HG13	2.32	0.55
1:C:187:LYS:HE3	1:C:258:LEU:O	2.06	0.55
1:D:53:SER:C	1:D:55:LYS:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ILE:HG22	1:B:381:ILE:O	2.07	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: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:A:188:MET:HE1	1:A:224:ARG:O	2.08	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:D:92:GLU:HA	1:D:93:PRO:C	2.31	0.54
1:B:379:ASP:O	1:B:380:ARG:C	2.50	0.54
1:B:79:THR:HA	1:B:82:LEU:HB2	1.89	0.54
1:B:85:VAL:C	1:B:87:SER:N	2.64	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:A:212:GLU:CD	1:A:217:LYS:HD2	2.33	0.54
1:B:1:MET:HG3	1:B:2:TRP:N	2.12	0.54
1:B:188:MET:HE1	1:B:226:VAL:HG21	1.88	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:174:LYS:C	1:D:176:ARG:H	2.16	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:108:LYS:HE3	1:A:118:MET:CE	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:146:LYS:C	1:D:178:LEU:HD23	2.34	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:345:LYS:NZ	1:A:353:LYS:O	2.39	0.52
1:B:188:MET:HE1	1:B:226:VAL:HG22	1.90	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: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: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:A:230:ILE:O	1:A:231:ASN:C	2.53	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: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:A:254:GLU:OE1	1:A:273:HIS:NE2	2.43	0.51
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:188:MET:CE	1:B:190:LEU:HD21	2.36	0.51
1:B:281:GLU:OE2	1:B:339:SER:OG	2.27	0.51
1:D:28:ILE:C	7:D:587:HOH:O	2.51	0.51
1:D:322:PRO:C	1:D:348:ALA:HB3	2.35	0.51
1:C:324:THR:O	1:C:325:HIS:C	2.53	0.51
1:D:74:ILE:HD12	1:D:77:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LEU:HD12	1:D:237:LEU:C	2.34	0.51
1:B:38:SER:O	1:B:39:PRO:C	2.51	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
1:C:64:ALA:C	1:C:66:THR:H	2.19	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:119:ALA:O	7:D:545:HOH:O	2.19	0.51
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ARG:HH11	1:D:61:ARG:CD	2.24	0.50
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:D:85:VAL:C	1:D:87:SER:H	2.20	0.49
1:D:126:GLU:HG2	1:D:131:GLU:CD	2.36	0.49
1:A:61:ARG:HH22	1:A:84:GLU:CD	2.19	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:141:TYR:HA	1:B:142:PRO:C	2.38	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: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: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:14:GLN:HB3	1:D:343:TYR:CD1	2.48	0.49
1:D:171:GLU:CD	1:D:172:ALA:N	2.71	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:TYR:CD2	1:D:278:TYR:C	2.91	0.48
1:B:47:ASP:C	7:B:579:HOH:O	2.56	0.48
1:D:58:GLU:O	1:D:59:ALA:C	2.56	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: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	1.91	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:205:PRO:CG	1:C:307:ILE:HD12	2.40	0.48
1:C:255:MET:HE3	1:C:255:MET:HB2	1.66	0.48
1:D:9:VAL:HG13	1:D:9:VAL:O	2.14	0.48
1:D:50:VAL:CG1	1:D:51:THR:N	2.68	0.48
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:324:THR:O	1:D:325:HIS:C	2.57	0.47
1:B:215:ILE:O	1:B:216:CYS:C	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:PHE:HE1	1:C:121:HIS:CD2	2.32	0.47
1:A:368:GLU:HG2	7:A:633:HOH:O	2.15	0.47
1:B:170:LEU:O	1:B:171:GLU:C	2.56	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:B:233[B]:LYS:NZ	7:B:657:HOH:O	2.34	0.47
1:C:2:TRP:CE3	1:C:3:ASN:HB3	2.49	0.47
1:B:192:VAL:CG2	1:B:255:MET:HE1	2.44	0.46
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:119:ALA:N	1:A:264:MET:HE3	2.30	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:A:118:MET:HE3	1:A:118:MET:HB3	1.85	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:C:233:LYS:HA	1:C:236[B]:GLU:CD	2.41	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:B:126:GLU:O	1:B:127:ASN:C	2.57	0.46
1:B:281:GLU:CD	1:B:339:SER:HG	2.23	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:D:34:ASP:C	1:D:35:ALA:O	2.59	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:D:41:LYS:HZ1	1:D:51:THR:HA	1.81	0.46
1:D:141:TYR:HA	1:D:142:PRO:C	2.41	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: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:108:LYS:O	1:C:109:GLU:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:111:LEU:HB2	1:C:118:MET:HE1	1.98	0.45
1:D:83:GLU:O	1:D:86:ALA:HB3	2.17	0.45
1:A:189:GLU:OE2	4:A:400:ADP:O3'	2.26	0.45
1:B:33:LEU:HB3	1:B:63:LEU:HD13	1.89	0.45
1:B:317:ILE:O	1:B:318:GLY:C	2.60	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:131:GLU:O	1:B:132:LEU:C	2.58	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:B:324:THR:O	1:B:325:HIS:C	2.57	0.44
1:C:187:LYS:HE2	1:C:259:GLU:CA	2.46	0.44
1:D:85:VAL:C	1:D:87:SER:N	2.74	0.44
1:D:230:ILE:O	1:D:231:ASN:C	2.58	0.44
1:C:106:ASN:O	1:C:107:GLN:C	2.58	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:204:TYR:CZ	1:A:305:LEU:HD22	2.53	0.44
1:B:112:ARG:C	1:B:114:TYR:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:321:ALA:C	1:C:323:ASP:H	2.24	0.44
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:78[A]:ASP:CG	1:B:81:ALA:HB2	2.43	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: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:A:258:LEU:C	1:A:260:ASP:N	2.76	0.43
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: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:B:126:GLU:H	1:B:131:GLU:CD	2.26	0.43
1:C:2:TRP:NE1	1:D:330:GLU:HB2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:346:GLY:O	1:C:347:ALA:C	2.60	0.43
1:D:171:GLU:OE1	1:D:172:ALA:CA	2.63	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:C:241:ALA:O	1:C:244:ALA:HB3	2.19	0.43
1:B:197:THR:C	1:B:199:ASP:N	2.75	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:131:GLU:O	1:D:132:LEU:C	2.61	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:B:197:THR:OG1	1:B:200:GLU:N	2.36	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: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:239:ARG:O	1:C:240:LYS:C	2.61	0.42
1:C:321:ALA:C	1:C:323:ASP:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:CYS:SG	1:C:374:LEU:HD12	2.59	0.42
1:A:109:GLU:CD	1:A:112:ARG:NH1	2.77	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
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:132:LEU:O	1:D:133:ALA:C	2.61	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:D:112:ARG:CG	1:D:118:MET:HE1	2.40	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: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:B:121:HIS:CD2	1:B:121:HIS:C	2.97	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:263:ILE:CG2	1:A:264:MET:N	2.82	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:62:GLN:O	1:C:62:GLN:HG3	2.12	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
1:A:34:ASP:O	1:A:41:LYS:NZ	2.53	0.41
1:A:150:MET:HE3	1:A:150:MET:HB3	1.88	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:A:278:TYR:CD2	1:A:278:TYR:C	2.97	0.41
1:C:15:LEU:HD13	1:C:272:ILE:HG13	2.01	0.41
1:C:259:GLU:C	1:C:261:ASP:H	2.27	0.41
1:D:59:ALA:O	1:D:62:GLN:CB	2.69	0.41
1:D:314:LEU:HD21	1:D:378:VAL:HG21	2.02	0.41
1:A:227:SER:C	1:A:229:ALA:N	2.78	0.41
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.84	0.41
1:C:128:THR:HA	1:C:129:PRO:HD3	1.70	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:A:62:GLN:O	1:A:63:LEU:C	2.60	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:C:187:LYS:HE2	1:C:259:GLU:C	2.46	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:119:ALA:CA	1:A:264:MET:HE3	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:B:9:VAL:O	1:B:9:VAL:HG13	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:221:ALA:HA	1:B:222:PRO:HA	1.60	0.41
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:D:171:GLU:CD	1:D:172:ALA:H	2.29	0.41
1:A:92:GLU:HA	1:A:93:PRO:C	2.45	0.40
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:B:274:ASN:C	1:B:274:ASN:ND2	2.77	0.40
1:D:191:ALA:O	1:D:207:VAL:HG22	2.20	0.40
1:B:103:ASN:C	1:B:103:ASN:OD1	2.64	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:D:50:VAL:HG12	1:D:51:THR:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ALA:HA	1:C:322:PRO:HD3	1.78	0.40
1:C:327:GLN:O	1:C:328:ALA:C	2.63	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%)	36	35
1	B	378/403 (94%)	346 (92%)	28 (7%)	4 (1%)	11	7
1	C	386/403 (96%)	368 (95%)	16 (4%)	2 (0%)	24	21
1	D	368/403 (91%)	344 (94%)	18 (5%)	6 (2%)	7	3
All	All	1516/1612 (94%)	1423 (94%)	80 (5%)	13 (1%)	14	9

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

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Mol	Chain	Res	Type
1	C	34	ASP
1	D	175	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/336 (96%)	282 (88%)	40 (12%)	4	2
1	B	320/336 (95%)	253 (79%)	67 (21%)	1	0
1	C	324/336 (96%)	280 (86%)	44 (14%)	3	2
1	D	312/336 (93%)	257 (82%)	55 (18%)	2	1
All	All	1278/1344 (95%)	1072 (84%)	206 (16%)	2	1

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	SER
1	A	6	LYS
1	A	10	LEU
1	A	28	ILE
1	A	57	ARG
1	A	73	GLU
1	A	75	GLU
1	A	77	VAL
1	A	84	GLU
1	A	87	SER
1	A	108	LYS
1	A	109	GLU
1	A	112	ARG
1	A	118	MET
1	A	123	GLU
1	A	126	GLU
1	A	131	GLU
1	A	132	LEU

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Mol	Chain	Res	Type
1	A	139	LEU
1	A	174	LYS
1	A	181	GLU
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	250	VAL
1	A	259	GLU
1	A	264	MET
1	A	272	ILE
1	A	275	SER
1	A	303	GLN
1	A	344	SER
1	A	364	MET
1	A	377	VAL
1	A	378	VAL
1	B	1	MET
1	B	5	ARG
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	87	SER
1	B	88	GLU
1	B	90	LYS
1	B	94	SER

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Mol	Chain	Res	Type
1	B	102	GLN
1	B	104	LYS
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	182	LYS
1	B	190	LEU
1	B	196	LYS
1	B	198	LYS
1	B	200	GLU
1	B	211	GLN
1	B	225	ASN
1	B	232	GLN
1	B	237	LEU
1	B	250	VAL
1	B	259[A]	GLU
1	B	259[B]	GLU
1	B	264	MET
1	B	272	ILE
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	357	ILE

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Mol	Chain	Res	Type
1	B	369	THR
1	B	372	GLN
1	B	378	VAL
1	B	380	ARG
1	C	6	LYS
1	C	15	LEU
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	88	GLU
1	C	89	VAL
1	C	98	ILE
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	134	LYS
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	242	VAL
1	C	248	LYS
1	C	255	MET
1	C	260	ASP
1	C	264	MET
1	C	265	LEU
1	C	280	ILE
1	C	292	LEU
1	C	307	ILE
1	C	317	ILE

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Mol	Chain	Res	Type
1	C	323	ASP
1	C	330	GLU
1	C	339	SER
1	C	357	ILE
1	C	377	VAL
1	C	378	VAL
1	D	1	MET
1	D	5	ARG
1	D	37	ASN
1	D	38	SER
1	D	47	ASP
1	D	55	LYS
1	D	57	ARG
1	D	61	ARG
1	D	65	LYS
1	D	69	VAL
1	D	74	ILE
1	D	85	VAL
1	D	88	GLU
1	D	89	VAL
1	D	104	LYS
1	D	108	LYS
1	D	122	ARG
1	D	124	LEU
1	D	126	GLU
1	D	129	PRO
1	D	132	LEU
1	D	134	LYS
1	D	137	GLU
1	D	143	LEU
1	D	144	MET
1	D	145	LEU
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

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Mol	Chain	Res	Type
1	D	202	LEU
1	D	208	GLU
1	D	213	ASP
1	D	218	LEU
1	D	225	ASN
1	D	246	ASP
1	D	295	ILE
1	D	301	PRO
1	D	308	ARG
1	D	314	LEU
1	D	317	ILE
1	D	344	SER
1	D	350	PRO
1	D	352	ARG
1	D	353	LYS
1	D	366	GLU
1	D	375	ILE
1	D	378	VAL
1	D	380	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	121	HIS
1	A	127	ASN
1	A	225	ASN
1	B	96	GLN
1	B	107	GLN
1	B	127	ASN
1	C	37	ASN
1	C	62	GLN
1	C	106	ASN
1	C	225	ASN
1	C	232	GLN
1	C	327	GLN
1	C	337	ASN
1	C	365	HIS
1	D	42	GLN
1	D	96	GLN
1	D	102	GLN
1	D	106	ASN

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Mol	Chain	Res	Type
1	D	110	HIS
1	D	157	ASN
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 oligosaccharides 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$
3	NHE	C	384	-	13,13,13	1.08	1 (7%)	16,17,17	3.04	5 (31%)
3	NHE	A	385	-	13,13,13	1.16	1 (7%)	16,17,17	2.31	6 (37%)
4	ADP	B	400	5	28,29,29	1.20	3 (10%)	43,45,45	1.82	12 (27%)
6	AIR	B	402	-	19,20,20	0.66	0	27,30,30	2.46	11 (40%)
6	AIR	C	402	-	19,20,20	0.90	1 (5%)	27,30,30	1.83	11 (40%)
4	ADP	D	400	5	28,29,29	1.20	3 (10%)	43,45,45	2.13	11 (25%)
4	ADP	C	400	5	28,29,29	1.24	4 (14%)	43,45,45	1.92	13 (30%)
6	AIR	D	402	-	19,20,20	0.76	0	27,30,30	1.83	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	AIR	A	402	-	19,20,20	1.00	2 (10%)	27,30,30	2.28	12 (44%)
4	ADP	A	400	5	28,29,29	1.36	3 (10%)	43,45,45	2.59	21 (48%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	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	B	400	5	-	1/16/32/32	0/3/3/3
6	AIR	B	402	-	-	6/10/26/26	0/2/2/2
6	AIR	C	402	-	-	1/10/26/26	0/2/2/2
4	ADP	D	400	5	-	1/16/32/32	0/3/3/3
4	ADP	C	400	5	-	2/16/32/32	0/3/3/3
6	AIR	D	402	-	-	2/10/26/26	0/2/2/2
6	AIR	A	402	-	1/1/5/5	7/10/26/26	0/2/2/2
4	ADP	A	400	5	-	3/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	ADP	C6-N6	-5.03	1.21	1.34
4	D	400	ADP	C6-N6	-3.59	1.25	1.34
4	B	400	ADP	C6-N6	-3.53	1.25	1.34
3	A	385	NHE	C2-S	3.28	1.82	1.77
4	B	400	ADP	C2-N1	3.24	1.39	1.33
4	C	400	ADP	C6-N6	-3.05	1.26	1.34
6	A	402	AIR	C4-C5	2.95	1.39	1.36
4	D	400	ADP	C2-N1	2.89	1.39	1.33
4	C	400	ADP	PA-O3A	2.88	1.62	1.59
4	A	400	ADP	C2-N1	2.86	1.39	1.33
3	C	384	NHE	C2-S	2.61	1.81	1.77
4	D	400	ADP	C2-N3	-2.46	1.29	1.33
4	C	400	ADP	C2-N1	2.32	1.38	1.33
4	B	400	ADP	C8-N7	2.27	1.36	1.31
6	C	402	AIR	C4-C5	2.25	1.38	1.36
6	A	402	AIR	P-O6	2.16	1.62	1.54
4	A	400	ADP	C8-N7	2.12	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	400	ADP	C8-N7	2.04	1.35	1.31

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	384	NHE	O1-S-C2	9.10	120.48	106.73
6	A	402	AIR	C5'-C4'-C3'	6.25	137.71	115.21
4	D	400	ADP	C2-N1-C6	6.01	128.61	118.73
4	D	400	ADP	C6-C5-C4	6.01	125.39	117.18
4	A	400	ADP	O3B-PB-O1B	5.95	134.00	110.83
6	B	402	AIR	N1-C2-N3	5.79	117.17	111.68
4	A	400	ADP	N3-C2-N1	-5.66	120.02	128.58
3	A	385	NHE	O3-S-O2	-5.39	97.92	111.40
4	A	400	ADP	O4'-C1'-N9	5.30	118.27	108.09
4	C	400	ADP	N3-C2-N1	-5.27	120.60	128.58
4	D	400	ADP	C5-C6-N1	-5.08	104.61	117.51
3	C	384	NHE	C1-N-C1'	-5.07	104.42	114.18
4	A	400	ADP	C5-C6-N6	5.06	135.81	123.29
4	B	400	ADP	N3-C2-N1	-4.71	121.45	128.58
6	B	402	AIR	C4-N3-C2	-4.60	99.23	105.24
4	C	400	ADP	O2A-PA-O3A	4.37	119.09	107.27
4	A	400	ADP	N6-C6-N1	-4.35	108.68	118.38
4	B	400	ADP	O2'-C2'-C1'	-4.33	95.20	110.10
4	D	400	ADP	N6-C6-N1	4.30	127.95	118.38
4	D	400	ADP	C6-C5-N7	-4.12	124.14	132.09
3	A	385	NHE	O2-S-O1	4.12	127.22	113.82
6	B	402	AIR	O4'-C4'-C3'	-3.95	97.32	105.15
4	C	400	ADP	C4-N9-C8	3.89	109.83	105.74
3	C	384	NHE	O3-S-O1	-3.83	101.81	111.40
6	A	402	AIR	N1-C2-N3	3.81	115.29	111.68
6	B	402	AIR	C5-C4-N3	3.75	113.91	109.66
6	B	402	AIR	C2-N1-C5	-3.71	103.74	106.60
4	A	400	ADP	O2B-PB-O1B	-3.57	96.91	110.83
4	C	400	ADP	N9-C8-N7	-3.56	108.88	113.94
4	B	400	ADP	O3'-C3'-C2'	3.55	123.21	111.82
4	A	400	ADP	C4-N9-C8	3.55	109.46	105.74
6	D	402	AIR	C4-C5-N1	-3.52	104.73	107.48
6	A	402	AIR	C3'-C2'-C1'	-3.48	94.87	101.46
4	B	400	ADP	N9-C8-N7	-3.48	108.99	113.94
6	C	402	AIR	C5'-C4'-C3'	3.44	127.61	115.21
3	A	385	NHE	C1-N-C1'	-3.33	107.78	114.18
4	A	400	ADP	C2-N1-C6	3.33	124.19	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	402	AIR	C4-C5-N6	-3.30	127.07	131.28
4	C	400	ADP	C2-N1-C6	3.29	124.14	118.73
4	A	400	ADP	C3'-C2'-C1'	-3.25	95.32	101.46
6	D	402	AIR	O2'-C2'-C1'	-3.23	98.99	110.10
6	C	402	AIR	O6-P-O5'	-3.21	98.31	106.67
6	A	402	AIR	O4'-C4'-C5'	3.20	119.58	109.33
6	D	402	AIR	O5'-P-O8	3.18	115.02	106.44
4	A	400	ADP	O2'-C2'-C1'	-3.15	99.26	110.10
4	B	400	ADP	O2A-PA-O3A	3.03	115.46	107.27
6	D	402	AIR	C5-C4-N3	2.99	113.05	109.66
4	B	400	ADP	C4-N9-C8	2.99	108.88	105.74
4	A	400	ADP	C5-C4-N9	-2.91	102.64	105.81
6	C	402	AIR	N1-C2-N3	2.90	114.43	111.68
4	A	400	ADP	C4-C5-N7	2.88	113.88	110.58
3	C	384	NHE	O3-S-O2	-2.85	104.28	111.40
4	A	400	ADP	N3-C4-N9	2.83	131.98	127.17
6	D	402	AIR	C4-N3-C2	-2.83	101.55	105.24
6	D	402	AIR	O3'-C3'-C2'	2.83	120.88	111.82
6	A	402	AIR	O2'-C2'-C1'	2.81	119.79	110.10
4	A	400	ADP	C2'-C1'-N9	-2.78	106.39	113.30
4	D	400	ADP	O2A-PA-O3A	2.76	114.74	107.27
6	B	402	AIR	O6-P-O5'	2.76	113.87	106.67
3	C	384	NHE	O3-S-C2	-2.68	100.76	106.00
6	C	402	AIR	O2'-C2'-C3'	2.68	120.40	111.82
6	B	402	AIR	O5'-P-O8	2.67	113.67	106.44
4	D	400	ADP	O2'-C2'-C1'	-2.67	100.92	110.10
3	A	385	NHE	O2-S-C2	-2.66	102.70	106.73
6	A	402	AIR	O3'-C3'-C4'	2.65	118.71	111.08
6	B	402	AIR	O4'-C4'-C5'	2.64	117.80	109.33
4	D	400	ADP	O3'-C3'-C4'	2.63	118.65	111.08
4	A	400	ADP	C2-N3-C4	2.63	118.26	111.83
4	B	400	ADP	O4'-C4'-C3'	-2.63	99.93	105.15
6	B	402	AIR	C4-C5-N1	-2.62	105.44	107.48
4	A	400	ADP	O2A-PA-O3A	2.62	114.35	107.27
3	A	385	NHE	O3-S-C2	2.60	111.09	106.00
4	C	400	ADP	C2'-C1'-N9	-2.52	107.03	113.30
4	B	400	ADP	C5'-C4'-C3'	-2.50	106.20	115.21
6	D	402	AIR	N1-C2-N3	2.46	114.02	111.68
4	D	400	ADP	O3'-C3'-C2'	2.40	119.50	111.82
4	D	400	ADP	O5'-PA-O1A	2.39	118.40	108.94
6	C	402	AIR	O7-P-O6	2.38	116.71	107.80
6	C	402	AIR	C4-C5-N1	-2.37	105.63	107.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	ADP	C2-N1-C6	2.37	122.62	118.73
3	A	385	NHE	C2-C1-N	-2.37	104.64	111.40
6	C	402	AIR	O5'-P-O8	2.36	112.81	106.44
6	A	402	AIR	C1'-N1-C2	2.33	133.36	126.73
6	A	402	AIR	O4'-C1'-N1	-2.33	103.09	108.36
4	C	400	ADP	C2-N3-C4	2.29	117.43	111.83
4	B	400	ADP	C5-N7-C8	2.28	107.03	103.45
4	C	400	ADP	C5-C6-N6	2.27	128.91	123.29
6	A	402	AIR	C4-C5-N1	-2.25	105.72	107.48
4	A	400	ADP	O4'-C4'-C3'	-2.24	100.70	105.15
4	A	400	ADP	O3'-C3'-C4'	-2.24	104.64	111.08
6	B	402	AIR	O2'-C2'-C1'	-2.24	102.39	110.10
4	C	400	ADP	O4'-C1'-C2'	2.24	111.40	106.62
4	C	400	ADP	C5-N7-C8	2.22	106.94	103.45
6	C	402	AIR	C2'-C3'-C4'	-2.19	98.37	102.61
6	C	402	AIR	C5-C4-N3	2.19	112.14	109.66
6	D	402	AIR	C4-C5-N6	-2.15	128.53	131.28
6	A	402	AIR	O4'-C4'-C3'	-2.15	100.88	105.15
6	A	402	AIR	C4-N3-C2	-2.15	102.43	105.24
6	C	402	AIR	C1'-N1-C2	2.14	132.81	126.73
6	A	402	AIR	C2-N1-C5	-2.12	104.97	106.60
4	C	400	ADP	O3B-PB-O2B	-2.10	99.91	107.80
4	B	400	ADP	O2B-PB-O3A	2.10	111.67	104.64
4	A	400	ADP	N9-C8-N7	-2.10	110.96	113.94
4	A	400	ADP	O3B-PB-O2B	-2.07	100.02	107.80
4	C	400	ADP	C1'-N9-C8	-2.07	122.50	127.09
4	C	400	ADP	O2B-PB-O1B	2.05	118.81	110.83
4	B	400	ADP	N6-C6-N1	2.04	122.93	118.38
4	A	400	ADP	O3B-PB-O3A	-2.03	97.83	104.64
4	D	400	ADP	O3A-PA-O1A	-2.00	104.68	110.70
6	C	402	AIR	C2-N1-C5	-2.00	105.06	106.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	402	AIR	C4'

All (30) 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

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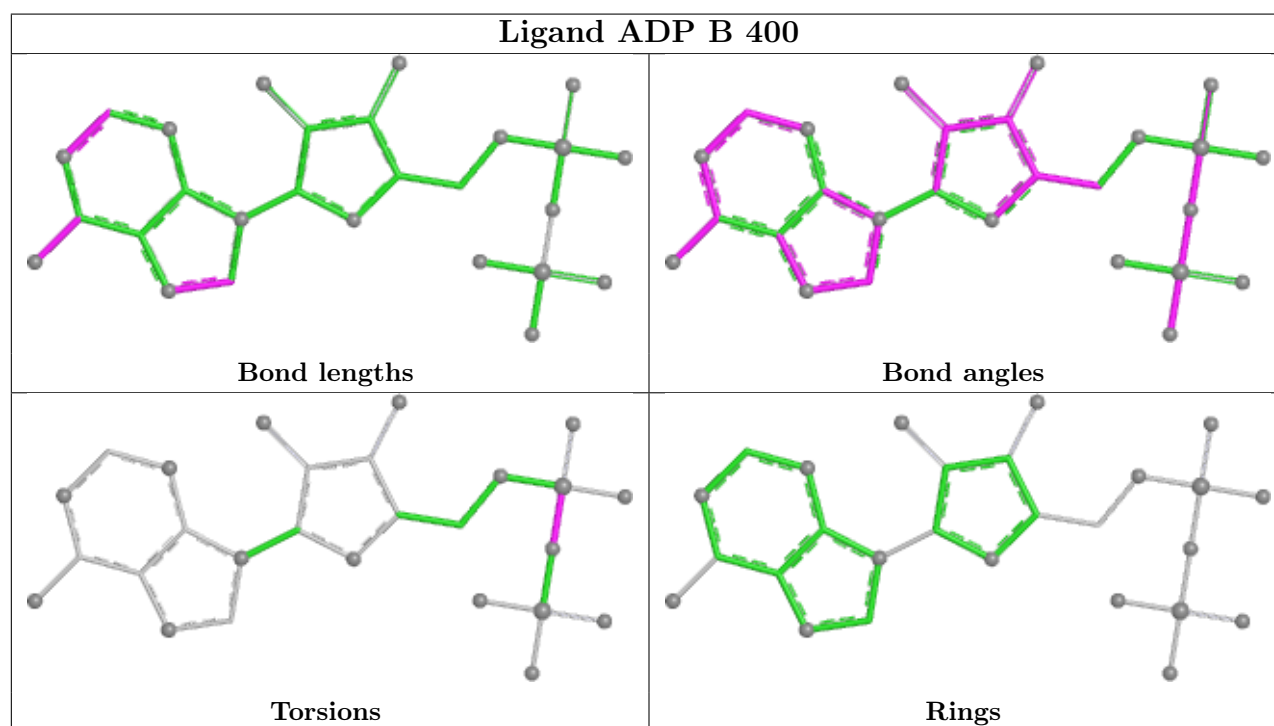
Mol	Chain	Res	Type	Atoms
3	C	384	NHE	C1-C2-S-O2
4	A	400	ADP	PA-O3A-PB-O3B
6	A	402	AIR	C5'-O5'-P-O6
6	A	402	AIR	C5'-O5'-P-O7
6	A	402	AIR	C5'-O5'-P-O8
6	B	402	AIR	C5'-O5'-P-O7
6	B	402	AIR	C5'-O5'-P-O8
6	A	402	AIR	C3'-C4'-C5'-O5'
6	A	402	AIR	O4'-C4'-C5'-O5'
6	B	402	AIR	O4'-C4'-C5'-O5'
6	B	402	AIR	C3'-C4'-C5'-O5'
3	C	384	NHE	C1-C2-S-O3
3	C	384	NHE	C2-C1-N-C1'
6	B	402	AIR	O4'-C1'-N1-C5
3	C	384	NHE	C1-C2-S-O1
4	C	400	ADP	C3'-C4'-C5'-O5'
4	A	400	ADP	PA-O3A-PB-O1B
6	C	402	AIR	C2'-C1'-N1-C2
4	C	400	ADP	O4'-C4'-C5'-O5'
6	A	402	AIR	C2'-C1'-N1-C5
3	A	385	NHE	C2'-C1'-N-C1
6	A	402	AIR	C2'-C1'-N1-C2
6	B	402	AIR	C5'-O5'-P-O6
6	D	402	AIR	C2'-C1'-N1-C5
6	D	402	AIR	C2'-C1'-N1-C2
4	A	400	ADP	PB-O3A-PA-O2A
4	B	400	ADP	PB-O3A-PA-O2A
4	D	400	ADP	PB-O3A-PA-O2A

There are no ring outliers.

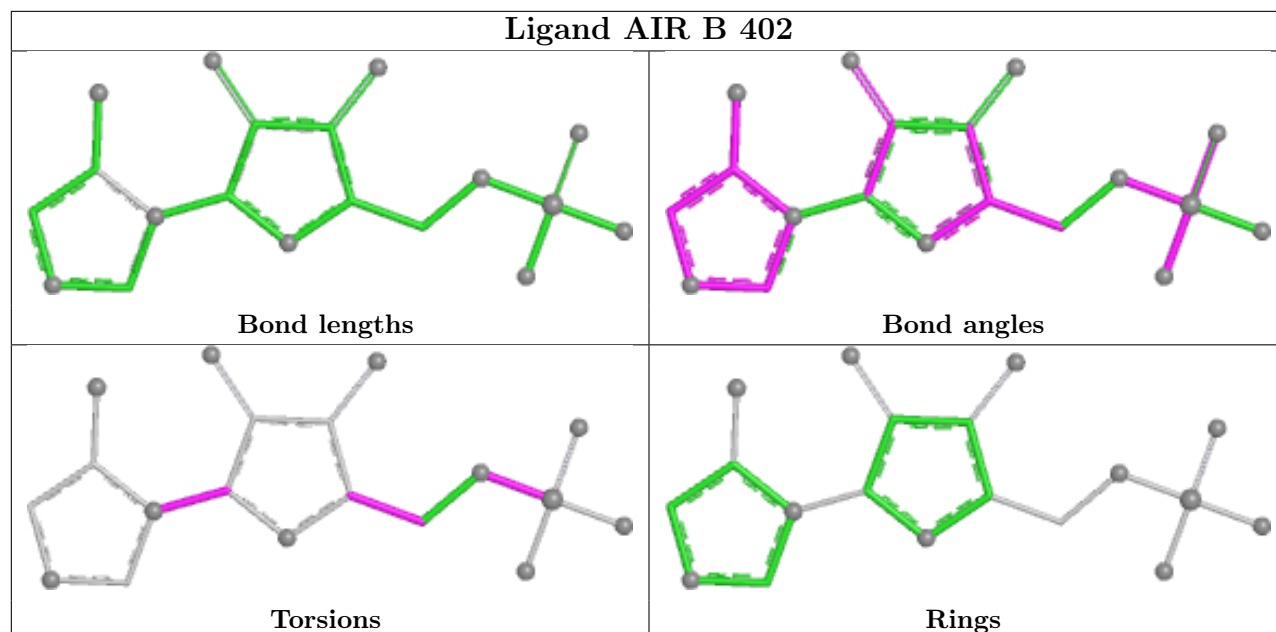
9 monomers are involved in 19 short contacts:

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

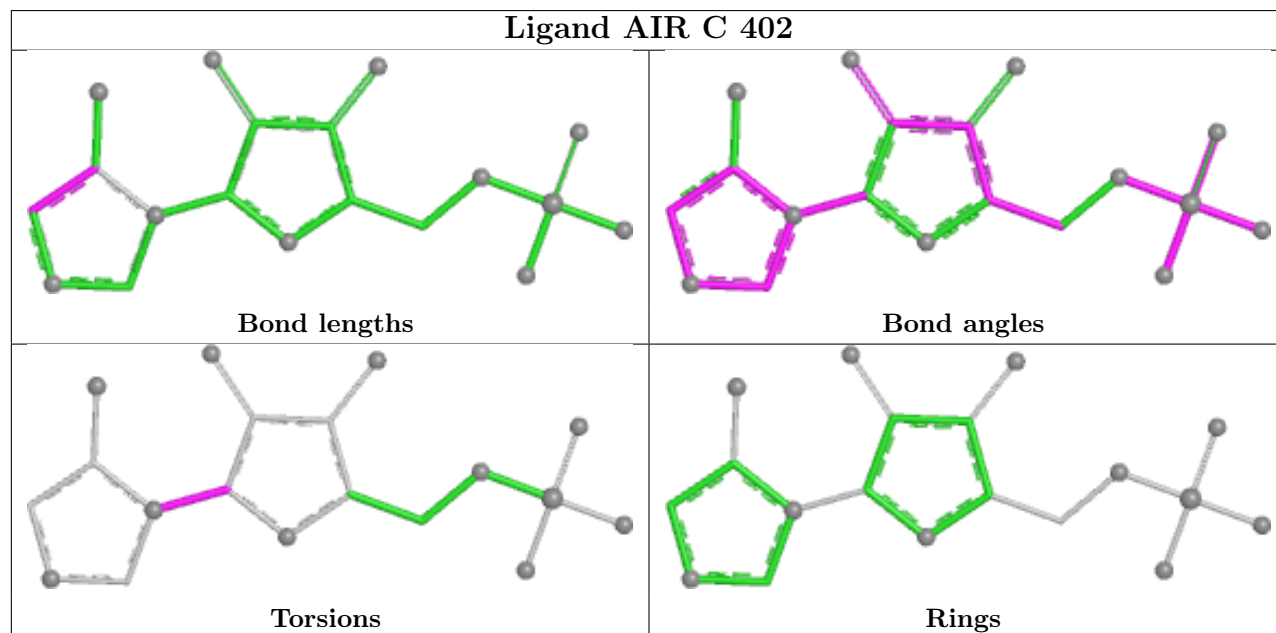
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

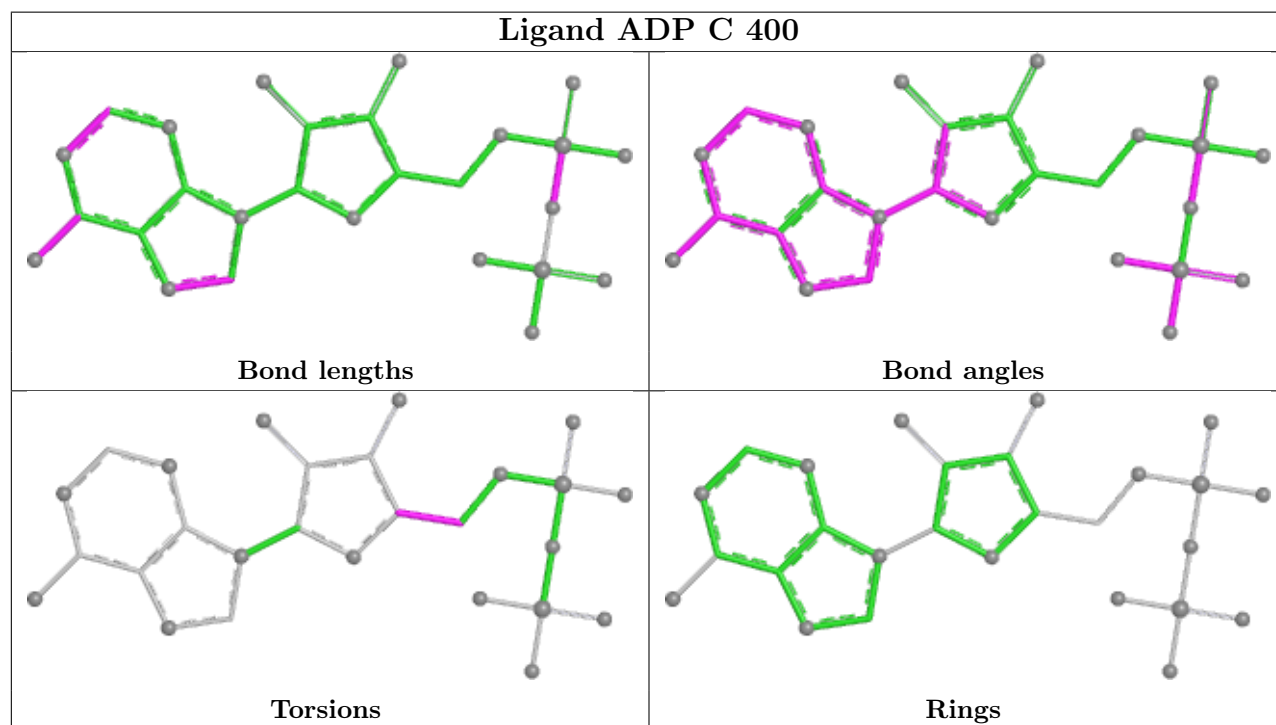
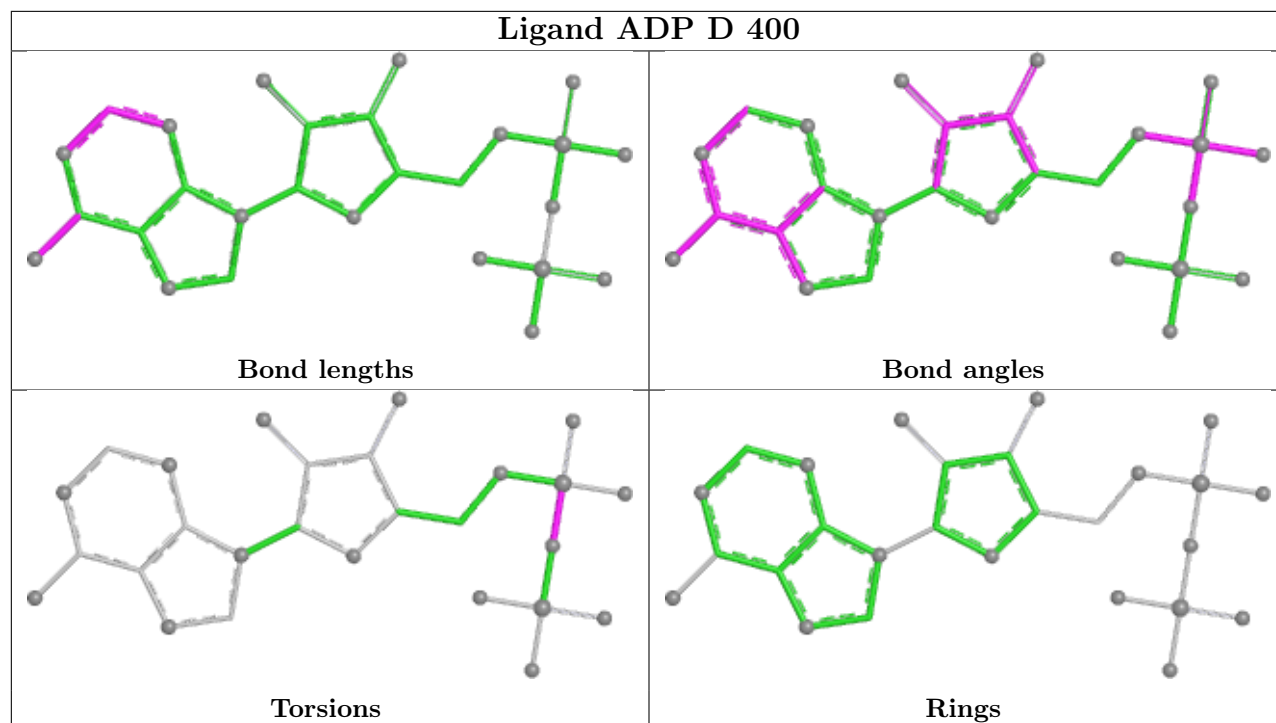


Ligand AIR B 402

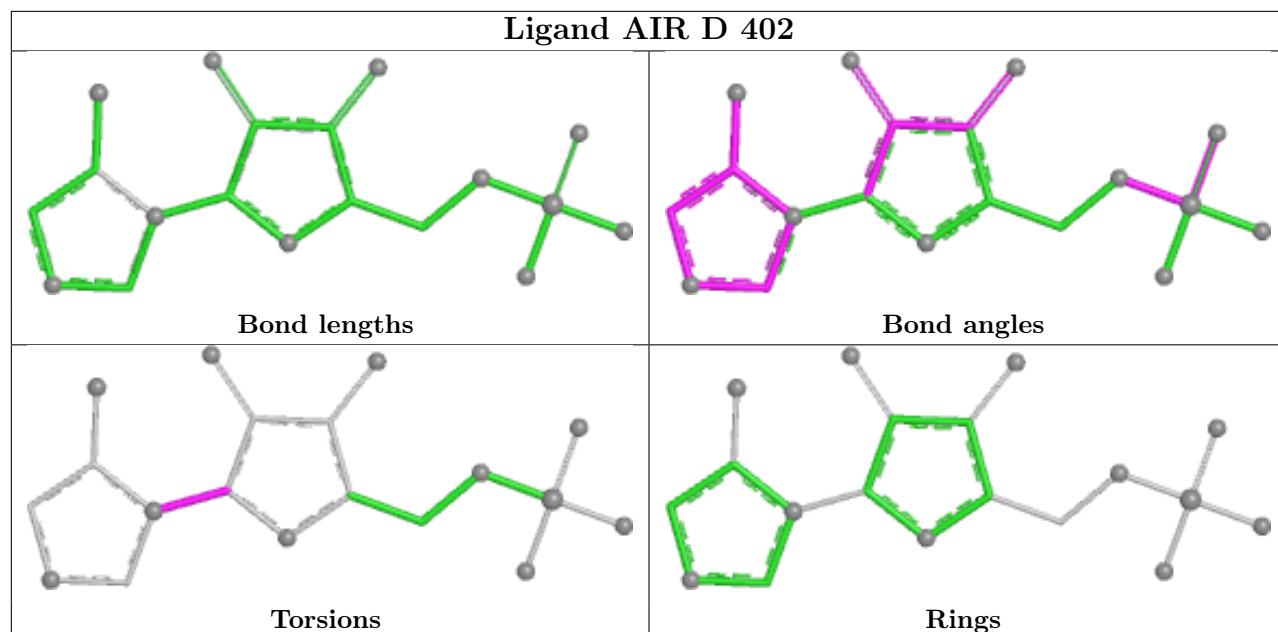


Ligand AIR C 402

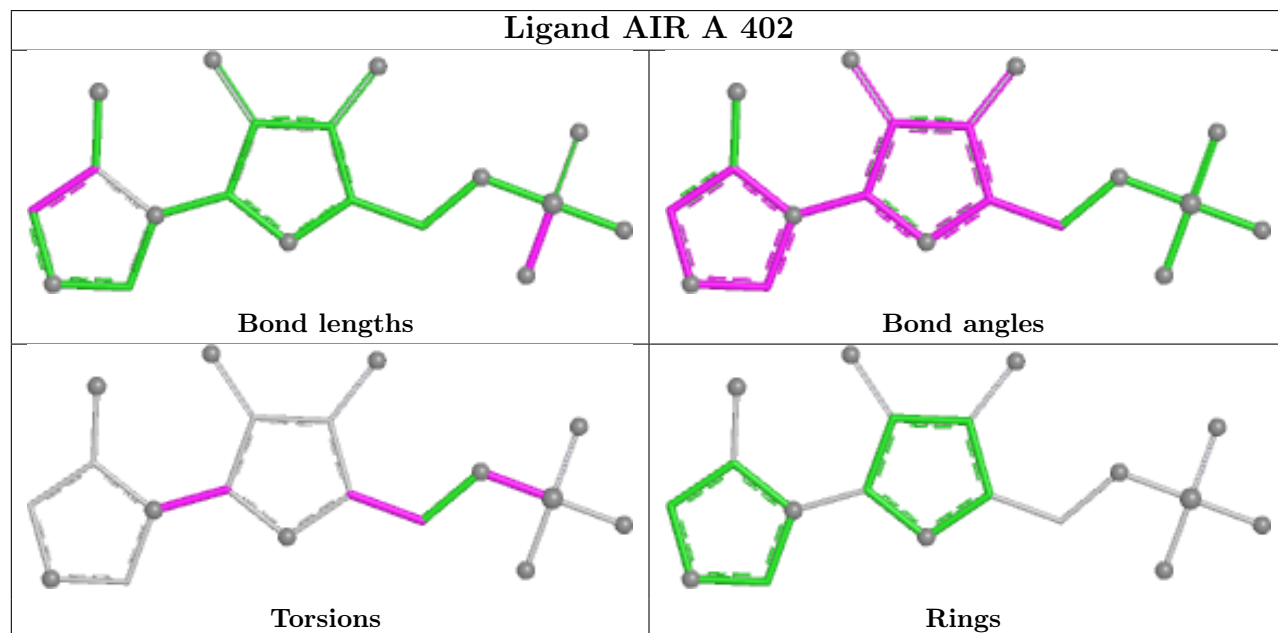


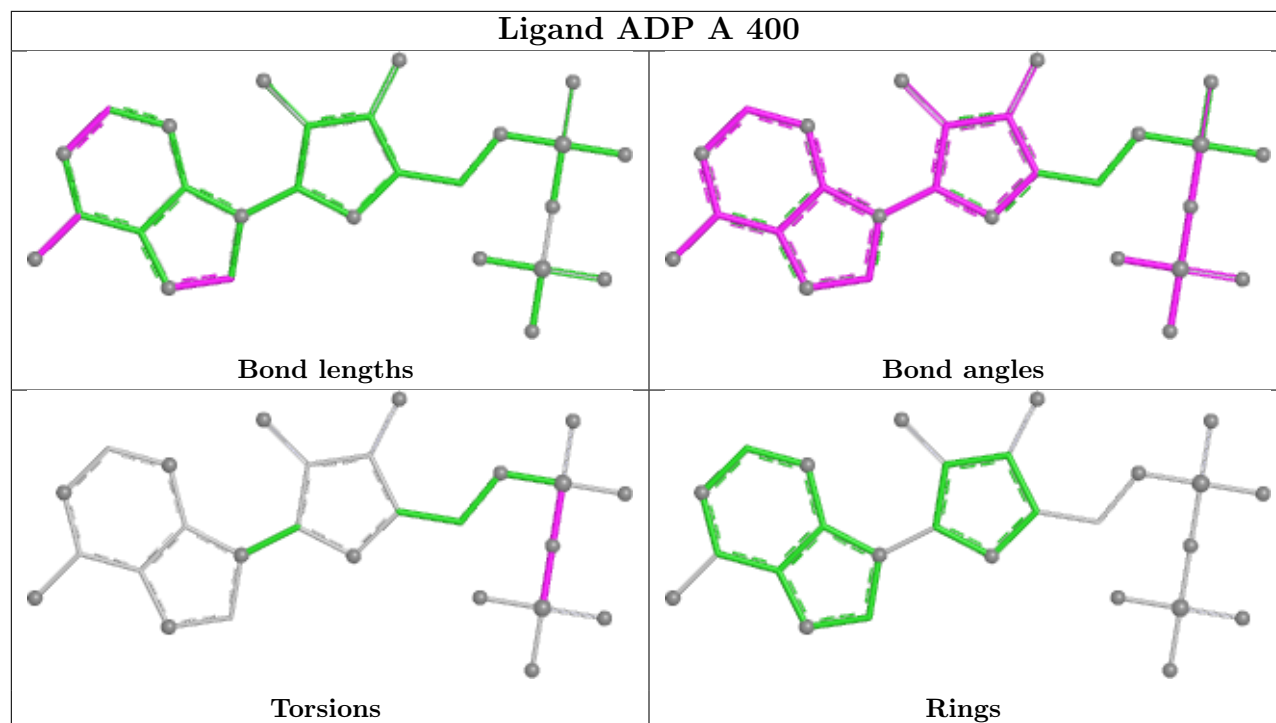


Ligand AIR D 402



Ligand AIR A 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	381/403 (94%)	0.19	26 (6%) 23 22	7, 25, 59, 79	5 (1%)
1	B	376/403 (93%)	0.46	42 (11%) 10 9	8, 28, 72, 93	6 (1%)
1	C	382/403 (94%)	0.26	23 (6%) 27 26	10, 26, 61, 84	6 (1%)
1	D	373/403 (92%)	0.51	43 (11%) 9 8	10, 29, 71, 90	1 (0%)
All	All	1512/1612 (93%)	0.35	134 (8%) 15 14	7, 27, 67, 93	18 (1%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	319	GLY	4.8
1	D	322	PRO	4.7
1	D	35	ALA	4.4
1	B	322	PRO	4.3
1	B	320	ALA	4.3
1	B	75	GLU	4.3
1	D	156	GLY	4.1
1	B	54	PHE	3.9
1	C	37	ASN	3.9
1	D	150	MET	3.9
1	C	381	ILE	3.8
1	A	381	ILE	3.8
1	D	1	MET	3.8
1	A	125	VAL	3.7
1	A	324	THR	3.7
1	B	129	PRO	3.6
1	D	74	ILE	3.5
1	C	125	VAL	3.5
1	C	325	HIS	3.4
1	D	164	ASP	3.4
1	C	87	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	322	PRO	3.3
1	D	320	ALA	3.3
1	A	322	PRO	3.3
1	B	133	ALA	3.2
1	D	175	ASP	3.2
1	B	85	VAL	3.2
1	A	321	ALA	3.1
1	B	346	GLY	3.1
1	B	1	MET	3.1
1	D	47	ASP	3.1
1	C	321	ALA	3.1
1	D	163	GLN	3.1
1	B	172	ALA	3.0
1	B	125	VAL	3.0
1	B	226	VAL	3.0
1	D	170	LEU	3.0
1	B	80	TYR	3.0
1	D	52	GLY	2.9
1	D	325	HIS	2.9
1	B	177	PRO	2.9
1	B	81	ALA	2.9
1	C	324	THR	2.9
1	A	246	ASP	2.8
1	D	54	PHE	2.8
1	B	89	VAL	2.8
1	A	4	SER	2.8
1	A	129	PRO	2.8
1	C	67	CYS	2.8
1	D	177	PRO	2.8
1	A	320	ALA	2.8
1	B	52	GLY	2.7
1	A	180	ALA	2.7
1	A	114	TYR	2.7
1	D	112	ARG	2.7
1	B	163	GLN	2.7
1	C	89	VAL	2.7
1	D	66	THR	2.6
1	B	86	ALA	2.6
1	A	112	ARG	2.6
1	D	85	VAL	2.6
1	D	171	GLU	2.6
1	A	347	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	143	LEU	2.6
1	A	141	TYR	2.5
1	B	158	PHE	2.5
1	B	325	HIS	2.5
1	B	37	ASN	2.5
1	C	380	ARG	2.5
1	D	176	ARG	2.5
1	B	323	ASP	2.5
1	B	149	THR	2.5
1	D	128	THR	2.5
1	D	158	PHE	2.5
1	C	163	GLN	2.5
1	B	175	ASP	2.4
1	B	324	THR	2.4
1	C	61	ARG	2.4
1	C	1	MET	2.4
1	A	1	MET	2.4
1	D	65	LYS	2.4
1	D	129	PRO	2.4
1	C	65[A]	LYS	2.3
1	C	166	ILE	2.3
1	A	183	TRP	2.3
1	B	95	TRP	2.3
1	B	321	ALA	2.3
1	B	380	ARG	2.3
1	D	174	LYS	2.3
1	D	162	SER	2.3
1	B	176	ARG	2.3
1	D	380	ARG	2.3
1	A	184	ALA	2.3
1	A	323	ASP	2.3
1	A	258	LEU	2.3
1	B	135	VAL	2.2
1	D	50	VAL	2.2
1	B	231	ASN	2.2
1	D	135	VAL	2.2
1	D	178	LEU	2.2
1	D	95	TRP	2.2
1	D	172	ALA	2.2
1	D	173	LEU	2.2
1	B	47	ASP	2.2
1	A	137	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	351	GLY	2.1
1	A	130	ALA	2.1
1	A	185	TYR	2.1
1	B	157	ASN	2.1
1	A	232	GLN	2.1
1	B	381	ILE	2.1
1	D	272	ILE	2.1
1	D	81	ALA	2.1
1	B	174	LYS	2.1
1	D	36	ASP	2.1
1	C	185	TYR	2.1
1	B	112	ARG	2.1
1	B	155	ARG	2.1
1	A	65[A]	LYS	2.1
1	C	88	GLU	2.1
1	A	167	PRO	2.1
1	C	129	PRO	2.1
1	D	57	ARG	2.1
1	D	77	VAL	2.1
1	B	59	ALA	2.1
1	C	172	ALA	2.1
1	A	225	ASN	2.0
1	D	37	ASN	2.0
1	C	382	ARG	2.0
1	C	198	LYS	2.0
1	C	140	GLY	2.0
1	B	348	ALA	2.0
1	B	90	LYS	2.0
1	B	114	TYR	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 oligosaccharides in this entry.

6.4 Ligands

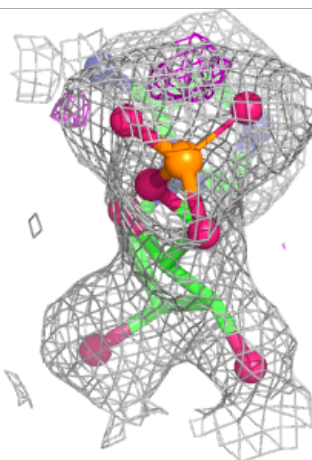
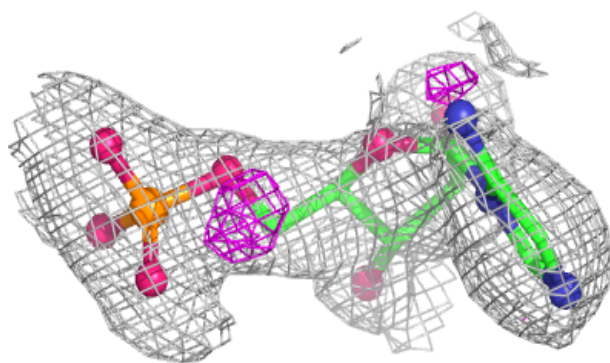
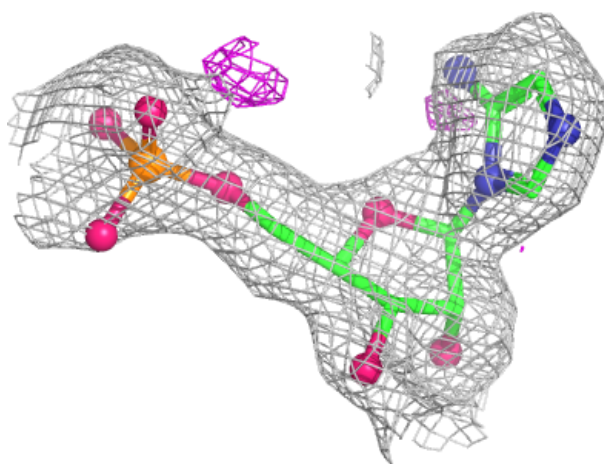
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	384	1/1	0.90	0.09	37,37,37,37	0
6	AIR	D	402	19/19	0.92	0.12	14,45,99,99	0
4	ADP	D	400	27/27	0.95	0.08	8,29,56,98	0
4	ADP	B	400	27/27	0.95	0.09	4,35,63,99	0
3	NHE	C	384	13/13	0.96	0.12	17,37,56,77	0
6	AIR	B	402	19/19	0.96	0.09	2,34,99,99	0
3	NHE	A	385	13/13	0.96	0.12	15,30,99,99	0
6	AIR	A	402	19/19	0.97	0.05	1,15,23,23	0
5	MG	B	401	1/1	0.97	0.05	27,27,27,27	0
6	AIR	C	402	19/19	0.97	0.06	4,13,32,38	0
5	MG	D	401	1/1	0.97	0.03	31,31,31,31	0
5	MG	C	401	1/1	0.98	0.04	18,18,18,18	0
5	MG	A	401	1/1	0.98	0.03	14,14,14,14	0
4	ADP	C	400	27/27	0.98	0.06	4,21,41,47	0
4	ADP	A	400	27/27	0.99	0.06	6,19,31,99	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.

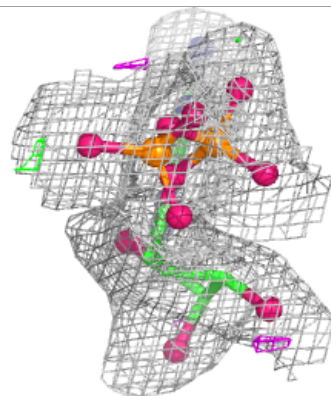
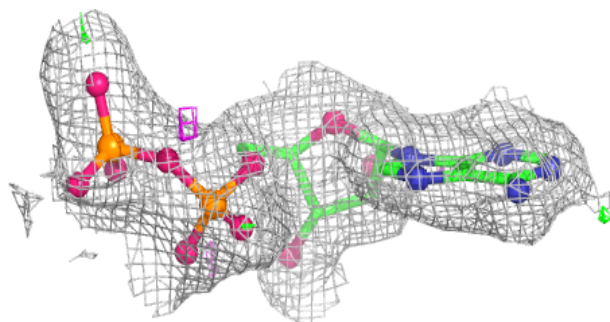
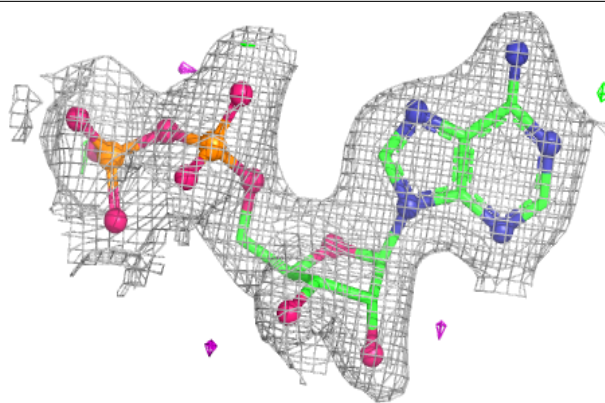
Electron density around AIR D 402:

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

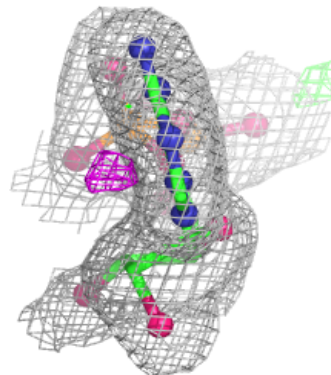
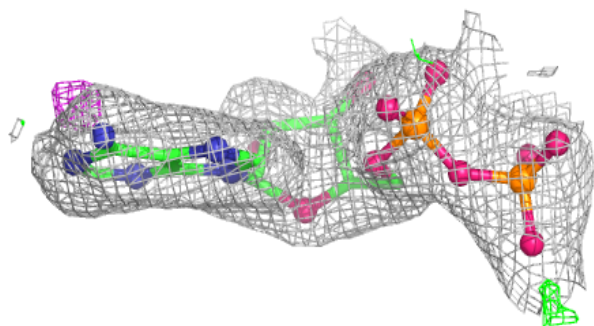
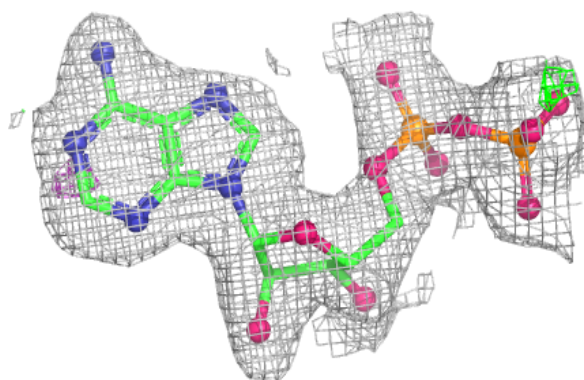


Electron density around ADP D 400:

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

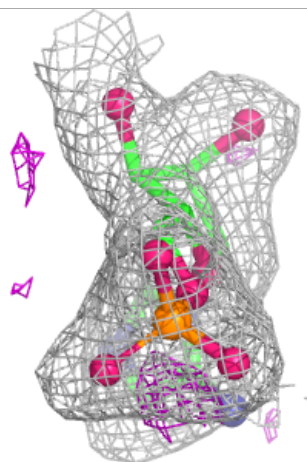
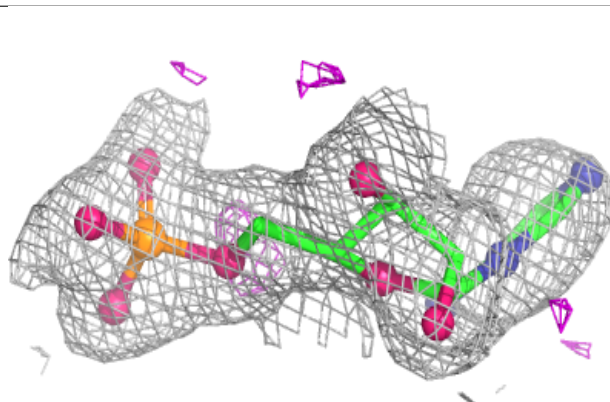
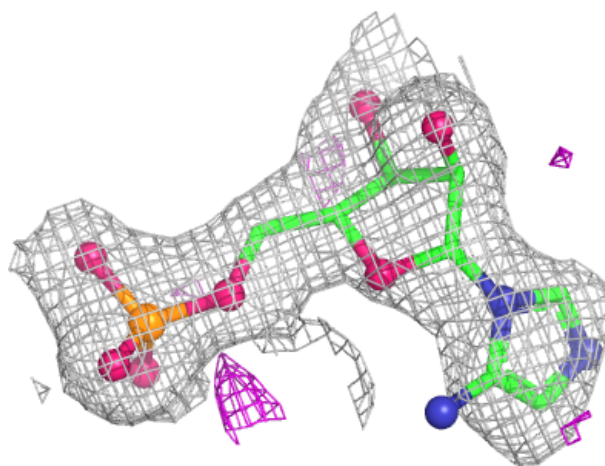
**Electron density around ADP B 400:**

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and green (positive)



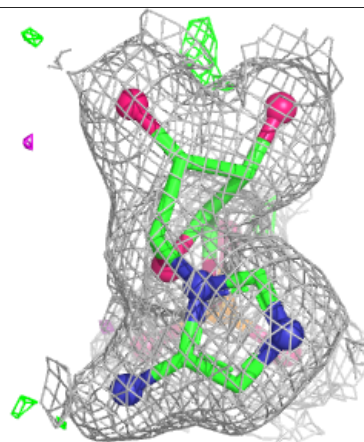
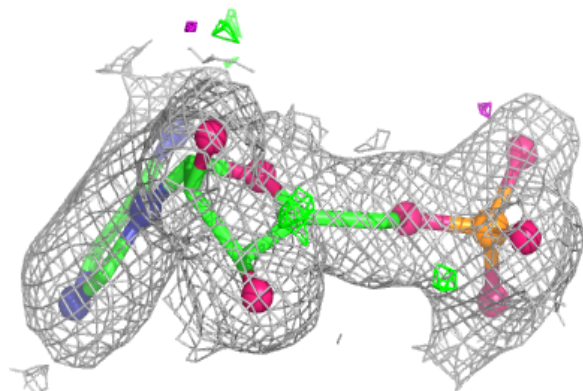
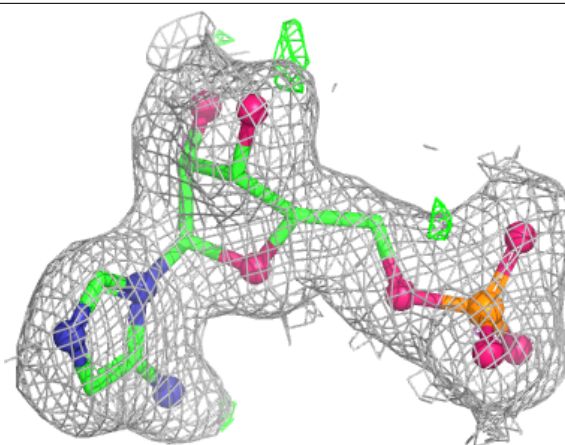
Electron density around AIR B 402:

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



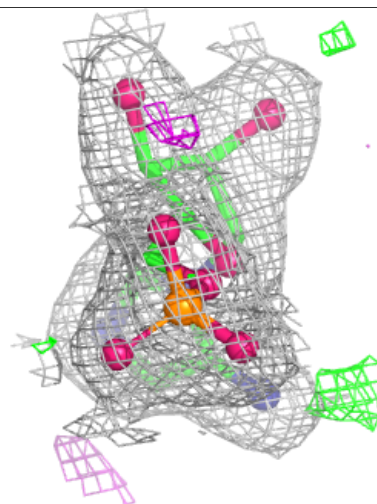
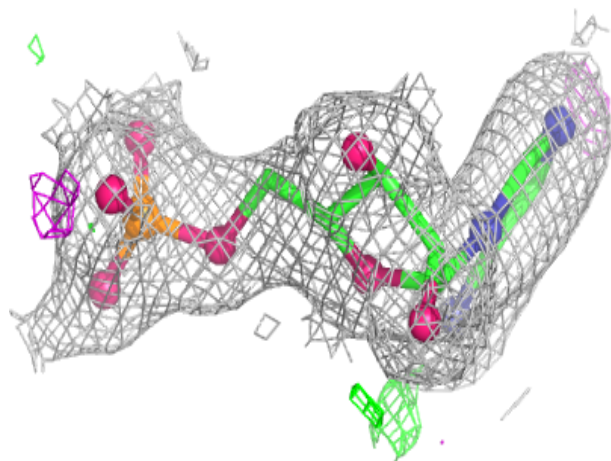
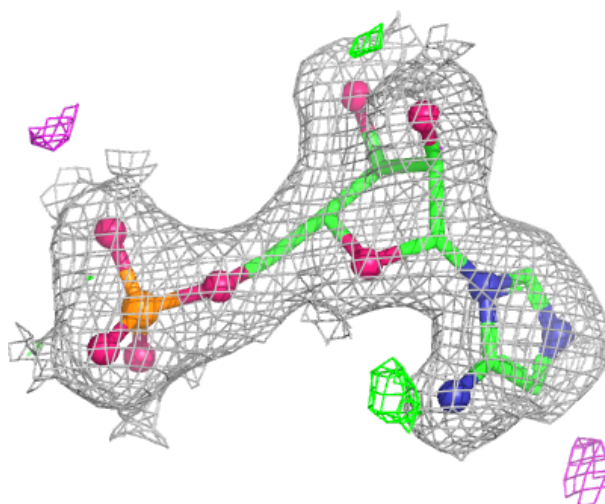
Electron density around AIR A 402:

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



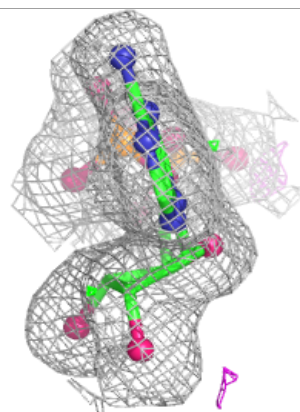
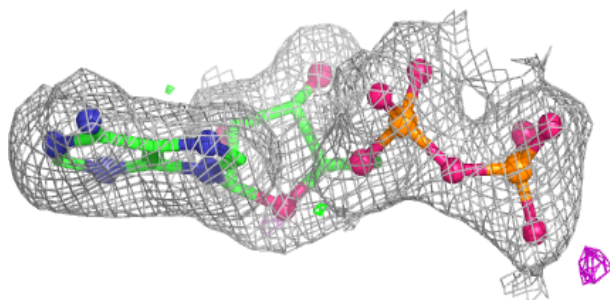
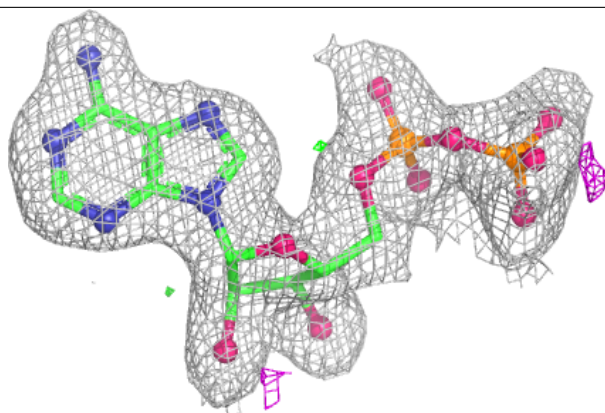
Electron density around AIR C 402:

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

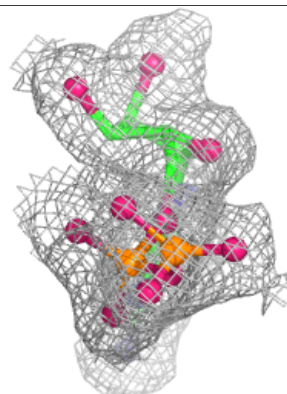
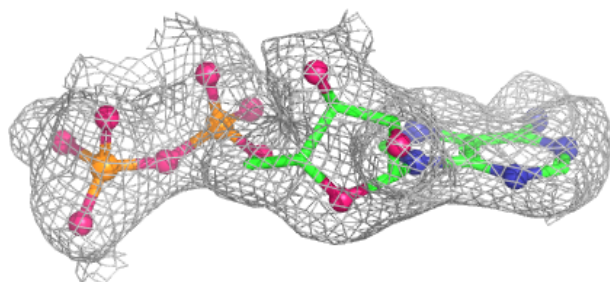
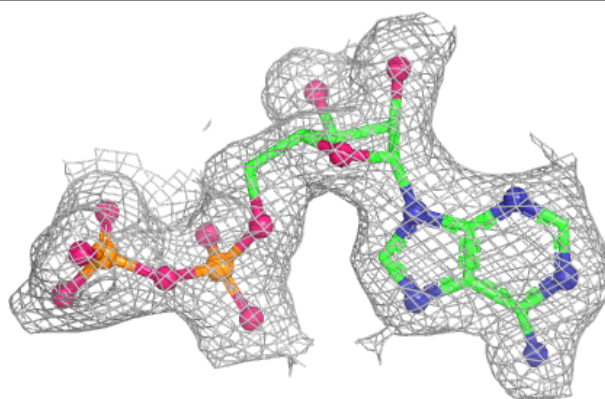


Electron density around ADP C 400:

$2mF_o-DF_c$ (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.