



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:22 AM UTC

PDB ID : 4XRU / pdb_00004xru
Title : Structure of Pnkp1/Rnl/Hen1 complex
Authors : Wang, P.
Deposited on : 2015-01-21
Resolution : 3.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

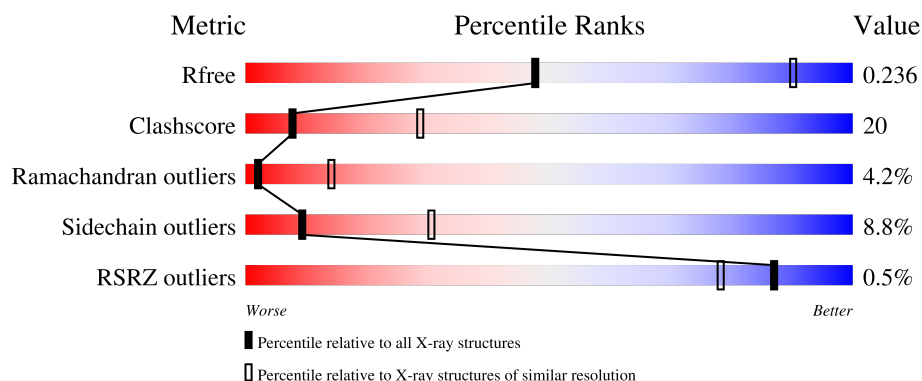
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	312	50% 38% 7%
1	D	312	50% 36% 6% 8%
2	B	394	% 54% 36% 8% %
2	E	394	% 49% 41% 8% %
3	C	436	54% 36% 6% %

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Mol	Chain	Length	Quality of chain
3	F	436	51% 37% 8% ••

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18713 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 Pnkp1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	Se	0	0	0
			2388	1524	405	448	3	8			
1	D	287	Total	C	N	O	S	Se	0	0	0
			2358	1506	399	443	2	8			

- Molecule 2 is a protein called Rnl.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S		0	0	0
			3290	2117	556	608	9				
2	E	393	Total	C	N	O	S		0	0	0
			3282	2112	555	607	8				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	THR	ALA	conflict	UNP C2M8N4
B	329	GLU	GLN	conflict	UNP C2M8N4
E	269	THR	ALA	conflict	UNP C2M8N4
E	329	GLU	GLN	conflict	UNP C2M8N4

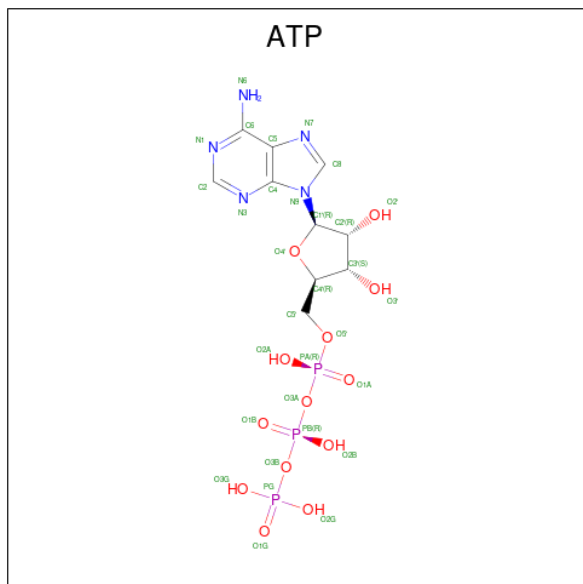
- Molecule 3 is a protein called Hen1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	424	Total	C	N	O	S		0	0	0
			3536	2286	579	654	17				
3	F	424	Total	C	N	O	S		0	0	0
			3536	2286	579	654	17				

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 5 13 3	0	0
5	B	1	Total C N O P 31 10 5 13 3	0	0
5	D	1	Total C N O P 31 10 5 13 3	0	0
5	E	1	Total C N O P 31 10 5 13 3	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



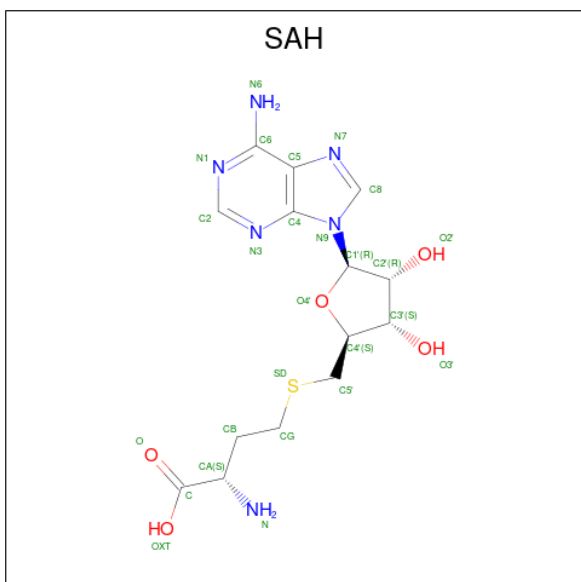
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	E	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		
8	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
9	F	1	Total	C	N	O	S	5	0
			26	14	6	5	1		

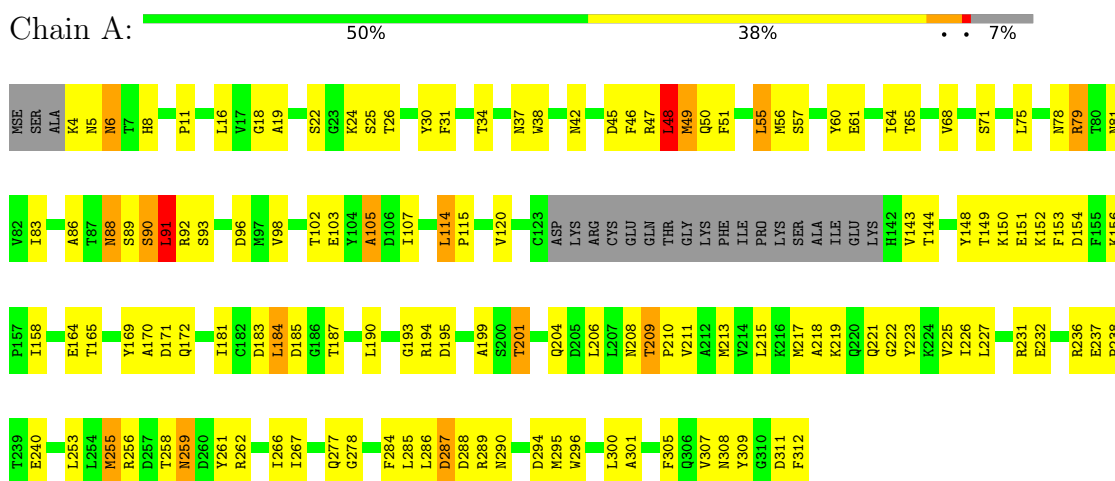
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	8	Total	O	0	0
			8	8		
10	B	28	Total	O	0	0
			28	28		
10	C	16	Total	O	0	0
			16	16		
10	D	10	Total	O	0	0
			10	10		
10	E	17	Total	O	0	0
			17	17		
10	F	13	Total	O	0	0
			13	13		

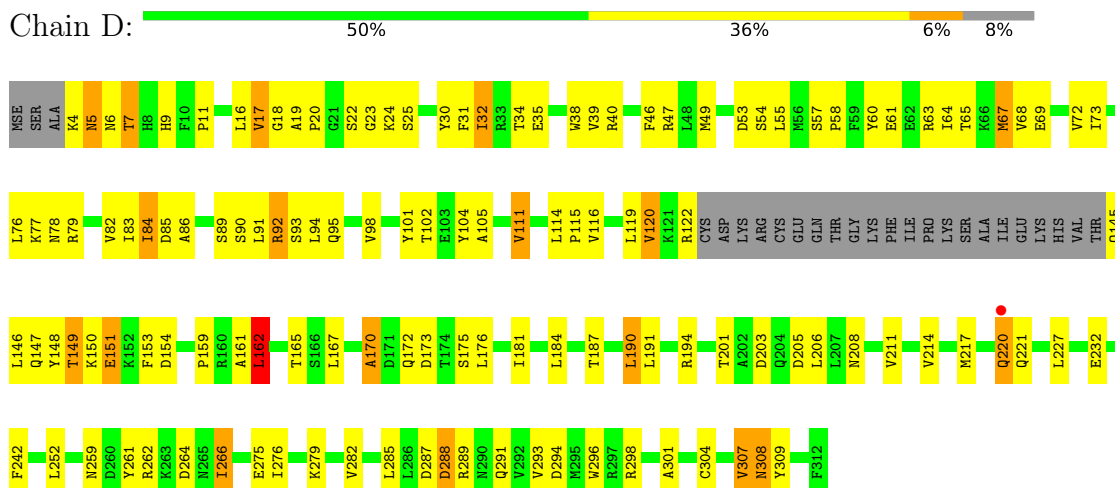
3 Residue-property plots

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

• Molecule 1: Pnkp1

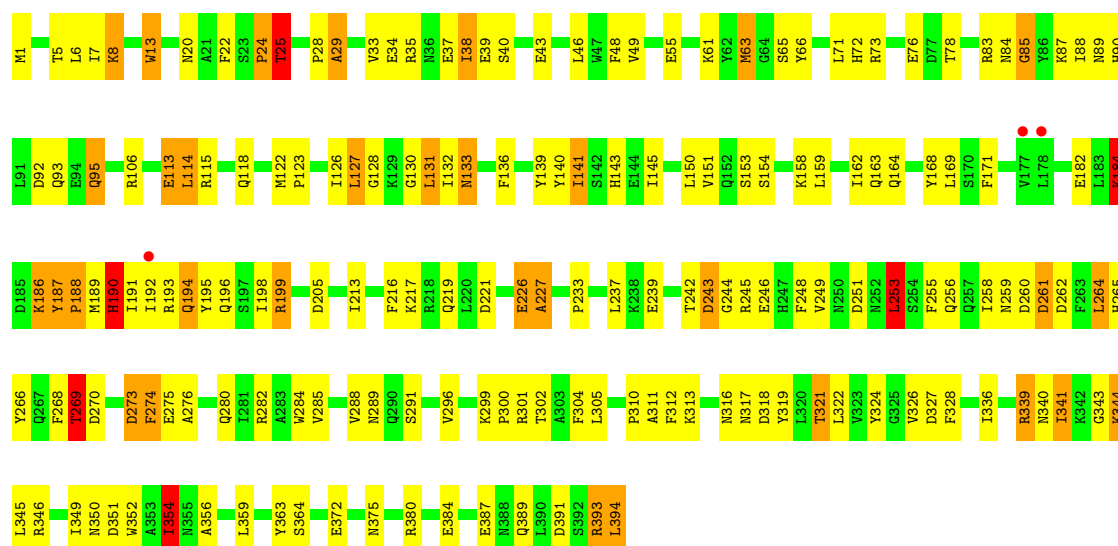


• Molecule 1: Pnkp1

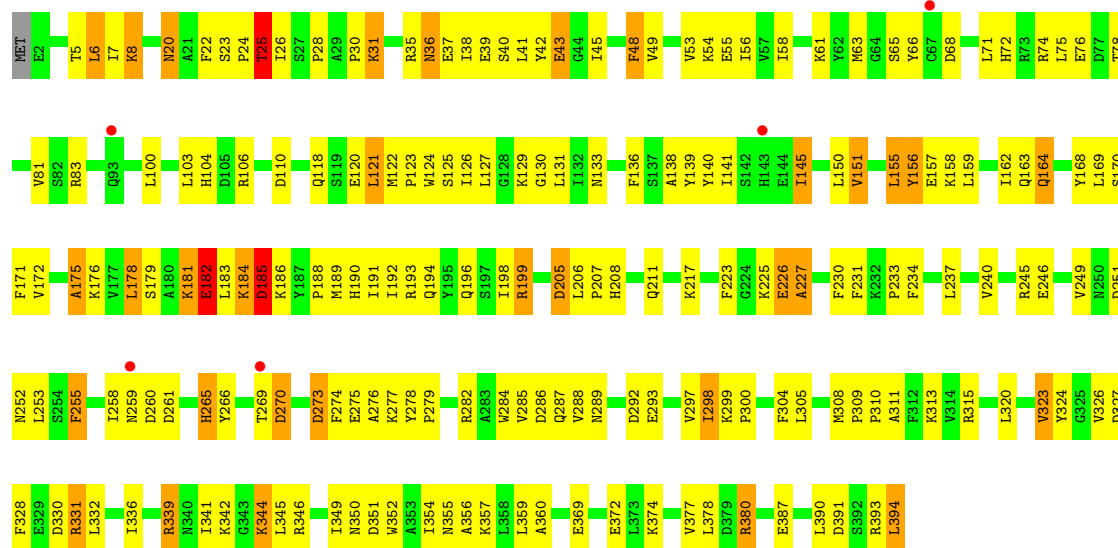


• Molecule 2: Rnl

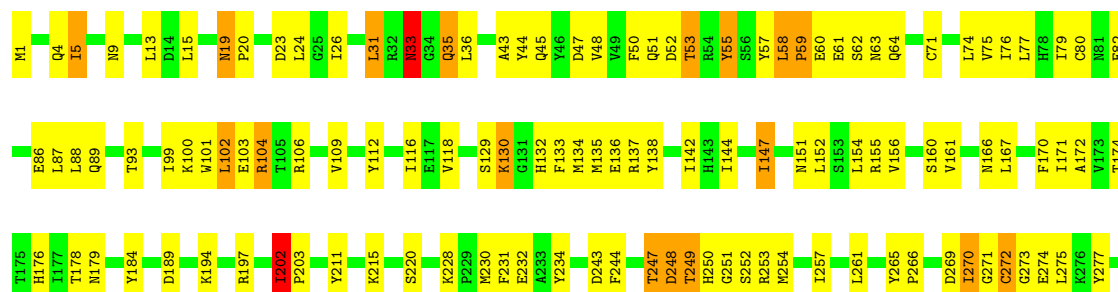


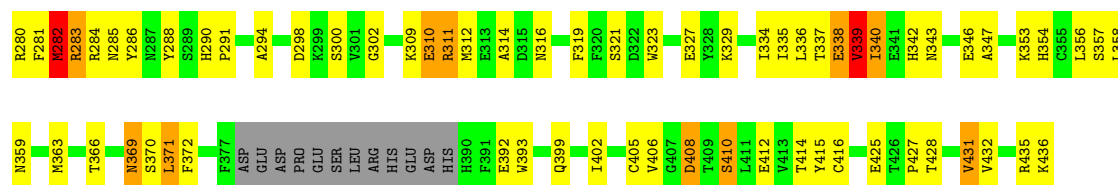


• Molecule 2: Rnl



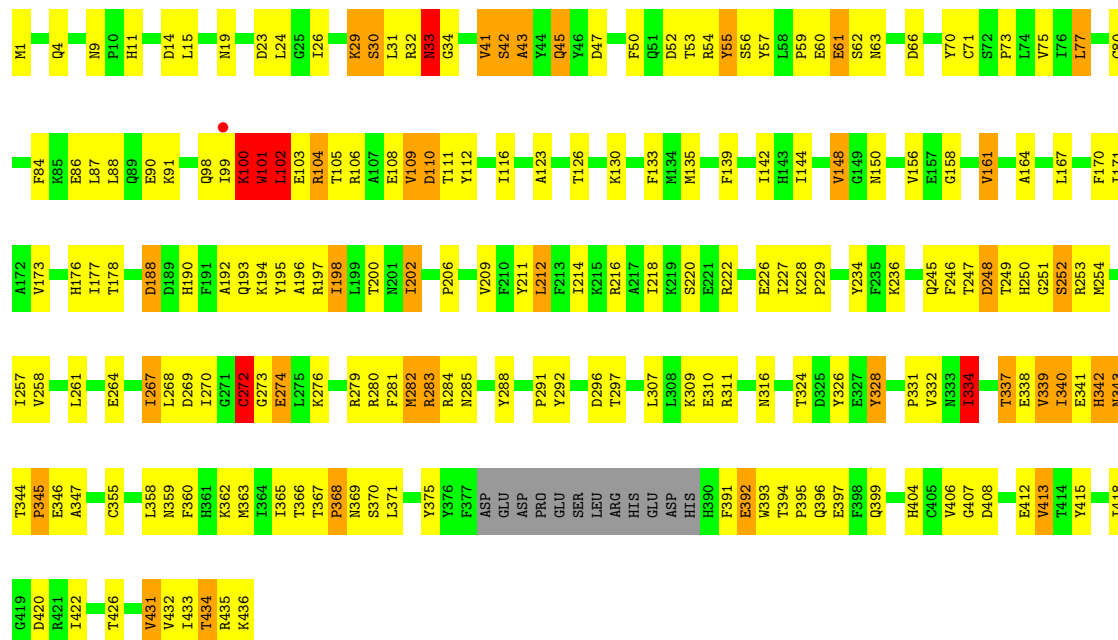
• Molecule 3: Hen1





• Molecule 3: Hen1

Chain F: 51% 37% 8% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.48Å 187.25Å 112.00Å 90.00° 106.04° 90.00°	Depositor
Resolution (Å)	42.93 – 3.41 42.93 – 3.41	Depositor EDS
% Data completeness (in resolution range)	98.2 (42.93-3.41) 94.8 (42.93-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.176 , 0.233 0.182 , 0.236	Depositor DCC
R_{free} test set	2178 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	103.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for l,k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18713	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: MES, GOL, PO4, ATP, SAH, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/2427	0.98	12/3266 (0.4%)
1	D	0.55	0/2396	1.02	9/3223 (0.3%)
2	B	0.70	1/3367 (0.0%)	1.13	20/4547 (0.4%)
2	E	0.60	0/3359	1.07	16/4537 (0.4%)
3	C	0.62	1/3634 (0.0%)	1.11	23/4928 (0.5%)
3	F	0.68	0/3634	1.17	28/4928 (0.6%)
All	All	0.62	2/18817 (0.0%)	1.09	108/25429 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	2
3	C	0	2
3	F	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	338	GLU	CA-C	-6.12	1.49	1.52
2	B	269	THR	CA-CB	5.57	1.62	1.53

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194	LYS	N-CA-C	-12.77	100.07	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	194	LYS	N-CA-C	-11.48	100.28	114.75
3	F	273	GLY	N-CA-C	-11.45	97.89	112.54
3	F	43	ALA	N-CA-C	-10.09	97.51	110.53
3	C	202	ILE	CA-C-N	-9.72	107.69	119.84
3	C	202	ILE	C-N-CA	-9.72	107.69	119.84
3	F	347	ALA	N-CA-C	-9.62	101.22	113.16
2	B	131	LEU	N-CA-C	-9.45	101.06	111.36
3	C	347	ALA	N-CA-C	-8.59	102.70	113.01
1	D	93	SER	N-CA-C	-8.35	102.65	113.17
1	D	19	ALA	CA-C-N	8.09	129.96	119.84
1	D	19	ALA	C-N-CA	8.09	129.96	119.84
1	D	151	GLU	N-CA-C	7.96	120.22	108.60
3	F	272	CYS	N-CA-C	7.76	120.99	107.49
3	F	202	ILE	CA-C-N	-7.51	112.47	120.66
3	F	202	ILE	C-N-CA	-7.51	112.47	120.66
3	F	161	VAL	N-CA-C	-7.51	103.47	110.53
3	C	252	SER	N-CA-C	-7.50	103.08	111.71
3	F	274	GLU	N-CA-C	7.38	121.98	113.19
3	C	265	TYR	CA-C-N	7.34	127.38	119.90
3	C	265	TYR	C-N-CA	7.34	127.38	119.90
1	A	156	LYS	CA-C-N	7.33	127.37	119.90
1	A	156	LYS	C-N-CA	7.33	127.37	119.90
2	B	273	ASP	N-CA-C	-7.22	104.28	113.23
3	C	132	HIS	N-CA-C	7.22	120.85	109.81
3	F	248	ASP	N-CA-C	7.15	118.62	108.54
3	C	43	ALA	N-CA-C	-7.13	100.52	110.35
2	E	261	ASP	N-CA-C	-7.10	104.61	113.20
1	D	5	ASN	N-CA-C	7.08	118.52	108.54
2	B	29	ALA	CA-C-N	7.05	127.08	119.89
2	B	29	ALA	C-N-CA	7.05	127.08	119.89
3	C	272	CYS	N-CA-C	6.87	119.69	107.80
2	E	273	ASP	N-CA-C	-6.75	104.52	112.89
3	F	55	TYR	N-CA-C	6.73	120.78	111.90
2	B	88	ILE	CB-CA-C	-6.72	102.72	111.25
2	E	176	LYS	N-CA-C	-6.65	105.17	113.28
2	E	131	LEU	N-CA-C	-6.62	104.14	111.36
3	C	33	ASN	N-CA-C	6.58	120.00	112.57
2	E	226	GLU	CA-C-N	6.56	133.51	121.70
2	E	226	GLU	C-N-CA	6.56	133.51	121.70
3	F	66	ASP	N-CA-C	6.52	120.08	110.30
3	C	310	GLU	N-CA-C	6.52	120.89	112.41
3	C	58	LEU	CA-C-N	6.49	127.95	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	58	LEU	C-N-CA	6.49	127.95	119.84
3	F	310	GLU	N-CA-C	-6.37	106.22	112.97
2	B	85	GLY	N-CA-C	6.35	123.19	115.31
3	F	45	GLN	N-CA-C	6.33	119.01	108.13
2	B	136	PHE	N-CA-C	6.25	117.76	111.07
2	B	133	ASN	N-CA-C	6.22	118.61	111.02
2	E	136	PHE	N-CA-C	6.20	117.71	111.07
2	B	261	ASP	N-CA-C	-6.14	104.90	113.37
3	F	252	SER	N-CA-C	-6.12	104.61	111.28
3	F	19	ASN	CA-C-N	6.04	125.92	119.28
3	F	19	ASN	C-N-CA	6.04	125.92	119.28
1	A	105	ALA	N-CA-C	6.02	117.38	108.60
3	C	248	ASP	N-CA-C	6.01	118.56	107.73
3	F	42	SER	N-CA-C	-5.97	99.45	107.88
1	A	6	ASN	N-CA-C	5.96	119.30	110.48
1	A	48	LEU	N-CA-C	-5.87	105.88	114.39
3	F	63	ASN	N-CA-C	5.84	118.83	110.24
2	B	354	ILE	N-CA-C	-5.80	104.68	111.00
3	F	102	LEU	N-CA-C	5.78	123.11	110.80
2	E	25	THR	N-CA-C	-5.76	103.10	110.53
2	B	25	THR	N-CA-C	-5.72	102.44	110.50
2	B	253	LEU	N-CA-C	-5.62	106.08	113.17
3	C	270	ILE	N-CA-C	5.62	116.68	111.45
2	E	323	VAL	CB-CA-C	-5.61	104.69	112.04
2	B	274	PHE	N-CA-C	-5.60	102.73	110.35
1	D	307	VAL	CB-CA-C	-5.57	103.03	111.33
3	C	147	ILE	N-CA-C	-5.55	106.27	111.48
1	A	195	ASP	CA-C-N	5.52	124.98	119.24
1	A	195	ASP	C-N-CA	5.52	124.98	119.24
1	A	164	GLU	N-CA-C	5.51	118.17	107.71
3	F	61	GLU	N-CA-C	-5.49	99.11	110.80
1	A	307	VAL	N-CA-C	5.47	116.13	110.82
2	E	182	GLU	N-CA-C	5.45	122.41	110.80
2	E	145	ILE	CB-CA-C	-5.45	105.00	111.97
2	E	139	TYR	N-CA-C	-5.43	105.05	110.97
1	A	114	LEU	CA-C-N	5.39	126.58	119.84
1	A	114	LEU	C-N-CA	5.39	126.58	119.84
2	B	226	GLU	CA-C-N	5.39	131.41	121.70
2	B	226	GLU	C-N-CA	5.39	131.41	121.70
1	D	49	MSE	N-CA-C	-5.38	106.22	112.89
2	B	340	ASN	N-CA-C	5.33	116.13	107.23
3	C	33	ASN	CA-C-N	5.30	131.23	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	33	ASN	C-N-CA	5.30	131.23	121.70
2	B	145	ILE	CB-CA-C	-5.28	104.95	111.70
3	F	394	THR	CA-C-N	-5.25	115.17	120.21
3	F	394	THR	C-N-CA	-5.25	115.17	120.21
3	F	426	THR	CA-C-N	-5.25	113.27	119.84
3	F	426	THR	C-N-CA	-5.25	113.27	119.84
2	B	393	ARG	N-CA-C	-5.24	105.60	112.41
3	C	19	ASN	CA-C-N	5.19	125.27	119.87
3	C	19	ASN	C-N-CA	5.19	125.27	119.87
1	D	275	GLU	N-CA-C	5.18	117.72	111.40
1	A	49	MSE	N-CA-C	-5.17	105.55	111.14
3	C	371	LEU	N-CA-C	-5.17	106.81	113.01
2	B	344	LYS	N-CA-C	-5.10	105.41	110.97
3	F	334	ILE	N-CA-C	5.08	115.79	108.48
2	E	265	HIS	N-CA-C	5.07	116.00	108.60
1	D	58	PRO	N-CA-C	-5.06	107.54	113.86
2	E	270	ASP	N-CA-C	5.06	116.77	108.52
2	B	384	GLU	N-CA-C	-5.05	105.66	111.07
3	F	367	THR	CA-C-N	5.02	126.11	119.84
3	F	367	THR	C-N-CA	5.02	126.11	119.84
2	E	292	ASP	N-CA-C	5.01	118.70	112.58
3	C	130	LYS	N-CA-C	5.01	116.99	110.43
2	E	276	ALA	N-CA-C	-5.00	107.02	113.23

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	129	SER	Peptide
3	C	342	HIS	Peptide
1	D	92	ARG	Peptide
2	E	181	LYS	Peptide
2	E	185	ASP	Peptide
3	F	101	TRP	Peptide
3	F	272	CYS	Peptide

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	2388	0	2380	84	0
1	D	2358	0	2352	87	0
2	B	3290	0	3251	135	0
2	E	3282	0	3239	170	0
3	C	3536	0	3410	131	0
3	F	3536	0	3410	169	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	31	0	12	2	0
5	B	31	0	12	5	0
5	D	31	0	12	2	0
5	E	31	0	12	5	0
6	B	12	0	12	3	0
7	B	12	0	16	2	0
8	B	5	0	0	0	0
8	C	5	0	0	0	0
8	E	5	0	0	1	0
8	F	10	0	0	0	0
9	C	26	0	19	1	0
9	F	26	0	19	1	0
10	A	8	0	0	1	0
10	B	28	0	0	1	0
10	C	16	0	0	1	0
10	D	10	0	0	0	0
10	E	17	0	0	1	0
10	F	13	0	0	0	0
All	All	18713	0	18156	734	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 20.

All (734) 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)
2:B:339:ARG:HG3	2:B:339:ARG:HH11	1.01	1.09
2:E:72:HIS:H	2:E:78:THR:HG22	1.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:ARG:HH22	2:E:394:LEU:HA	1.29	0.95
2:B:339:ARG:HG3	2:B:339:ARG:NH1	1.76	0.92
2:B:72:HIS:H	2:B:78:THR:HG22	1.31	0.92
2:E:125:SER:HB2	2:E:129:LYS:HB2	1.53	0.91
3:F:142:ILE:HD12	3:F:171:ILE:HD11	1.51	0.91
3:F:334:ILE:HB	3:F:363:MET:HG3	1.54	0.89
2:E:391:ASP:HB3	2:E:394:LEU:HD11	1.57	0.87
3:F:80:CYS:HB3	3:F:88:LEU:HD11	1.57	0.84
3:C:251:GLY:HA2	3:C:254:MET:HB3	1.60	0.83
3:F:267:ILE:HG21	3:F:280:ARG:HH12	1.43	0.82
1:D:173:ASP:OD2	1:D:175:SER:OG	1.99	0.81
2:B:130:GLY:HA2	2:B:133:ASN:HB2	1.63	0.80
2:E:269:THR:HB	2:E:274:PHE:HB2	1.64	0.80
3:C:269:ASP:OD2	3:C:272:CYS:HB3	1.81	0.79
2:B:196:GLN:HG3	2:B:199:ARG:HH21	1.48	0.78
3:F:369:ASN:O	3:F:369:ASN:ND2	2.15	0.78
2:B:193:ARG:HH21	2:B:194:GLN:HG3	1.47	0.77
2:E:25:THR:OG1	2:E:387:GLU:OE2	2.03	0.76
2:E:35:ARG:O	2:E:36:ASN:ND2	2.16	0.76
2:E:158:LYS:HD3	3:F:24:LEU:HB3	1.68	0.74
3:F:274:GLU:OE2	3:F:274:GLU:HA	1.86	0.74
2:B:380:ARG:NH2	2:B:387:GLU:OE2	2.21	0.73
3:C:33:ASN:O	3:C:53:THR:OG1	2.06	0.73
1:A:262:ARG:HH21	3:F:291:PRO:HD3	1.53	0.72
2:B:122:MET:HG3	2:B:123:PRO:HA	1.71	0.72
3:F:413:VAL:HG22	3:F:433:ILE:HG12	1.72	0.72
2:E:182:GLU:HB3	2:E:183:LEU:C	2.14	0.72
2:E:61:LYS:HZ1	5:E:501:ATP:PA	2.13	0.72
1:A:114:LEU:HD12	1:A:115:PRO:HD2	1.70	0.72
2:E:30:PRO:O	2:E:40:SER:OG	2.07	0.72
2:B:393:ARG:HH11	3:C:63:ASN:HB3	1.55	0.72
3:C:9:ASN:HD22	3:C:112:TYR:HB2	1.54	0.72
3:F:84:PHE:HB3	3:F:87:LEU:HD12	1.72	0.72
3:F:393:TRP:HB3	3:F:397:GLU:HB3	1.71	0.72
3:C:80:CYS:HB3	3:C:88:LEU:HD11	1.70	0.71
3:F:133:PHE:HB2	3:F:144:ILE:HG13	1.72	0.71
3:C:253:ARG:HG2	3:C:257:ILE:HD11	1.71	0.71
3:F:342:HIS:O	3:F:343:ASN:ND2	2.23	0.71
3:C:86:GLU:N	3:C:86:GLU:OE2	2.24	0.70
2:E:74:ARG:HD2	2:E:76:GLU:OE2	1.91	0.70
2:B:269:THR:HB	2:B:274:PHE:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:91:LYS:NZ	3:F:91:LYS:HB3	2.07	0.69
2:B:237:LEU:HD13	2:B:359:LEU:HD11	1.73	0.69
2:B:339:ARG:HH11	2:B:339:ARG:CG	1.91	0.69
2:E:226:GLU:HA	2:E:227:ALA:HB2	1.75	0.69
3:C:228:LYS:HE3	3:C:232:GLU:OE2	1.91	0.69
3:F:369:ASN:O	3:F:371:LEU:N	2.26	0.68
2:B:310:PRO:HB3	2:B:352:TRP:CG	2.29	0.68
2:E:342:LYS:HB3	2:E:346:ARG:NH1	2.09	0.68
3:F:267:ILE:HD11	3:F:292:TYR:CE1	2.29	0.67
3:F:251:GLY:HA2	3:F:254:MET:HB3	1.75	0.67
3:C:156:VAL:HG13	3:C:167:LEU:HD23	1.75	0.67
2:E:315:ARG:NH2	2:E:394:LEU:HA	2.06	0.67
1:A:184:LEU:HD11	1:A:227:LEU:HD13	1.76	0.67
2:B:246:GLU:OE2	2:B:363:TYR:N	2.27	0.67
1:D:25:SER:HB2	5:D:402:ATP:O2B	1.95	0.66
2:E:38:ILE:HG21	2:E:328:PHE:HZ	1.60	0.66
3:F:50:PHE:CE2	3:F:52:ASP:HB2	2.29	0.66
1:D:78:ASN:O	1:D:78:ASN:ND2	2.24	0.66
2:E:61:LYS:NZ	5:E:501:ATP:O5'	2.27	0.66
3:F:195:TYR:O	3:F:198:ILE:HG23	1.96	0.66
3:F:337:THR:O	3:F:366:THR:HB	1.95	0.66
2:E:178:LEU:HB2	2:E:181:LYS:HD2	1.78	0.65
3:C:9:ASN:HA	3:C:112:TYR:HD2	1.62	0.65
1:D:184:LEU:HD21	1:D:227:LEU:HD13	1.78	0.65
1:A:19:ALA:O	1:A:22:SER:OG	2.14	0.65
2:E:122:MET:HG3	2:E:123:PRO:HA	1.79	0.64
3:C:310:GLU:N	3:C:311:ARG:HA	2.12	0.64
2:E:273:ASP:OD1	2:E:277:LYS:NZ	2.31	0.64
3:F:135:MET:HE2	3:F:170:PHE:HE2	1.62	0.64
2:E:61:LYS:NZ	5:E:501:ATP:PA	2.69	0.64
3:F:100:LYS:HD3	3:F:102:LEU:H	1.62	0.64
2:E:189:MET:O	2:E:191:ILE:N	2.31	0.64
2:E:342:LYS:HB3	2:E:346:ARG:HH12	1.63	0.64
3:F:105:THR:HG22	3:F:108:GLU:HG3	1.80	0.63
1:A:193:GLY:N	1:D:165:THR:OG1	2.31	0.63
2:E:66:TYR:HD2	2:E:83:ARG:HA	1.63	0.63
1:A:49:MSE:O	1:D:40:ARG:HD3	1.99	0.63
2:E:189:MET:O	2:E:192:ILE:N	2.31	0.63
2:E:274:PHE:HA	2:E:277:LYS:HB2	1.81	0.63
2:B:72:HIS:N	2:B:78:THR:HG22	2.11	0.63
2:B:61:LYS:NZ	5:B:501:ATP:O5'	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:VAL:O	1:A:102:THR:HG22	1.99	0.63
3:F:267:ILE:HD11	3:F:292:TYR:CZ	2.34	0.63
2:B:71:LEU:HD12	2:B:78:THR:HG21	1.81	0.62
2:E:61:LYS:HB2	2:E:297:VAL:HG23	1.80	0.62
3:C:62:SER:HB3	3:C:184:TYR:CE2	2.35	0.62
2:E:285:VAL:O	2:E:289:ASN:ND2	2.32	0.62
3:F:52:ASP:OD2	3:F:53:THR:N	2.33	0.62
1:A:256:ARG:HG3	1:A:267:ILE:HG12	1.82	0.62
3:C:399:GLN:HG2	3:C:415:TYR:CE1	2.35	0.62
1:D:116:VAL:HG11	1:D:146:LEU:HA	1.80	0.62
3:F:281:PHE:HE1	3:F:288:TYR:CD2	2.16	0.62
3:F:9:ASN:HB2	3:F:112:TYR:HB2	1.81	0.62
3:F:264:GLU:OE1	3:F:264:GLU:N	2.31	0.62
2:E:41:LEU:HD11	2:E:285:VAL:HG21	1.82	0.62
3:F:188:ASP:OD1	3:F:190:HIS:N	2.26	0.61
2:E:28:PRO:HA	2:E:313:LYS:HG2	1.82	0.61
2:B:63:MET:N	2:B:122:MET:HE1	2.16	0.61
2:E:245:ARG:NH2	8:E:503:PO4:O1	2.33	0.61
3:C:174:THR:O	3:C:178:THR:HG22	2.01	0.61
3:F:368:PRO:HB2	3:F:392:GLU:HG2	1.82	0.61
2:B:55:GLU:OE1	2:B:266:TYR:OH	2.17	0.61
1:A:92:ARG:O	1:A:96:ASP:HB2	2.01	0.61
2:B:141:ILE:HG21	3:C:147:ILE:HG21	1.83	0.61
2:B:192:ILE:O	2:B:196:GLN:HB2	2.01	0.61
1:D:262:ARG:HH11	1:D:262:ARG:HG2	1.66	0.61
2:E:310:PRO:HB3	2:E:352:TRP:CD2	2.36	0.61
3:F:100:LYS:HD3	3:F:101:TRP:H	1.65	0.61
3:C:281:PHE:O	3:C:283:ARG:N	2.33	0.61
2:E:58:ILE:HD11	2:E:298:ILE:HD12	1.83	0.61
2:B:140:TYR:CZ	2:B:217:LYS:HD3	2.36	0.61
2:E:45:ILE:HG12	2:E:298:ILE:HD13	1.83	0.61
2:E:68:ASP:HB2	2:E:81:VAL:HG23	1.83	0.60
3:C:215:LYS:NZ	3:C:248:ASP:HA	2.16	0.60
3:F:279:ARG:HG3	3:F:279:ARG:HH11	1.67	0.60
3:C:302:GLY:HA2	3:C:319:PHE:CE2	2.36	0.60
1:D:89:SER:HA	1:D:94:LEU:HD21	1.84	0.60
3:C:369:ASN:O	3:C:369:ASN:ND2	2.35	0.60
1:A:217:MSE:HB2	1:D:221:GLN:HG3	1.84	0.60
3:F:106:ARG:HG2	3:F:106:ARG:HH11	1.67	0.60
2:B:171:PHE:HZ	2:B:192:ILE:HG23	1.66	0.59
1:D:214:VAL:HA	1:D:217:MSE:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:354:HIS:O	3:C:357:SER:OG	2.17	0.59
1:D:114:LEU:HB3	1:D:119:LEU:HD13	1.85	0.59
2:E:324:TYR:CE1	2:E:393:ARG:NH1	2.66	0.59
3:C:280:ARG:HB2	3:C:280:ARG:HH11	1.68	0.59
3:F:156:VAL:HG13	3:F:167:LEU:HD23	1.84	0.59
2:B:61:LYS:HE3	2:B:313:LYS:HB2	1.85	0.58
2:B:196:GLN:CG	2:B:199:ARG:HH21	2.15	0.58
2:E:23:SER:O	2:E:380:ARG:NH1	2.36	0.58
1:A:181:ILE:HD13	1:A:226:ILE:HB	1.84	0.58
1:A:221:GLN:O	1:A:223:TYR:N	2.36	0.58
2:E:249:VAL:HG12	2:E:251:ASP:H	1.69	0.58
2:B:61:LYS:NZ	5:B:501:ATP:PA	2.76	0.58
3:C:271:GLY:HA3	3:C:339:VAL:HG22	1.85	0.58
1:D:98:VAL:O	1:D:102:THR:OG1	2.16	0.58
3:F:104:ARG:HD2	3:F:108:GLU:CD	2.28	0.58
3:F:268:LEU:HB3	3:F:334:ILE:HG23	1.86	0.58
2:E:168:TYR:OH	2:E:199:ARG:HB2	2.03	0.57
2:E:255:PHE:CE2	2:E:260:ASP:HB3	2.39	0.57
1:A:308:ASN:CG	1:A:309:TYR:H	2.11	0.57
1:D:95:GLN:OE1	1:D:95:GLN:N	2.35	0.57
3:C:197:ARG:HG3	3:C:230:MET:SD	2.43	0.57
1:A:262:ARG:NH2	3:F:291:PRO:HD3	2.17	0.57
3:C:277:TYR:CE1	3:C:281:PHE:HE2	2.22	0.57
1:D:187:THR:HG22	1:D:211:VAL:HG11	1.84	0.57
2:E:68:ASP:HB2	2:E:81:VAL:CG2	2.34	0.57
2:E:304:PHE:CE1	2:E:356:ALA:HB2	2.39	0.57
2:E:344:LYS:HD2	2:E:394:LEU:HB2	1.87	0.57
2:E:320:LEU:HD23	2:E:323:VAL:HG21	1.86	0.57
3:F:346:GLU:N	3:F:346:GLU:OE1	2.37	0.57
3:F:32:ARG:HB2	3:F:56:SER:HB3	1.86	0.57
3:F:341:GLU:O	3:F:343:ASN:N	2.36	0.57
1:A:232:GLU:OE2	1:D:4:LYS:HG2	2.05	0.57
2:B:106:ARG:NH2	2:B:261:ASP:OD1	2.38	0.56
2:E:192:ILE:O	2:E:196:GLN:HB2	2.05	0.56
3:F:177:ILE:O	3:F:216:ARG:HD2	2.04	0.56
2:B:268:PHE:O	2:B:270:ASP:N	2.38	0.56
3:C:248:ASP:O	3:C:250:HIS:N	2.38	0.56
3:C:410:SER:O	3:C:410:SER:OG	2.17	0.56
3:F:338:GLU:OE2	3:F:366:THR:HG22	2.05	0.56
3:C:353:LYS:HG3	3:C:405:CYS:HB2	1.86	0.56
3:F:412:GLU:HB2	3:F:436:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:336:LEU:HD12	3:C:340:ILE:HG22	1.87	0.56
2:E:35:ARG:C	2:E:36:ASN:HD22	2.09	0.56
2:E:63:MET:HG2	2:E:223:PHE:HB3	1.87	0.56
2:E:63:MET:HE3	2:E:124:TRP:CD2	2.41	0.56
1:A:294:ASP:HA	1:D:309:TYR:OH	2.06	0.56
1:D:149:THR:OG1	1:D:151:GLU:OE1	2.24	0.56
1:A:150:LYS:HG3	1:A:152:LYS:HD3	1.88	0.56
3:F:362:LYS:HG3	3:F:434:THR:CG2	2.36	0.56
2:E:54:LYS:HA	2:E:270:ASP:HB2	1.88	0.56
3:F:269:ASP:OD2	3:F:272:CYS:HB3	2.06	0.56
3:F:341:GLU:C	3:F:343:ASN:H	2.13	0.56
3:C:402:ILE:HG13	3:C:431:VAL:HG11	1.87	0.55
2:B:193:ARG:HH21	2:B:194:GLN:CG	2.17	0.55
3:C:133:PHE:HB2	3:C:144:ILE:HG13	1.88	0.55
3:C:283:ARG:HG3	3:C:284:ARG:H	1.71	0.55
3:F:250:HIS:CE1	3:F:254:MET:HE2	2.42	0.55
1:A:30:TYR:CZ	1:A:34:THR:HG21	2.42	0.55
2:B:13:TRP:HA	2:B:13:TRP:CE3	2.41	0.55
2:B:280:GLN:N	2:B:280:GLN:OE1	2.39	0.55
3:C:215:LYS:NZ	3:C:247:THR:O	2.39	0.55
2:E:183:LEU:O	2:E:185:ASP:N	2.39	0.55
3:F:33:ASN:OD1	3:F:33:ASN:N	2.38	0.55
2:E:123:PRO:HD2	2:E:126:ILE:HG12	1.88	0.55
3:F:32:ARG:C	3:F:34:GLY:H	2.15	0.55
2:B:226:GLU:HA	2:B:227:ALA:HB2	1.88	0.55
2:E:158:LYS:HB3	3:F:26:ILE:HD11	1.88	0.55
1:A:218:ALA:O	1:A:223:TYR:HB2	2.07	0.54
2:B:171:PHE:CZ	2:B:192:ILE:HA	2.42	0.54
2:E:24:PRO:HA	2:E:351:ASP:HB3	1.89	0.54
1:A:98:VAL:HG13	1:A:107:ILE:HD12	1.89	0.54
3:F:222:ARG:NH1	3:F:226:GLU:OE2	2.41	0.54
3:F:248:ASP:O	3:F:250:HIS:N	2.39	0.54
2:B:128:GLY:O	2:B:132:ILE:HG13	2.08	0.54
3:C:282:MET:O	3:C:285:ASN:HB2	2.08	0.54
3:C:346:GLU:N	3:C:346:GLU:OE1	2.40	0.54
2:E:320:LEU:HD22	2:E:324:TYR:HE2	1.73	0.54
2:B:66:TYR:OH	2:B:118:GLN:NE2	2.39	0.54
3:C:62:SER:C	3:C:64:GLN:H	2.15	0.54
3:C:323:TRP:CZ3	3:C:358:LEU:HD21	2.43	0.54
2:E:310:PRO:HB3	2:E:352:TRP:CE2	2.42	0.54
3:C:135:MET:HE2	3:C:170:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:135:MET:HE2	3:F:170:PHE:CE2	2.41	0.54
3:F:254:MET:HA	3:F:276:LYS:NZ	2.23	0.54
1:A:165:THR:HB	1:D:191:LEU:HB2	1.90	0.54
2:E:71:LEU:HD23	2:E:78:THR:HG21	1.90	0.54
2:E:106:ARG:NE	2:E:259:ASN:H	2.06	0.54
2:E:182:GLU:HB3	2:E:183:LEU:O	2.07	0.54
3:F:281:PHE:HZ	3:F:316:ASN:HD21	1.55	0.54
3:C:48:VAL:HG11	3:C:79:ILE:HD13	1.89	0.53
2:B:162:ILE:HD11	3:C:23:ASP:O	2.08	0.53
2:B:310:PRO:HB3	2:B:352:TRP:CD2	2.43	0.53
2:E:178:LEU:HD12	2:E:181:LYS:HB2	1.91	0.53
2:E:207:PRO:O	2:E:211:GLN:HG2	2.09	0.53
3:F:257:ILE:HD13	3:F:276:LYS:HZ2	1.73	0.53
2:B:113:GLU:HG2	2:B:242:THR:HG22	1.90	0.53
2:B:233:PRO:O	2:B:260:ASP:OD2	2.27	0.53
3:F:178:THR:O	3:F:178:THR:OG1	2.22	0.53
3:F:282:MET:O	3:F:285:ASN:N	2.40	0.53
1:A:18:GLY:O	1:A:24:LYS:HE2	2.08	0.53
2:B:61:LYS:HZ1	5:B:501:ATP:PA	2.32	0.53
2:B:313:LYS:NZ	5:B:501:ATP:O1A	2.41	0.53
2:B:158:LYS:HD3	3:C:24:LEU:HB3	1.91	0.53
3:C:266:PRO:HG3	3:C:290:HIS:HB3	1.91	0.53
2:E:72:HIS:N	2:E:78:THR:HG22	2.09	0.53
2:E:140:TYR:CE1	2:E:217:LYS:HB2	2.43	0.53
2:E:43:GLU:OE2	10:E:611:HOH:O	2.18	0.53
1:A:289:ARG:NH2	1:A:312:PHE:O	2.36	0.53
2:E:141:ILE:O	2:E:145:ILE:HG13	2.08	0.53
3:F:343:ASN:HB2	9:F:501:SAH:H8	1.89	0.52
1:A:190:LEU:HD12	1:A:190:LEU:H	1.75	0.52
2:B:140:TYR:CE2	2:B:217:LYS:HD3	2.44	0.52
2:B:255:PHE:CE2	2:B:260:ASP:HB3	2.44	0.52
2:E:162:ILE:C	2:E:164:GLN:H	2.17	0.52
2:E:274:PHE:O	2:E:275:GLU:HB2	2.09	0.52
3:F:296:ASP:OD1	3:F:297:THR:N	2.42	0.52
2:B:217:LYS:HE3	2:B:221:ASP:OD2	2.10	0.52
3:F:31:LEU:HB3	3:F:50:PHE:HE1	1.74	0.52
3:F:291:PRO:HA	3:F:316:ASN:HB2	1.91	0.52
2:B:249:VAL:HG12	2:B:251:ASP:H	1.74	0.52
1:D:116:VAL:HG21	1:D:146:LEU:HD23	1.92	0.52
3:C:211:TYR:CE1	3:C:215:LYS:HE3	2.45	0.52
3:C:338:GLU:OE2	10:C:616:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:ARG:HG3	2:E:35:ARG:HH11	1.74	0.52
1:D:79:ARG:HD2	3:F:311:ARG:NH1	2.25	0.52
2:B:304:PHE:CD1	2:B:356:ALA:HB2	2.45	0.52
2:B:37:GLU:HG3	2:B:40:SER:HB2	1.91	0.52
3:C:5:ILE:HG23	3:C:116:ILE:HB	1.92	0.52
1:D:149:THR:HG23	1:D:150:LYS:HA	1.91	0.52
3:F:109:VAL:O	3:F:111:THR:HG22	2.09	0.52
1:A:237:GLU:HB3	1:A:238:PRO:HD3	1.93	0.51
2:E:162:ILE:O	2:E:164:GLN:N	2.43	0.51
3:C:277:TYR:CE1	3:C:281:PHE:CE2	2.99	0.51
3:C:291:PRO:HA	3:C:316:ASN:HB2	1.92	0.51
1:D:220:GLN:O	1:D:221:GLN:NE2	2.44	0.51
3:F:267:ILE:HG21	3:F:280:ARG:NH1	2.19	0.51
3:C:74:LEU:HD13	3:C:176:HIS:CE1	2.45	0.51
3:F:139:PHE:O	3:F:142:ILE:HG12	2.11	0.51
1:A:30:TYR:HB2	2:B:375:ASN:ND2	2.25	0.51
2:B:93:GLN:HG3	7:B:504:GOL:H2	1.92	0.51
3:C:249:THR:O	3:C:253:ARG:N	2.43	0.51
1:D:94:LEU:O	1:D:98:VAL:HG23	2.10	0.51
3:F:99:ILE:O	3:F:101:TRP:N	2.44	0.51
1:D:79:ARG:HD2	3:F:311:ARG:HH11	1.75	0.51
1:A:55:LEU:HD23	1:A:56:MSE:N	2.26	0.51
2:E:31:LYS:HZ2	2:E:341:ILE:HD12	1.75	0.51
2:E:274:PHE:CE1	2:E:278:TYR:HB2	2.46	0.51
1:A:55:LEU:HD23	1:A:56:MSE:H	1.76	0.51
2:E:5:THR:HG23	2:E:6:LEU:HD12	1.91	0.51
5:A:402:ATP:O2G	5:A:402:ATP:O2B	2.28	0.51
3:C:13:LEU:HD13	3:C:20:PRO:HB3	1.92	0.51
2:E:175:ALA:HA	2:E:184:LYS:HZ1	1.76	0.51
2:E:193:ARG:HD2	3:F:29:LYS:HG2	1.93	0.51
2:B:187:TYR:O	2:B:189:MET:N	2.44	0.51
3:F:98:GLN:HG2	3:F:101:TRP:CZ3	2.45	0.51
3:F:98:GLN:HG3	3:F:105:THR:HA	1.93	0.51
3:F:406:VAL:O	3:F:408:ASP:N	2.44	0.51
2:B:393:ARG:NH1	3:C:63:ASN:HB3	2.22	0.50
2:E:387:GLU:HA	2:E:390:LEU:HD13	1.93	0.50
3:F:98:GLN:HE21	3:F:101:TRP:HZ3	1.58	0.50
1:A:221:GLN:C	1:A:223:TYR:H	2.19	0.50
3:C:52:ASP:OD1	3:C:53:THR:N	2.44	0.50
2:B:92:ASP:HB3	2:B:95:GLN:HB2	1.93	0.50
2:B:153:SER:OG	2:B:154:SER:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:PHE:HB3	2:E:53:VAL:HG21	1.93	0.50
3:F:282:MET:O	3:F:284:ARG:N	2.45	0.50
1:A:261:TYR:CG	1:D:6:ASN:HB3	2.47	0.50
3:C:338:GLU:HB2	9:C:501:SAH:HG1	1.94	0.50
3:C:323:TRP:HZ3	3:C:358:LEU:HD21	1.75	0.50
1:A:51:PHE:CD2	1:A:51:PHE:N	2.79	0.50
1:D:11:PRO:HG3	3:F:311:ARG:HH12	1.76	0.50
1:D:146:LEU:O	1:D:147:GLN:NE2	2.41	0.50
2:B:46:LEU:HD13	2:B:274:PHE:HE2	1.76	0.50
2:E:341:ILE:HD12	2:E:341:ILE:H	1.77	0.50
2:B:318:ASP:O	2:B:321:THR:HB	2.12	0.50
2:B:344:LYS:HE2	2:B:394:LEU:CB	2.42	0.50
1:A:236:ARG:HH11	1:A:253:LEU:HD23	1.77	0.49
2:E:181:LYS:O	2:E:183:LEU:HA	2.11	0.49
3:F:214:ILE:HA	3:F:218:ILE:HD12	1.94	0.49
1:A:290:ASN:OD1	1:A:311:ASP:N	2.44	0.49
2:B:43:GLU:OE1	6:B:502:MES:H71	2.12	0.49
2:B:216:PHE:CE1	2:B:322:LEU:HA	2.47	0.49
2:E:39:GLU:OE2	2:E:315:ARG:NE	2.44	0.49
1:A:201:THR:O	1:A:204:GLN:HG3	2.12	0.49
2:B:55:GLU:HG3	2:B:268:PHE:HD1	1.76	0.49
3:F:253:ARG:HA	3:F:418:ILE:HG21	1.93	0.49
1:A:185:ASP:HB2	10:A:502:HOH:O	2.11	0.49
2:B:25:THR:HG21	2:B:344:LYS:HZ2	1.78	0.49
3:C:57:TYR:CZ	3:C:75:VAL:HG22	2.47	0.49
2:E:38:ILE:HG13	2:E:339:ARG:HD2	1.94	0.49
2:B:29:ALA:HA	2:B:312:PHE:CD1	2.48	0.49
1:D:73:ILE:HD11	1:D:101:TYR:HD1	1.77	0.49
2:E:150:LEU:HD22	2:E:156:TYR:CE2	2.47	0.49
2:E:304:PHE:CD1	2:E:356:ALA:HB2	2.48	0.49
2:E:56:ILE:HD13	2:E:298:ILE:HD11	1.95	0.49
3:F:365:ILE:HB	3:F:431:VAL:CG2	2.43	0.49
1:A:285:LEU:HD22	1:A:296:TRP:CE2	2.48	0.49
2:E:41:LEU:O	2:E:45:ILE:HG13	2.13	0.49
3:C:58:LEU:HD12	3:C:59:PRO:HD2	1.95	0.49
1:D:120:VAL:C	1:D:122:ARG:H	2.21	0.49
3:C:280:ARG:HB2	3:C:280:ARG:NH1	2.28	0.49
1:D:190:LEU:HD13	1:D:208:ASN:HB2	1.94	0.49
3:F:363:MET:HE3	3:F:365:ILE:HD11	1.93	0.49
1:A:46:PHE:C	1:A:48:LEU:H	2.21	0.49
3:C:88:LEU:O	3:C:197:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:75:LEU:HB2	2:E:104:HIS:CD2	2.48	0.49
1:A:232:GLU:OE1	1:A:258:THR:HA	2.13	0.48
1:A:305:PHE:CE1	1:D:307:VAL:HG13	2.48	0.48
3:C:215:LYS:HZ2	3:C:248:ASP:HA	1.77	0.48
2:E:122:MET:HB3	2:E:230:PHE:CE2	2.48	0.48
3:F:73:PRO:HG2	3:F:176:HIS:HB2	1.94	0.48
3:F:412:GLU:HB2	3:F:436:LYS:HZ2	1.78	0.48
2:E:168:TYR:O	2:E:169:LEU:HB2	2.13	0.48
2:E:282:ARG:NH1	2:E:286:ASP:OD1	2.45	0.48
3:F:101:TRP:O	3:F:103:GLU:N	2.45	0.48
3:C:33:ASN:OD1	3:C:33:ASN:N	2.46	0.48
3:C:135:MET:HE2	3:C:170:PHE:HE2	1.78	0.48
3:F:337:THR:OG1	3:F:338:GLU:N	2.30	0.48
2:B:273:ASP:O	2:B:276:ALA:HB3	2.13	0.48
2:E:25:THR:C	2:E:26:ILE:HD12	2.39	0.48
3:F:98:GLN:HG2	3:F:101:TRP:HZ3	1.77	0.48
1:A:170:ALA:HB2	1:A:301:ALA:HB3	1.95	0.48
2:B:310:PRO:HB3	2:B:352:TRP:CD1	2.49	0.48
2:B:324:TYR:HB2	2:B:328:PHE:HB2	1.95	0.48
1:D:4:LYS:NZ	1:D:5:ASN:H	2.11	0.48
2:E:286:ASP:HA	2:E:289:ASN:HD22	1.79	0.48
2:E:320:LEU:HA	2:E:323:VAL:HG23	1.96	0.48
3:F:109:VAL:O	3:F:111:THR:N	2.46	0.48
1:A:183:ASP:OD2	1:A:288:ASP:OD2	2.31	0.48
2:B:302:THR:HB	2:B:305:LEU:HD21	1.95	0.48
1:D:4:LYS:HZ3	1:D:5:ASN:H	1.60	0.48
1:D:76:LEU:HD22	1:D:105:ALA:HB2	1.96	0.48
1:D:90:SER:O	1:D:92:ARG:N	2.47	0.48
2:E:237:LEU:HD13	2:E:359:LEU:HD11	1.96	0.48
3:F:101:TRP:CZ3	3:F:104:ARG:HA	2.49	0.48
3:F:404:HIS:O	3:F:404:HIS:CG	2.66	0.48
1:A:286:LEU:HD23	1:A:305:PHE:HB2	1.95	0.48
2:E:48:PHE:HB3	2:E:53:VAL:CG2	2.44	0.48
1:D:203:ASP:HA	1:D:242:PHE:HB2	1.96	0.48
2:E:175:ALA:CB	2:E:184:LYS:HZ1	2.27	0.48
2:E:350:ASN:O	2:E:354:ILE:HG12	2.14	0.48
1:A:79:ARG:NH1	3:C:311:ARG:HD3	2.29	0.48
2:B:38:ILE:HB	2:B:336:ILE:HG12	1.96	0.48
2:B:63:MET:H	2:B:122:MET:HE1	1.79	0.48
1:D:11:PRO:HG3	3:F:311:ARG:HH22	1.79	0.48
3:F:41:VAL:HG12	3:F:45:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:HIS:HB3	2:B:213:ILE:HD11	1.96	0.47
1:D:35:GLU:OE2	2:E:8:LYS:HD3	2.14	0.47
1:D:53:ASP:OD2	1:D:54:SER:N	2.38	0.47
2:E:118:GLN:HG3	2:E:234:PHE:CE2	2.48	0.47
2:E:320:LEU:HD22	2:E:324:TYR:CE2	2.48	0.47
3:F:142:ILE:HD11	3:F:167:LEU:HD11	1.96	0.47
2:B:171:PHE:CE1	2:B:192:ILE:HA	2.48	0.47
2:E:282:ARG:O	2:E:282:ARG:HD3	2.14	0.47
3:F:1:MET:N	3:F:70:TYR:HA	2.30	0.47
3:F:23:ASP:O	3:F:24:LEU:HB2	2.14	0.47
3:C:154:LEU:HD12	3:C:155:ARG:H	1.80	0.47
2:E:184:LYS:O	2:E:186:LYS:N	2.47	0.47
1:A:4:LYS:O	1:A:5:ASN:HB3	2.14	0.47
1:D:17:VAL:O	1:D:111:VAL:HA	2.14	0.47
5:D:402:ATP:C5	2:E:372:GLU:HB2	2.49	0.47
2:E:20:ASN:O	2:E:20:ASN:ND2	2.45	0.47
2:E:206:LEU:HD23	2:E:206:LEU:HA	1.71	0.47
2:E:339:ARG:NH1	2:E:339:ARG:HG3	2.30	0.47
3:F:53:THR:C	3:F:54:ARG:HG3	2.38	0.47
2:B:24:PRO:HA	2:B:351:ASP:HB3	1.96	0.47
3:C:31:LEU:HB3	3:C:50:PHE:HE1	1.79	0.47
2:E:58:ILE:HD11	2:E:298:ILE:HB	1.95	0.47
2:B:242:THR:O	2:B:244:GLY:N	2.48	0.47
3:C:270:ILE:HB	3:C:336:LEU:HD22	1.97	0.47
1:D:30:TYR:CE1	2:E:374:LYS:HB3	2.50	0.47
1:D:77:LYS:HE2	1:D:104:TYR:HE1	1.79	0.47
3:F:29:LYS:HD3	3:F:30:SER:N	2.29	0.47
3:C:5:ILE:O	3:C:45:GLN:HA	2.15	0.47
3:C:142:ILE:CD1	3:C:171:ILE:HD11	2.45	0.47
2:E:178:LEU:HD11	2:E:184:LYS:HE3	1.95	0.47
3:F:52:ASP:OD2	3:F:54:ARG:N	2.48	0.47
3:F:100:LYS:NZ	3:F:102:LEU:HB2	2.30	0.47
1:D:289:ARG:O	1:D:293:VAL:HG23	2.15	0.47
2:E:377:VAL:O	2:E:380:ARG:N	2.47	0.47
3:F:192:ALA:HB1	3:F:227:ILE:HD11	1.96	0.47
3:F:369:ASN:ND2	3:F:395:PRO:HD3	2.30	0.47
3:C:298:ASP:OD1	3:C:300:SER:HB3	2.14	0.47
2:E:35:ARG:HG3	2:E:35:ARG:NH1	2.28	0.47
2:E:205:ASP:HB3	2:E:208:HIS:HB3	1.97	0.47
2:E:225:LYS:HA	2:E:225:LYS:HD3	1.65	0.47
1:A:8:HIS:O	1:A:8:HIS:ND1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:O	1:A:78:ASN:N	2.48	0.46
2:B:260:ASP:C	2:B:262:ASP:H	2.21	0.46
3:F:279:ARG:HG3	3:F:279:ARG:NH1	2.28	0.46
2:E:323:VAL:HB	2:E:324:TYR:CD2	2.50	0.46
3:F:375:TYR:CE1	3:F:422:ILE:HG21	2.50	0.46
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.80	0.46
3:F:11:HIS:HB3	3:F:14:ASP:HB2	1.98	0.46
2:B:168:TYR:O	2:B:169:LEU:HB2	2.16	0.46
2:B:260:ASP:C	2:B:262:ASP:N	2.73	0.46
3:C:309:LYS:NZ	3:C:314:ALA:O	2.48	0.46
2:E:22:PHE:N	2:E:355:ASN:OD1	2.42	0.46
2:E:159:LEU:HD23	3:F:26:ILE:HD13	1.98	0.46
3:F:254:MET:HA	3:F:276:LYS:HZ3	1.80	0.46
3:F:341:GLU:HG3	3:F:368:PRO:HG2	1.97	0.46
2:E:151:VAL:HG23	2:E:206:LEU:HD13	1.98	0.46
2:E:299:LYS:HG2	2:E:311:ALA:HB2	1.98	0.46
2:B:256:GLN:HB3	2:B:264:LEU:HD22	1.98	0.46
2:B:299:LYS:HE3	5:B:501:ATP:N1	2.30	0.46
2:B:351:ASP:OD2	2:B:380:ARG:NH2	2.48	0.46
3:C:286:TYR:O	3:C:288:TYR:N	2.49	0.46
2:E:140:TYR:CZ	2:E:217:LYS:HD3	2.51	0.46
1:A:209:THR:N	1:A:210:PRO:HD2	2.31	0.46
2:B:1:MET:O	2:B:7:ILE:HD11	2.16	0.46
3:C:76:ILE:HD11	3:C:118:VAL:HG11	1.97	0.46
2:B:28:PRO:HB3	2:B:39:GLU:HG2	1.97	0.46
3:C:231:PHE:O	3:C:234:TYR:HB3	2.16	0.46
3:F:331:PRO:HA	3:F:359:ASN:O	2.15	0.46
1:A:71:SER:O	1:A:75:LEU:HD12	2.16	0.46
1:A:261:TYR:CD2	1:D:6:ASN:HB3	2.50	0.46
3:C:100:LYS:HE2	3:C:101:TRP:CZ2	2.50	0.46
3:F:369:ASN:HD22	3:F:369:ASN:C	2.11	0.46
2:B:114:LEU:HD12	2:B:115:ARG:N	2.31	0.46
3:C:425:GLU:HA	3:C:425:GLU:OE2	2.16	0.46
2:E:278:TYR:N	2:E:279:PRO:HD2	2.30	0.46
3:F:59:PRO:HA	3:F:60:GLU:HA	1.65	0.46
3:F:360:PHE:O	3:F:435:ARG:HD2	2.16	0.46
2:B:126:ILE:HG22	2:B:127:LEU:HD13	1.98	0.45
3:F:193:GLN:H	3:F:196:ALA:HB2	1.80	0.45
3:F:345:PRO:C	3:F:346:GLU:OE1	2.59	0.45
2:B:48:PHE:CZ	2:B:300:PRO:HD3	2.51	0.45
2:B:113:GLU:OE2	2:B:242:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:250:HIS:O	3:F:252:SER:N	2.46	0.45
3:F:355:CYS:O	3:F:358:LEU:HB2	2.16	0.45
2:B:22:PHE:CG	2:B:380:ARG:HG2	2.52	0.45
2:B:243:ASP:OD2	2:B:245:ARG:HG2	2.16	0.45
3:C:57:TYR:CE2	3:C:75:VAL:HG22	2.51	0.45
1:D:6:ASN:OD1	1:D:7:THR:N	2.49	0.45
2:E:120:GLU:OE2	5:E:501:ATP:H1'	2.16	0.45
2:E:171:PHE:CZ	2:E:192:ILE:HA	2.51	0.45
2:E:324:TYR:HB2	2:E:328:PHE:HB2	1.98	0.45
1:A:57:SER:HB3	1:A:60:TYR:HD1	1.81	0.45
3:C:31:LEU:H	3:C:35:GLN:H	1.63	0.45
3:C:202:ILE:HD12	3:C:202:ILE:HA	1.82	0.45
3:F:60:GLU:H	3:F:62:SER:H	1.64	0.45
1:A:308:ASN:ND2	1:D:167:LEU:HD21	2.32	0.45
3:C:370:SER:HB3	3:C:393:TRP:O	2.17	0.45
1:D:18:GLY:O	1:D:24:LYS:NZ	2.50	0.45
1:D:79:ARG:CZ	3:F:311:ARG:HD2	2.47	0.45
2:E:308:MET:C	2:E:349:ILE:HG22	2.42	0.45
2:E:357:LYS:O	2:E:360:ALA:HB3	2.17	0.45
3:F:86:GLU:H	3:F:86:GLU:CD	2.23	0.45
1:A:11:PRO:N	3:C:311:ARG:HH22	2.15	0.45
1:A:208:ASN:HD22	1:A:211:VAL:HG23	1.80	0.45
3:C:1:MET:HE3	3:C:76:ILE:HG13	1.99	0.45
3:C:15:LEU:HD23	3:C:106:ARG:HH21	1.82	0.45
3:C:87:LEU:HD21	3:C:161:VAL:HG12	1.97	0.45
1:D:73:ILE:HD11	1:D:101:TYR:CD1	2.51	0.45
2:E:38:ILE:HG13	2:E:339:ARG:CD	2.47	0.45
2:E:121:LEU:HD11	2:E:126:ILE:HG21	1.99	0.45
2:E:162:ILE:C	2:E:164:GLN:N	2.75	0.45
3:F:395:PRO:O	3:F:396:GLN:HB3	2.17	0.45
1:A:258:THR:O	3:F:328:TYR:HA	2.16	0.45
2:B:25:THR:HG21	2:B:344:LYS:NZ	2.30	0.45
2:B:284:TRP:O	2:B:288:VAL:HG23	2.16	0.45
2:E:351:ASP:OD2	2:E:380:ARG:NH2	2.50	0.45
2:B:162:ILE:CD1	3:C:23:ASP:HB3	2.47	0.45
2:B:184:LYS:NZ	2:B:186:LYS:HE2	2.32	0.45
3:C:353:LYS:HA	3:C:356:LEU:HD12	1.98	0.45
3:C:412:GLU:HB2	3:C:436:LYS:NZ	2.31	0.45
2:E:172:VAL:HG13	2:E:199:ARG:HD2	1.98	0.45
2:E:285:VAL:HG12	2:E:289:ASN:HD21	1.81	0.45
2:E:339:ARG:HG3	2:E:339:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:TYR:O	1:D:64:ILE:HG13	2.16	0.45
1:D:73:ILE:CG2	1:D:77:LYS:HE3	2.47	0.45
2:E:162:ILE:HD11	3:F:23:ASP:O	2.17	0.44
2:E:198:ILE:O	2:E:199:ARG:HB3	2.17	0.44
3:F:274:GLU:OE2	3:F:274:GLU:CA	2.62	0.44
3:F:344:THR:HA	3:F:345:PRO:HD3	1.73	0.44
1:A:31:PHE:HE2	1:A:38:TRP:CD2	2.35	0.44
2:B:304:PHE:CE1	2:B:352:TRP:CE2	3.06	0.44
1:D:194:ARG:NH1	1:D:205:ASP:OD2	2.46	0.44
3:F:100:LYS:HE2	3:F:100:LYS:HB2	1.80	0.44
1:A:90:SER:OG	1:A:91:LEU:N	2.48	0.44
1:A:183:ASP:HB2	1:A:287:ASP:OD2	2.17	0.44
3:C:130:LYS:HE2	3:C:130:LYS:HB3	1.64	0.44
3:C:354:HIS:O	3:C:358:LEU:HD13	2.18	0.44
2:E:63:MET:N	2:E:122:MET:HE1	2.31	0.44
3:F:391:PHE:CE1	3:F:393:TRP:CE2	3.05	0.44
2:B:141:ILE:HD13	2:B:141:ILE:HA	1.57	0.44
1:D:16:LEU:HD11	1:D:83:ILE:HD11	2.00	0.44
1:D:72:VAL:HG22	1:D:82:VAL:HG11	2.00	0.44
2:E:345:LEU:HA	2:E:345:LEU:HD12	1.68	0.44
3:F:362:LYS:HG3	3:F:434:THR:HG22	1.99	0.44
2:E:327:ASP:O	2:E:331:ARG:HG2	2.18	0.44
3:F:42:SER:OG	3:F:43:ALA:O	2.20	0.44
1:A:236:ARG:O	1:A:240:GLU:HG3	2.18	0.44
2:B:191:ILE:HG23	2:B:195:TYR:CD1	2.53	0.44
3:C:36:LEU:HD21	3:C:79:ILE:HG12	2.00	0.44
3:C:253:ARG:HG2	3:C:257:ILE:CD1	2.42	0.44
2:E:8:LYS:HB2	2:E:8:LYS:HE3	1.82	0.44
2:E:122:MET:HG2	2:E:230:PHE:CZ	2.53	0.44
3:F:200:THR:HG23	3:F:234:TYR:HD1	1.83	0.44
1:A:150:LYS:H	1:A:152:LYS:NZ	2.16	0.44
2:B:162:ILE:HD13	3:C:23:ASP:HB3	2.00	0.44
2:B:285:VAL:HG22	2:B:296:VAL:HG11	2.00	0.44
3:C:166:ASN:HB3	3:C:202:ILE:HD13	2.00	0.44
3:C:353:LYS:HE3	3:C:405:CYS:HA	2.00	0.44
3:C:435:ARG:HH11	3:C:435:ARG:HG2	1.83	0.44
1:D:151:GLU:HB2	1:D:153:PHE:CD1	2.53	0.44
1:D:176:LEU:HD22	1:D:279:LYS:C	2.43	0.44
2:E:22:PHE:HB3	2:E:23:SER:H	1.59	0.44
2:B:188:PRO:C	2:B:190:HIS:H	2.26	0.44
2:B:189:MET:O	2:B:192:ILE:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLN:O	2:B:198:ILE:HG13	2.18	0.43
2:E:37:GLU:HG3	2:E:40:SER:HB3	1.99	0.43
2:E:130:GLY:HA2	2:E:133:ASN:HB2	2.00	0.43
3:F:29:LYS:HD3	3:F:30:SER:H	1.82	0.43
3:F:41:VAL:HG11	3:F:45:GLN:CD	2.43	0.43
3:F:57:TYR:CZ	3:F:75:VAL:HG22	2.53	0.43
3:F:200:THR:HG23	3:F:234:TYR:CD1	2.52	0.43
1:A:194:ARG:NH1	1:A:199:ALA:HA	2.33	0.43
2:B:115:ARG:HG2	2:B:239:GLU:HG2	2.00	0.43
2:B:196:GLN:HG3	2:B:199:ARG:NH2	2.24	0.43
3:C:283:ARG:CG	3:C:284:ARG:H	2.30	0.43
3:C:372:PHE:CD2	3:C:427:PRO:HB3	2.53	0.43
1:D:92:ARG:NH2	1:D:95:GLN:HG3	2.33	0.43
1:D:170:ALA:HB2	1:D:301:ALA:HB3	2.00	0.43
2:E:100:LEU:HG	2:E:231:PHE:CE2	2.53	0.43
3:C:99:ILE:HG22	3:C:100:LYS:HG2	2.00	0.43
3:C:137:ARG:HB3	3:C:138:TYR:CD2	2.53	0.43
3:F:4:GLN:HG2	3:F:47:ASP:OD1	2.19	0.43
1:A:16:LEU:HD11	1:A:83:ILE:HD11	2.00	0.43
1:A:284:PHE:CZ	1:D:217:MSE:HE1	2.54	0.43
2:B:106:ARG:CZ	2:B:259:ASN:HA	2.48	0.43
2:B:189:MET:HA	2:B:192:ILE:HD12	1.99	0.43
2:B:344:LYS:HE2	2:B:394:LEU:HB3	2.00	0.43
3:C:156:VAL:CG1	3:C:167:LEU:HD23	2.45	0.43
3:C:327:GLU:O	3:C:329:LYS:HG3	2.18	0.43
3:F:206:PRO:HG2	3:F:209:VAL:HG23	1.99	0.43
1:A:60:TYR:O	1:A:64:ILE:HG12	2.17	0.43
2:B:8:LYS:HB2	2:B:8:LYS:HE3	1.69	0.43
3:C:100:LYS:HG3	3:C:101:TRP:CD2	2.53	0.43
1:D:65:THR:O	1:D:69:GLU:HG3	2.18	0.43
3:F:90:GLU:HG2	3:F:197:ARG:HD2	2.00	0.43
3:F:158:GLY:HA3	3:F:164:ALA:HB2	2.00	0.43
2:B:253:LEU:HD11	2:B:266:TYR:CE2	2.54	0.43
2:B:299:LYS:HG2	2:B:311:ALA:HB2	2.00	0.43
3:C:270:ILE:HB	3:C:335:ILE:O	2.18	0.43
3:F:339:VAL:O	3:F:341:GLU:N	2.51	0.43
1:A:71:SER:HB3	1:D:67:MSE:HB2	2.01	0.43
1:A:215:LEU:HD22	1:A:225:VAL:CG1	2.48	0.43
1:A:236:ARG:NH1	1:A:253:LEU:HD23	2.34	0.43
2:B:317:ASN:OD1	7:B:503:GOL:H12	2.19	0.43
3:F:178:THR:HG22	3:F:212:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASN:O	1:A:81:ASN:HB2	2.19	0.43
2:B:344:LYS:HE2	2:B:394:LEU:HB2	2.01	0.43
3:C:77:LEU:HD12	3:C:77:LEU:HA	1.63	0.43
1:D:308:ASN:OD1	1:D:309:TYR:N	2.52	0.43
2:E:48:PHE:CZ	2:E:300:PRO:HD3	2.53	0.43
3:F:399:GLN:HG2	3:F:415:TYR:CE1	2.53	0.43
2:B:343:GLY:HA2	2:B:346:ARG:HB3	2.01	0.43
3:C:100:LYS:HG3	3:C:101:TRP:CE3	2.54	0.43
2:E:231:PHE:C	2:E:233:PRO:HD3	2.43	0.43
2:E:240:VAL:HG13	2:E:246:GLU:HG2	1.99	0.43
3:F:105:THR:O	3:F:109:VAL:HG23	2.18	0.43
1:D:32:ILE:HD12	1:D:32:ILE:HA	1.87	0.43
1:D:46:PHE:CD2	1:D:68:VAL:HG22	2.54	0.43
1:D:69:GLU:O	1:D:73:ILE:HG12	2.19	0.43
2:E:42:TYR:HD1	2:E:278:TYR:CD1	2.37	0.43
3:C:337:THR:HA	3:C:366:THR:HB	2.00	0.42
1:D:101:TYR:O	1:D:104:TYR:N	2.41	0.42
2:E:138:ALA:HA	2:E:141:ILE:HG22	2.00	0.42
1:A:47:ARG:NH1	1:A:61:GLU:OE1	2.51	0.42
2:B:33:VAL:HG22	6:B:502:MES:O1	2.19	0.42
2:B:163:GLN:HA	2:B:168:TYR:CD2	2.55	0.42
3:C:19:ASN:HA	3:C:20:PRO:HD2	1.89	0.42
3:C:62:SER:HB2	3:C:64:GLN:HG3	2.01	0.42
3:F:91:LYS:HB3	3:F:91:LYS:HZ3	1.83	0.42
2:E:155:LEU:O	2:E:157:GLU:N	2.52	0.42
2:B:13:TRP:HA	2:B:13:TRP:HE3	1.82	0.42
2:E:369:GLU:OE1	2:E:369:GLU:N	2.45	0.42
1:D:114:LEU:HD12	1:D:115:PRO:HD2	2.01	0.42
1:D:287:ASP:OD2	1:D:288:ASP:N	2.44	0.42
3:F:123:ALA:O	3:F:150:ASN:HB3	2.19	0.42
3:F:198:ILE:HG21	3:F:198:ILE:HD13	1.72	0.42
1:A:153:PHE:HZ	1:A:158:ILE:HD11	1.85	0.42
2:B:139:TYR:OH	2:B:326:VAL:HG13	2.20	0.42
3:C:334:ILE:HG23	3:C:363:MET:HG3	2.01	0.42
1:D:31:PHE:HE2	1:D:38:TRP:CD2	2.37	0.42
1:D:262:ARG:HG2	1:D:262:ARG:NH1	2.33	0.42
3:F:280:ARG:HD3	3:F:280:ARG:HA	1.65	0.42
1:A:295:MSE:HE3	1:A:295:MSE:HB3	2.01	0.42
2:B:189:MET:O	2:B:191:ILE:N	2.52	0.42
1:D:161:ALA:O	1:D:162:LEU:HB2	2.20	0.42
2:E:288:VAL:HG13	2:E:293:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:52:ASP:OD1	3:F:56:SER:OG	2.37	0.42
1:A:172:GLN:H	1:A:172:GLN:HG2	1.62	0.42
2:B:163:GLN:HA	2:B:168:TYR:CE2	2.54	0.42
3:C:369:ASN:O	3:C:371:LEU:N	2.45	0.42
1:D:293:VAL:HG13	1:D:304:CYS:SG	2.60	0.42
2:E:170:SER:OG	2:E:171:PHE:N	2.53	0.42
2:B:193:ARG:NH2	2:B:194:GLN:HG3	2.24	0.42
2:B:248:PHE:HZ	2:B:304:PHE:CD2	2.37	0.42
2:B:391:ASP:HB3	2:B:394:LEU:HD13	2.02	0.42
3:C:9:ASN:HB2	3:C:112:TYR:HB2	2.00	0.42
2:B:251:ASP:C	2:B:253:LEU:H	2.28	0.42
3:C:55:TYR:CE1	3:C:60:GLU:HG3	2.55	0.42
1:D:79:ARG:HB3	3:F:311:ARG:CZ	2.49	0.42
1:D:206:LEU:HA	1:D:206:LEU:HD23	1.81	0.42
1:A:165:THR:CG2	1:D:191:LEU:H	2.33	0.41
2:B:83:ARG:NH2	10:B:611:HOH:O	2.53	0.41
3:F:104:ARG:HD2	3:F:108:GLU:OE2	2.20	0.41
3:F:257:ILE:HD13	3:F:276:LYS:NZ	2.35	0.41
2:B:282:ARG:HD3	2:B:282:ARG:O	2.20	0.41
3:C:55:TYR:CD1	3:C:60:GLU:HA	2.55	0.41
3:C:272:CYS:SG	3:C:294:ALA:HB1	2.60	0.41
2:E:252:ASN:CG	2:E:299:LYS:HD3	2.46	0.41
3:F:77:LEU:HD12	3:F:77:LEU:HA	1.67	0.41
3:F:101:TRP:CH2	3:F:104:ARG:HA	2.55	0.41
3:F:253:ARG:HD3	3:F:366:THR:HG21	2.03	0.41
3:F:326:TYR:HE2	3:F:358:LEU:HD22	1.85	0.41
1:A:51:PHE:H	1:A:51:PHE:HD2	1.66	0.41
3:C:311:ARG:HG2	3:C:312:MET:O	2.20	0.41
3:F:362:LYS:HG3	3:F:434:THR:HG23	2.03	0.41
2:B:34:GLU:HB2	6:B:502:MES:C2	2.51	0.41
2:B:84:ASN:OD1	2:B:85:GLY:N	2.54	0.41
2:B:219:GLN:HG2	2:B:319:TYR:HA	2.02	0.41
3:C:9:ASN:ND2	3:C:112:TYR:HB2	2.28	0.41
3:C:133:PHE:HE1	3:C:152:LEU:HD21	1.84	0.41
3:C:261:LEU:HD23	3:C:261:LEU:HA	1.64	0.41
1:D:181:ILE:HD11	1:D:282:VAL:HG22	2.02	0.41
2:E:309:PRO:N	2:E:349:ILE:HG22	2.35	0.41
2:E:332:LEU:O	2:E:336:ILE:HG13	2.20	0.41
3:F:258:VAL:HG22	3:F:280:ARG:HE	1.85	0.41
3:F:281:PHE:O	3:F:282:MET:C	2.62	0.41
1:D:30:TYR:CE1	1:D:34:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ASN:HD22	1:D:78:ASN:C	2.19	0.41
1:D:294:ASP:O	1:D:298:ARG:HG2	2.20	0.41
2:E:58:ILE:HB	2:E:265:HIS:CE1	2.56	0.41
2:E:184:LYS:HE2	2:E:184:LYS:HB3	1.94	0.41
2:E:206:LEU:N	2:E:207:PRO:HD2	2.36	0.41
3:F:334:ILE:HD11	3:F:360:PHE:HB3	2.02	0.41
1:A:11:PRO:HG2	1:A:105:ALA:HB2	2.02	0.41
1:A:47:ARG:NH1	1:A:61:GLU:OE2	2.54	0.41
1:A:289:ARG:HH21	1:A:312:PHE:C	2.27	0.41
2:B:24:PRO:HG3	2:B:352:TRP:CE3	2.56	0.41
2:B:73:ARG:HE	2:B:73:ARG:HB2	1.52	0.41
2:B:150:LEU:HD11	3:C:51:GLN:HE21	1.86	0.41
2:B:341:ILE:HD12	2:B:345:LEU:HB2	2.02	0.41
2:E:188:PRO:HA	2:E:189:MET:HA	1.67	0.41
2:E:330:ASP:O	2:E:332:LEU:N	2.46	0.41
3:F:261:LEU:HA	3:F:261:LEU:HD23	1.64	0.41
3:F:309:LYS:C	3:F:311:ARG:H	2.29	0.41
1:A:259:ASN:HA	1:A:261:TYR:CZ	2.56	0.41
3:C:4:GLN:HG2	3:C:47:ASP:CG	2.46	0.41
3:C:274:GLU:O	3:C:277:TYR:HB3	2.21	0.41
3:F:57:TYR:CE2	3:F:75:VAL:HG22	2.56	0.41
3:F:246:PHE:CD1	3:F:246:PHE:C	2.98	0.41
1:A:277:GLN:HE21	1:A:278:GLY:N	2.18	0.41
2:B:158:LYS:HB3	3:C:26:ILE:HD11	2.02	0.41
1:D:72:VAL:HG21	1:D:84:ILE:HD11	2.02	0.41
1:A:6:ASN:HB3	1:D:261:TYR:CE1	2.55	0.41
1:A:25:SER:OG	5:A:402:ATP:O2B	2.28	0.41
2:B:242:THR:C	2:B:244:GLY:H	2.29	0.41
3:C:50:PHE:CE2	3:C:52:ASP:HB2	2.55	0.41
3:C:77:LEU:HD13	3:C:172:ALA:CB	2.51	0.41
3:C:151:ASN:ND2	3:C:151:ASN:N	2.69	0.41
3:C:178:THR:HG23	3:C:178:THR:O	2.21	0.41
1:D:266:ILE:H	1:D:266:ILE:HG13	1.68	0.41
2:E:66:TYR:HE1	2:E:118:GLN:HB2	1.86	0.41
2:E:162:ILE:HD12	3:F:26:ILE:HD12	2.02	0.41
2:E:284:TRP:O	2:E:287:GLN:HB3	2.21	0.41
3:F:100:LYS:CD	3:F:101:TRP:H	2.32	0.41
3:F:170:PHE:O	3:F:173:VAL:HG12	2.21	0.41
3:F:228:LYS:N	3:F:229:PRO:HD2	2.36	0.41
3:F:234:TYR:CD2	3:F:234:TYR:C	2.99	0.41
2:B:35:ARG:HB2	2:B:37:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:61:LYS:NZ	5:E:501:ATP:O2A	2.54	0.41
2:E:155:LEU:HD23	2:E:156:TYR:HD2	1.86	0.41
2:E:304:PHE:O	2:E:305:LEU:HD23	2.20	0.41
1:A:88:ASN:HB3	1:A:93:SER:OG	2.21	0.40
3:C:61:GLU:O	3:C:62:SER:C	2.64	0.40
3:C:103:GLU:O	3:C:104:ARG:HB2	2.22	0.40
1:D:77:LYS:C	1:D:79:ARG:H	2.29	0.40
1:D:285:LEU:HD22	1:D:296:TRP:CD2	2.56	0.40
2:E:54:LYS:HG3	2:E:270:ASP:HB2	2.03	0.40
2:E:71:LEU:HD11	2:E:103:LEU:HG	2.03	0.40
2:E:123:PRO:HD2	2:E:126:ILE:CG1	2.51	0.40
2:E:305:LEU:HD12	2:E:308:MET:HE3	2.02	0.40
1:A:42:ASN:HB3	1:A:45:ASP:HB2	2.03	0.40
2:B:289:ASN:OD1	2:B:316:ASN:HB3	2.20	0.40
2:B:350:ASN:O	2:B:354:ILE:HG13	2.21	0.40
3:C:273:GLY:O	3:C:274:GLU:HB2	2.21	0.40
3:C:402:ILE:O	3:C:406:VAL:HG12	2.21	0.40
1:D:47:ARG:NH1	1:D:61:GLU:OE2	2.55	0.40
2:E:155:LEU:O	2:E:156:TYR:C	2.64	0.40
3:F:211:TYR:O	3:F:214:ILE:N	2.55	0.40
3:F:245:GLN:N	3:F:420:ASP:OD1	2.54	0.40
1:A:231:ARG:HB2	1:A:255:MSE:CE	2.50	0.40
2:B:38:ILE:HD11	2:B:339:ARG:CZ	2.52	0.40
2:B:159:LEU:HD23	2:B:159:LEU:HA	1.89	0.40
3:C:243:ASP:O	3:C:244:PHE:HB2	2.22	0.40
3:C:254:MET:HA	3:C:257:ILE:HD12	2.03	0.40
3:F:52:ASP:CG	3:F:56:SER:HG	2.30	0.40
3:F:283:ARG:C	3:F:285:ASN:H	2.28	0.40
3:C:151:ASN:N	3:C:151:ASN:HD22	2.20	0.40
3:F:34:GLY:HA3	3:F:52:ASP:HA	2.03	0.40
1:A:50:GLN:CD	1:A:50:GLN:N	2.80	0.40
2:E:41:LEU:CD1	2:E:285:VAL:HG11	2.51	0.40
2:E:55:GLU:OE1	2:E:266:TYR:OH	2.36	0.40
3:F:15:LEU:HD22	3:F:110:ASP:HB2	2.02	0.40
3:F:270:ILE:HD13	3:F:355:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/312 (92%)	235 (82%)	40 (14%)	12 (4%)	2	14
1	D	283/312 (91%)	220 (78%)	47 (17%)	16 (6%)	1	9
2	B	392/394 (100%)	330 (84%)	48 (12%)	14 (4%)	2	16
2	E	391/394 (99%)	323 (83%)	55 (14%)	13 (3%)	3	17
3	C	420/436 (96%)	344 (82%)	61 (14%)	15 (4%)	2	16
3	F	420/436 (96%)	342 (81%)	56 (13%)	22 (5%)	1	10
All	All	2193/2284 (96%)	1794 (82%)	307 (14%)	92 (4%)	2	14

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	151	GLU
1	A	154	ASP
2	B	184	LYS
2	B	186	LYS
2	B	187	TYR
2	B	188	PRO
2	B	190	HIS
2	B	227	ALA
2	B	243	ASP
2	B	269	THR
3	C	89	GLN
3	C	282	MET
3	C	343	ASN
1	D	7	THR
1	D	55	LEU
1	D	86	ALA
1	D	162	LEU
1	D	170	ALA
2	E	184	LYS

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Mol	Chain	Res	Type
2	E	190	HIS
2	E	227	ALA
3	F	61	GLU
3	F	102	LEU
3	F	104	ARG
3	F	283	ARG
3	F	345	PRO
3	F	407	GLY
1	A	86	ALA
1	A	88	ASN
1	A	91	LEU
1	A	144	THR
1	A	148	TYR
1	A	222	GLY
2	B	264	LEU
2	B	275	GLU
3	C	71	CYS
3	C	249	THR
3	C	359	ASN
3	C	408	ASP
1	D	20	PRO
1	D	22	SER
1	D	91	LEU
1	D	220	GLN
1	D	308	ASN
2	E	155	LEU
2	E	163	GLN
2	E	175	ALA
2	E	182	GLU
2	E	185	ASP
3	F	100	LYS
3	F	101	TRP
3	F	148	VAL
3	F	337	THR
3	F	343	ASN
1	A	89	SER
1	A	90	SER
1	A	169	TYR
2	B	95	GLN
3	C	102	LEU
3	C	104	ARG
1	D	148	TYR

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Mol	Chain	Res	Type
1	D	154	ASP
1	D	264	ASP
2	E	31	LYS
3	F	33	ASN
3	F	249	THR
3	F	342	HIS
2	B	291	SER
3	C	179	ASN
2	E	156	TYR
2	E	205	ASP
2	E	255	PHE
3	F	71	CYS
3	F	282	MET
3	F	328	TYR
2	B	205	ASP
3	C	203	PRO
1	D	23	GLY
2	E	331	ARG
3	F	110	ASP
3	F	368	PRO
3	C	283	ARG
3	C	416	CYS
1	D	159	PRO
1	D	291	GLN
3	F	370	SER
3	C	59	PRO
3	F	340	ILE
2	B	24	PRO
3	C	339	VAL
3	F	339	VAL

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	265/274 (97%)	242 (91%)	23 (9%)	9 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	261/274 (95%)	239 (92%)	22 (8%)	10	33
2	B	359/359 (100%)	319 (89%)	40 (11%)	6	21
2	E	358/359 (100%)	328 (92%)	30 (8%)	10	33
3	C	387/399 (97%)	355 (92%)	32 (8%)	10	34
3	F	387/399 (97%)	356 (92%)	31 (8%)	11	35
All	All	2017/2064 (98%)	1839 (91%)	178 (9%)	9	30

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	48	LEU
1	A	55	LEU
1	A	65	THR
1	A	68	VAL
1	A	79	ARG
1	A	91	LEU
1	A	120	VAL
1	A	143	VAL
1	A	149	THR
1	A	171	ASP
1	A	184	LEU
1	A	187	THR
1	A	201	THR
1	A	206	LEU
1	A	209	THR
1	A	213	MSE
1	A	219	LYS
1	A	255	MSE
1	A	259	ASN
1	A	266	ILE
1	A	287	ASP
1	A	300	LEU
2	B	5	THR
2	B	6	LEU
2	B	8	LYS
2	B	13	TRP
2	B	20	ASN
2	B	25	THR
2	B	38	ILE

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Mol	Chain	Res	Type
2	B	49	VAL
2	B	63	MET
2	B	65	SER
2	B	76	GLU
2	B	87	LYS
2	B	89	ASN
2	B	90	HIS
2	B	113	GLU
2	B	114	LEU
2	B	127	LEU
2	B	131	LEU
2	B	141	ILE
2	B	151	VAL
2	B	164	GLN
2	B	182	GLU
2	B	184	LYS
2	B	190	HIS
2	B	194	GLN
2	B	199	ARG
2	B	253	LEU
2	B	258	ILE
2	B	265	HIS
2	B	301	ARG
2	B	321	THR
2	B	327	ASP
2	B	339	ARG
2	B	341	ILE
2	B	349	ILE
2	B	354	ILE
2	B	364	SER
2	B	372	GLU
2	B	389	GLN
2	B	394	LEU
3	C	5	ILE
3	C	31	LEU
3	C	33	ASN
3	C	35	GLN
3	C	44	TYR
3	C	53	THR
3	C	55	TYR
3	C	82	GLU
3	C	93	THR

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Mol	Chain	Res	Type
3	C	102	LEU
3	C	109	VAL
3	C	134	MET
3	C	136	GLU
3	C	160	SER
3	C	189	ASP
3	C	202	ILE
3	C	220	SER
3	C	247	THR
3	C	275	LEU
3	C	282	MET
3	C	311	ARG
3	C	321	SER
3	C	339	VAL
3	C	340	ILE
3	C	369	ASN
3	C	392	GLU
3	C	408	ASP
3	C	410	SER
3	C	414	THR
3	C	428	THR
3	C	431	VAL
3	C	432	VAL
1	D	9	HIS
1	D	17	VAL
1	D	32	ILE
1	D	39	VAL
1	D	57	SER
1	D	67	MSE
1	D	84	ILE
1	D	85	ASP
1	D	111	VAL
1	D	120	VAL
1	D	145	GLN
1	D	149	THR
1	D	162	LEU
1	D	172	GLN
1	D	190	LEU
1	D	201	THR
1	D	232	GLU
1	D	252	LEU
1	D	259	ASN

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Mol	Chain	Res	Type
1	D	266	ILE
1	D	276	ILE
1	D	288	ASP
2	E	6	LEU
2	E	7	ILE
2	E	8	LYS
2	E	20	ASN
2	E	25	THR
2	E	36	ASN
2	E	43	GLU
2	E	48	PHE
2	E	49	VAL
2	E	65	SER
2	E	110	ASP
2	E	121	LEU
2	E	127	LEU
2	E	151	VAL
2	E	164	GLN
2	E	178	LEU
2	E	179	SER
2	E	182	GLU
2	E	185	ASP
2	E	194	GLN
2	E	199	ARG
2	E	253	LEU
2	E	258	ILE
2	E	298	ILE
2	E	326	VAL
2	E	339	ARG
2	E	344	LYS
2	E	378	LEU
2	E	380	ARG
2	E	394	LEU
3	F	29	LYS
3	F	30	SER
3	F	33	ASN
3	F	41	VAL
3	F	55	TYR
3	F	77	LEU
3	F	100	LYS
3	F	109	VAL
3	F	116	ILE

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Mol	Chain	Res	Type
3	F	126	THR
3	F	130	LYS
3	F	148	VAL
3	F	161	VAL
3	F	188	ASP
3	F	198	ILE
3	F	202	ILE
3	F	212	LEU
3	F	220	SER
3	F	236	LYS
3	F	247	THR
3	F	267	ILE
3	F	307	LEU
3	F	324	THR
3	F	332	VAL
3	F	334	ILE
3	F	340	ILE
3	F	392	GLU
3	F	413	VAL
3	F	431	VAL
3	F	432	VAL
3	F	434	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	8	HIS
2	B	20	ASN
2	B	36	ASN
2	B	51	ASN
2	B	118	GLN
2	B	208	HIS
2	B	235	ASN
2	B	389	GLN
3	C	4	GLN
3	C	11	HIS
3	C	132	HIS
3	C	287	ASN
3	C	333	ASN
3	C	369	ASN
3	C	399	GLN

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Mol	Chain	Res	Type
1	D	198	ASN
2	E	84	ASN
2	E	118	GLN
2	E	235	ASN
2	E	280	GLN
3	F	35	GLN
3	F	143	HIS
3	F	151	ASN
3	F	343	ASN
3	F	359	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z > 2$
5	ATP	D	402	-	32,33,33	1.54	7 (21%)	48,52,52	1.73	8 (16%)
8	PO4	E	503	-	4,4,4	0.99	0	6,6,6	0.37	0
8	PO4	F	504	-	4,4,4	0.93	0	6,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MES	B	502	-	12,12,12	2.05	1 (8%)	15,16,16	2.47	8 (53%)
7	GOL	B	503	-	5,5,5	0.42	0	5,5,5	0.72	0
5	ATP	E	501	4	32,33,33	1.65	7 (21%)	48,52,52	1.79	10 (20%)
9	SAH	F	501	-	27,28,28	1.13	3 (11%)	36,40,40	2.15	11 (30%)
8	PO4	B	506	-	4,4,4	0.94	0	6,6,6	0.49	0
9	SAH	C	501	-	27,28,28	1.14	4 (14%)	36,40,40	2.22	11 (30%)
7	GOL	B	504	-	5,5,5	0.41	0	5,5,5	0.23	0
8	PO4	F	503	-	4,4,4	0.87	0	6,6,6	0.46	0
5	ATP	B	501	4	32,33,33	1.76	7 (21%)	48,52,52	1.75	10 (20%)
8	PO4	C	503	-	4,4,4	0.95	0	6,6,6	0.44	0
5	ATP	A	402	-	32,33,33	1.54	7 (21%)	48,52,52	1.75	9 (18%)

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
5	ATP	D	402	-	-	5/22/38/38	0/3/3/3
6	MES	B	502	-	-	3/6/14/14	0/1/1/1
7	GOL	B	503	-	-	0/4/4/4	-
5	ATP	E	501	4	-	10/22/38/38	0/3/3/3
9	SAH	F	501	-	-	4/15/31/31	0/3/3/3
9	SAH	C	501	-	-	7/15/31/31	0/3/3/3
7	GOL	B	504	-	-	4/4/4/4	-
5	ATP	B	501	4	-	11/22/38/38	0/3/3/3
5	ATP	A	402	-	-	4/22/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	MES	C8-S	-6.76	1.68	1.77
5	E	501	ATP	C5-C4	5.25	1.48	1.39
5	D	402	ATP	C5-C4	5.01	1.48	1.39
5	B	501	ATP	C5-C4	4.84	1.47	1.39
5	A	402	ATP	C5-C4	4.68	1.47	1.39
5	B	501	ATP	PA-O3A	4.27	1.64	1.59
5	B	501	ATP	PB-O3A	3.95	1.63	1.59
5	E	501	ATP	PA-O3A	3.88	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	501	ATP	PB-O3A	3.48	1.63	1.59
5	D	402	ATP	C5-C6	3.02	1.49	1.41
5	D	402	ATP	PA-O3A	2.97	1.62	1.59
5	A	402	ATP	C5-C6	2.95	1.49	1.41
5	A	402	ATP	PA-O3A	2.93	1.62	1.59
5	B	501	ATP	PB-O3B	2.92	1.62	1.59
9	C	501	SAH	C2-N3	2.87	1.39	1.33
5	B	501	ATP	C5-N7	-2.73	1.34	1.39
9	F	501	SAH	C2-N3	2.69	1.38	1.33
5	E	501	ATP	C5-C6	2.60	1.48	1.41
9	F	501	SAH	C2-N1	2.59	1.38	1.33
5	A	402	ATP	PB-O3B	2.57	1.62	1.59
9	F	501	SAH	C8-N7	2.57	1.36	1.31
5	A	402	ATP	PB-O3A	2.45	1.62	1.59
9	C	501	SAH	C2-N1	2.41	1.38	1.33
5	A	402	ATP	C8-N7	2.39	1.36	1.31
5	B	501	ATP	C5-C6	2.37	1.47	1.41
5	D	402	ATP	C8-N7	2.32	1.36	1.31
9	C	501	SAH	C8-N7	2.31	1.36	1.31
5	A	402	ATP	C5-N7	-2.23	1.35	1.39
5	D	402	ATP	PB-O3A	2.16	1.61	1.59
5	B	501	ATP	C8-N7	2.12	1.35	1.31
5	E	501	ATP	C5-N7	-2.11	1.35	1.39
5	E	501	ATP	C8-N7	2.11	1.35	1.31
5	E	501	ATP	C4-N9	-2.08	1.33	1.37
5	D	402	ATP	PB-O3B	2.07	1.61	1.59
5	D	402	ATP	C5-N7	-2.04	1.35	1.39
9	C	501	SAH	OXT-C	-2.02	1.24	1.30

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	ATP	C5-C4-N3	-6.06	118.38	126.72
5	B	501	ATP	C5-C4-N3	-5.97	118.50	126.72
5	D	402	ATP	C5-C4-N3	-5.84	118.67	126.72
9	F	501	SAH	N3-C2-N1	-5.81	119.78	128.58
9	C	501	SAH	C5-C4-N3	-5.72	118.85	126.72
9	C	501	SAH	N3-C2-N1	-5.61	120.10	128.58
5	E	501	ATP	C5-C4-N3	-5.27	119.46	126.72
5	E	501	ATP	N3-C4-N9	5.10	135.84	127.17
5	B	501	ATP	N3-C4-N9	5.03	135.72	127.17
9	F	501	SAH	C5-C4-N3	-4.90	119.97	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	502	MES	C5-N4-C3	4.88	119.35	108.84
5	A	402	ATP	N3-C4-N9	4.60	135.00	127.17
5	D	402	ATP	N3-C4-N9	4.51	134.83	127.17
9	C	501	SAH	C5'-SD-CG	-4.41	89.16	102.26
9	C	501	SAH	C2-N3-C4	3.97	121.52	111.83
9	F	501	SAH	C2-N3-C4	3.85	121.22	111.83
5	A	402	ATP	C4-C5-N7	-3.82	106.21	110.58
6	B	502	MES	C2-C3-N4	-3.77	104.39	110.12
5	A	402	ATP	C2-N3-C4	3.75	120.98	111.83
9	C	501	SAH	N3-C4-N9	3.73	133.50	127.17
5	D	402	ATP	C2-N3-C4	3.60	120.63	111.83
9	F	501	SAH	O4'-C1'-N9	3.60	115.01	108.09
5	D	402	ATP	C4-C5-N7	-3.56	106.51	110.58
9	F	501	SAH	N9-C8-N7	-3.52	108.95	113.94
6	B	502	MES	C6-C5-N4	-3.49	104.81	110.12
9	C	501	SAH	C5-N7-C8	3.41	108.81	103.45
9	C	501	SAH	N9-C8-N7	-3.39	109.12	113.94
5	E	501	ATP	C2-N3-C4	3.39	120.11	111.83
5	E	501	ATP	C4-N9-C8	3.37	109.28	105.74
9	F	501	SAH	C5-N7-C8	3.29	108.63	103.45
5	B	501	ATP	C2-N3-C4	3.28	119.83	111.83
9	F	501	SAH	OXT-C-O	-3.17	116.89	124.08
5	E	501	ATP	N3-C2-N1	-3.05	123.96	128.58
6	B	502	MES	C7-N4-C3	3.03	119.32	111.24
5	A	402	ATP	N3-C2-N1	-2.94	124.14	128.58
5	A	402	ATP	C5-N7-C8	2.84	107.91	103.45
5	D	402	ATP	N3-C2-N1	-2.82	124.32	128.58
9	F	501	SAH	N3-C4-N9	2.80	131.94	127.17
6	B	502	MES	C7-N4-C5	2.79	118.68	111.24
9	C	501	SAH	OXT-C-O	-2.74	117.86	124.08
9	F	501	SAH	C4-C5-N7	-2.69	107.50	110.58
5	B	501	ATP	C3'-C2'-C1'	2.60	106.39	101.46
6	B	502	MES	O1S-S-C8	2.58	110.63	106.73
6	B	502	MES	O2S-S-C8	2.55	110.58	106.73
5	B	501	ATP	C4-C5-N7	-2.52	107.70	110.58
9	C	501	SAH	O4'-C1'-N9	2.48	112.86	108.09
5	D	402	ATP	C5-N7-C8	2.44	107.29	103.45
5	A	402	ATP	C4-N9-C8	2.41	108.27	105.74
5	B	501	ATP	O5'-C5'-C4'	-2.40	100.82	108.99
9	C	501	SAH	C4-C5-N7	-2.39	107.85	110.58
9	F	501	SAH	C5'-SD-CG	-2.35	95.29	102.26
6	B	502	MES	O2S-S-O1S	-2.32	106.28	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	501	ATP	O2'-C2'-C1'	-2.31	102.14	110.10
5	A	402	ATP	C6-C5-N7	2.27	136.46	132.09
5	D	402	ATP	C4-N9-C8	2.24	108.09	105.74
5	B	501	ATP	N3-C2-N1	-2.21	125.24	128.58
5	B	501	ATP	O2'-C2'-C1'	-2.20	102.52	110.10
5	E	501	ATP	C3'-C2'-C1'	2.19	105.61	101.46
5	B	501	ATP	C4-N9-C8	2.14	107.98	105.74
5	B	501	ATP	O2B-PB-O3A	2.12	113.00	107.27
9	F	501	SAH	C5-C4-N9	2.09	108.09	105.81
5	A	402	ATP	N9-C8-N7	-2.08	110.99	113.94
5	E	501	ATP	C2'-C3'-C4'	-2.07	98.60	102.61
5	D	402	ATP	C6-C5-N7	2.06	136.06	132.09
5	E	501	ATP	C4-C5-N7	-2.04	108.25	110.58
9	C	501	SAH	C6-C5-C4	2.02	119.94	117.18
5	E	501	ATP	N6-C6-N1	2.00	122.84	118.38

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	501	ATP	C5'-O5'-PA-O2A
7	B	504	GOL	O1-C1-C2-C3
7	B	504	GOL	C1-C2-C3-O3
9	C	501	SAH	C-CA-CB-CG
9	F	501	SAH	N-CA-CB-CG
9	F	501	SAH	C-CA-CB-CG
5	D	402	ATP	O4'-C4'-C5'-O5'
7	B	504	GOL	O1-C1-C2-O2
7	B	504	GOL	O2-C2-C3-O3
5	D	402	ATP	C3'-C4'-C5'-O5'
9	C	501	SAH	OXT-C-CA-CB
5	D	402	ATP	PB-O3B-PG-O1G
6	B	502	MES	C8-C7-N4-C5
9	C	501	SAH	O-C-CA-CB
9	F	501	SAH	CA-CB-CG-SD
5	E	501	ATP	C4'-C5'-O5'-PA
5	E	501	ATP	C3'-C4'-C5'-O5'
5	A	402	ATP	PB-O3B-PG-O2G
6	B	502	MES	N4-C7-C8-S
5	B	501	ATP	PG-O3B-PB-O2B
9	C	501	SAH	OXT-C-CA-N
5	E	501	ATP	O4'-C4'-C5'-O5'

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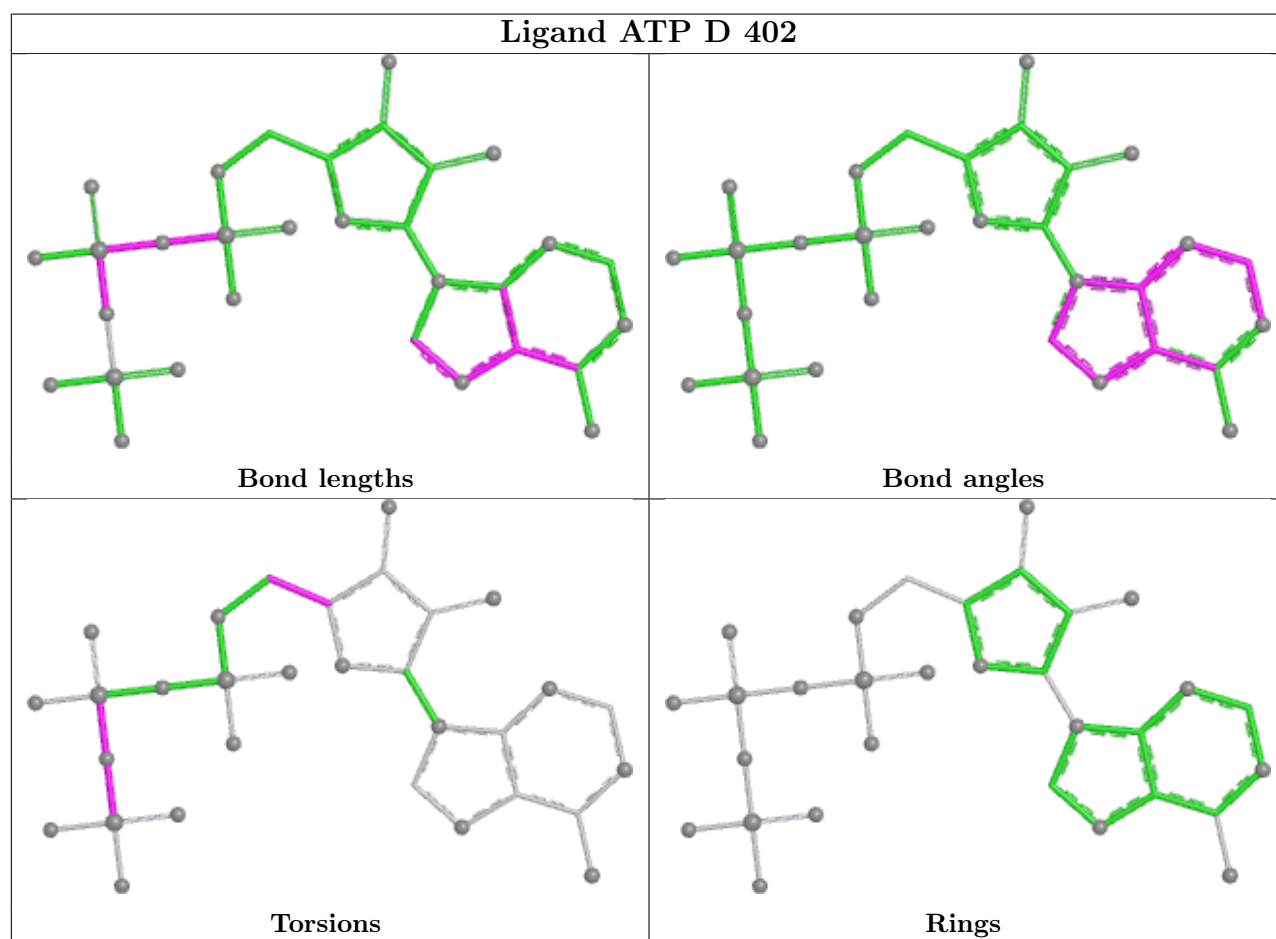
Mol	Chain	Res	Type	Atoms
5	B	501	ATP	C5'-O5'-PA-O1A
5	B	501	ATP	C5'-O5'-PA-O2A
5	B	501	ATP	C5'-O5'-PA-O3A
5	E	501	ATP	C5'-O5'-PA-O1A
5	E	501	ATP	C5'-O5'-PA-O3A
5	B	501	ATP	C4'-C5'-O5'-PA
5	E	501	ATP	C2'-C1'-N9-C8
5	B	501	ATP	PA-O3A-PB-O2B
5	B	501	ATP	C2'-C1'-N9-C4
5	E	501	ATP	C2'-C1'-N9-C4
5	B	501	ATP	C2'-C1'-N9-C8
9	F	501	SAH	CB-CG-SD-C5'
9	C	501	SAH	O-C-CA-N
5	A	402	ATP	PG-O3B-PB-O2B
5	B	501	ATP	O4'-C1'-N9-C8
6	B	502	MES	C8-C7-N4-C3
5	A	402	ATP	PB-O3B-PG-O3G
5	E	501	ATP	O4'-C1'-N9-C8
5	A	402	ATP	PG-O3B-PB-O1B
5	B	501	ATP	PB-O3A-PA-O2A
5	D	402	ATP	PG-O3B-PB-O1B
5	D	402	ATP	PG-O3B-PB-O2B
5	E	501	ATP	PA-O3A-PB-O2B
9	C	501	SAH	C2'-C1'-N9-C8
9	C	501	SAH	CB-CG-SD-C5'
5	B	501	ATP	PG-O3B-PB-O1B

There are no ring outliers.

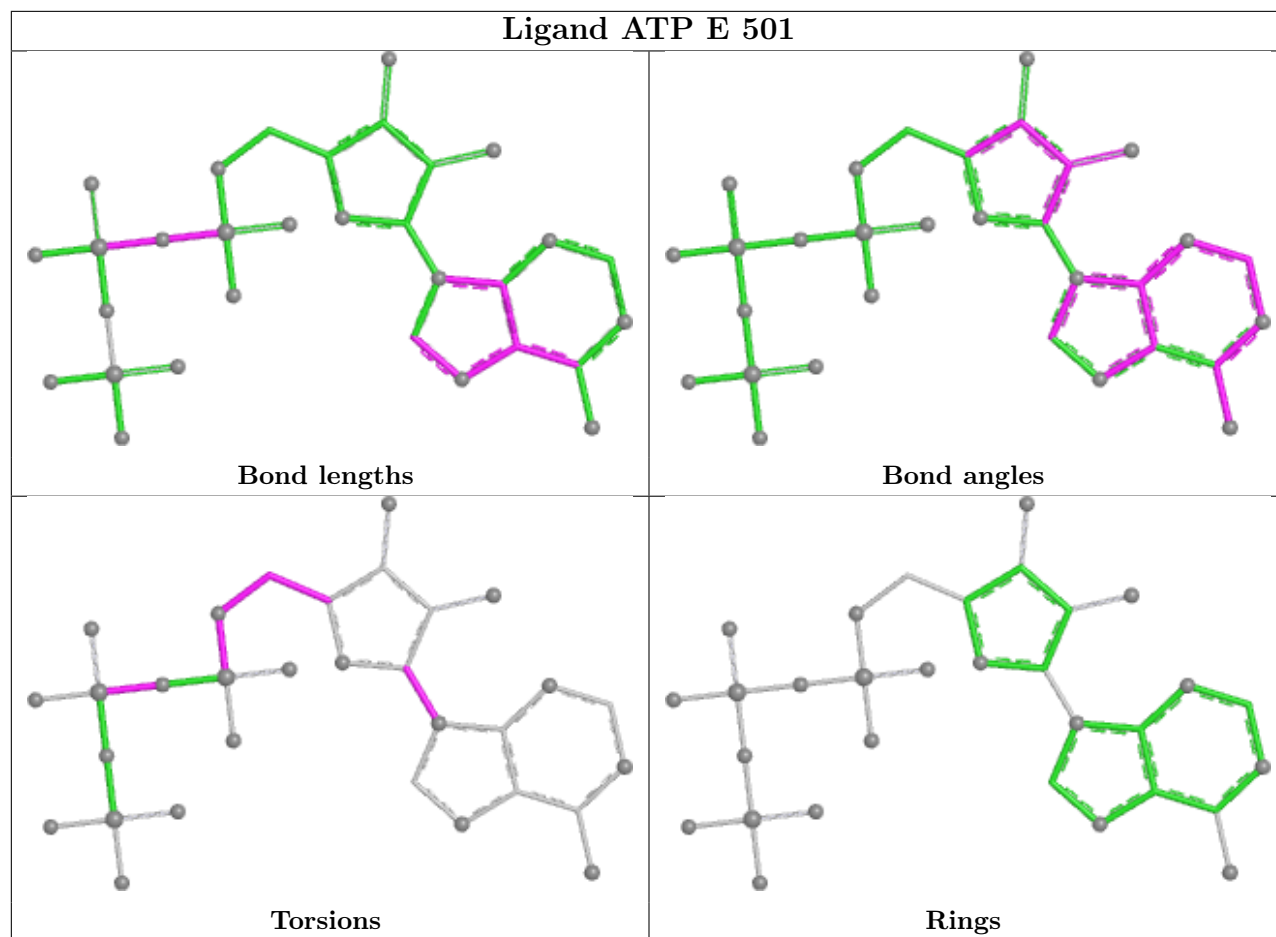
10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	402	ATP	2	0
8	E	503	PO4	1	0
6	B	502	MES	3	0
7	B	503	GOL	1	0
5	E	501	ATP	5	0
9	F	501	SAH	1	0
9	C	501	SAH	1	0
7	B	504	GOL	1	0
5	B	501	ATP	5	0
5	A	402	ATP	2	0

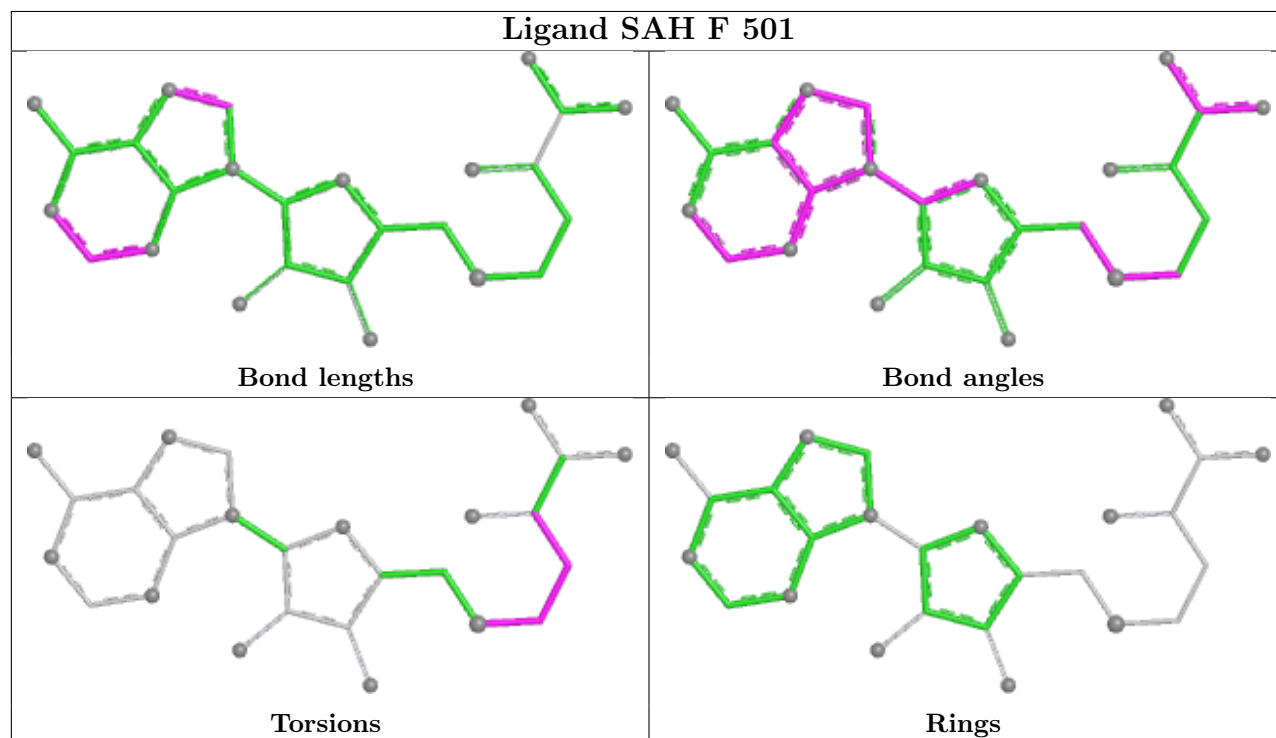
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



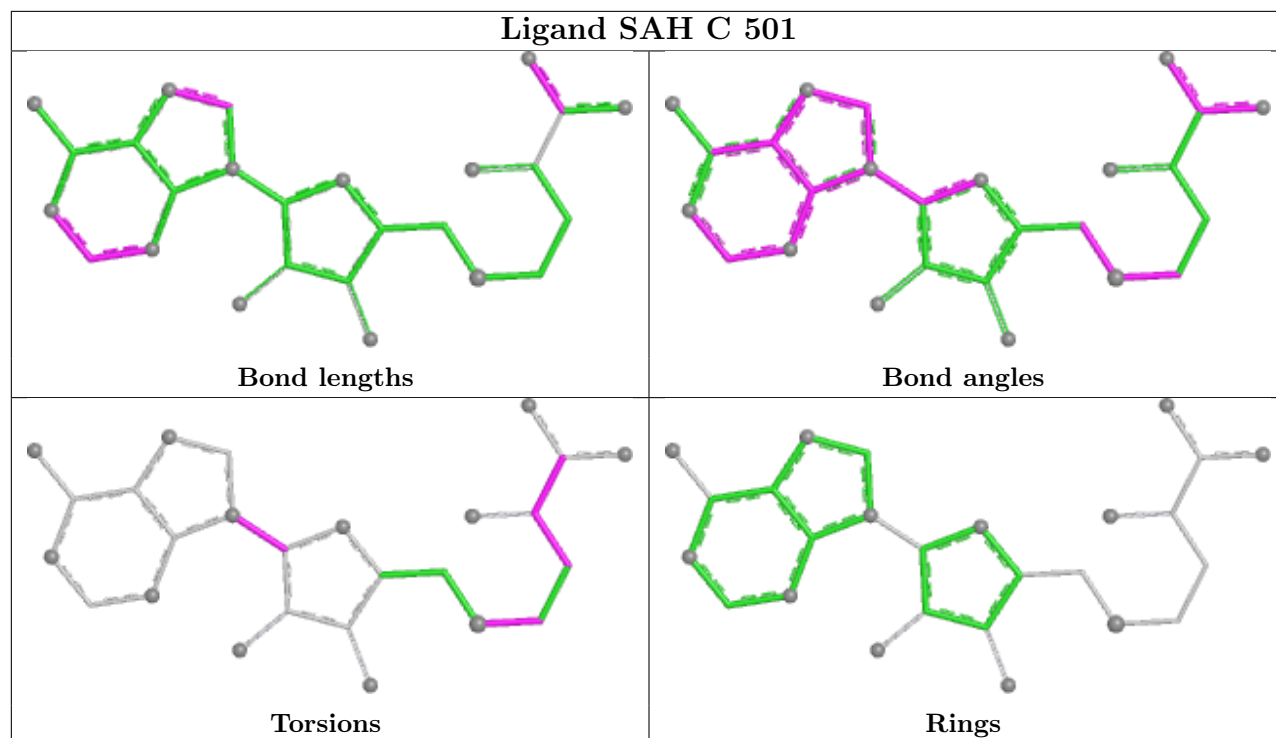
Ligand ATP E 501



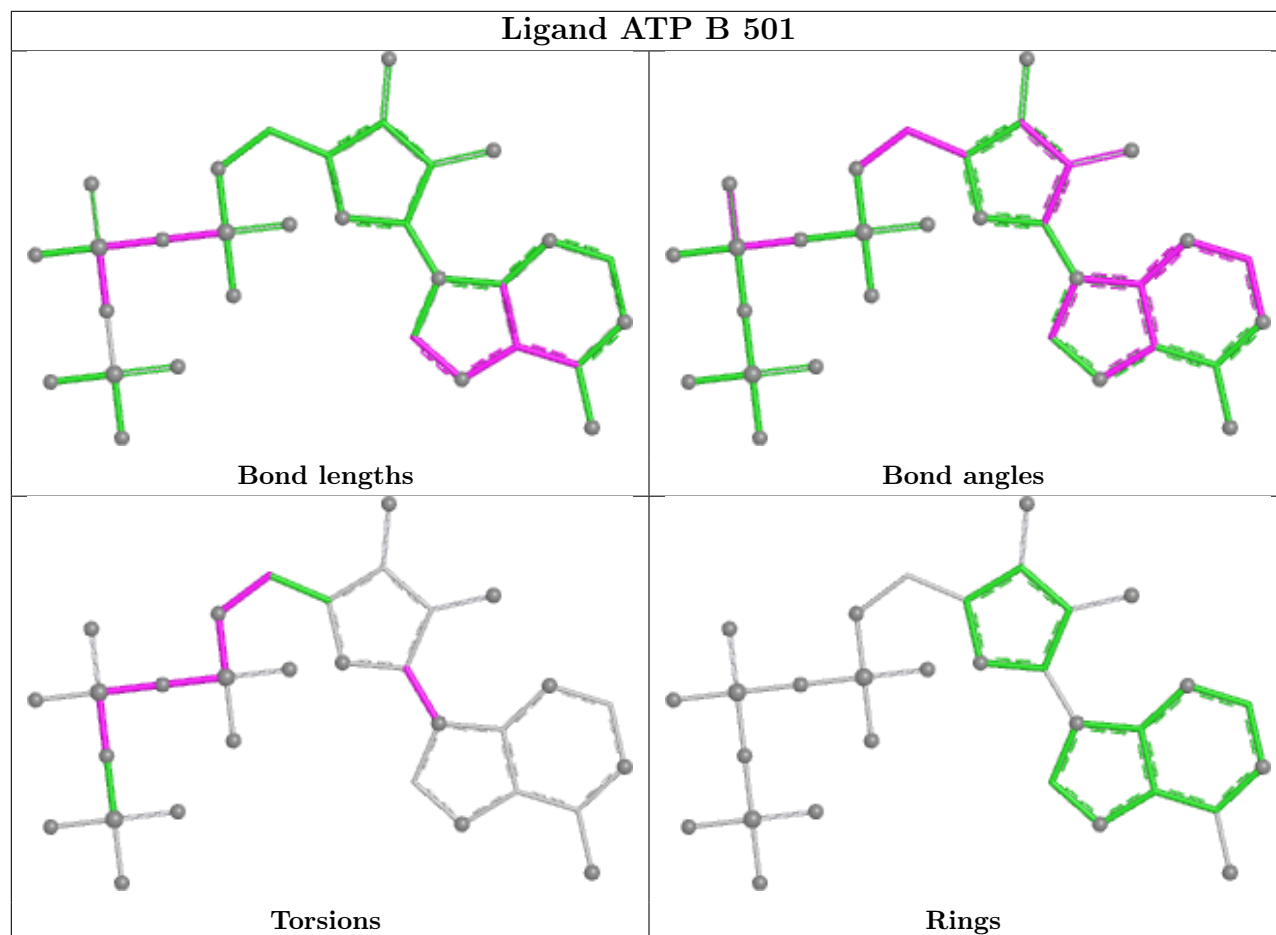
Ligand SAH F 501

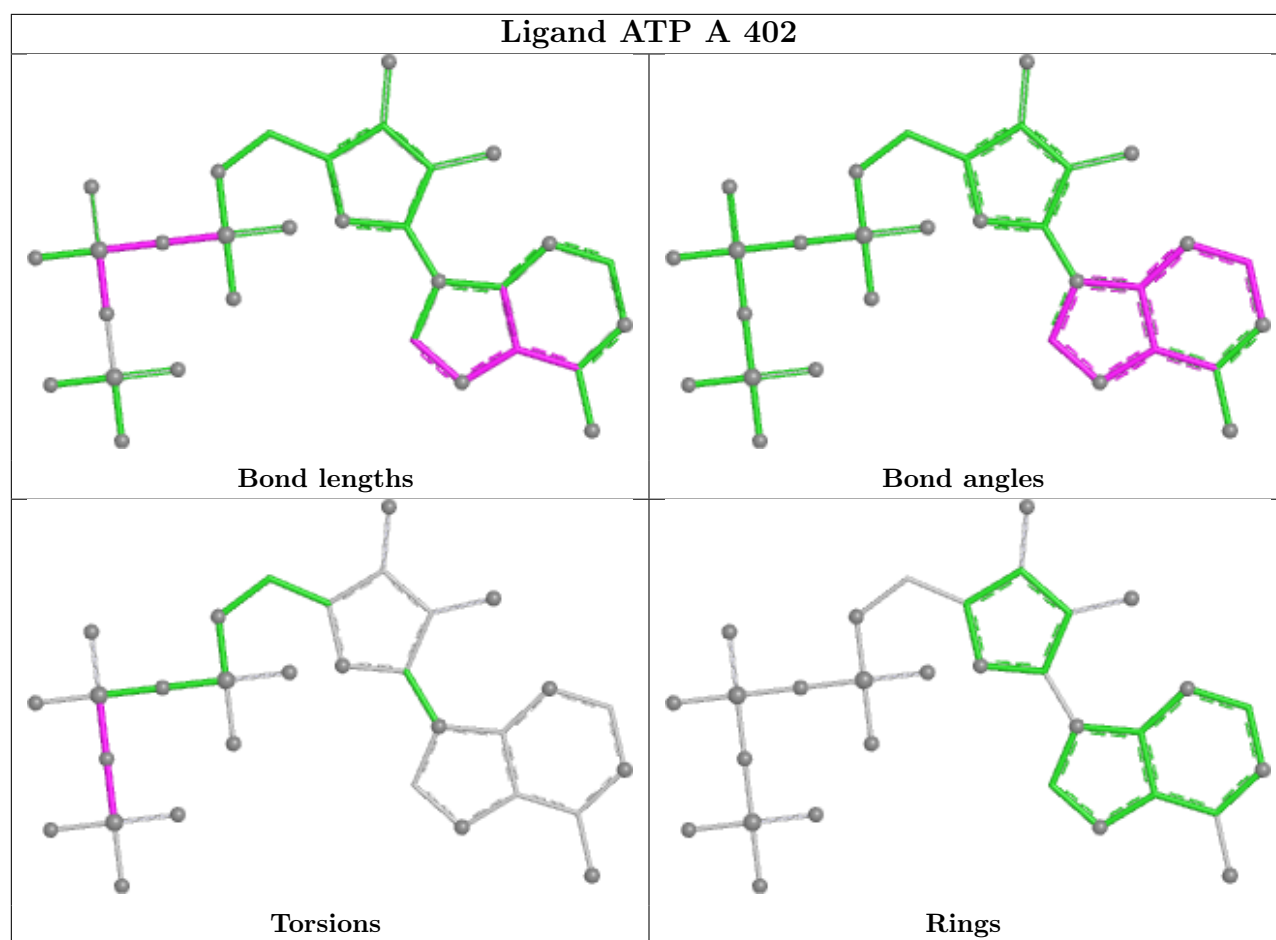


Ligand SAH C 501



Ligand ATP B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/312 (90%)	-0.57	0 100 100	51, 87, 134, 147	0
1	D	279/312 (89%)	-0.47	1 (0%) 88 81	51, 92, 136, 163	0
2	B	394/394 (100%)	-0.63	3 (0%) 82 71	42, 63, 128, 159	0
2	E	393/394 (99%)	-0.37	5 (1%) 75 61	55, 93, 128, 149	0
3	C	424/436 (97%)	-0.55	0 100 100	44, 82, 122, 147	0
3	F	424/436 (97%)	-0.60	1 (0%) 91 88	49, 74, 120, 145	0
All	All	2197/2284 (96%)	-0.53	10 (0%) 87 78	42, 82, 129, 163	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	269	THR	4.5
2	B	177	VAL	3.2
2	E	259	ASN	2.6
2	B	192	ILE	2.4
2	B	178	LEU	2.4
1	D	220	GLN	2.3
2	E	93	GLN	2.2
2	E	67	CYS	2.1
2	E	143	HIS	2.0
3	F	99	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

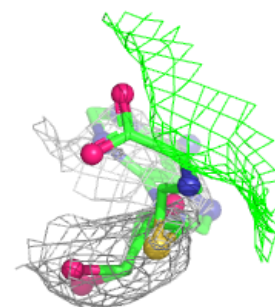
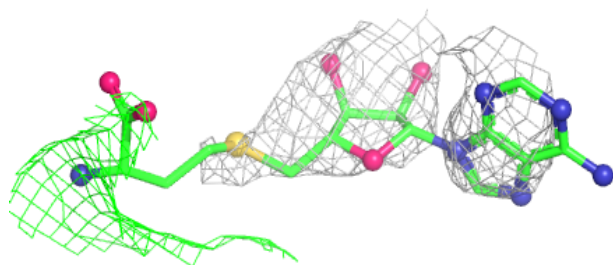
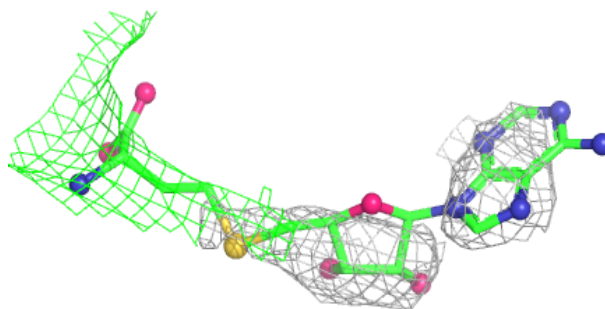
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PO4	E	503	5/5	0.72	0.16	166,168,170,171	0
6	MES	B	502	12/12	0.74	0.13	64,80,120,122	0
8	PO4	B	506	5/5	0.80	0.12	136,137,139,141	0
9	SAH	F	501	26/26	0.82	0.16	83,101,121,196	9
9	SAH	C	501	26/26	0.83	0.12	124,138,150,188	0
8	PO4	C	503	5/5	0.85	0.18	145,146,146,148	0
5	ATP	D	402	31/31	0.89	0.07	121,127,140,179	0
8	PO4	F	503	5/5	0.90	0.17	115,117,120,125	0
8	PO4	F	504	5/5	0.90	0.14	134,135,135,137	0
5	ATP	A	402	31/31	0.91	0.06	98,119,150,150	0
5	ATP	E	501	31/31	0.91	0.09	57,67,171,189	0
7	GOL	B	504	6/6	0.93	0.20	95,103,106,108	0
4	MG	A	401	1/1	0.94	0.17	54,54,54,54	0
4	MG	F	502	1/1	0.95	0.08	54,54,54,54	0
7	GOL	B	503	6/6	0.95	0.08	58,77,81,82	0
4	MG	C	502	1/1	0.96	0.14	41,41,41,41	0
5	ATP	B	501	31/31	0.96	0.07	39,53,168,198	0
4	MG	E	502	1/1	0.97	0.12	68,68,68,68	0
4	MG	D	401	1/1	0.97	0.13	56,56,56,56	0
4	MG	B	505	1/1	0.99	0.08	48,48,48,48	0

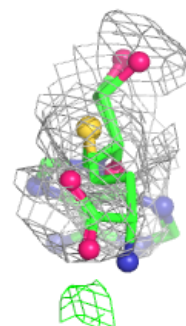
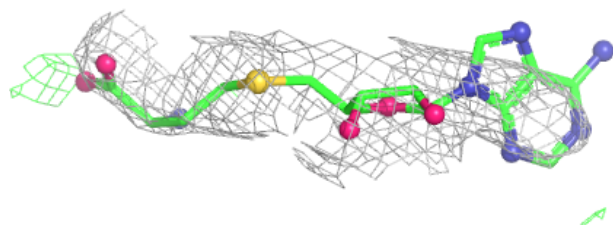
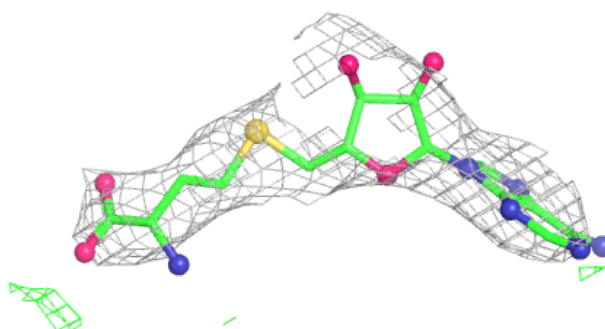
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH F 501:

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

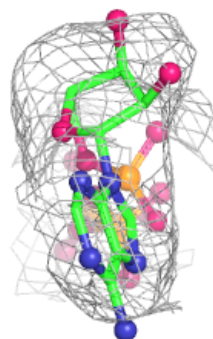
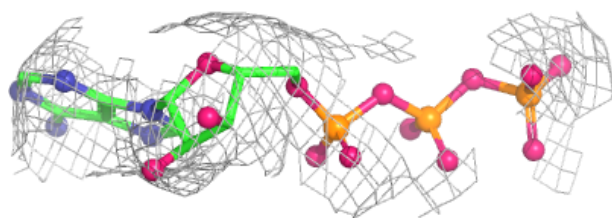
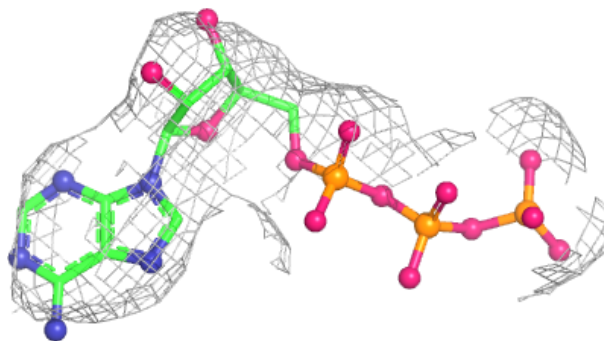
**Electron density around SAH C 501:**

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

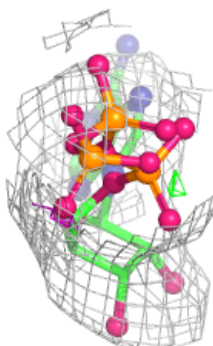
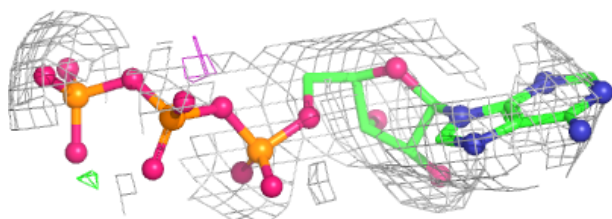
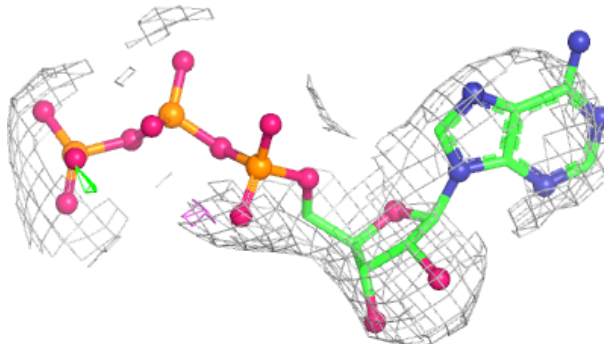


Electron density around ATP D 402:

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

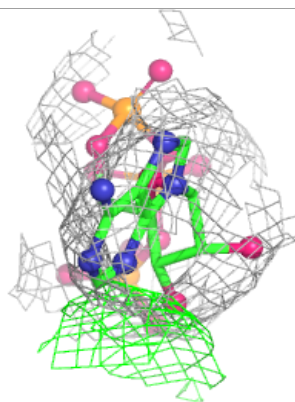
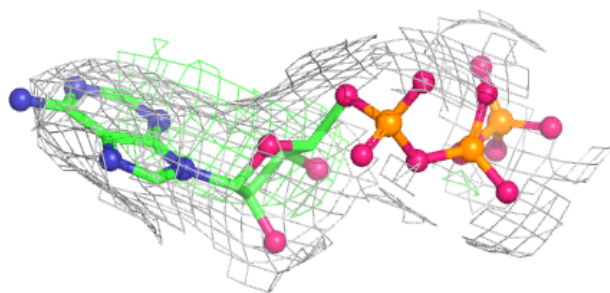
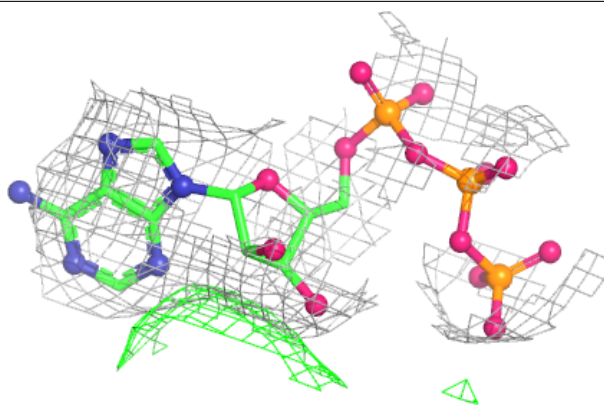
**Electron density around ATP A 402:**

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

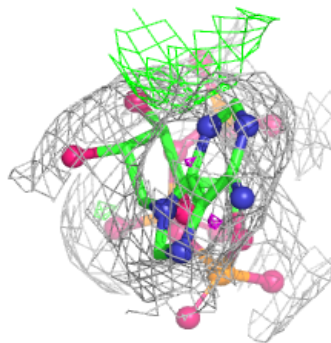
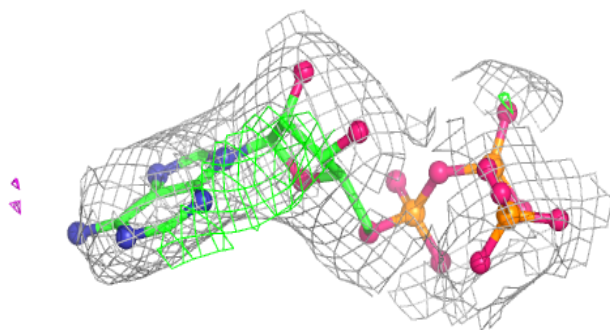
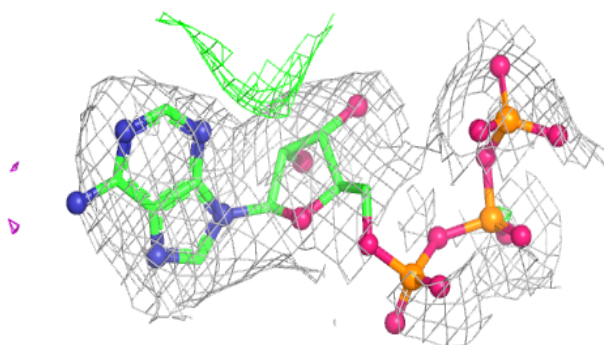


Electron density around ATP E 501:

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

**Electron density around ATP B 501:**

$2mF_o-DF_c$ (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.