



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:38 pm BST

PDB ID : 5KNN
Title : Evolutionary gain of alanine mischarging to non-cognate tRNAs with a G4:U69 base pair
Authors : Sun, L.; He, W.; Yang, X.-L.
Deposited on : 2016-06-28
Resolution : 2.68 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

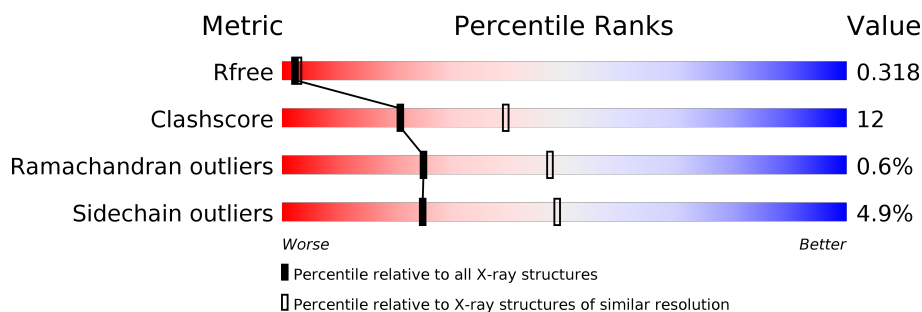
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	450	78% 19% .
1	B	450	73% 22% . .
1	C	450	66% 26% 5% . .
1	D	450	72% 23% . .
1	E	450	74% 22% . .
1	F	450	74% 23% . .
1	G	450	73% 24% . .

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Mol	Chain	Length	Quality of chain
1	H	450	<div><div></div><div>69%</div><div>25%</div><div></div><div>.</div><div>..</div></div>

2 Entry composition

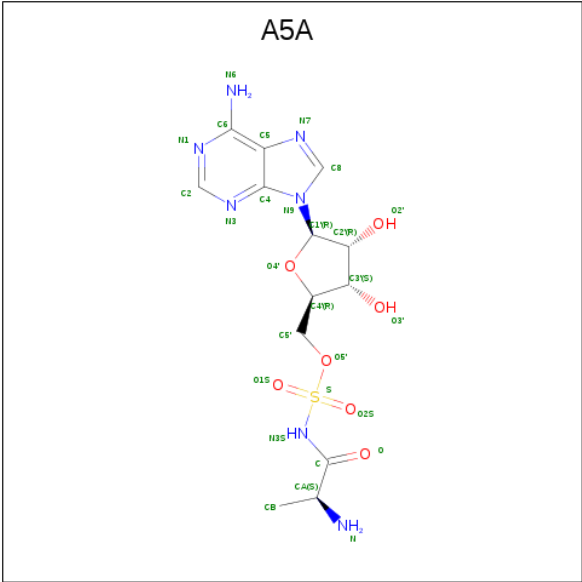
There are 2 unique types of molecules in this entry. The entry contains 28584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alanine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	B	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	C	444	Total	C	N	O	S	0	0	0
			3514	2227	604	667	16			
1	D	447	Total	C	N	O	S	0	0	0
			3536	2241	608	671	16			
1	E	450	Total	C	N	O	S	0	0	0
			3560	2255	613	676	16			
1	F	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	G	449	Total	C	N	O	S	0	0	0
			3551	2250	611	674	16			
1	H	446	Total	C	N	O	S	0	0	0
			3528	2235	607	670	16			

- Molecule 2 is '5'-O-(N-(L-ALANYL)-SULFAMOYL)ADENOSINE (three-letter code: A5A) (formula: C₁₃H₁₉N₇O₇S).

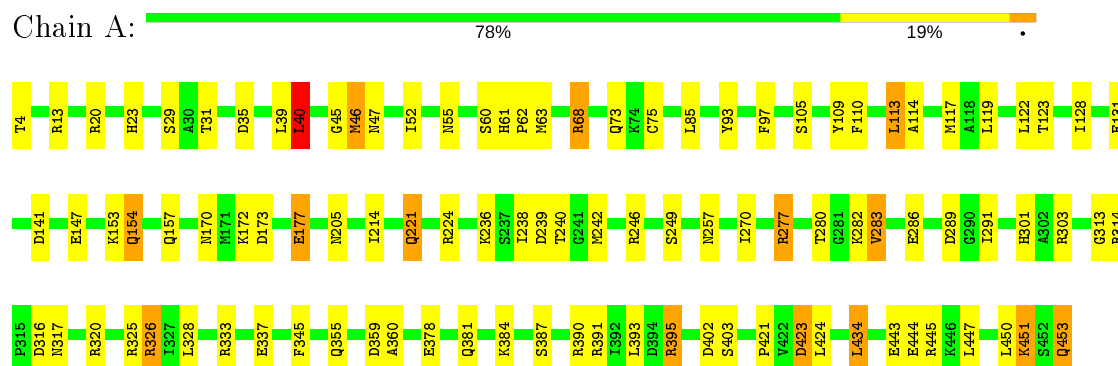


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	B	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	C	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	D	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	E	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	F	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	G	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	H	1	Total	C	N	O	S	0	0
			28	13	7	7	1		

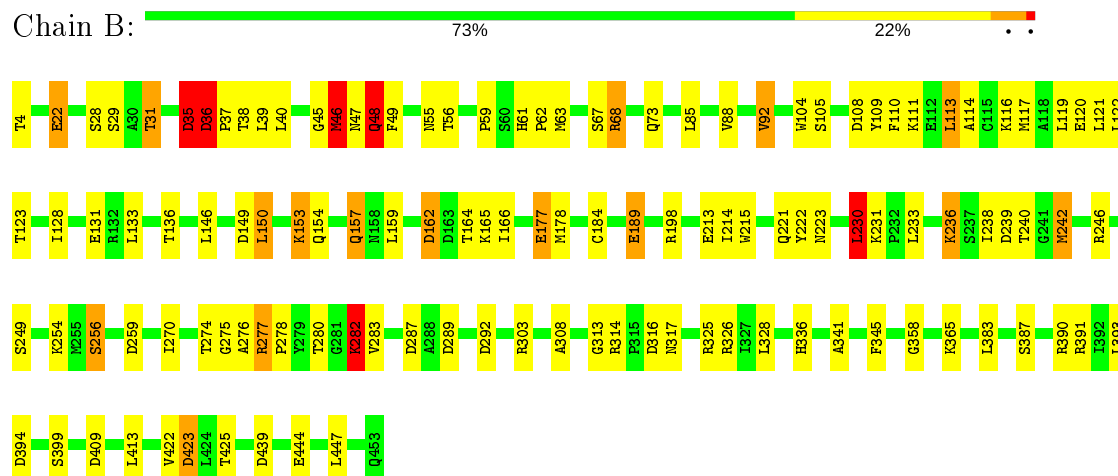
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

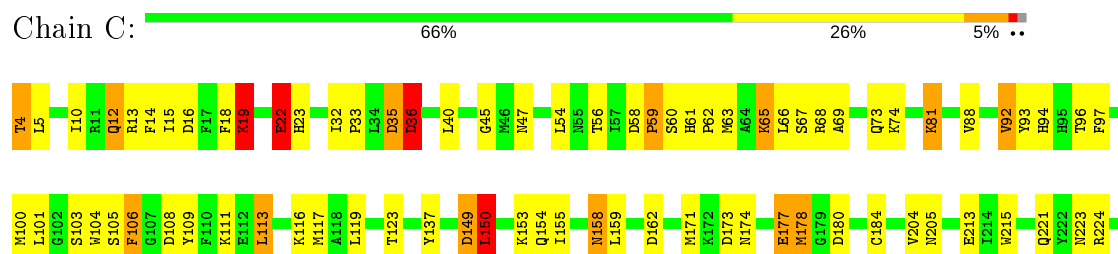
- Molecule 1: Alanine-tRNA ligase, cytoplasmic

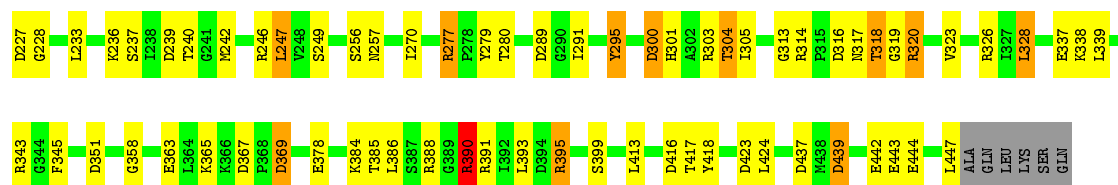


- Molecule 1: Alanine-tRNA ligase, cytoplasmic



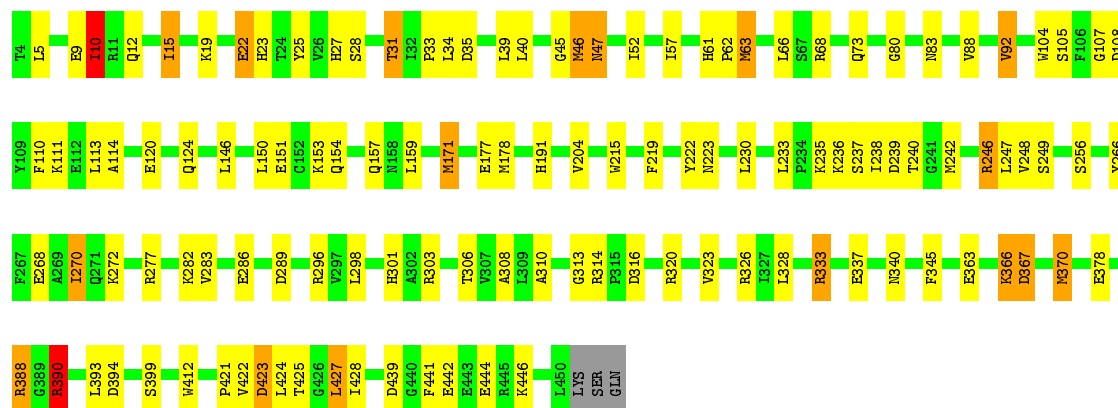
- Molecule 1: Alanine-tRNA ligase, cytoplasmic





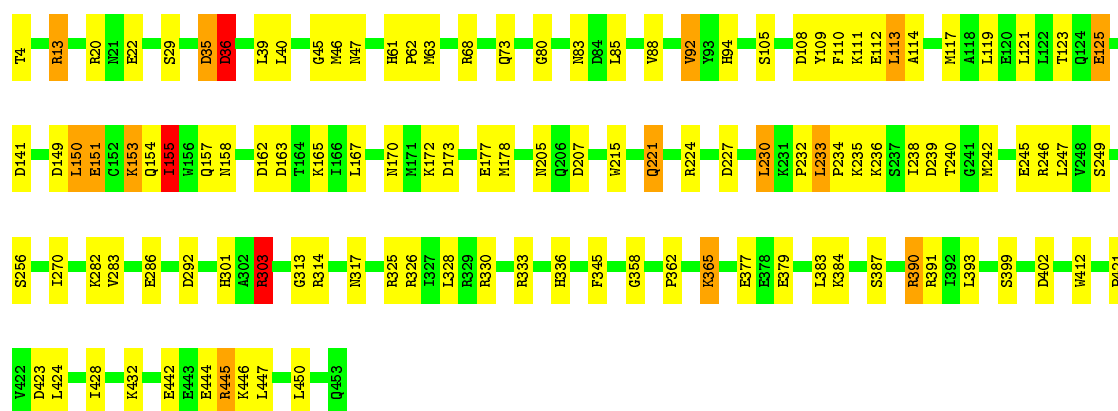
- Molecule 1: Alanine-tRNA ligase, cytoplasmic

Chain D: 72% 23%



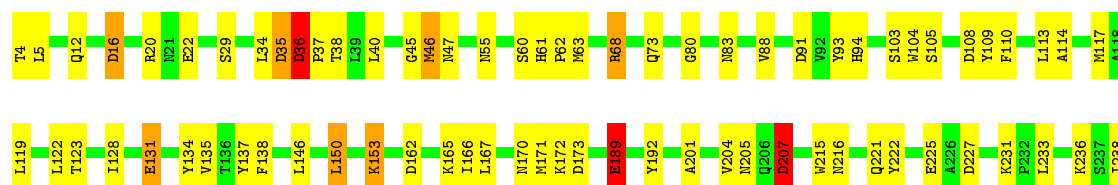
- Molecule 1: Alanine-tRNA ligase, cytoplasmic

Chain E: 74% 22%



- Molecule 1: Alanine-tRNA ligase, cytoplasmic

Chain F: 74% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.17 Å 98.26 Å 201.38 Å 90.07° 89.95° 90.11°	Depositor
Resolution (Å)	49.13 – 2.68 49.13 – 2.68	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.13-2.68) 99.4 (49.13-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.216 , 0.254 0.282 , 0.318	Depositor DCC
R_{free} test set	5439 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l 0.079 for -h,k,-l 0.146 for -h,-k,l	Xtriage
Reported twinning fraction	0.441 for H, K, L 0.076 for -h,-k,l 0.275 for h,-k,-l 0.209 for -H, K, -L	Depositor
Outliers	0 of 112184 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: A5A

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	0.77	1/3635 (0.0%)	1.01	22/4915 (0.4%)
1	B	0.78	4/3635 (0.1%)	1.01	26/4915 (0.5%)
1	C	0.86	6/3589 (0.2%)	1.16	39/4854 (0.8%)
1	D	0.81	2/3611 (0.1%)	1.11	29/4884 (0.6%)
1	E	0.79	2/3635 (0.1%)	1.04	26/4915 (0.5%)
1	F	0.80	1/3626 (0.0%)	0.99	22/4903 (0.4%)
1	G	0.81	0/3626	1.08	28/4903 (0.6%)
1	H	0.87	5/3603 (0.1%)	1.16	36/4873 (0.7%)
All	All	0.81	21/28960 (0.1%)	1.07	228/39162 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	4
All	All	0	12

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	151	GLU	C-O	-7.96	1.08	1.23
1	C	149	ASP	CG-OD2	-7.35	1.08	1.25
1	C	442	GLU	CD-OE1	7.21	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	GLU	CD-OE1	6.73	1.33	1.25
1	B	177	GLU	CD-OE1	-6.72	1.18	1.25
1	C	177	GLU	CG-CD	-6.71	1.41	1.51
1	F	134	TYR	CB-CG	-6.40	1.42	1.51
1	B	189	GLU	CD-OE1	-6.30	1.18	1.25
1	H	102	GLY	N-CA	5.79	1.54	1.46
1	B	256	SER	CA-CB	5.63	1.61	1.52
1	B	213	GLU	CG-CD	5.57	1.60	1.51
1	C	19	LYS	CB-CG	5.50	1.67	1.52
1	C	439	ASP	CB-CG	-5.39	1.40	1.51
1	D	366	LYS	CA-CB	5.34	1.65	1.53
1	H	101	LEU	C-O	-5.33	1.13	1.23
1	H	115	CYS	CB-SG	-5.27	1.73	1.81
1	A	177	GLU	CD-OE1	-5.23	1.19	1.25
1	C	74	LYS	CD-CE	5.16	1.64	1.51
1	E	46	MET	CG-SD	-5.08	1.68	1.81
1	H	249	SER	CA-CB	5.01	1.60	1.52
1	E	125	GLU	CD-OE2	-5.00	1.20	1.25

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ASP	CB-CG-OD1	13.34	130.31	118.30
1	E	402	ASP	CB-CG-OD2	-12.89	106.70	118.30
1	H	303	ARG	NE-CZ-NH1	11.53	126.07	120.30
1	D	367	ASP	CB-CG-OD1	11.23	128.41	118.30
1	D	367	ASP	CB-CG-OD2	-10.24	109.09	118.30
1	A	277	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	E	163	ASP	CB-CG-OD2	9.83	127.15	118.30
1	E	365	LYS	CD-CE-NZ	-9.75	89.27	111.70
1	B	68	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	E	230	LEU	CB-CG-CD1	9.45	127.06	111.00
1	C	300	ASP	CB-CG-OD2	9.23	126.61	118.30
1	A	277	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	C	162	ASP	CB-CG-OD2	9.03	126.43	118.30
1	D	146	LEU	CB-CG-CD1	9.03	126.35	111.00
1	H	102	GLY	N-CA-C	8.94	135.46	113.10
1	F	36	ASP	CB-CG-OD1	8.71	126.14	118.30
1	D	439	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	H	388	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	303	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	B	242	MET	CG-SD-CE	8.35	113.57	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	35	ASP	CB-CG-OD1	-8.35	110.78	118.30
1	H	90	LYS	CB-CG-CD	8.35	133.31	111.60
1	H	103	SER	N-CA-C	8.34	133.53	111.00
1	C	390	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	G	130	ILE	CA-CB-CG2	8.31	127.52	110.90
1	H	242	MET	CG-SD-CE	8.30	113.47	100.20
1	G	325	ARG	CG-CD-NE	8.26	129.15	111.80
1	E	36	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	326	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	295	TYR	CB-CG-CD1	8.23	125.94	121.00
1	H	391	ARG	CA-CB-CG	8.20	131.44	113.40
1	E	303	ARG	CG-CD-NE	-8.16	94.66	111.80
1	G	439	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	G	329	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	E	402	ASP	CB-CG-OD1	8.01	125.50	118.30
1	G	316	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	H	117	MET	CA-CB-CG	7.99	126.88	113.30
1	H	224	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	H	35	ASP	CB-CG-OD2	7.91	125.42	118.30
1	F	35	ASP	CB-CG-OD1	7.87	125.38	118.30
1	B	146	LEU	CB-CG-CD1	7.85	124.34	111.00
1	F	146	LEU	CB-CG-CD1	7.84	124.34	111.00
1	B	35	ASP	CB-CG-OD1	7.84	125.36	118.30
1	H	212	LEU	CA-CB-CG	7.78	133.19	115.30
1	B	36	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	H	91	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	36	ASP	CB-CG-OD2	7.55	125.09	118.30
1	H	388	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	171	MET	CG-SD-CE	7.52	112.23	100.20
1	C	247	LEU	CB-CG-CD2	-7.46	98.31	111.00
1	B	230	LEU	CA-CB-CG	-7.42	98.22	115.30
1	D	390	ARG	CD-NE-CZ	7.30	133.82	123.60
1	F	35	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	C	22	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	E	35	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	C	149	ASP	OD1-CG-OD2	-7.25	109.53	123.30
1	C	277	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	B	40	LEU	CB-CG-CD1	7.20	123.23	111.00
1	H	36	ASP	CB-CG-OD1	7.19	124.78	118.30
1	H	46	MET	CB-CG-SD	7.18	133.93	112.40
1	E	35	ASP	CB-CG-OD1	7.13	124.72	118.30
1	H	343	ARG	NE-CZ-NH1	7.13	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	316	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	G	316	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	221	GLN	N-CA-CB	-7.10	97.82	110.60
1	D	22	GLU	N-CA-C	6.99	129.88	111.00
1	F	16	ASP	CB-CG-OD2	6.97	124.58	118.30
1	C	13	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	G	329	ARG	CD-NE-CZ	6.95	133.33	123.60
1	D	316	ASP	CB-CG-OD1	6.94	124.54	118.30
1	C	395	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	343	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	F	40	LEU	CB-CG-CD1	6.84	122.63	111.00
1	G	445	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	36	ASP	C-N-CD	-6.80	105.64	120.60
1	G	36	ASP	CB-CG-OD1	6.74	124.36	118.30
1	G	233	LEU	CA-CB-CG	6.71	130.73	115.30
1	A	40	LEU	CB-CG-CD2	6.65	122.31	111.00
1	D	108	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	B	48	GLN	CB-CG-CD	6.64	128.87	111.60
1	C	106	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	D	63	MET	CG-SD-CE	6.62	110.80	100.20
1	C	150	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	445	ARG	CG-CD-NE	6.54	125.55	111.80
1	E	121	LEU	CB-CG-CD2	-6.52	99.91	111.00
1	F	68	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	338	LYS	CD-CE-NZ	6.49	126.62	111.70
1	B	68	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	C	416	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	120	GLU	OE1-CD-OE2	-6.47	115.54	123.30
1	G	282	LYS	CD-CE-NZ	-6.43	96.91	111.70
1	B	35	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	G	293	MET	CA-CB-CG	6.41	124.19	113.30
1	C	390	ARG	CD-NE-CZ	6.37	132.52	123.60
1	D	316	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	D	388	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	E	13	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	E	163	ASP	OD1-CG-OD2	-6.31	111.31	123.30
1	G	270	ILE	CA-CB-CG1	6.31	122.98	111.00
1	G	88	VAL	N-CA-C	6.30	128.00	111.00
1	C	295	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	63	MET	CG-SD-CE	6.17	110.08	100.20
1	F	447	LEU	CA-CB-CG	6.16	129.47	115.30
1	C	439	ASP	CB-CG-OD1	-6.15	112.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	225	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	H	104	TRP	N-CA-C	6.14	127.59	111.00
1	H	68	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	277	ARG	CB-CA-C	6.08	122.57	110.40
1	E	141	ASP	CB-CG-OD2	6.08	123.77	118.30
1	H	40	LEU	CB-CG-CD2	-6.06	100.69	111.00
1	B	162	ASP	CB-CG-OD1	6.05	123.75	118.30
1	E	153	LYS	N-CA-CB	6.05	121.48	110.60
1	H	224	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	E	292	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	20	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	F	131	GLU	CB-CA-C	5.93	122.26	110.40
1	A	434	LEU	CB-CG-CD2	5.90	121.04	111.00
1	A	141	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	40	LEU	CB-CG-CD2	-5.89	100.98	111.00
1	D	246	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	270	ILE	CA-CB-CG1	5.87	122.15	111.00
1	F	63	MET	CA-CB-CG	5.87	123.27	113.30
1	G	223	ASN	N-CA-CB	-5.87	100.04	110.60
1	C	390	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	F	303	ARG	CG-CD-NE	5.83	124.05	111.80
1	B	213	GLU	OE1-CD-OE2	-5.81	116.32	123.30
1	D	370	MET	CB-CG-SD	5.81	129.82	112.40
1	C	108	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	296	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	328	LEU	CA-CB-CG	-5.77	102.02	115.30
1	H	303	ARG	CD-NE-CZ	5.76	131.67	123.60
1	A	154	GLN	CA-CB-CG	5.74	126.03	113.40
1	D	439	ASP	CB-CG-OD1	5.74	123.47	118.30
1	G	68	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	106	PHE	CB-CG-CD2	5.71	124.79	120.80
1	H	57	ILE	CA-CB-CG2	5.70	122.30	110.90
1	A	393	LEU	CB-CG-CD2	5.69	120.67	111.00
1	C	393	LEU	CB-CG-CD2	5.68	120.66	111.00
1	D	10	ILE	CA-CB-CG2	5.68	122.27	110.90
1	C	162	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	D	246	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	439	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	171	MET	CA-CB-CG	5.65	122.91	113.30
1	A	326	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	F	134	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	E	167	LEU	CA-CB-CG	5.63	128.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	177	GLU	CG-CD-OE2	5.61	129.52	118.30
1	F	303	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	E	390	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	236	LYS	N-CA-CB	-5.58	100.55	110.60
1	B	236	LYS	CA-CB-CG	5.58	125.67	113.40
1	D	427	LEU	CB-CA-C	-5.58	99.61	110.20
1	B	277	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	H	343	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	F	40	LEU	CB-CG-CD2	-5.57	101.54	111.00
1	B	63	MET	CA-CB-CG	5.56	122.76	113.30
1	C	22	GLU	N-CA-C	5.56	126.00	111.00
1	F	162	ASP	CB-CG-OD1	5.56	123.30	118.30
1	H	103	SER	CB-CA-C	-5.53	99.60	110.10
1	F	393	LEU	CB-CG-CD2	5.52	120.38	111.00
1	A	177	GLU	CG-CD-OE1	-5.51	107.28	118.30
1	B	150	LEU	CB-CG-CD1	5.50	120.36	111.00
1	F	150	LEU	CB-CG-CD1	5.50	120.35	111.00
1	B	120	GLU	CG-CD-OE1	5.50	129.30	118.30
1	C	304	THR	CA-CB-CG2	-5.50	104.70	112.40
1	G	22	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	E	150	LEU	CB-CG-CD1	5.49	120.33	111.00
1	D	124	GLN	N-CA-CB	5.48	120.46	110.60
1	A	316	ASP	CB-CG-OD1	5.46	123.21	118.30
1	H	40	LEU	CB-CG-CD1	5.42	120.21	111.00
1	E	46	MET	CG-SD-CE	5.41	108.86	100.20
1	F	207	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	H	391	ARG	CB-CA-C	-5.40	99.60	110.40
1	A	13	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	388	ARG	N-CA-CB	5.39	120.30	110.60
1	F	153	LYS	CD-CE-NZ	5.39	124.09	111.70
1	F	189	GLU	CA-CB-CG	5.38	125.25	113.40
1	E	113	LEU	CB-CG-CD2	5.37	120.13	111.00
1	C	424	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	E	155	ILE	CG1-CB-CG2	5.34	123.15	111.40
1	B	46	MET	CG-SD-CE	5.33	108.73	100.20
1	H	303	ARG	CG-CD-NE	5.33	123.00	111.80
1	G	390	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	35	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	G	19	LYS	CD-CE-NZ	5.29	123.86	111.70
1	C	320	ARG	CG-CD-NE	-5.26	100.75	111.80
1	H	246	ARG	N-CA-CB	-5.26	101.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	22	GLU	N-CA-C	5.25	125.18	111.00
1	C	247	LEU	CB-CG-CD1	5.25	119.92	111.00
1	B	157	GLN	N-CA-CB	5.23	120.01	110.60
1	E	393	LEU	CB-CG-CD2	5.22	119.88	111.00
1	H	395	ARG	N-CA-CB	5.21	119.97	110.60
1	E	379	GLU	N-CA-CB	5.19	119.95	110.60
1	E	227	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	450	LEU	CB-CG-CD2	5.19	119.82	111.00
1	F	20	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	H	110	PHE	CB-CA-C	5.17	120.75	110.40
1	G	277	ARG	CG-CD-NE	-5.17	100.94	111.80
1	G	293	MET	CB-CA-C	-5.17	100.06	110.40
1	D	333	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	282	LYS	CD-CE-NZ	5.16	123.57	111.70
1	H	391	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	G	37	PRO	N-CA-C	5.15	125.49	112.10
1	E	303	ARG	CB-CA-C	5.15	120.69	110.40
1	C	318	THR	CA-CB-CG2	5.14	119.59	112.40
1	D	303	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	F	36	ASP	OD1-CG-OD2	-5.13	113.55	123.30
1	H	247	LEU	CB-CG-CD1	5.12	119.71	111.00
1	C	395	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	113	LEU	CB-CG-CD2	5.11	119.68	111.00
1	H	68	ARG	N-CA-CB	-5.10	101.42	110.60
1	D	34	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	141	ASP	OD1-CG-OD2	-5.09	113.62	123.30
1	C	213	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	D	159	LEU	CB-CG-CD1	5.08	119.64	111.00
1	E	108	ASP	CB-CG-OD1	5.08	122.88	118.30
1	G	450	LEU	CB-CG-CD2	5.08	119.64	111.00
1	C	65	LYS	CA-CB-CG	5.08	124.57	113.40
1	A	283	VAL	CA-CB-CG2	5.07	118.51	110.90
1	C	439	ASP	N-CA-CB	5.06	119.70	110.60
1	D	35	ASP	CB-CG-OD1	5.05	122.84	118.30
1	G	434	LEU	CB-CG-CD2	5.03	119.55	111.00
1	B	113	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	240	THR	N-CA-CB	5.01	119.83	110.30
1	H	303	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	G	81	LYS	N-CA-C	5.01	124.52	111.00
1	C	19	LYS	CD-CE-NZ	5.00	123.21	111.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	LYS	Peptide
1	B	277	ARG	Peptide
1	B	36	ASP	Peptide
1	C	22	GLU	Peptide
1	C	36	ASP	Peptide
1	E	36	ASP	Peptide
1	F	36	ASP	Peptide
1	G	36	ASP	Peptide
1	H	117	MET	Peptide
1	H	150	LEU	Peptide
1	H	151	GLU	Peptide
1	H	36	ASP	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	3560	0	3499	56	1
1	B	3560	0	3499	90	0
1	C	3514	0	3449	127	0
1	D	3536	0	3473	79	1
1	E	3560	0	3499	79	2
1	F	3551	0	3491	79	2
1	G	3551	0	3491	86	1
1	H	3528	0	3462	119	1
2	A	28	0	19	1	0
2	B	28	0	19	0	0
2	C	28	0	19	3	0
2	D	28	0	19	1	0
2	E	28	0	19	2	0
2	F	28	0	19	0	0
2	G	28	0	19	0	0
2	H	28	0	19	0	0
All	All	28584	0	28015	692	4

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 12.

All (692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH2	1:A:289:ASP:OD2	1.76	1.18
1:H:40:LEU:O	1:H:320:ARG:NH1	1.84	1.10
1:H:10:ILE:HD11	1:H:251:LEU:HD12	1.16	1.09
1:F:153:LYS:CE	1:F:166:ILE:HG23	1.86	1.04
1:B:222:TYR:HB3	1:B:230:LEU:HD22	1.39	1.01
1:C:54:LEU:HD22	1:C:223:ASN:HD22	1.27	0.98
1:F:153:LYS:HE2	1:F:166:ILE:HG23	1.46	0.97
1:B:222:TYR:HB3	1:B:230:LEU:CD2	1.95	0.97
1:G:233:LEU:O	1:G:236:LYS:NZ	1.99	0.96
1:E:442:GLU:O	1:E:445:ARG:NH1	2.04	0.91
1:H:10:ILE:HD11	1:H:251:LEU:CD1	2.01	0.91
1:H:52:ILE:O	1:H:235:LYS:NZ	2.06	0.89
1:F:381:GLN:OE1	1:F:384:LYS:NZ	2.05	0.89
1:D:233:LEU:O	1:D:236:LYS:NZ	2.07	0.88
1:G:31:THR:OG1	1:G:311:ASP:OD2	1.92	0.88
1:G:74:LYS:NZ	1:G:311:ASP:OD2	2.08	0.87
1:C:242:MET:HE1	1:C:247:LEU:HD12	1.56	0.85
1:H:70:ALA:HA	1:H:104:TRP:CE3	2.13	0.84
1:F:153:LYS:HE3	1:F:166:ILE:HG23	1.57	0.84
1:C:116:LYS:HA	1:C:159:LEU:HD21	1.60	0.84
1:D:326:ARG:NE	1:D:423:ASP:OD2	2.11	0.84
1:C:18:PHE:O	1:C:23:HIS:N	2.09	0.84
1:G:10:ILE:HD11	1:G:251:LEU:HD12	1.60	0.83
1:H:7:ALA:O	1:H:10:ILE:HG22	1.78	0.83
1:G:7:ALA:O	1:G:10:ILE:HG22	1.79	0.81
1:C:10:ILE:CG2	1:C:247:LEU:HD21	2.09	0.81
1:C:22:GLU:HB3	1:C:23:HIS:ND1	1.95	0.81
1:F:36:ASP:O	1:F:38:THR:N	2.13	0.81
1:E:358:GLY:O	1:E:365:LYS:NZ	2.12	0.81
1:H:40:LEU:HD21	1:H:323:VAL:HG21	1.63	0.81
1:B:282:LYS:HG3	1:B:292:ASP:OD2	1.80	0.81
1:H:141:ASP:H	1:H:146:LEU:HD11	1.46	0.80
1:H:39:LEU:O	1:H:320:ARG:NH2	2.14	0.80
1:F:189:GLU:OE1	1:F:216:ASN:ND2	2.11	0.80
1:H:113:LEU:HA	1:H:116:LYS:HB2	1.62	0.80
1:H:10:ILE:CD1	1:H:251:LEU:HD12	2.06	0.80
1:E:215:TRP:HE1	1:E:240:THR:HG23	1.48	0.79
1:G:105:SER:O	1:G:237:SER:OG	2.00	0.79
1:F:215:TRP:HE1	1:F:240:THR:HG23	1.47	0.79
1:H:409:ASP:OD1	1:H:444:GLU:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:SER:O	1:H:237:SER:OG	2.01	0.78
1:D:105:SER:O	1:D:237:SER:OG	2.01	0.78
1:G:10:ILE:CD1	1:G:251:LEU:HD12	2.14	0.78
1:B:68:ARG:HH11	1:B:109:TYR:HD2	1.30	0.78
1:G:40:LEU:HD21	1:G:323:VAL:HG21	1.66	0.78
1:H:70:ALA:HA	1:H:104:TRP:CZ3	2.18	0.78
1:H:36:ASP:O	1:H:38:THR:N	2.14	0.77
1:G:10:ILE:HG21	1:G:248:VAL:HG22	1.66	0.77
1:C:385:THR:HG21	1:C:418:TYR:O	1.84	0.77
1:C:105:SER:O	1:C:237:SER:OG	2.02	0.77
1:A:277:ARG:NH2	1:A:291:ILE:HD12	2.00	0.76
1:B:131:GLU:O	1:B:165:LYS:NZ	2.17	0.76
1:C:242:MET:CE	1:C:247:LEU:HD12	2.14	0.76
1:B:36:ASP:O	1:B:38:THR:N	2.15	0.76
1:D:40:LEU:HD21	1:D:323:VAL:HG21	1.66	0.76
1:B:68:ARG:HD3	1:B:109:TYR:CE2	2.21	0.76
1:C:279:TYR:HB2	1:C:295:TYR:CD2	2.21	0.76
1:C:40:LEU:HD21	1:C:323:VAL:HG21	1.67	0.76
1:G:326:ARG:NE	1:G:423:ASP:OD2	2.19	0.76
1:E:233:LEU:HG	1:E:235:LYS:O	1.86	0.76
1:E:224:ARG:HH21	1:E:230:LEU:HD11	1.49	0.75
1:C:96:THR:HB	1:C:304:THR:HG21	1.68	0.75
1:C:81:LYS:NZ	1:C:180:ASP:OD1	2.19	0.75
1:D:268:GLU:O	1:D:272:LYS:HG3	1.86	0.75
1:G:114:ALA:HB2	1:G:238:ILE:HD13	1.69	0.74
1:G:268:GLU:O	1:G:272:LYS:HG3	1.87	0.74
1:B:128:ILE:HD11	1:B:133:LEU:HD11	1.70	0.74
1:B:215:TRP:HE1	1:B:240:THR:HG23	1.51	0.74
1:C:277:ARG:NH1	1:C:289:ASP:OD2	2.21	0.74
1:D:215:TRP:HE1	1:D:240:THR:HG23	1.51	0.74
1:G:215:TRP:HE1	1:G:240:THR:HG23	1.52	0.74
1:H:102:GLY:O	1:H:104:TRP:CD2	2.41	0.74
1:H:215:TRP:HE1	1:H:240:THR:HG23	1.53	0.74
1:C:4:THR:HG22	1:C:5:LEU:HD12	1.68	0.73
1:B:114:ALA:HB2	1:B:238:ILE:HD13	1.69	0.73
1:C:337:GLU:OE1	1:C:390:ARG:NH1	2.20	0.73
1:D:114:ALA:HB2	1:D:238:ILE:HD13	1.70	0.73
1:H:10:ILE:HG21	1:H:248:VAL:HG22	1.70	0.73
1:C:246:ARG:HA	1:C:257:ASN:OD1	1.88	0.73
1:F:280:THR:HG23	1:F:282:LYS:HG3	1.71	0.73
1:E:61:HIS:HA	1:G:340:ASN:HD21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ARG:NH1	1:F:289:ASP:OD2	2.21	0.73
1:H:151:GLU:HA	1:H:154:GLN:H	1.54	0.72
1:E:13:ARG:NH1	1:E:20:ARG:HH12	1.87	0.72
1:G:223:ASN:HD22	1:G:233:LEU:HD12	1.54	0.72
1:G:22:GLU:O	1:G:68:ARG:NH1	2.23	0.71
1:A:61:HIS:HA	1:D:340:ASN:HD21	1.54	0.71
1:E:215:TRP:HE1	1:E:240:THR:CG2	2.03	0.71
1:E:282:LYS:HD2	1:E:286:GLU:O	1.91	0.71
1:B:122:LEU:HB3	1:B:128:ILE:HG12	1.71	0.71
1:C:215:TRP:HE1	1:C:240:THR:HG23	1.54	0.71
1:D:110:PHE:HE1	1:D:219:PHE:HB3	1.56	0.71
1:F:114:ALA:HB2	1:F:238:ILE:HD13	1.70	0.71
1:D:110:PHE:CE1	1:D:219:PHE:HB3	2.25	0.71
1:F:215:TRP:HE1	1:F:240:THR:CG2	2.04	0.71
1:F:204:VAL:O	1:F:205:ASN:HB3	1.90	0.71
1:E:114:ALA:HB2	1:E:238:ILE:HD13	1.70	0.70
1:E:150:LEU:HA	1:E:153:LYS:HG3	1.72	0.70
2:C:500:A5A:H5'1	2:C:500:A5A:H8	1.72	0.70
1:A:114:ALA:HB2	1:A:238:ILE:HD13	1.73	0.70
1:H:67:SER:HB2	1:H:108:ASP:HB2	1.73	0.70
1:H:116:LYS:O	1:H:117:MET:HG2	1.92	0.70
1:B:215:TRP:HE1	1:B:240:THR:CG2	2.05	0.70
1:C:177:GLU:HG3	1:C:184:CYS:HB3	1.74	0.70
1:G:61:HIS:CD2	1:G:62:PRO:HD2	2.27	0.69
1:F:61:HIS:HA	1:H:340:ASN:HD21	1.57	0.69
1:C:391:ARG:HE	1:C:395:ARG:HD2	1.57	0.69
1:H:19:LYS:HA	1:H:23:HIS:H	1.58	0.69
1:D:63:MET:HA	1:D:66:LEU:HD13	1.74	0.69
1:A:337:GLU:OE1	1:A:390:ARG:NH1	2.26	0.69
1:C:137:TYR:C	1:C:174:ASN:HD22	1.96	0.69
1:H:117:MET:HB3	1:H:120:GLU:HB2	1.75	0.69
1:C:23:HIS:HA	1:C:68:ARG:HG3	1.75	0.68
1:F:34:LEU:HB3	1:H:277:ARG:NH2	2.09	0.68
1:G:424:LEU:HD12	1:G:427:LEU:HD11	1.75	0.68
1:G:22:GLU:HB3	1:G:68:ARG:CZ	2.23	0.68
1:A:280:THR:HG23	1:A:282:LYS:HG3	1.76	0.68
1:C:279:TYR:HB2	1:C:295:TYR:CE2	2.28	0.68
1:C:33:PRO:HB2	1:C:36:ASP:OD2	1.93	0.68
1:C:351:ASP:OD2	1:E:232:PRO:HD3	1.95	0.67
1:B:85:LEU:O	1:B:88:VAL:HG22	1.93	0.67
1:H:19:LYS:HB2	1:H:23:HIS:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:TRP:HE1	1:H:240:THR:CG2	2.06	0.67
1:E:13:ARG:HD2	1:E:125:GLU:OE1	1.94	0.67
1:F:35:ASP:HB2	1:H:277:ARG:HB2	1.77	0.67
1:C:385:THR:HG21	1:C:418:TYR:CA	2.24	0.67
1:E:221:GLN:HB2	1:E:236:LYS:HD2	1.77	0.67
1:B:68:ARG:HD3	1:B:109:TYR:HE2	1.59	0.67
1:C:215:TRP:HE1	1:C:240:THR:CG2	2.08	0.66
1:D:215:TRP:HE1	1:D:240:THR:CG2	2.08	0.66
1:G:85:LEU:HD11	1:G:330:ARG:HH12	1.60	0.66
1:G:85:LEU:HD11	1:G:330:ARG:NH1	2.11	0.66
1:A:282:LYS:HD2	1:A:286:GLU:O	1.96	0.66
1:C:10:ILE:HG21	1:C:247:LEU:HD21	1.76	0.66
1:D:266:TYR:O	1:D:270:ILE:HG12	1.96	0.66
1:G:215:TRP:HE1	1:G:240:THR:CG2	2.09	0.66
1:H:40:LEU:O	1:H:320:ARG:CZ	2.44	0.65
1:C:100:MET:HE2	2:C:500:A5A:H5'2	1.76	0.65
1:C:113:LEU:O	1:C:117:MET:HG2	1.96	0.65
1:C:19:LYS:HG2	1:C:23:HIS:O	1.97	0.65
1:G:68:ARG:HB2	1:G:68:ARG:NH1	2.12	0.65
1:E:221:GLN:O	1:E:221:GLN:HG3	1.96	0.65
1:A:40:LEU:O	1:A:320:ARG:HD3	1.95	0.64
1:H:141:ASP:H	1:H:146:LEU:CD1	2.09	0.64
1:G:68:ARG:HH11	1:G:68:ARG:HB2	1.62	0.64
1:C:54:LEU:HD22	1:C:223:ASN:ND2	2.05	0.64
1:C:119:LEU:O	1:C:123:THR:OG1	2.16	0.64
1:A:119:LEU:O	1:A:123:THR:OG1	2.14	0.64
1:A:289:ASP:OD1	1:A:289:ASP:N	2.30	0.64
1:B:119:LEU:O	1:B:123:THR:OG1	2.15	0.64
1:D:235:LYS:HD2	1:D:236:LYS:H	1.62	0.64
1:E:215:TRP:NE1	1:E:240:THR:HG23	2.13	0.64
1:E:119:LEU:O	1:E:123:THR:OG1	2.15	0.63
1:F:221:GLN:HG2	1:F:236:LYS:HD3	1.79	0.63
1:E:442:GLU:OE2	1:E:445:ARG:HD3	1.98	0.63
1:H:117:MET:HA	1:H:119:LEU:H	1.64	0.63
1:D:19:LYS:HB2	1:D:23:HIS:O	1.99	0.63
1:C:351:ASP:OD2	1:E:232:PRO:CD	2.47	0.63
1:G:330:ARG:HH21	1:G:423:ASP:CB	2.11	0.63
1:F:119:LEU:O	1:F:123:THR:OG1	2.16	0.63
1:H:141:ASP:N	1:H:146:LEU:HD11	2.14	0.63
1:F:215:TRP:NE1	1:F:240:THR:HG23	2.14	0.62
1:H:120:GLU:HG2	1:H:124:GLN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LYS:HG2	1:C:23:HIS:C	2.18	0.62
1:A:277:ARG:CZ	1:A:291:ILE:HD12	2.29	0.62
1:E:412:TRP:CD2	1:E:444:GLU:OE1	2.52	0.62
1:H:388:ARG:O	1:H:391:ARG:HB2	1.98	0.62
1:G:403:SER:O	1:G:404:LYS:HD3	1.98	0.62
1:B:326:ARG:HD3	1:B:423:ASP:OD2	1.99	0.62
1:C:177:GLU:HG3	1:C:184:CYS:CB	2.30	0.62
1:C:23:HIS:HD2	1:C:69:ALA:O	1.82	0.61
1:B:274:THR:O	1:B:276:ALA:N	2.33	0.61
1:F:326:ARG:HG2	1:F:421:PRO:HB3	1.80	0.61
1:C:63:MET:HG3	1:C:66:LEU:HD13	1.82	0.61
1:E:173:ASP:CG	1:E:205:ASN:HD21	2.04	0.61
1:B:122:LEU:O	1:B:128:ILE:HG13	2.00	0.61
1:H:23:HIS:CD2	1:H:68:ARG:HG3	2.36	0.61
1:E:326:ARG:HG2	1:E:421:PRO:HB3	1.81	0.61
1:G:133:LEU:O	1:G:165:LYS:NZ	2.20	0.61
1:A:221:GLN:HG3	1:A:236:LYS:HD2	1.83	0.61
1:B:222:TYR:HB3	1:B:230:LEU:HD21	1.81	0.60
1:C:173:ASP:CG	1:C:205:ASN:HD21	2.05	0.60
1:C:277:ARG:HH21	1:C:280:THR:HG22	1.65	0.60
1:C:385:THR:O	1:C:385:THR:HG22	1.99	0.60
1:D:444:GLU:O	1:D:444:GLU:HG3	2.01	0.60
1:H:111:LYS:NZ	1:H:149:ASP:OD1	2.34	0.60
1:A:277:ARG:HH22	1:A:289:ASP:CG	2.05	0.60
1:F:93:TYR:OH	1:F:207:ASP:OD1	2.19	0.60
1:G:266:TYR:O	1:G:270:ILE:HG12	1.99	0.60
1:E:173:ASP:OD2	1:E:205:ASN:ND2	2.34	0.60
1:F:12:GLN:HG3	1:F:16:ASP:OD2	2.02	0.60
1:E:336:HIS:CD2	1:E:383:LEU:HD21	2.37	0.60
1:C:111:LYS:NZ	1:C:149:ASP:OD1	2.35	0.60
1:C:224:ARG:HE	1:C:228:GLY:HA2	1.65	0.60
1:B:215:TRP:NE1	1:B:240:THR:HG23	2.15	0.60
1:D:47:ASN:H	1:D:47:ASN:HD22	1.48	0.60
1:C:277:ARG:HH21	1:C:280:THR:CG2	2.15	0.59
1:B:68:ARG:NH1	1:B:108:ASP:OD1	2.35	0.59
1:C:385:THR:HG21	1:C:418:TYR:C	2.22	0.59
1:C:385:THR:HG21	1:C:418:TYR:HA	1.83	0.59
1:A:326:ARG:NE	1:A:423:ASP:OD2	2.35	0.59
1:H:102:GLY:O	1:H:104:TRP:CE3	2.55	0.59
1:H:19:LYS:HA	1:H:23:HIS:N	2.17	0.59
1:H:227:ASP:OD2	1:H:229:ILE:HD12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:OD1	1:A:325:ARG:NH2	2.35	0.59
1:G:136:THR:HB	1:G:174:ASN:HD21	1.68	0.59
1:B:36:ASP:OD2	1:B:39:LEU:HB2	2.01	0.59
1:A:61:HIS:HA	1:D:340:ASN:ND2	2.17	0.59
1:H:326:ARG:HG2	1:H:421:PRO:HB3	1.85	0.58
1:C:155:ILE:O	1:C:158:ASN:HB3	2.03	0.58
1:C:15:ILE:HG13	1:C:16:ASP:N	2.17	0.58
1:D:390:ARG:NH1	1:D:394:ASP:OD2	2.36	0.58
1:G:277:ARG:NH1	1:G:289:ASP:OD2	2.36	0.58
1:B:222:TYR:CB	1:B:230:LEU:HD22	2.25	0.58
1:B:29:SER:H	1:B:48:GLN:HE21	1.50	0.58
1:H:22:GLU:HB2	1:H:68:ARG:HH21	1.68	0.58
1:F:153:LYS:HE3	1:F:166:ILE:CG2	2.29	0.58
1:C:391:ARG:NE	1:C:395:ARG:HD2	2.19	0.58
1:D:424:LEU:O	1:D:427:LEU:HB2	2.04	0.58
1:E:233:LEU:HD12	1:E:234:PRO:CD	2.34	0.58
1:B:116:LYS:HA	1:B:159:LEU:HD21	1.84	0.58
1:D:33:PRO:HD2	1:D:320:ARG:NH1	2.20	0.57
1:E:239:ASP:OD2	2:E:500:A5A:N	2.36	0.57
1:B:128:ILE:HD12	1:B:128:ILE:O	2.04	0.57
1:C:173:ASP:OD2	1:C:205:ASN:ND2	2.31	0.57
1:H:62:PRO:O	1:H:65:LYS:HB2	2.04	0.57
1:C:32:ILE:HG23	1:C:320:ARG:HH11	1.69	0.57
1:G:270:ILE:HD12	1:G:298:LEU:HD23	1.85	0.57
1:H:102:GLY:HA3	1:H:240:THR:O	2.05	0.57
1:A:93:TYR:HA	1:A:257:ASN:ND2	2.20	0.57
1:E:162:ASP:H	1:E:165:LYS:HE2	1.69	0.57
1:C:323:VAL:HG22	1:C:326:ARG:HH21	1.69	0.57
1:H:117:MET:SD	1:H:120:GLU:HB2	2.44	0.57
1:D:215:TRP:NE1	1:D:240:THR:HG23	2.20	0.57
1:C:215:TRP:NE1	1:C:240:THR:HG23	2.20	0.56
1:D:110:PHE:HD2	1:D:111:LYS:CG	2.18	0.56
1:F:326:ARG:NE	1:F:423:ASP:OD2	2.38	0.56
1:A:333:ARG:HD3	1:A:424:LEU:HD11	1.86	0.56
1:A:326:ARG:HG2	1:A:421:PRO:HB3	1.87	0.56
1:C:154:GLN:O	1:C:158:ASN:HB2	2.04	0.56
1:E:362:PRO:HA	1:E:365:LYS:NZ	2.21	0.56
1:E:61:HIS:HA	1:G:340:ASN:ND2	2.18	0.56
1:G:424:LEU:HA	1:G:427:LEU:HG	1.88	0.56
1:A:173:ASP:CG	1:A:205:ASN:HD21	2.08	0.56
1:D:22:GLU:HB2	1:D:68:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:ARG:NH2	1:H:125:GLU:OE1	2.39	0.56
1:H:138:PHE:CE2	1:H:146:LEU:HD22	2.41	0.56
1:F:153:LYS:HE3	1:F:166:ILE:HG12	1.88	0.56
1:G:333:ARG:HD3	1:G:424:LEU:HD11	1.86	0.56
1:H:18:PHE:CE1	1:H:103:SER:HB3	2.41	0.56
1:H:33:PRO:HG2	1:H:320:ARG:HH22	1.70	0.56
1:H:270:ILE:HA	1:H:345:PHE:HZ	1.70	0.56
1:H:112:GLU:O	1:H:116:LYS:N	2.39	0.55
1:B:28:SER:HB3	1:B:73:GLN:HA	1.89	0.55
1:E:246:ARG:NH1	2:E:500:A5A:O2'	2.40	0.55
1:B:221:GLN:HG2	1:B:236:LYS:HE3	1.86	0.55
1:B:280:THR:OG1	1:B:282:LYS:HE3	2.07	0.55
1:H:215:TRP:NE1	1:H:240:THR:HG23	2.19	0.55
1:D:239:ASP:OD2	2:D:500:A5A:N	2.39	0.55
1:G:19:LYS:HB2	1:G:23:HIS:O	2.05	0.55
1:E:317:ASN:OD1	1:E:325:ARG:NH2	2.40	0.55
1:G:215:TRP:NE1	1:G:240:THR:HG23	2.21	0.55
1:F:128:ILE:HD11	1:F:192:TYR:CE2	2.42	0.55
1:F:122:LEU:C	1:F:128:ILE:HG22	2.26	0.55
1:H:313:GLY:O	1:H:314:ARG:NH1	2.37	0.55
1:A:451:LYS:HA	1:A:453:GLN:H	1.71	0.54
1:B:68:ARG:HD3	1:B:109:TYR:CD2	2.42	0.54
1:H:117:MET:HB3	1:H:120:GLU:H	1.72	0.54
1:B:128:ILE:CD1	1:B:133:LEU:HD11	2.35	0.54
1:G:10:ILE:HD11	1:G:247:LEU:HG	1.88	0.54
1:D:333:ARG:NH1	1:D:337:GLU:OE1	2.40	0.54
1:D:46:MET:HG3	1:D:47:ASN:N	2.23	0.54
1:D:33:PRO:HG2	1:D:320:ARG:HH12	1.73	0.54
1:F:46:MET:HG3	1:F:47:ASN:N	2.23	0.54
1:H:333:ARG:HD3	1:H:424:LEU:HD11	1.89	0.54
1:B:358:GLY:HA3	1:B:365:LYS:HE3	1.90	0.54
1:D:111:LYS:HE3	1:D:151:GLU:OE2	2.08	0.54
1:F:358:GLY:HA3	1:F:365:LYS:HE3	1.90	0.54
1:B:56:THR:HA	1:E:154:GLN:NE2	2.23	0.54
1:C:10:ILE:HG21	1:C:247:LEU:CD2	2.37	0.54
1:D:367:ASP:OD2	1:D:370:MET:HB2	2.08	0.54
1:H:19:LYS:HD3	1:H:22:GLU:HA	1.89	0.54
1:H:71:ASN:OD1	1:H:104:TRP:CH2	2.61	0.54
1:E:301:HIS:HE1	1:E:330:ARG:HE	1.54	0.53
1:G:22:GLU:HB3	1:G:68:ARG:NH1	2.24	0.53
1:H:33:PRO:HD2	1:H:320:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LYS:O	1:D:157:GLN:HG3	2.08	0.53
1:D:277:ARG:NH1	1:D:289:ASP:OD2	2.42	0.53
1:H:116:LYS:O	1:H:159:LEU:HD21	2.08	0.53
1:C:62:PRO:O	1:C:65:LYS:HB3	2.09	0.53
1:H:409:ASP:OD1	1:H:444:GLU:CG	2.54	0.53
1:D:328:LEU:CD2	1:D:378:GLU:HB3	2.39	0.53
1:B:55:ASN:ND2	1:E:158:ASN:OD1	2.41	0.53
1:F:173:ASP:CG	1:F:205:ASN:HD21	2.10	0.53
1:D:110:PHE:HD2	1:D:111:LYS:HG2	1.74	0.53
1:C:150:LEU:O	1:C:153:LYS:HB3	2.09	0.53
1:B:223:ASN:O	1:B:230:LEU:HD23	2.08	0.53
1:C:301:HIS:HA	1:C:304:THR:OG1	2.09	0.53
1:E:242:MET:HE1	1:E:247:LEU:HD13	1.91	0.53
1:H:86:ASP:O	1:H:90:LYS:HD3	2.08	0.53
1:F:172:LYS:HG3	1:F:173:ASP:N	2.23	0.53
1:F:22:GLU:OE1	1:F:68:ARG:NH1	2.42	0.53
1:F:242:MET:HE1	1:F:247:LEU:HD13	1.91	0.52
1:A:328:LEU:CD2	1:A:378:GLU:HB3	2.39	0.52
1:E:94:HIS:HD2	1:E:246:ARG:NH2	2.07	0.52
1:F:333:ARG:NH1	1:F:337:GLU:OE1	2.42	0.52
1:G:33:PRO:HG2	1:G:320:ARG:NH2	2.24	0.52
1:E:387:SER:OG	1:E:391:ARG:NH2	2.42	0.52
1:F:105:SER:HB2	1:F:109:TYR:CE2	2.45	0.52
1:F:61:HIS:CA	1:H:340:ASN:HD21	2.23	0.52
1:B:282:LYS:CG	1:B:292:ASP:OD2	2.55	0.52
1:D:12:GLN:O	1:D:15:ILE:HG23	2.09	0.52
1:E:444:GLU:OE1	1:E:444:GLU:C	2.48	0.52
1:A:173:ASP:OD2	1:A:205:ASN:ND2	2.38	0.52
1:C:19:LYS:CG	1:C:23:HIS:O	2.57	0.52
1:D:310:ALA:O	1:D:366:LYS:NZ	2.25	0.52
1:G:81:LYS:NZ	1:G:180:ASP:OD1	2.42	0.52
1:H:57:ILE:HD13	1:H:64:ALA:HB2	1.92	0.52
1:B:22:GLU:CG	1:B:68:ARG:HE	2.22	0.52
1:C:93:TYR:HA	1:C:257:ASN:ND2	2.25	0.52
1:D:222:TYR:CE1	1:D:230:LEU:HD13	2.45	0.52
1:G:242:MET:HE1	1:G:247:LEU:HD13	1.92	0.52
1:A:313:GLY:O	1:A:314:ARG:NH1	2.42	0.52
1:B:336:HIS:CD2	1:B:383:LEU:HD21	2.44	0.52
1:D:242:MET:HE1	1:D:247:LEU:HD13	1.92	0.52
1:G:246:ARG:O	1:G:249:SER:OG	2.18	0.52
1:C:385:THR:HG23	1:C:418:TYR:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:O	1:D:249:SER:OG	2.18	0.52
1:F:131:GLU:HB3	1:F:165:LYS:CE	2.40	0.52
1:H:19:LYS:HE2	1:H:24:THR:HA	1.91	0.52
1:B:128:ILE:HD11	1:B:133:LEU:CD1	2.40	0.51
1:D:47:ASN:HD22	1:D:47:ASN:N	2.07	0.51
1:A:387:SER:OG	1:A:391:ARG:NH2	2.43	0.51
1:C:313:GLY:O	1:C:314:ARG:NH1	2.41	0.51
1:D:39:LEU:HD21	1:D:47:ASN:OD1	2.11	0.51
1:H:12:GLN:OE1	1:H:15:ILE:HD11	2.10	0.51
1:E:61:HIS:CA	1:G:340:ASN:HD21	2.22	0.51
1:B:122:LEU:C	1:B:128:ILE:HG13	2.31	0.51
1:H:117:MET:HB3	1:H:120:GLU:CB	2.38	0.51
1:F:61:HIS:HA	1:H:340:ASN:ND2	2.24	0.51
1:H:358:GLY:HA3	1:H:365:LYS:HE3	1.93	0.51
1:F:280:THR:HG21	1:F:282:LYS:HE3	1.91	0.51
1:G:45:GLY:HA2	1:G:73:GLN:HG2	1.92	0.51
1:C:413:LEU:O	1:C:417:THR:OG1	2.28	0.51
1:A:381:GLN:OE1	1:A:384:LYS:NZ	2.38	0.51
1:C:100:MET:CE	2:C:500:A5A:H5'2	2.40	0.51
1:C:22:GLU:C	1:C:68:ARG:HD2	2.31	0.51
1:G:236:LYS:N	1:G:236:LYS:HD3	2.26	0.50
1:B:313:GLY:O	1:B:314:ARG:NH1	2.43	0.50
1:D:270:ILE:HD12	1:D:298:LEU:HD23	1.92	0.50
1:F:4:THR:OG1	1:F:5:LEU:N	2.42	0.50
1:G:85:LEU:CD1	1:G:330:ARG:HH12	2.23	0.50
1:D:236:LYS:N	1:D:236:LYS:HD3	2.25	0.50
1:F:280:THR:CG2	1:F:282:LYS:HE3	2.41	0.50
1:G:11:ARG:NH1	1:G:99:GLU:OE2	2.45	0.50
1:E:446:LYS:HZ2	1:E:450:LEU:HD11	1.76	0.50
1:G:132:ARG:HH21	1:G:196:GLY:HA3	1.77	0.50
1:E:412:TRP:CG	1:E:444:GLU:OE1	2.64	0.50
1:F:313:GLY:O	1:F:314:ARG:NH1	2.43	0.50
1:H:413:LEU:O	1:H:417:THR:OG1	2.29	0.50
1:C:12:GLN:O	1:C:15:ILE:HG13	2.11	0.50
1:D:222:TYR:CD1	1:D:230:LEU:HD13	2.46	0.50
1:D:45:GLY:HA2	1:D:73:GLN:HG2	1.94	0.50
1:A:52:ILE:HD11	1:A:63:MET:HG2	1.93	0.50
1:E:22:GLU:HB2	1:E:68:ARG:HH11	1.75	0.50
1:H:33:PRO:HD2	1:H:320:ARG:CZ	2.41	0.50
1:G:413:LEU:O	1:G:417:THR:OG1	2.30	0.50
1:C:47:ASN:OD1	1:C:178:MET:SD	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:TRP:CD1	1:D:444:GLU:HG2	2.46	0.49
1:F:317:ASN:OD1	1:F:325:ARG:NH2	2.45	0.49
1:C:10:ILE:HG22	1:C:247:LEU:HD21	1.94	0.49
1:D:282:LYS:HD3	1:D:286:GLU:HB3	1.94	0.49
1:H:33:PRO:CG	1:H:320:ARG:HH22	2.25	0.49
1:H:51:PRO:HB2	1:H:57:ILE:CG2	2.42	0.49
1:A:391:ARG:O	1:A:395:ARG:HG2	2.11	0.49
1:C:385:THR:HG23	1:C:418:TYR:CD2	2.46	0.49
1:A:110:PHE:C	1:A:238:ILE:HD11	2.33	0.49
1:A:46:MET:HG3	1:A:47:ASN:N	2.26	0.49
1:C:358:GLY:HA3	1:C:365:LYS:HE3	1.93	0.49
1:A:170:ASN:ND2	1:A:172:LYS:HE3	2.28	0.49
1:B:154:GLN:HA	1:B:157:GLN:HG2	1.94	0.49
1:E:245:GLU:OE2	1:E:303:ARG:NH2	2.43	0.49
1:G:367:ASP:HB2	1:G:370:MET:HB3	1.93	0.49
1:H:337:GLU:HG2	1:H:390:ARG:HH11	1.77	0.49
1:C:23:HIS:NE2	1:C:109:TYR:OH	2.46	0.49
1:D:57:ILE:HD11	1:D:61:HIS:HD2	1.78	0.49
1:G:128:ILE:HA	1:G:128:ILE:HD13	1.66	0.49
1:E:233:LEU:HD12	1:E:234:PRO:HD2	1.93	0.49
1:F:387:SER:OG	1:F:391:ARG:NH2	2.46	0.49
1:A:214:ILE:O	1:A:242:MET:HG3	2.13	0.48
1:H:153:LYS:HD2	1:H:153:LYS:C	2.33	0.48
1:A:61:HIS:ND1	1:A:62:PRO:HD2	2.28	0.48
1:D:333:ARG:NH1	1:D:428:ILE:HG12	2.28	0.48
1:E:153:LYS:O	1:E:157:GLN:HG3	2.13	0.48
1:E:270:ILE:HA	1:E:345:PHE:HZ	1.76	0.48
1:F:270:ILE:HA	1:F:345:PHE:HZ	1.76	0.48
1:B:104:TRP:CD1	1:B:239:ASP:HA	2.47	0.48
1:A:61:HIS:CA	1:D:340:ASN:HD21	2.23	0.48
1:H:102:GLY:O	1:H:104:TRP:CE2	2.66	0.48
1:B:387:SER:OG	1:B:391:ARG:NH2	2.46	0.48
1:C:277:ARG:NH1	1:C:291:ILE:HB	2.28	0.48
1:C:18:PHE:O	1:C:22:GLU:HB2	2.13	0.48
1:F:91:ASP:OD2	1:F:94:HIS:ND1	2.38	0.48
1:G:277:ARG:NH2	1:G:292:ASP:OD1	2.45	0.48
1:A:451:LYS:HD3	1:A:453:GLN:O	2.14	0.48
1:B:390:ARG:NH1	1:B:394:ASP:OD1	2.36	0.48
1:F:170:ASN:OD1	1:F:171:MET:N	2.45	0.48
1:F:289:ASP:O	1:F:338:LYS:NZ	2.27	0.48
1:H:393:LEU:HD11	1:H:425:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:LEU:CG	1:G:330:ARG:HH12	2.27	0.48
1:H:117:MET:C	1:H:119:LEU:H	2.16	0.48
1:F:93:TYR:CE1	1:F:94:HIS:CE1	3.02	0.48
1:B:128:ILE:HD13	1:B:133:LEU:HG	1.96	0.48
1:C:316:ASP:OD1	1:C:317:ASN:N	2.46	0.48
1:D:27:HIS:CD2	1:D:28:SER:H	2.32	0.48
1:A:277:ARG:HH22	1:A:289:ASP:CB	2.27	0.48
1:B:46:MET:HG3	1:B:47:ASN:N	2.28	0.48
1:C:23:HIS:CD2	1:C:69:ALA:O	2.65	0.48
1:B:270:ILE:HA	1:B:345:PHE:HZ	1.79	0.47
1:C:45:GLY:HA2	1:C:73:GLN:HG2	1.96	0.47
1:D:363:GLU:O	1:D:366:LYS:HG3	2.14	0.47
1:B:45:GLY:HA2	1:B:73:GLN:HG2	1.94	0.47
1:C:40:LEU:HD12	1:C:320:ARG:HG2	1.95	0.47
1:F:390:ARG:NH1	1:F:394:ASP:OD1	2.36	0.47
1:C:270:ILE:HA	1:C:345:PHE:HZ	1.80	0.47
1:D:52:ILE:HD11	1:D:63:MET:HG2	1.95	0.47
1:F:189:GLU:CD	1:F:216:ASN:HD22	2.08	0.47
1:B:22:GLU:HG2	1:B:68:ARG:HE	1.80	0.47
1:C:221:GLN:HG2	1:C:236:LYS:HD2	1.96	0.47
1:D:110:PHE:CD2	1:D:111:LYS:HG2	2.49	0.47
1:F:167:LEU:HD11	1:F:201:ALA:HB1	1.96	0.47
1:H:33:PRO:HD2	1:H:320:ARG:NH1	2.29	0.47
1:C:22:GLU:HA	1:C:68:ARG:HH11	1.79	0.47
1:E:105:SER:HB2	1:E:109:TYR:CE2	2.50	0.47
1:E:170:ASN:OD1	1:E:172:LYS:HG2	2.14	0.47
1:C:437:ASP:OD1	1:C:439:ASP:OD1	2.32	0.47
1:E:207:ASP:OD1	1:E:207:ASP:N	2.44	0.47
1:G:313:GLY:O	1:G:314:ARG:NH1	2.45	0.47
1:H:254:LYS:NZ	1:H:259:ASP:O	2.46	0.47
1:A:444:GLU:HA	1:A:447:LEU:HG	1.97	0.47
1:B:223:ASN:HB3	1:B:231:LYS:HG2	1.96	0.47
1:C:318:THR:O	1:C:318:THR:HG23	2.15	0.47
1:D:313:GLY:O	1:D:314:ARG:NH1	2.48	0.47
1:E:111:LYS:NZ	1:E:151:GLU:HG2	2.29	0.47
1:C:204:VAL:O	1:C:205:ASN:HB3	2.15	0.47
1:E:149:ASP:OD1	1:E:151:GLU:HB3	2.15	0.47
1:B:274:THR:OG1	1:B:274:THR:O	2.29	0.47
1:E:313:GLY:O	1:E:314:ARG:NH1	2.46	0.47
1:H:57:ILE:HD13	1:H:64:ALA:CB	2.45	0.47
1:B:246:ARG:O	1:B:249:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ARG:O	1:C:249:SER:OG	2.19	0.46
1:G:67:SER:HB2	1:G:108:ASP:HB2	1.98	0.46
1:G:68:ARG:HH11	1:G:68:ARG:CB	2.27	0.46
1:B:29:SER:N	1:B:48:GLN:HE21	2.13	0.46
1:E:333:ARG:HD3	1:E:424:LEU:HD11	1.97	0.46
1:B:317:ASN:OD1	1:B:325:ARG:NH2	2.48	0.46
1:G:23:HIS:CD2	1:G:68:ARG:HB3	2.50	0.46
1:G:442:GLU:HA	1:G:445:ARG:HG3	1.96	0.46
1:H:263:PHE:CZ	1:H:303:ARG:NH1	2.83	0.46
1:C:384:LYS:O	1:C:388:ARG:NH1	2.43	0.46
1:C:385:THR:O	1:C:385:THR:CG2	2.64	0.46
1:C:390:ARG:HD2	1:C:390:ARG:HA	1.62	0.46
1:C:61:HIS:ND1	1:C:62:PRO:HD2	2.31	0.46
1:G:169:GLY:HA3	1:G:174:ASN:ND2	2.30	0.46
1:H:102:GLY:C	1:H:104:TRP:CZ3	2.88	0.46
1:H:214:ILE:O	1:H:242:MET:HG3	2.15	0.46
1:H:23:HIS:CE1	1:H:68:ARG:HD2	2.50	0.46
1:H:367:ASP:OD1	1:H:369:ASP:OD1	2.34	0.46
1:A:239:ASP:OD2	2:A:500:A5A:N	2.48	0.46
1:C:367:ASP:OD1	1:C:369:ASP:OD1	2.33	0.46
1:E:177:GLU:OE2	1:E:224:ARG:CZ	2.64	0.46
1:G:40:LEU:HD12	1:G:320:ARG:HG2	1.98	0.46
1:H:138:PHE:CZ	1:H:146:LEU:HD22	2.50	0.46
1:H:23:HIS:HA	1:H:68:ARG:HG2	1.97	0.46
1:G:382:PHE:CE2	1:G:386:LEU:HD13	2.51	0.46
1:H:45:GLY:HA2	1:H:73:GLN:HG2	1.97	0.46
1:F:131:GLU:HB3	1:F:165:LYS:HZ2	1.80	0.46
1:A:85:LEU:HD23	1:A:326:ARG:NH2	2.30	0.46
1:B:289:ASP:OD1	1:B:289:ASP:N	2.48	0.46
1:B:316:ASP:OD1	1:B:317:ASN:N	2.48	0.46
1:C:23:HIS:CE1	1:C:109:TYR:OH	2.69	0.46
1:C:15:ILE:HG13	1:C:16:ASP:H	1.79	0.46
1:G:330:ARG:HH21	1:G:423:ASP:HB2	1.81	0.46
1:G:326:ARG:HH21	1:G:330:ARG:HH22	1.63	0.46
1:A:45:GLY:HA2	1:A:73:GLN:HG2	1.97	0.46
1:C:22:GLU:O	1:C:68:ARG:HD2	2.16	0.46
1:D:31:THR:HG21	1:D:308:ALA:HA	1.98	0.46
1:F:222:TYR:C	1:F:233:LEU:HD13	2.35	0.46
1:G:137:TYR:O	1:G:174:ASN:ND2	2.49	0.46
1:C:153:LYS:HE3	1:C:154:GLN:HB2	1.98	0.45
1:H:249:SER:OG	1:H:257:ASN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:HD11	1:B:425:THR:HG23	1.98	0.45
1:C:113:LEU:HD23	1:C:117:MET:SD	2.56	0.45
1:G:403:SER:C	1:G:404:LYS:HD3	2.37	0.45
1:H:117:MET:CB	1:H:120:GLU:HB2	2.45	0.45
1:C:385:THR:CG2	1:C:418:TYR:O	2.60	0.45
1:D:442:GLU:O	1:D:446:LYS:HG3	2.15	0.45
1:F:135:VAL:HG23	1:F:153:LYS:HZ1	1.81	0.45
1:F:289:ASP:N	1:F:289:ASP:OD1	2.49	0.45
1:F:61:HIS:ND1	1:F:62:PRO:HD2	2.31	0.45
1:B:136:THR:OG1	1:B:189:GLU:HG3	2.15	0.45
1:C:223:ASN:CG	1:C:233:LEU:HD21	2.37	0.45
1:C:444:GLU:HA	1:C:447:LEU:HB3	1.98	0.45
1:D:154:GLN:HA	1:D:157:GLN:HG3	1.98	0.45
1:H:117:MET:CG	1:H:120:GLU:HB2	2.47	0.45
1:E:333:ARG:CD	1:E:424:LEU:HD11	2.46	0.45
1:E:45:GLY:HA2	1:E:73:GLN:HG2	1.98	0.45
1:F:110:PHE:C	1:F:238:ILE:HD11	2.37	0.45
1:G:110:PHE:C	1:G:238:ILE:HD11	2.36	0.45
1:H:444:GLU:O	1:H:448:ALA:N	2.48	0.45
1:C:23:HIS:HD2	1:C:104:TRP:H	1.65	0.45
1:E:444:GLU:O	1:E:447:LEU:HB3	2.17	0.45
1:D:10:ILE:HG12	1:D:248:VAL:HG22	1.98	0.45
1:D:223:ASN:HB2	1:D:233:LEU:HD21	1.99	0.45
1:H:46:MET:SD	1:H:176:TRP:HZ3	2.39	0.45
1:H:51:PRO:HB2	1:H:57:ILE:HG23	1.99	0.45
1:A:270:ILE:HA	1:A:345:PHE:HZ	1.82	0.45
1:B:444:GLU:HA	1:B:447:LEU:HG	1.99	0.45
1:G:10:ILE:HD11	1:G:251:LEU:CD1	2.41	0.45
1:H:102:GLY:HA2	1:H:240:THR:HG22	1.99	0.45
1:B:110:PHE:C	1:B:238:ILE:HD11	2.37	0.44
1:B:48:GLN:OE1	1:B:49:PHE:CE2	2.70	0.44
1:H:71:ASN:H	1:H:104:TRP:HZ3	1.64	0.44
1:F:246:ARG:O	1:F:249:SER:HB3	2.16	0.44
1:A:246:ARG:O	1:A:249:SER:HB3	2.17	0.44
1:D:92:VAL:CG1	1:D:256:SER:HA	2.47	0.44
1:A:170:ASN:HD22	1:A:172:LYS:HE3	1.82	0.44
1:A:177:GLU:OE2	1:A:224:ARG:NH1	2.51	0.44
1:D:422:VAL:HG21	1:D:441:PHE:CE2	2.52	0.44
1:D:393:LEU:HD11	1:D:425:THR:HG23	1.99	0.44
1:B:28:SER:CB	1:B:73:GLN:HA	2.48	0.44
1:C:14:PHE:CE2	1:C:101:LEU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:MET:C	1:C:65:LYS:N	2.71	0.44
1:H:71:ASN:N	1:H:104:TRP:CZ3	2.84	0.44
1:A:39:LEU:O	1:A:320:ARG:NH1	2.51	0.44
1:B:214:ILE:O	1:B:242:MET:HG3	2.17	0.44
1:E:61:HIS:CE1	1:E:63:MET:HG2	2.52	0.44
1:D:191:HIS:CD2	1:D:204:VAL:HG13	2.53	0.44
1:D:92:VAL:HG13	1:D:256:SER:HA	2.00	0.44
1:F:122:LEU:HB3	1:F:128:ILE:HG21	1.99	0.44
1:F:135:VAL:HG23	1:F:153:LYS:NZ	2.32	0.44
1:F:138:PHE:CZ	1:F:171:MET:HE3	2.53	0.44
1:H:141:ASP:HB3	1:H:146:LEU:HD21	2.00	0.44
1:C:328:LEU:HD22	1:C:378:GLU:HB3	1.99	0.44
1:E:246:ARG:O	1:E:249:SER:HB3	2.17	0.44
1:F:138:PHE:HZ	1:F:171:MET:HE3	1.82	0.44
1:G:397:ILE:HD13	1:G:432:LYS:HD3	1.99	0.44
1:H:15:ILE:HG13	1:H:16:ASP:N	2.33	0.44
1:A:384:LYS:CE	1:B:409:ASP:OD2	2.66	0.44
1:B:55:ASN:O	1:E:154:GLN:NE2	2.51	0.44
1:H:146:LEU:C	1:H:146:LEU:HD12	2.39	0.44
1:A:105:SER:HB2	1:A:109:TYR:CE2	2.52	0.43
1:A:359:ASP:OD1	1:A:360:ALA:N	2.49	0.43
1:E:112:GLU:HG3	1:E:155:ILE:CD1	2.48	0.43
1:B:223:ASN:HD22	1:B:231:LYS:HE3	1.82	0.43
1:B:31:THR:HG21	1:B:308:ALA:HA	2.00	0.43
1:C:58:ASP:OD1	1:C:59:PRO:HD2	2.18	0.43
1:D:326:ARG:HG2	1:D:421:PRO:HB3	2.00	0.43
1:F:282:LYS:N	1:F:292:ASP:OD2	2.47	0.43
1:G:105:SER:HB2	1:G:109:TYR:CE2	2.54	0.43
1:G:337:GLU:OE2	1:G:390:ARG:HG3	2.18	0.43
1:B:105:SER:HB2	1:B:109:TYR:CE2	2.52	0.43
1:B:92:VAL:CG1	1:B:256:SER:HA	2.48	0.43
1:C:337:GLU:CD	1:C:390:ARG:HH11	2.22	0.43
1:F:45:GLY:HA2	1:F:73:GLN:HG2	2.00	0.43
1:C:92:VAL:CG1	1:C:256:SER:HA	2.48	0.43
1:G:224:ARG:NH2	1:G:230:LEU:HD11	2.33	0.43
1:H:146:LEU:HB2	1:H:147:GLU:H	1.52	0.43
1:B:230:LEU:HD23	1:B:230:LEU:HA	1.70	0.43
1:D:422:VAL:CG2	1:D:441:PHE:CZ	3.01	0.43
1:F:153:LYS:HA	1:F:153:LYS:HD2	1.09	0.43
1:G:326:ARG:HG2	1:G:421:PRO:HB3	1.99	0.43
1:B:254:LYS:NZ	1:B:259:ASP:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LEU:HA	1:E:40:LEU:HD12	1.73	0.43
1:E:80:GLY:N	1:E:83:ASN:HB2	2.33	0.43
1:H:246:ARG:HG3	1:H:257:ASN:HD21	1.84	0.43
1:F:35:ASP:CG	1:H:278:PRO:HD2	2.39	0.43
1:D:27:HIS:HD2	1:D:28:SER:H	1.64	0.43
1:F:35:ASP:OD2	1:H:277:ARG:HA	2.18	0.43
1:E:110:PHE:C	1:E:238:ILE:HD11	2.39	0.43
1:E:61:HIS:ND1	1:E:62:PRO:HD2	2.34	0.43
1:G:18:PHE:O	1:G:23:HIS:N	2.33	0.43
1:B:128:ILE:HD12	1:B:128:ILE:C	2.38	0.43
1:C:319:GLY:O	1:C:323:VAL:HG23	2.19	0.43
1:E:61:HIS:ND1	1:E:63:MET:HG2	2.33	0.43
1:F:110:PHE:CE1	1:F:236:LYS:HB3	2.54	0.43
1:F:316:ASP:OD1	1:F:317:ASN:N	2.52	0.43
1:D:104:TRP:CD1	1:D:239:ASP:HA	2.54	0.43
1:E:35:ASP:HB2	1:G:277:ARG:HB2	2.01	0.43
1:C:22:GLU:HG3	1:C:22:GLU:H	1.53	0.42
1:D:424:LEU:HD12	1:D:427:LEU:HD12	2.01	0.42
1:F:110:PHE:HZ	1:F:221:GLN:HE21	1.66	0.42
1:G:37:PRO:HA	1:G:320:ARG:HH22	1.84	0.42
1:H:117:MET:C	1:H:119:LEU:N	2.71	0.42
1:B:162:ASP:OD2	1:B:164:THR:OG1	2.24	0.42
1:C:67:SER:HA	1:C:106:PHE:HB2	2.01	0.42
1:F:104:TRP:CD1	1:F:239:ASP:HA	2.54	0.42
1:H:150:LEU:HA	1:H:153:LYS:HB3	1.99	0.42
1:H:18:PHE:O	1:H:23:HIS:ND1	2.47	0.42
1:H:33:PRO:HD2	1:H:320:ARG:HH22	1.84	0.42
1:B:231:LYS:HD2	1:B:233:LEU:HD23	2.01	0.42
1:B:92:VAL:HG13	1:B:256:SER:HA	2.01	0.42
1:B:35:ASP:HB2	1:C:277:ARG:HB2	2.00	0.42
1:F:225:GLU:OE2	1:F:231:LYS:HB2	2.19	0.42
1:D:107:GLY:HA2	1:D:235:LYS:HG3	2.01	0.42
1:G:169:GLY:HA3	1:G:174:ASN:HD22	1.84	0.42
1:H:270:ILE:HA	1:H:345:PHE:CZ	2.52	0.42
1:G:270:ILE:HA	1:G:345:PHE:HZ	1.84	0.42
1:H:93:TYR:CE2	1:H:94:HIS:CE1	3.07	0.42
1:B:111:LYS:NZ	1:B:149:ASP:OD1	2.53	0.42
1:C:103:SER:O	1:C:240:THR:HB	2.19	0.42
1:C:385:THR:CG2	1:C:418:TYR:HB3	2.49	0.42
1:H:110:PHE:CG	1:H:111:LYS:N	2.85	0.42
1:H:277:ARG:HH22	1:H:280:THR:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLN:HG3	1:B:48:GLN:H	1.66	0.42
1:C:204:VAL:O	1:C:205:ASN:CB	2.68	0.42
1:E:446:LYS:NZ	1:E:450:LEU:HD11	2.35	0.42
1:B:67:SER:HB2	1:B:108:ASP:HB2	2.01	0.42
1:B:282:LYS:HD2	1:B:287:ASP:OD1	2.19	0.42
1:C:22:GLU:HA	1:C:68:ARG:HD2	2.01	0.42
1:D:19:LYS:HA	1:D:23:HIS:H	1.85	0.42
1:H:105:SER:HB2	1:H:109:TYR:CE2	2.54	0.42
1:B:336:HIS:ND1	1:B:341:ALA:O	2.51	0.42
1:C:111:LYS:NZ	1:C:149:ASP:OD2	2.48	0.42
1:C:304:THR:HG1	1:C:305:ILE:H	1.67	0.42
1:C:413:LEU:HD12	1:C:417:THR:OG1	2.20	0.42
1:H:177:GLU:HG2	1:H:184:CYS:CB	2.49	0.42
1:A:172:LYS:HG3	1:A:173:ASP:N	2.35	0.42
1:B:177:GLU:HG2	1:B:184:CYS:CB	2.50	0.42
1:F:131:GLU:HB3	1:F:165:LYS:HE3	2.02	0.42
1:F:137:TYR:CD2	1:F:153:LYS:HE2	2.55	0.42
1:B:153:LYS:HD3	1:B:166:ILE:HG21	2.00	0.41
1:B:222:TYR:HD1	1:B:231:LYS:O	2.02	0.41
1:C:316:ASP:CG	1:C:318:THR:HG22	2.41	0.41
1:D:390:ARG:HG3	1:D:390:ARG:HH11	1.84	0.41
1:E:150:LEU:HD23	1:E:153:LYS:HD2	2.02	0.41
1:A:153:LYS:O	1:A:157:GLN:HG3	2.19	0.41
1:C:386:LEU:O	1:C:390:ARG:HG2	2.20	0.41
1:G:77:ARG:HD3	1:G:82:HIS:HB3	2.02	0.41
1:B:109:TYR:CE1	1:B:238:ILE:HD12	2.55	0.41
1:E:39:LEU:HD21	1:E:47:ASN:OD1	2.20	0.41
1:G:93:TYR:CE2	1:G:94:HIS:CE1	3.08	0.41
1:H:194:ARG:HH12	1:H:249:SER:HB3	1.86	0.41
1:F:62:PRO:HD3	1:H:340:ASN:OD1	2.20	0.41
1:E:109:TYR:CE1	1:E:238:ILE:HD12	2.55	0.41
1:E:390:ARG:NH1	1:E:428:ILE:HG21	2.36	0.41
1:G:22:GLU:HB3	1:G:68:ARG:HD2	2.01	0.41
1:A:75:CYS:O	1:A:97:PHE:HA	2.21	0.41
1:C:113:LEU:HD21	1:C:117:MET:HE1	2.01	0.41
1:D:15:ILE:HD12	1:D:25:TYR:CD1	2.55	0.41
1:D:61:HIS:ND1	1:D:62:PRO:HD2	2.35	0.41
1:E:13:ARG:CZ	1:E:20:ARG:HH12	2.33	0.41
1:E:35:ASP:CG	1:G:278:PRO:HD2	2.40	0.41
1:G:19:LYS:HD3	1:G:24:THR:HA	2.02	0.41
1:G:80:GLY:HA2	1:G:81:LYS:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:VAL:CG1	1:E:256:SER:HA	2.51	0.41
1:C:93:TYR:CE2	1:C:94:HIS:CE1	3.09	0.41
1:H:117:MET:CA	1:H:119:LEU:H	2.33	0.41
1:H:409:ASP:N	1:H:409:ASP:OD1	2.53	0.41
1:C:92:VAL:HG13	1:C:256:SER:HA	2.03	0.41
1:E:390:ARG:HH12	1:E:432:LYS:HE2	1.84	0.41
1:F:103:SER:O	1:F:240:THR:HB	2.21	0.41
1:H:413:LEU:HD12	1:H:417:THR:OG1	2.21	0.41
1:A:122:LEU:C	1:A:128:ILE:HG22	2.42	0.41
1:B:109:TYR:CD1	1:B:238:ILE:HD12	2.56	0.41
1:B:113:LEU:O	1:B:117:MET:HG3	2.21	0.41
1:C:295:TYR:HD1	1:C:339:LEU:HD21	1.85	0.41
1:D:27:HIS:HD2	1:D:28:SER:N	2.18	0.41
1:F:131:GLU:HB3	1:F:165:LYS:NZ	2.35	0.41
1:H:52:ILE:HD11	1:H:63:MET:HG2	2.02	0.41
1:B:59:PRO:HG2	1:E:150:LEU:HB2	2.02	0.41
1:C:277:ARG:HH12	1:C:289:ASP:CG	2.24	0.41
1:E:85:LEU:HD23	1:E:326:ARG:NH2	2.36	0.41
1:A:109:TYR:CE1	1:A:238:ILE:HD12	2.56	0.41
1:F:113:LEU:O	1:F:117:MET:HG3	2.21	0.41
1:A:113:LEU:O	1:A:117:MET:HG3	2.22	0.40
1:C:111:LYS:NZ	1:C:149:ASP:CG	2.75	0.40
1:D:19:LYS:HA	1:D:23:HIS:N	2.36	0.40
1:A:23:HIS:CD2	1:A:68:ARG:HB2	2.56	0.40
1:A:434:LEU:HD12	1:A:434:LEU:N	2.36	0.40
1:F:80:GLY:N	1:F:83:ASN:HB2	2.36	0.40
1:G:330:ARG:HD2	1:G:330:ARG:HH11	1.68	0.40
1:C:104:TRP:CD1	1:C:239:ASP:HA	2.56	0.40
1:D:270:ILE:HA	1:D:345:PHE:HZ	1.86	0.40
1:B:61:HIS:ND1	1:B:62:PRO:HD2	2.36	0.40
1:C:137:TYR:CA	1:C:174:ASN:HD22	2.34	0.40
1:G:14:PHE:CE1	1:G:18:PHE:HE2	2.40	0.40
1:C:300:ASP:C	1:C:300:ASP:OD1	2.60	0.40
1:C:97:PHE:CB	1:C:304:THR:HG22	2.52	0.40
1:D:80:GLY:N	1:D:83:ASN:HB2	2.37	0.40
1:E:113:LEU:O	1:E:117:MET:HG3	2.22	0.40
1:G:245:GLU:HG3	1:G:262:LEU:HD13	2.02	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:GLU:OE1	1:F:395:ARG:NH1[1_546]	1.89	0.31
1:A:154:GLN:NE2	1:F:55:ASN:O[1_545]	2.10	0.10
1:E:445:ARG:NE	1:G:405:THR:OG1[1_655]	2.12	0.08
1:D:388:ARG:NH2	1:H:366:LYS:O[1_645]	2.15	0.05

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	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	47	71
1	B	448/450 (100%)	431 (96%)	12 (3%)	5 (1%)	14	31
1	C	442/450 (98%)	426 (96%)	12 (3%)	4 (1%)	17	37
1	D	445/450 (99%)	431 (97%)	14 (3%)	0	100	100
1	E	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	47	71
1	F	447/450 (99%)	434 (97%)	11 (2%)	2 (0%)	34	58
1	G	447/450 (99%)	429 (96%)	15 (3%)	3 (1%)	22	44
1	H	444/450 (99%)	421 (95%)	18 (4%)	5 (1%)	14	31
All	All	3569/3600 (99%)	3444 (96%)	104 (3%)	21 (1%)	25	47

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	B	37	PRO
1	C	22	GLU
1	F	37	PRO
1	H	37	PRO
1	H	103	SER
1	H	104	TRP
1	C	158	ASN
1	G	37	PRO

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Mol	Chain	Res	Type
1	H	142	GLU
1	B	275	GLY
1	B	35	ASP
1	G	22	GLU
1	C	35	ASP
1	B	278	PRO
1	C	59	PRO
1	B	36	ASP
1	E	36	ASP
1	F	36	ASP
1	G	36	ASP
1	H	36	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	379/379 (100%)	360 (95%)	19 (5%)	24	47
1	B	379/379 (100%)	358 (94%)	21 (6%)	21	43
1	C	374/379 (99%)	355 (95%)	19 (5%)	24	46
1	D	376/379 (99%)	357 (95%)	19 (5%)	24	46
1	E	379/379 (100%)	363 (96%)	16 (4%)	30	55
1	F	378/379 (100%)	362 (96%)	16 (4%)	30	55
1	G	378/379 (100%)	361 (96%)	17 (4%)	27	52
1	H	375/379 (99%)	353 (94%)	22 (6%)	19	40
All	All	3018/3032 (100%)	2869 (95%)	149 (5%)	25	49

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	29	SER
1	A	31	THR

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Mol	Chain	Res	Type
1	A	40	LEU
1	A	46	MET
1	A	55	ASN
1	A	60	SER
1	A	68	ARG
1	A	131	GLU
1	A	147	GLU
1	A	283	VAL
1	A	301	HIS
1	A	355	GLN
1	A	395	ARG
1	A	402	ASP
1	A	403	SER
1	A	423	ASP
1	A	443	GLU
1	A	453	GLN
1	B	4	THR
1	B	22	GLU
1	B	31	THR
1	B	46	MET
1	B	48	GLN
1	B	92	VAL
1	B	121	LEU
1	B	150	LEU
1	B	153	LYS
1	B	178	MET
1	B	198	ARG
1	B	230	LEU
1	B	282	LYS
1	B	283	VAL
1	B	303	ARG
1	B	328	LEU
1	B	399	SER
1	B	413	LEU
1	B	422	VAL
1	B	423	ASP
1	B	439	ASP
1	C	4	THR
1	C	12	GLN
1	C	19	LYS
1	C	56	THR
1	C	60	SER

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Mol	Chain	Res	Type
1	C	81	LYS
1	C	88	VAL
1	C	92	VAL
1	C	113	LEU
1	C	150	LEU
1	C	178	MET
1	C	227	ASP
1	C	303	ARG
1	C	363	GLU
1	C	369	ASP
1	C	390	ARG
1	C	399	SER
1	C	423	ASP
1	C	443	GLU
1	D	5	LEU
1	D	9	GLU
1	D	10	ILE
1	D	15	ILE
1	D	31	THR
1	D	46	MET
1	D	47	ASN
1	D	88	VAL
1	D	92	VAL
1	D	113	LEU
1	D	150	LEU
1	D	171	MET
1	D	178	MET
1	D	283	VAL
1	D	301	HIS
1	D	306	THR
1	D	390	ARG
1	D	399	SER
1	D	423	ASP
1	E	4	THR
1	E	29	SER
1	E	88	VAL
1	E	92	VAL
1	E	151	GLU
1	E	155	ILE
1	E	178	MET
1	E	221	GLN
1	E	233	LEU

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Mol	Chain	Res	Type
1	E	283	VAL
1	E	303	ARG
1	E	328	LEU
1	E	384	LYS
1	E	399	SER
1	E	423	ASP
1	E	445	ARG
1	F	29	SER
1	F	46	MET
1	F	60	SER
1	F	88	VAL
1	F	108	ASP
1	F	150	LEU
1	F	189	GLU
1	F	207	ASP
1	F	227	ASP
1	F	283	VAL
1	F	301	HIS
1	F	303	ARG
1	F	328	LEU
1	F	403	SER
1	F	423	ASP
1	F	443	GLU
1	G	11	ARG
1	G	19	LYS
1	G	29	SER
1	G	31	THR
1	G	55	ASN
1	G	94	HIS
1	G	113	LEU
1	G	131	GLU
1	G	178	MET
1	G	198	ARG
1	G	301	HIS
1	G	303	ARG
1	G	328	LEU
1	G	365	LYS
1	G	399	SER
1	G	422	VAL
1	G	423	ASP
1	H	4	THR
1	H	29	SER

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Mol	Chain	Res	Type
1	H	81	LYS
1	H	88	VAL
1	H	104	TRP
1	H	116	LYS
1	H	120	GLU
1	H	146	LEU
1	H	153	LYS
1	H	154	GLN
1	H	230	LEU
1	H	236	LYS
1	H	249	SER
1	H	301	HIS
1	H	326	ARG
1	H	328	LEU
1	H	370	MET
1	H	386	LEU
1	H	388	ARG
1	H	423	ASP
1	H	439	ASP
1	H	442	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	205	ASN
1	B	48	GLN
1	C	154	GLN
1	C	174	ASN
1	C	205	ASN
1	C	223	ASN
1	D	27	HIS
1	D	47	ASN
1	D	174	ASN
1	D	191	HIS
1	D	340	ASN
1	E	94	HIS
1	E	154	GLN
1	E	205	ASN
1	E	301	HIS
1	G	55	ASN
1	G	124	GLN

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Mol	Chain	Res	Type
1	G	174	ASN
1	G	223	ASN
1	G	340	ASN
1	G	355	GLN
1	H	157	GLN
1	H	257	ASN
1	H	340	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A5A	H	500	-	26,30,30	1.40	5 (19%)	30,45,45	1.67	3 (10%)
2	A5A	B	500	-	26,30,30	1.72	5 (19%)	30,45,45	2.38	8 (26%)
2	A5A	C	500	-	26,30,30	1.83	7 (26%)	30,45,45	2.34	10 (33%)
2	A5A	A	500	-	26,30,30	1.59	3 (11%)	30,45,45	3.02	11 (36%)
2	A5A	F	500	-	26,30,30	2.04	6 (23%)	30,45,45	2.09	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A5A	G	500	-	26,30,30	1.40	4 (15%)	30,45,45	1.99	7 (23%)
2	A5A	D	500	-	26,30,30	1.35	5 (19%)	30,45,45	2.51	10 (33%)
2	A5A	E	500	-	26,30,30	1.48	5 (19%)	30,45,45	2.28	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A5A	H	500	-	-	0/14/35/35	0/3/3/3
2	A5A	B	500	-	-	5/14/35/35	0/3/3/3
2	A5A	C	500	-	-	4/14/35/35	0/3/3/3
2	A5A	A	500	-	-	4/14/35/35	0/3/3/3
2	A5A	F	500	-	-	5/14/35/35	0/3/3/3
2	A5A	G	500	-	-	2/14/35/35	0/3/3/3
2	A5A	D	500	-	-	3/14/35/35	0/3/3/3
2	A5A	E	500	-	-	4/14/35/35	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	A5A	O1S-S	5.99	1.47	1.42
2	F	500	A5A	O2S-S	4.80	1.46	1.42
2	B	500	A5A	O2S-S	4.74	1.46	1.42
2	A	500	A5A	O2S-S	4.72	1.46	1.42
2	C	500	A5A	O5'-S	-4.45	1.50	1.59
2	B	500	A5A	O5'-S	-3.96	1.51	1.59
2	E	500	A5A	O2S-S	3.84	1.45	1.42
2	A	500	A5A	O5'-S	-3.80	1.51	1.59
2	C	500	A5A	O1S-S	3.56	1.45	1.42
2	F	500	A5A	O5'-S	-3.51	1.52	1.59
2	G	500	A5A	C2'-C1'	-3.21	1.48	1.53
2	C	500	A5A	O2S-S	3.19	1.45	1.42
2	D	500	A5A	O2S-S	3.12	1.45	1.42
2	H	500	A5A	O4'-C1'	2.88	1.45	1.41
2	F	500	A5A	C5-C4	2.88	1.48	1.40
2	H	500	A5A	C2'-C1'	-2.84	1.49	1.53
2	G	500	A5A	O2S-S	2.70	1.44	1.42
2	C	500	A5A	C5-C4	2.69	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	A5A	C2'-C1'	-2.58	1.49	1.53
2	C	500	A5A	S-N3S	2.55	1.64	1.59
2	C	500	A5A	C2'-C1'	-2.49	1.50	1.53
2	G	500	A5A	O5'-S	-2.48	1.54	1.59
2	H	500	A5A	O5'-S	-2.47	1.54	1.59
2	H	500	A5A	O2S-S	2.44	1.44	1.42
2	E	500	A5A	O5'-S	-2.41	1.54	1.59
2	D	500	A5A	O5'-S	-2.35	1.54	1.59
2	F	500	A5A	S-N3S	2.21	1.63	1.59
2	E	500	A5A	O1S-S	2.17	1.44	1.42
2	F	500	A5A	C2-N3	2.16	1.35	1.32
2	D	500	A5A	C5-C4	2.16	1.46	1.40
2	C	500	A5A	O5'-C5'	-2.14	1.37	1.46
2	G	500	A5A	C5-C4	2.12	1.46	1.40
2	B	500	A5A	C2-N3	2.12	1.35	1.32
2	D	500	A5A	O4'-C1'	2.11	1.44	1.41
2	H	500	A5A	C5-C4	2.07	1.46	1.40
2	E	500	A5A	C6-C5	2.06	1.50	1.43
2	B	500	A5A	O1S-S	-2.04	1.40	1.42
2	E	500	A5A	C2-N3	2.03	1.35	1.32
2	D	500	A5A	C6-C5	2.02	1.50	1.43
2	B	500	A5A	O4'-C1'	2.02	1.43	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	A5A	O2S-S-O1S	-13.49	99.75	120.76
2	E	500	A5A	O2S-S-O1S	-9.56	105.87	120.76
2	B	500	A5A	O2S-S-O1S	-9.00	106.74	120.76
2	D	500	A5A	O2S-S-O1S	-8.75	107.13	120.76
2	G	500	A5A	O2S-S-O1S	-7.88	108.48	120.76
2	C	500	A5A	O2S-S-O1S	-7.41	109.21	120.76
2	F	500	A5A	O2S-S-O1S	-6.16	111.16	120.76
2	H	500	A5A	O2S-S-O1S	-6.09	111.28	120.76
2	A	500	A5A	N3-C2-N1	-4.99	120.88	128.68
2	D	500	A5A	N3-C2-N1	-4.70	121.34	128.68
2	B	500	A5A	N3-C2-N1	-4.48	121.67	128.68
2	C	500	A5A	CA-C-N3S	4.39	123.63	114.34
2	B	500	A5A	C2'-C3'-C4'	3.79	110.01	102.64
2	C	500	A5A	C-N3S-S	-3.67	118.66	124.61
2	D	500	A5A	CA-C-N3S	3.63	122.01	114.34
2	F	500	A5A	N3-C2-N1	-3.62	123.02	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	A5A	C2'-C3'-C4'	3.48	109.41	102.64
2	F	500	A5A	O4'-C1'-C2'	3.44	111.96	106.93
2	F	500	A5A	C4-C5-N7	-3.43	105.82	109.40
2	H	500	A5A	C4-C5-N7	-3.38	105.87	109.40
2	H	500	A5A	N3-C2-N1	-3.27	123.56	128.68
2	D	500	A5A	C1'-N9-C4	-3.26	120.91	126.64
2	C	500	A5A	N3-C2-N1	-3.21	123.66	128.68
2	E	500	A5A	C5-C6-N6	3.19	125.21	120.35
2	D	500	A5A	C4-C5-N7	-3.19	106.08	109.40
2	D	500	A5A	C5-C6-N6	3.16	125.15	120.35
2	G	500	A5A	N3-C2-N1	-3.15	123.76	128.68
2	A	500	A5A	O5'-S-O1S	3.14	115.18	105.59
2	C	500	A5A	C5-C6-N6	3.10	125.06	120.35
2	E	500	A5A	N3-C2-N1	-3.08	123.86	128.68
2	B	500	A5A	O4'-C1'-C2'	2.99	111.29	106.93
2	B	500	A5A	O-C-N3S	-2.93	117.36	123.00
2	C	500	A5A	C2-N1-C6	2.92	123.76	118.75
2	C	500	A5A	C4-C5-N7	-2.82	106.46	109.40
2	D	500	A5A	O4'-C1'-C2'	2.77	110.97	106.93
2	E	500	A5A	C-N3S-S	2.75	129.06	124.61
2	A	500	A5A	C4-C5-N7	-2.73	106.56	109.40
2	C	500	A5A	O5'-S-O1S	2.68	113.79	105.59
2	B	500	A5A	O5'-S-O2S	2.65	113.69	105.59
2	E	500	A5A	C4-C5-N7	-2.64	106.65	109.40
2	G	500	A5A	C4-C5-N7	-2.58	106.71	109.40
2	C	500	A5A	C1'-N9-C4	-2.47	122.30	126.64
2	G	500	A5A	O5'-S-O1S	2.43	113.02	105.59
2	D	500	A5A	C2-N1-C6	2.36	122.79	118.75
2	A	500	A5A	C2-N1-C6	2.35	122.78	118.75
2	A	500	A5A	C5-C6-N6	2.35	123.92	120.35
2	D	500	A5A	O5'-S-N3S	2.34	112.12	105.60
2	D	500	A5A	O5'-C5'-C4'	2.33	111.97	107.62
2	A	500	A5A	O4'-C4'-C3'	-2.31	100.54	105.11
2	A	500	A5A	C2'-C3'-C4'	2.31	107.13	102.64
2	B	500	A5A	C4-C5-N7	-2.29	107.01	109.40
2	A	500	A5A	O3'-C3'-C2'	-2.29	104.42	111.82
2	F	500	A5A	CA-C-N3S	2.27	119.15	114.34
2	G	500	A5A	CA-C-N3S	2.25	119.10	114.34
2	G	500	A5A	C1'-N9-C4	-2.17	122.82	126.64
2	F	500	A5A	C-N3S-S	-2.10	121.21	124.61
2	B	500	A5A	O-C-CA	2.08	125.13	120.52
2	G	500	A5A	C-N3S-S	-2.05	121.29	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	A5A	O-C-CA	-2.03	116.02	120.52
2	A	500	A5A	CA-C-N3S	2.03	118.63	114.34
2	E	500	A5A	C2'-C3'-C4'	2.01	106.55	102.64
2	A	500	A5A	O5'-S-N3S	2.01	111.20	105.60

There are no chirality outliers.

All (27) torsion outliers are listed below:

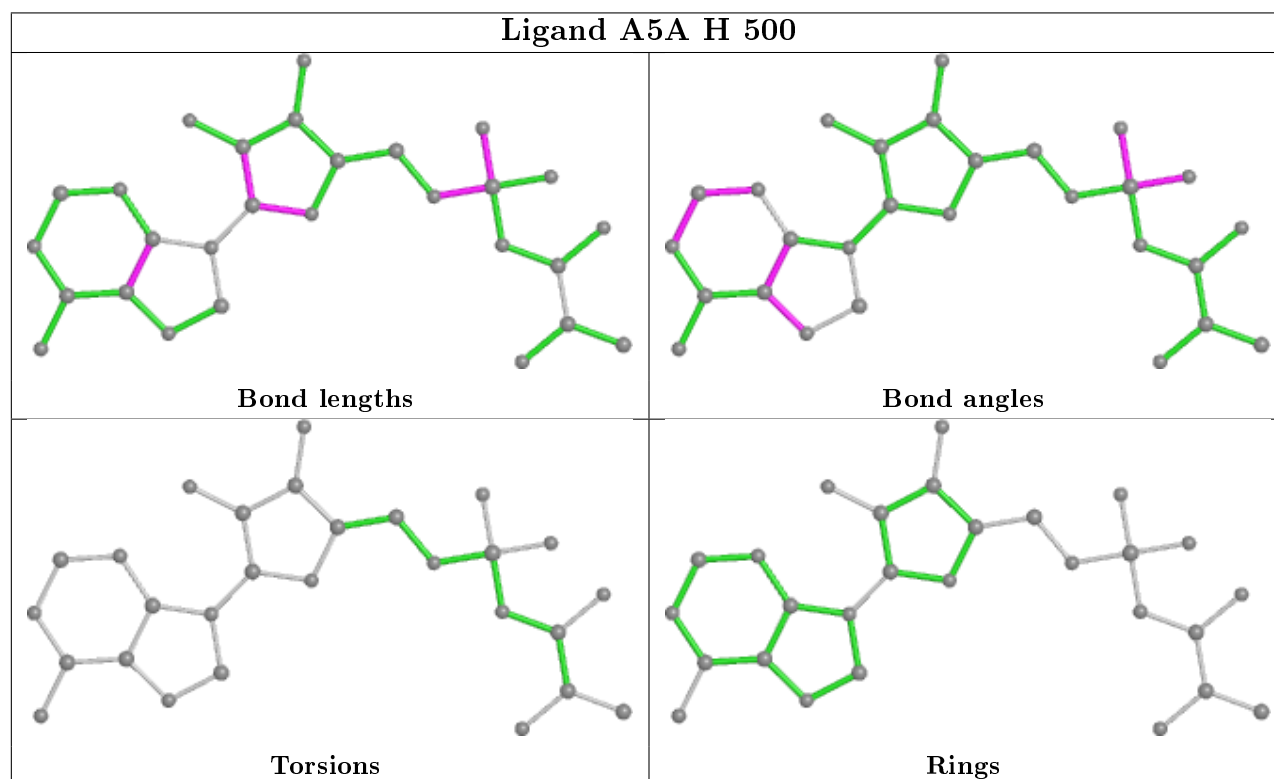
Mol	Chain	Res	Type	Atoms
2	B	500	A5A	C5'-O5'-S-N3S
2	C	500	A5A	C5'-O5'-S-N3S
2	C	500	A5A	C5'-O5'-S-O2S
2	C	500	A5A	C3'-C4'-C5'-O5'
2	A	500	A5A	C5'-O5'-S-N3S
2	A	500	A5A	C5'-O5'-S-O2S
2	F	500	A5A	O-C-CA-N
2	F	500	A5A	C5'-O5'-S-N3S
2	F	500	A5A	C5'-O5'-S-O2S
2	G	500	A5A	C-N3S-S-O1S
2	G	500	A5A	C5'-O5'-S-N3S
2	D	500	A5A	O4'-C4'-C5'-O5'
2	D	500	A5A	C3'-C4'-C5'-O5'
2	E	500	A5A	C5'-O5'-S-N3S
2	B	500	A5A	O-C-CA-N
2	B	500	A5A	N3S-C-CA-N
2	F	500	A5A	N3S-C-CA-N
2	A	500	A5A	N3S-C-CA-CB
2	E	500	A5A	N3S-C-CA-CB
2	C	500	A5A	C5'-O5'-S-O1S
2	F	500	A5A	C5'-O5'-S-O1S
2	E	500	A5A	O-C-CA-CB
2	B	500	A5A	C5'-O5'-S-O2S
2	E	500	A5A	C5'-O5'-S-O2S
2	D	500	A5A	C5'-O5'-S-N3S
2	A	500	A5A	O-C-CA-CB
2	B	500	A5A	C5'-O5'-S-O1S

There are no ring outliers.

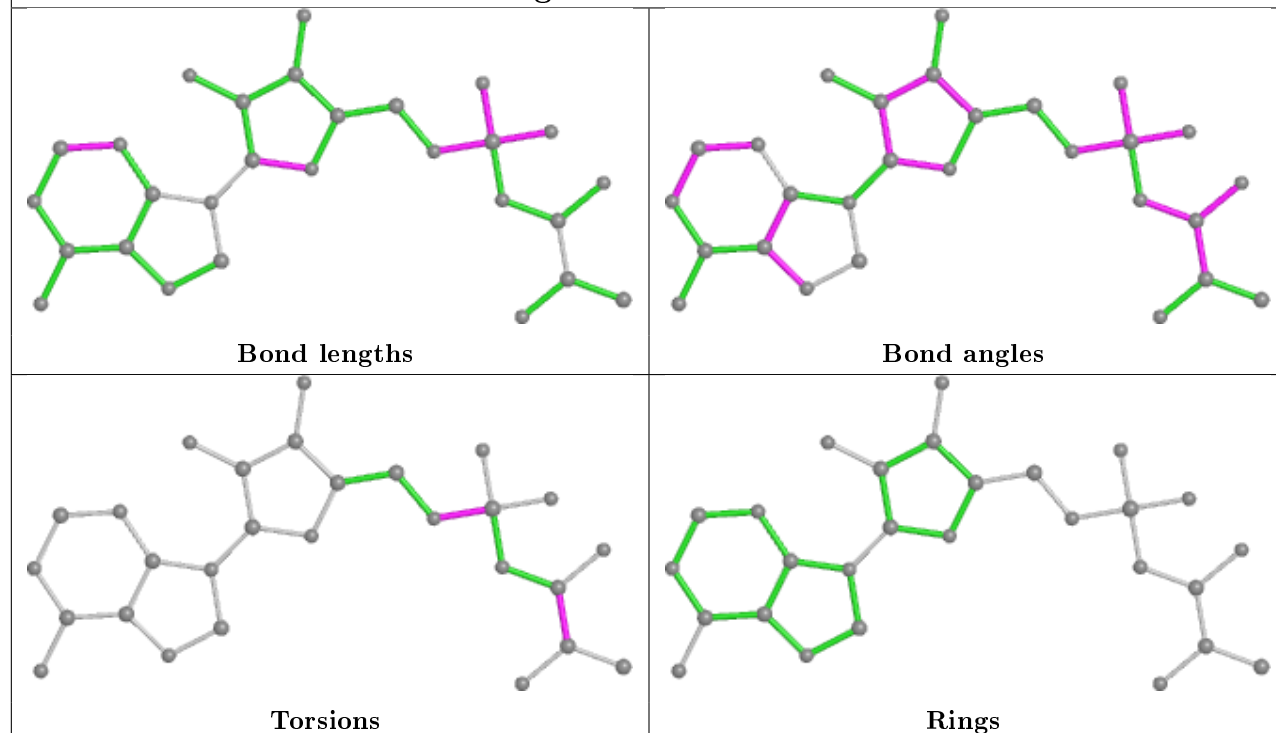
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	A5A	3	0
2	A	500	A5A	1	0
2	D	500	A5A	1	0
2	E	500	A5A	2	0

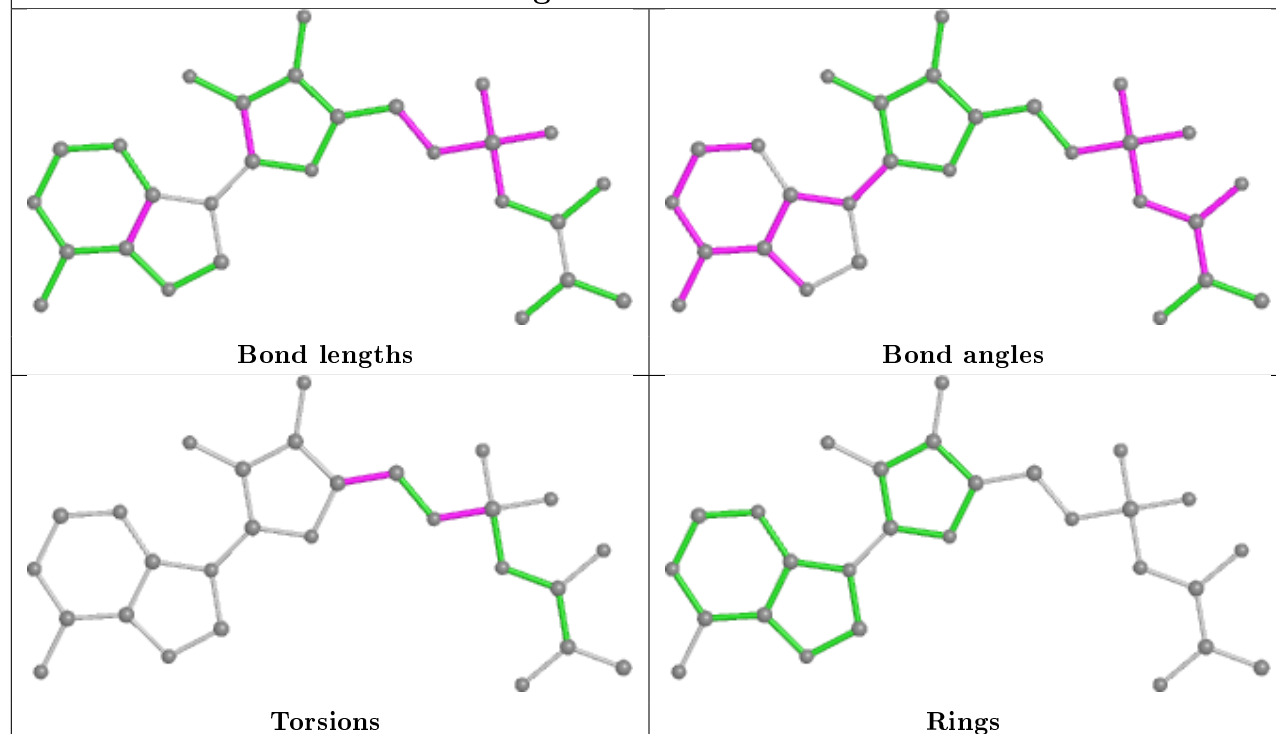
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



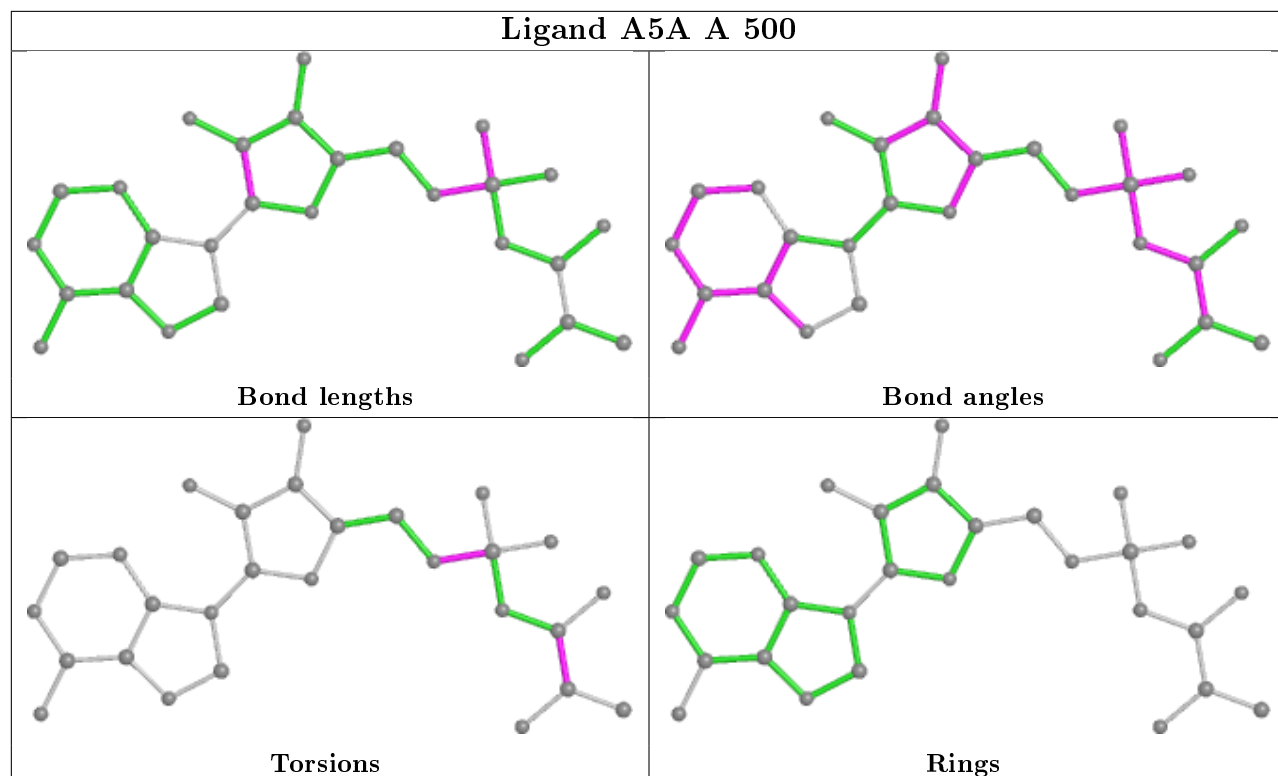
Ligand A5A B 500



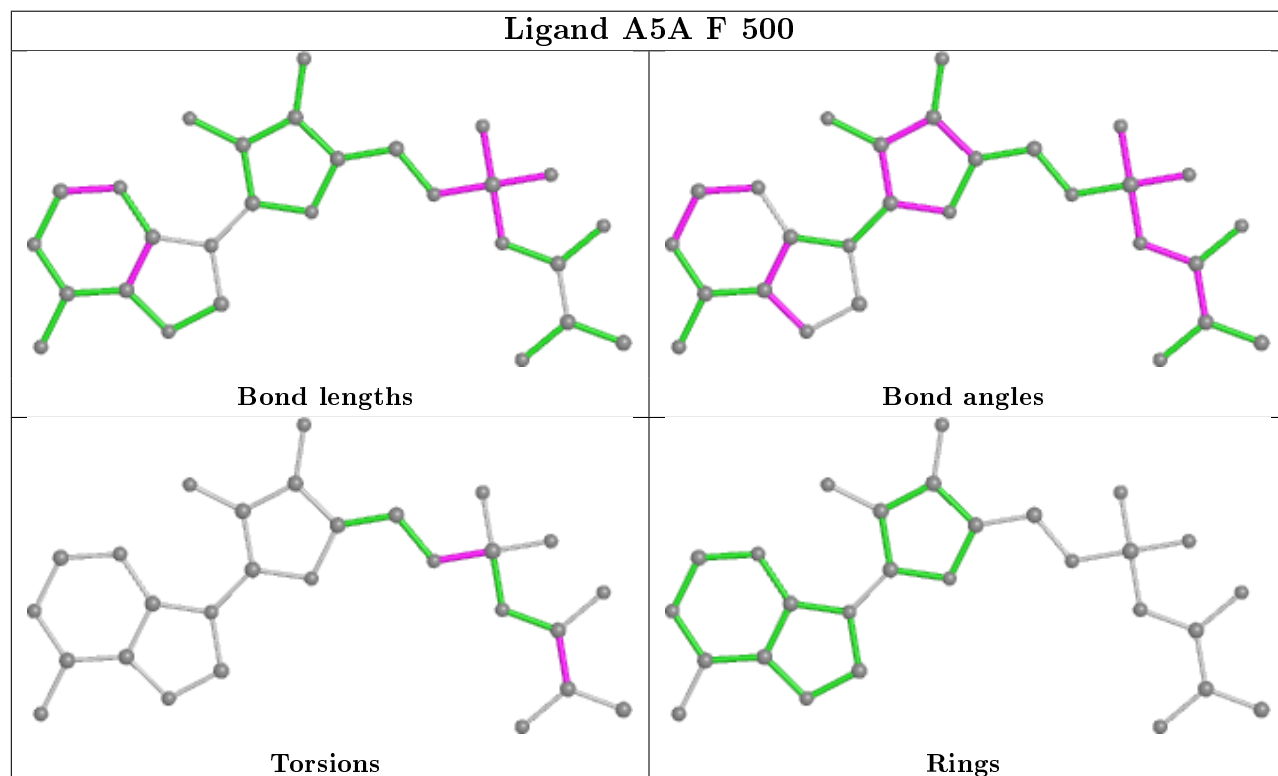
Ligand A5A C 500



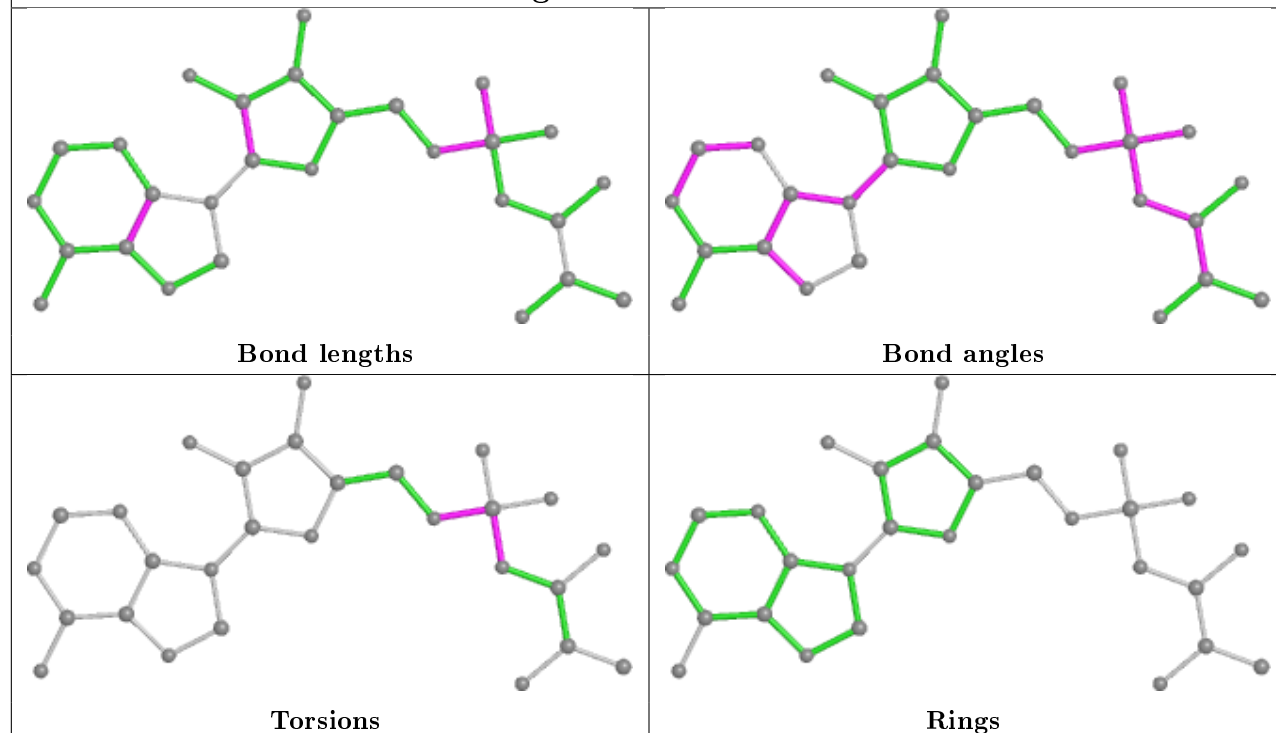
Ligand A5A A 500



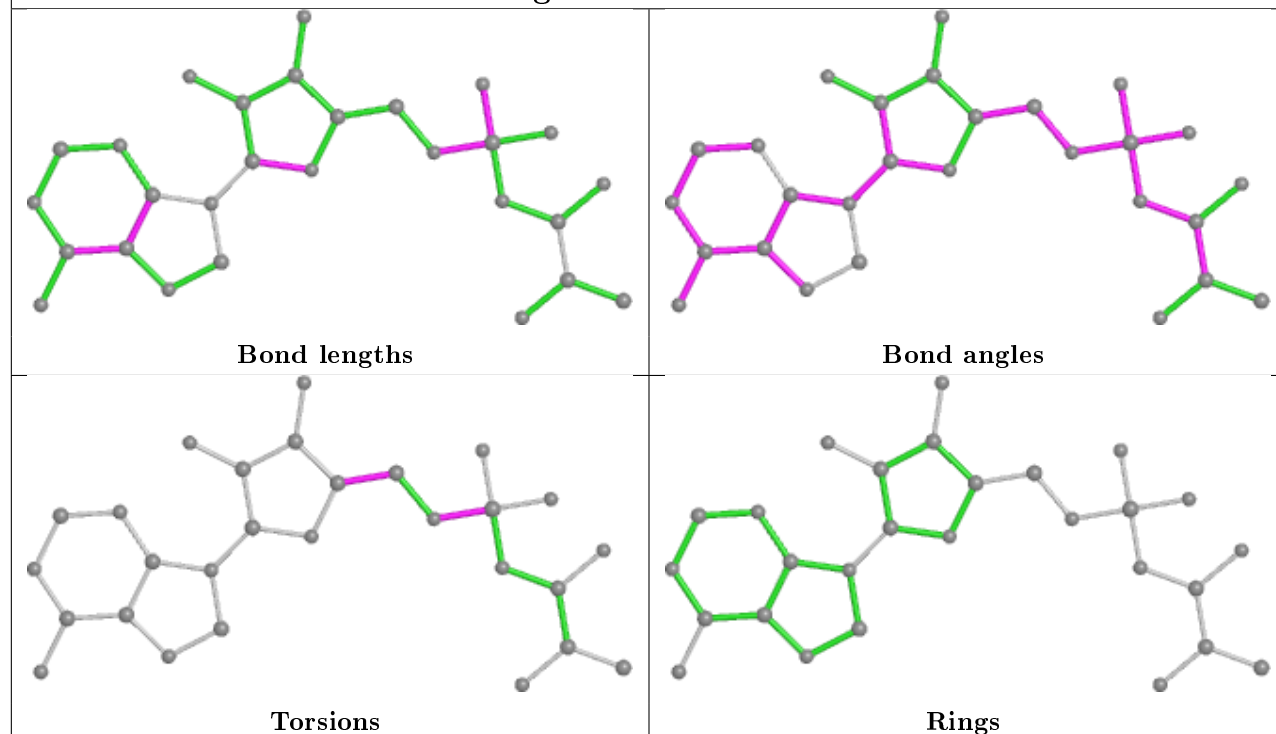
Ligand A5A F 500

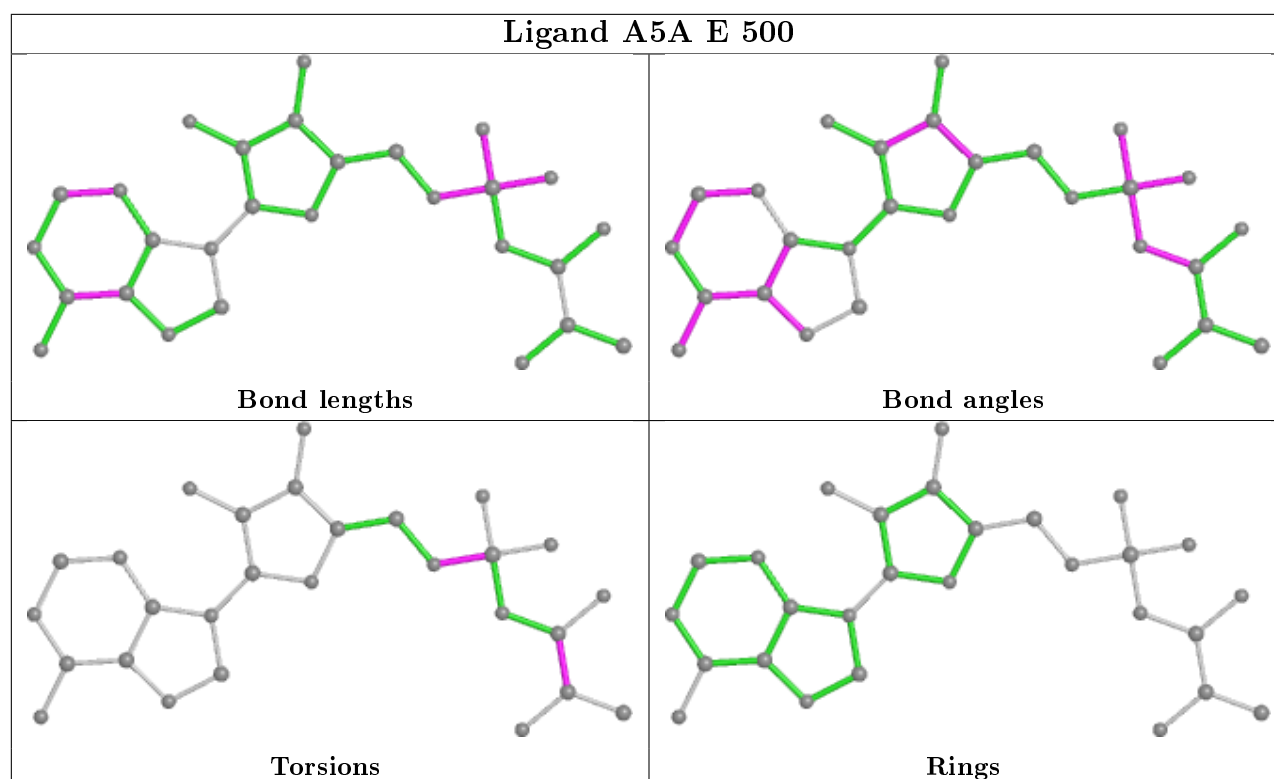


Ligand A5A G 500



Ligand A5A D 500





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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

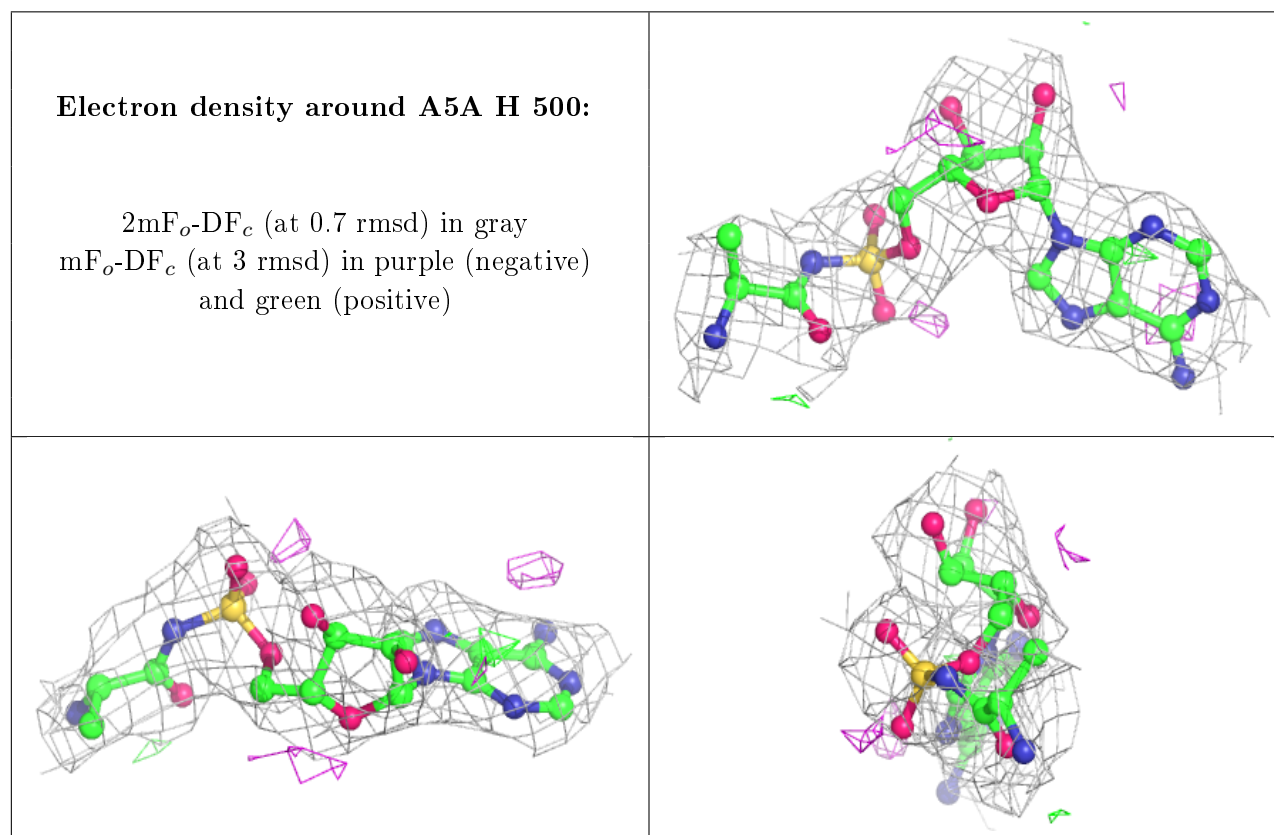
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

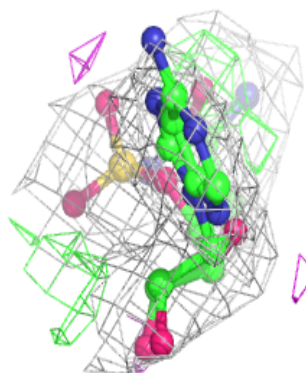
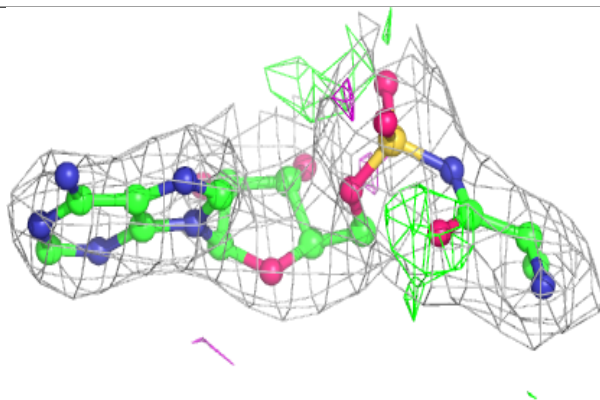
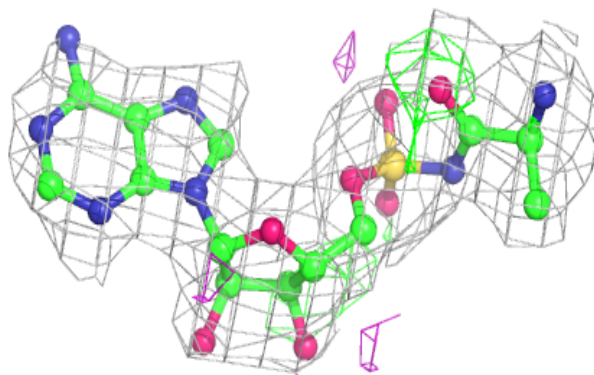
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

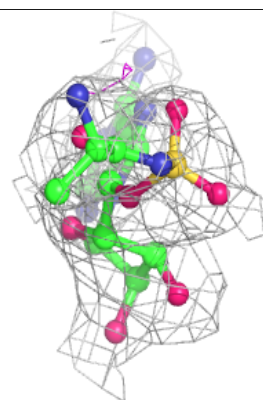
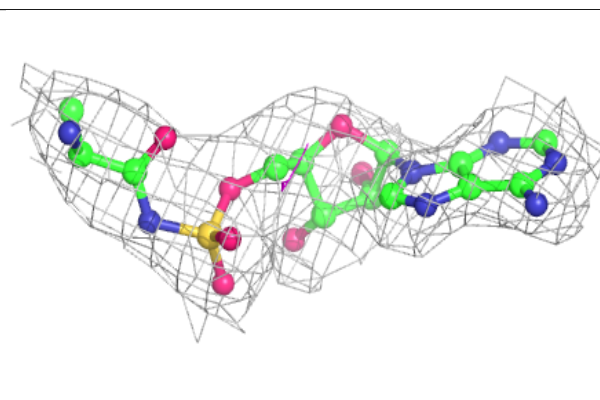
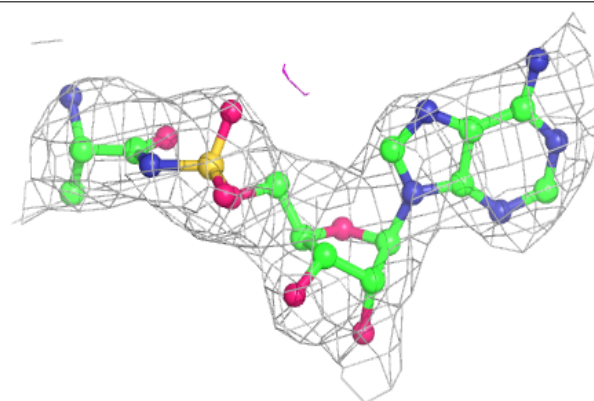


Electron density around A5A B 500:

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

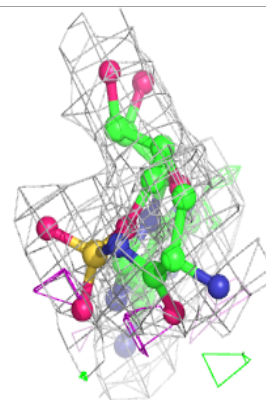
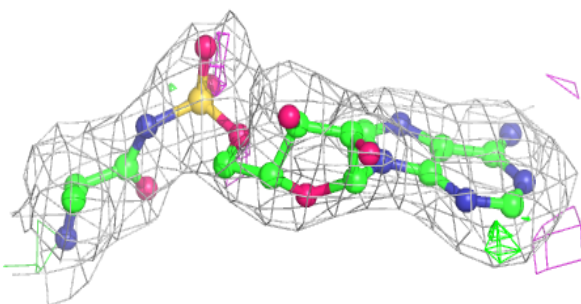
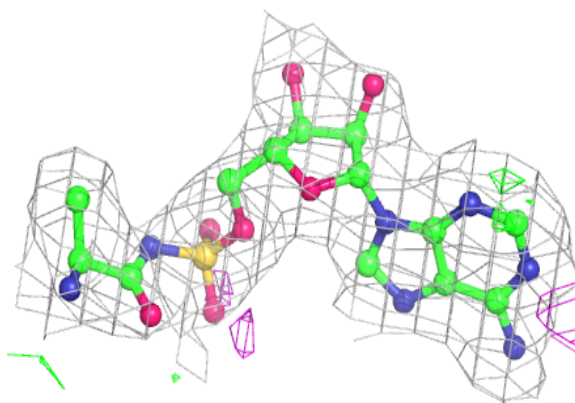
**Electron density around A5A C 500:**

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

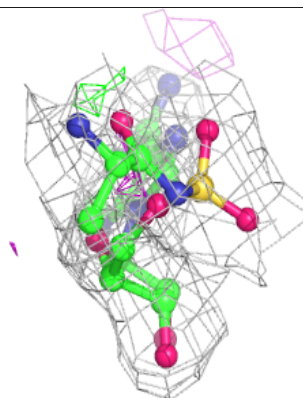
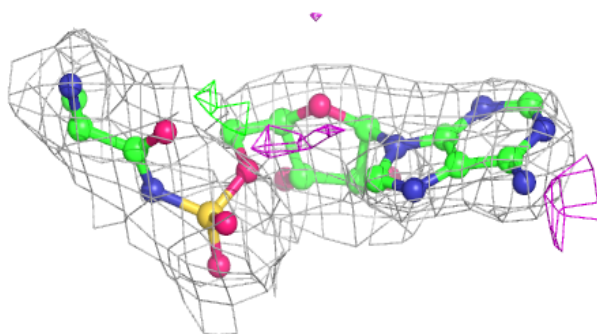
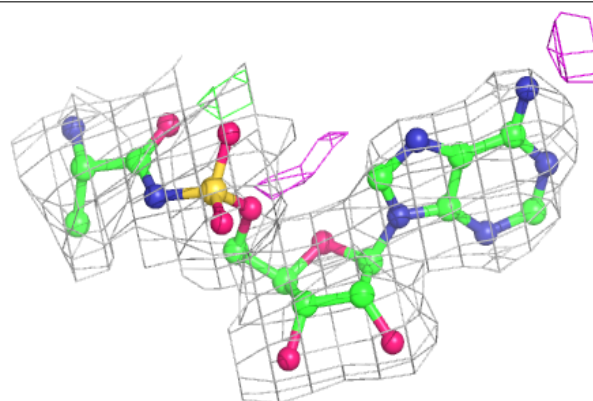


Electron density around A5A A 500:

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

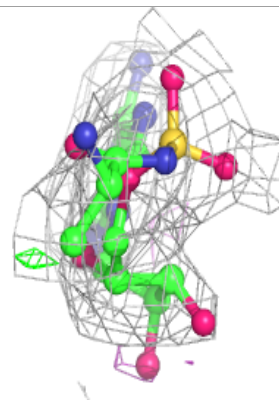
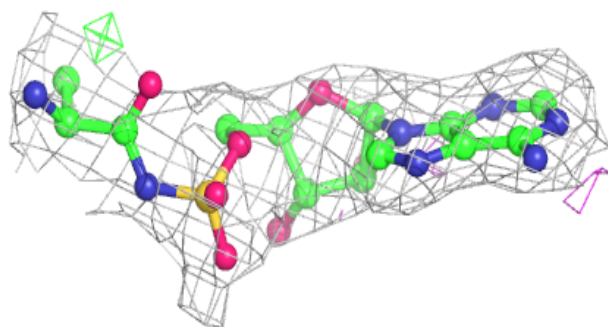
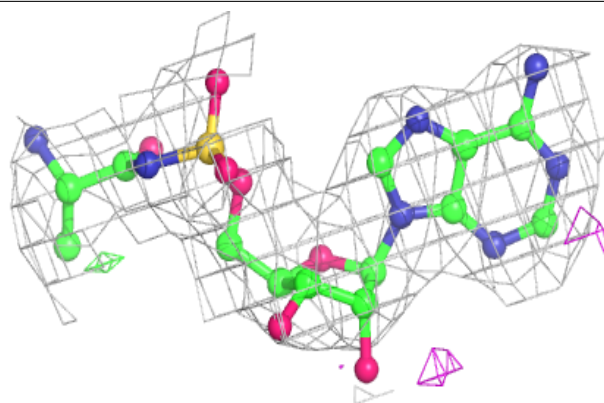
**Electron density around A5A F 500:**

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

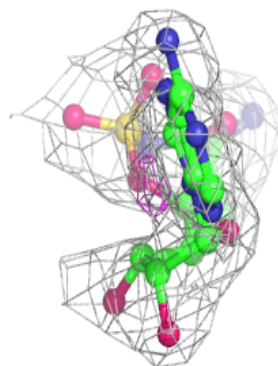
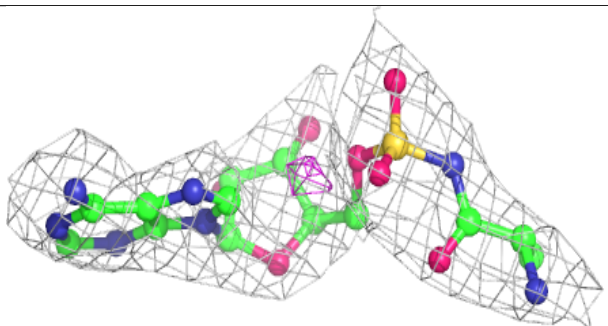
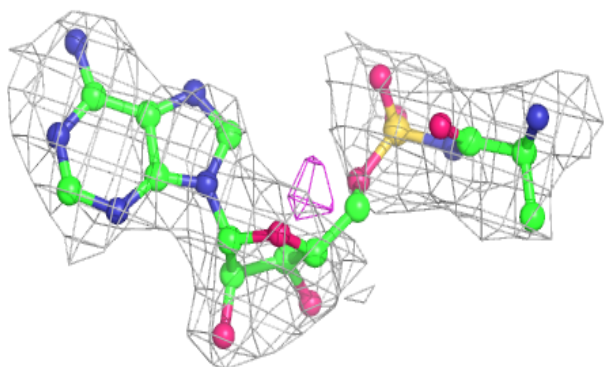


Electron density around A5A G 500:

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

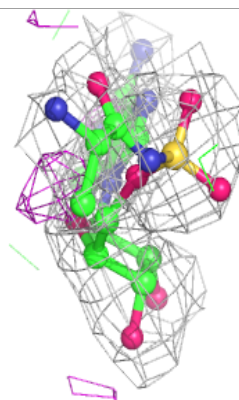
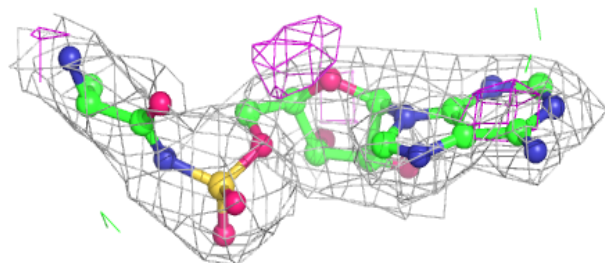
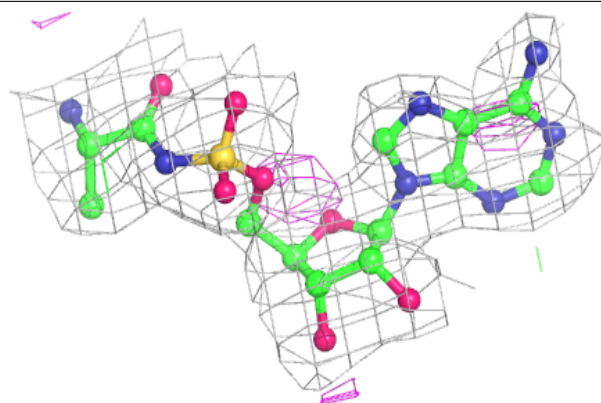
**Electron density around A5A D 500:**

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



Electron density around A5A E 500:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.