



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:40 AM UTC

PDB ID : 5KNN / pdb_00005knn
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 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

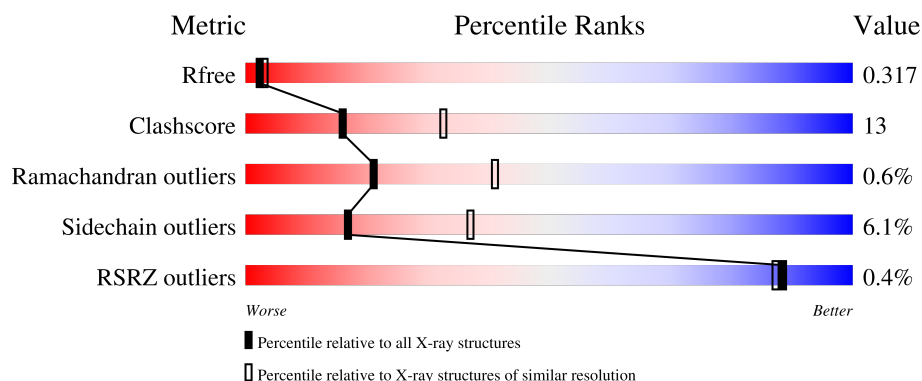
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

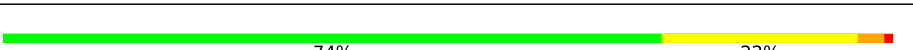
The reported resolution of this entry is 2.68 Å.

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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 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	450	
1	B	450	
1	C	450	
1	D	450	
1	E	450	

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Mol	Chain	Length	Quality of chain
1	F	450	73% 24% ..
1	G	450	% 72% 23% .
1	H	450	67% 24% 5% ..

2 Entry composition

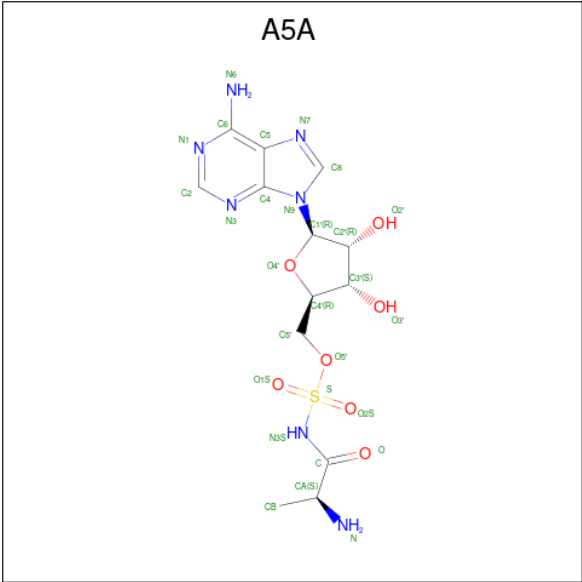
There are 2 unique types of molecules in this entry. The entry contains 28584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: A5A) (formula: C₁₃H₁₉N₇O₇S).

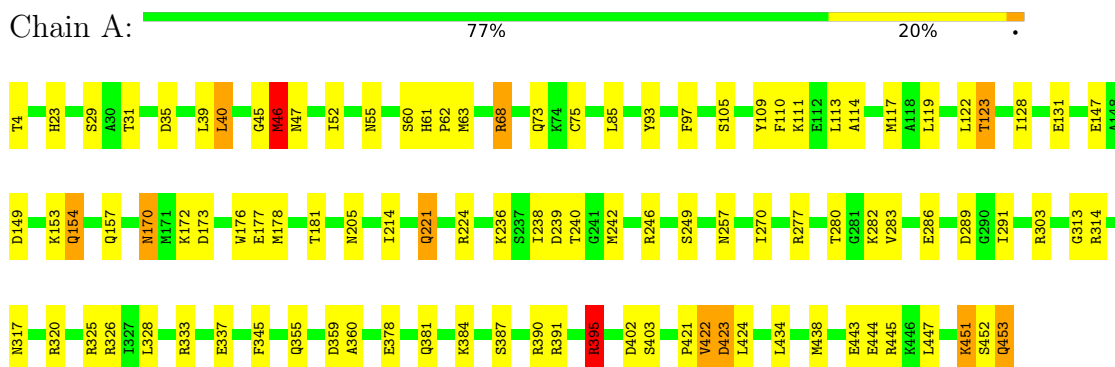


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	B	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	C	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	D	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	E	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	F	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
2	G	1	Total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

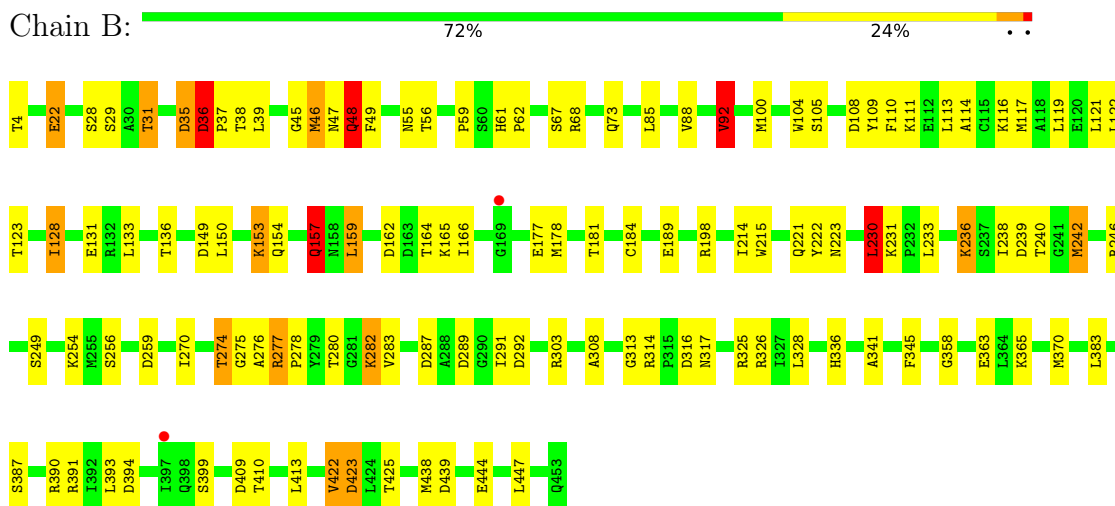
3 Residue-property plots [i](#)

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

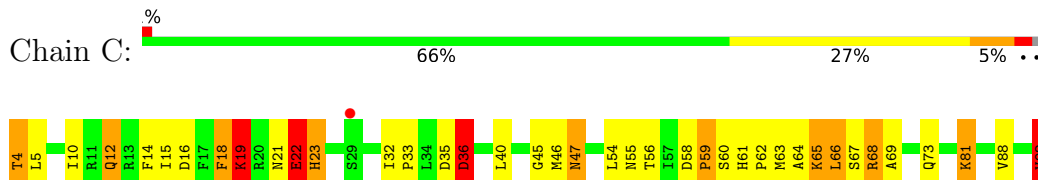
- Molecule 1: Alanine-tRNA ligase, cytoplasmic

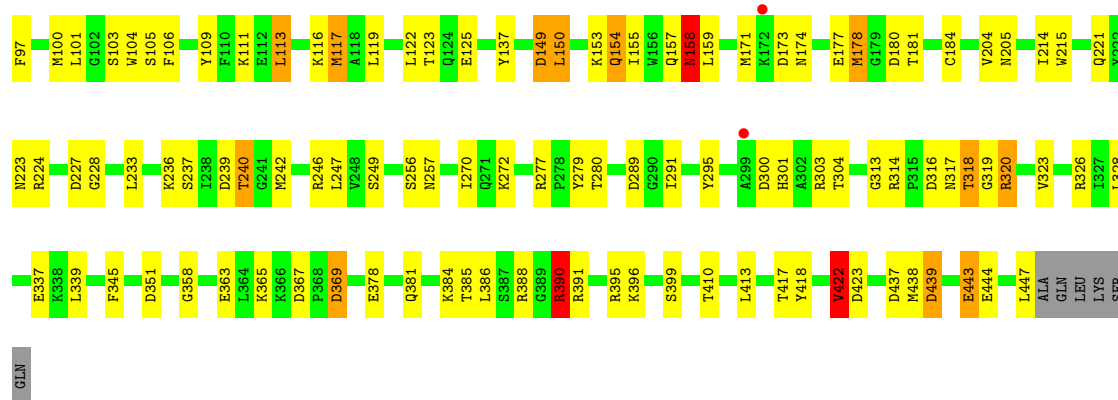


- Molecule 1: Alanine-tRNA ligase, cytoplasmic

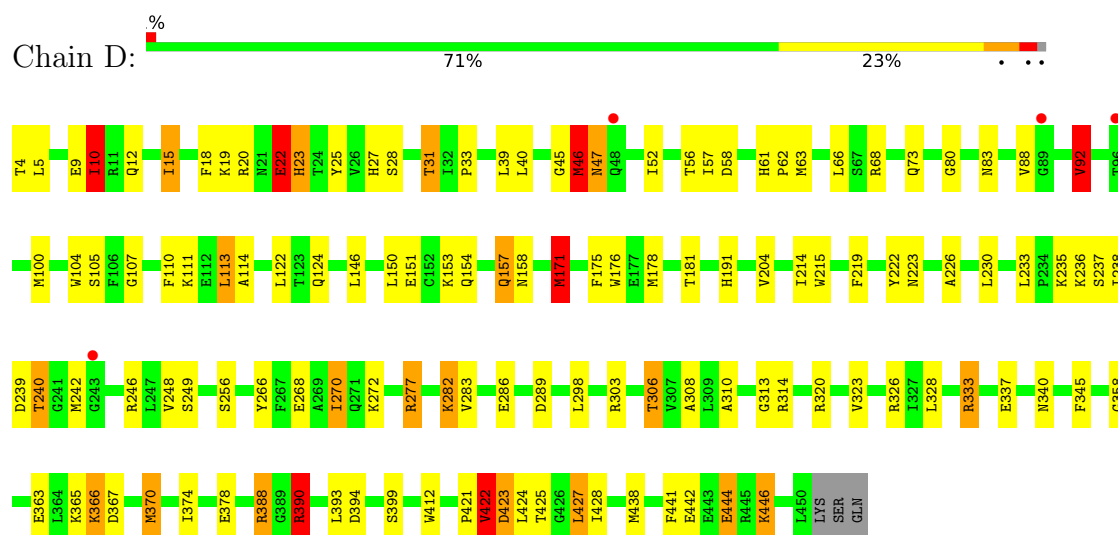


- Molecule 1: Alanine-tRNA ligase, cytoplasmic

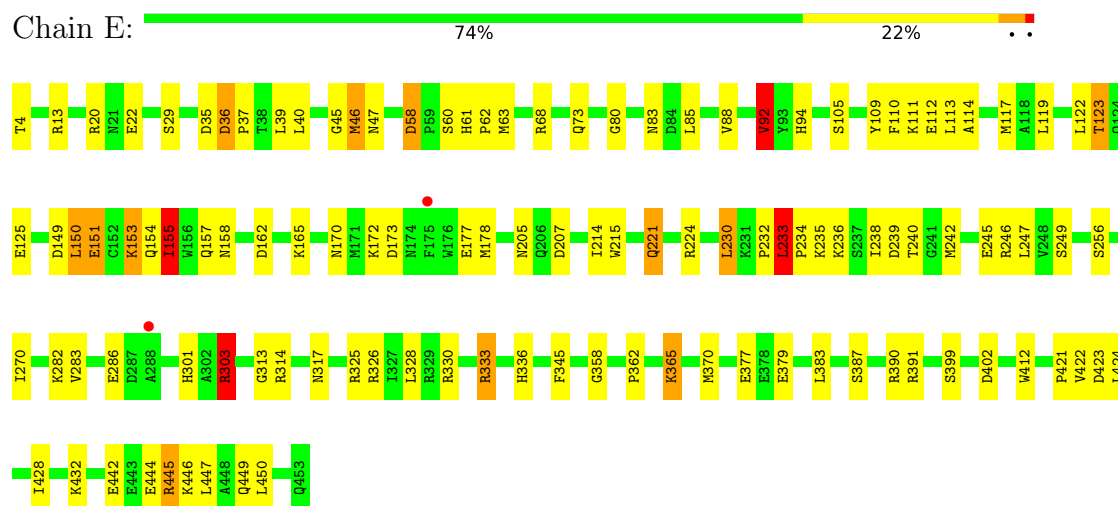




• Molecule 1: Alanine-tRNA ligase, cytoplasmic

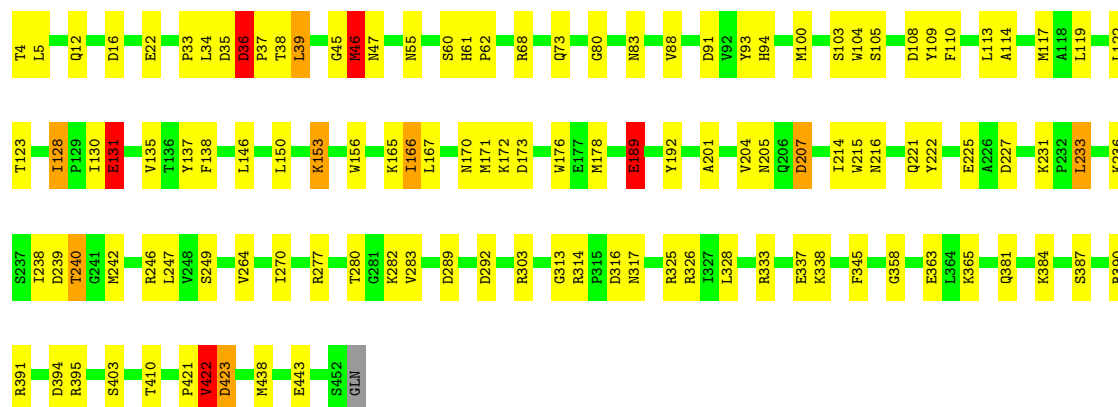


• Molecule 1: Alanine-tRNA ligase, cytoplasmic

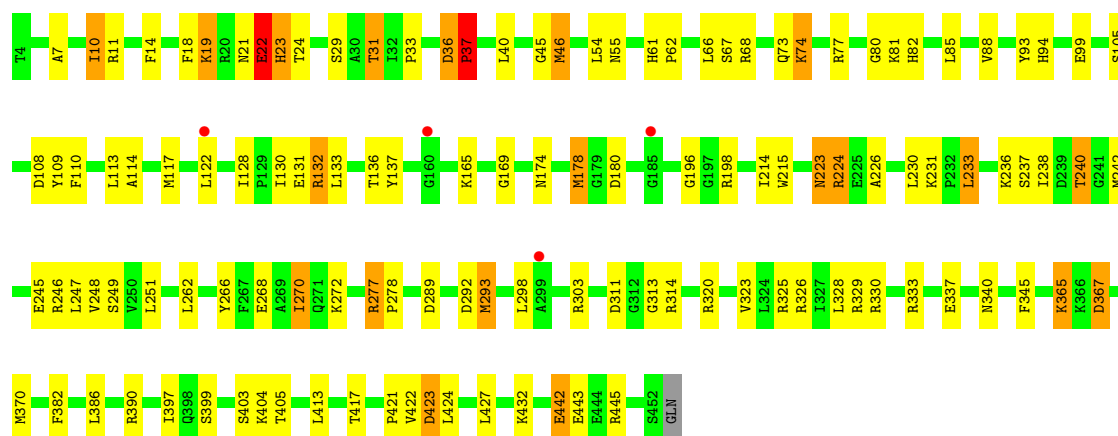
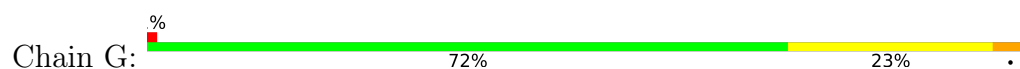


• Molecule 1: Alanine-tRNA ligase, cytoplasmic

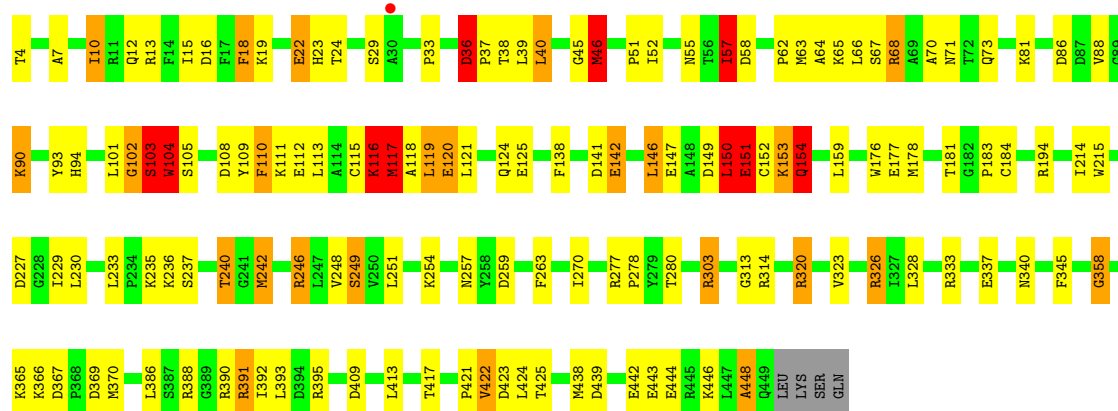




- Molecule 1: Alanine-tRNA ligase, cytoplasmic



- Molecule 1: Alanine-tRNA ligase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.17Å 98.26Å 201.38Å 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) 99.3 (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 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.216 , 0.254 0.284 , 0.317	Depositor DCC
R_{free} test set	5439 reflections (4.82%)	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)	0.33 , 42.3	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	0.91	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.*

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: 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	0.97	0/3635	1.13	9/4915 (0.2%)
1	B	0.97	3/3635 (0.1%)	1.16	14/4915 (0.3%)
1	C	1.07	12/3589 (0.3%)	1.26	28/4854 (0.6%)
1	D	1.04	11/3611 (0.3%)	1.27	30/4884 (0.6%)
1	E	0.99	3/3635 (0.1%)	1.16	14/4915 (0.3%)
1	F	1.01	3/3626 (0.1%)	1.15	14/4903 (0.3%)
1	G	1.05	8/3626 (0.2%)	1.26	21/4903 (0.4%)
1	H	1.15	18/3603 (0.5%)	1.35	40/4873 (0.8%)
All	All	1.03	58/28960 (0.2%)	1.22	170/39162 (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	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 (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	151	GLU	C-O	-16.17	1.08	1.24
1	H	104	TRP	CA-C	9.61	1.65	1.52
1	H	117	MET	CA-C	9.33	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	ASP	CG-OD2	-8.89	1.08	1.25
1	H	101	LEU	C-O	-8.74	1.13	1.24
1	D	366	LYS	CA-CB	7.82	1.65	1.53
1	H	103	SER	N-CA	7.74	1.56	1.46
1	D	22	GLU	CA-C	7.50	1.62	1.52
1	H	151	GLU	N-CA	-7.14	1.38	1.46
1	C	117	MET	C-O	-7.11	1.14	1.24
1	H	115	CYS	C-O	6.93	1.32	1.24
1	C	21	ASN	CA-CB	6.76	1.64	1.53
1	C	21	ASN	CA-C	6.70	1.61	1.52
1	G	443	GLU	CA-CB	6.67	1.63	1.53
1	C	21	ASN	C-O	6.57	1.32	1.24
1	H	142	GLU	N-CA	6.56	1.54	1.46
1	D	277	ARG	C-O	-6.47	1.16	1.24
1	H	102	GLY	N-CA	6.46	1.54	1.45
1	C	22	GLU	CA-C	6.28	1.61	1.52
1	B	48	GLN	CA-CB	6.28	1.64	1.53
1	H	119	LEU	C-O	-6.23	1.16	1.24
1	H	57	ILE	CA-CB	6.22	1.60	1.54
1	D	23	HIS	N-CA	6.18	1.53	1.46
1	C	171	MET	CA-CB	6.15	1.62	1.53
1	G	22	GLU	C-O	6.10	1.31	1.24
1	G	443	GLU	C-O	6.03	1.31	1.24
1	D	390	ARG	CD-NE	5.99	1.54	1.46
1	D	446	LYS	CA-CB	5.98	1.62	1.53
1	H	118	ALA	N-CA	5.95	1.54	1.46
1	G	22	GLU	CA-C	5.92	1.60	1.52
1	G	224	ARG	C-O	-5.91	1.16	1.24
1	H	151	GLU	CA-C	-5.90	1.44	1.52
1	C	443	GLU	C-O	-5.87	1.16	1.24
1	H	443	GLU	C-O	-5.66	1.16	1.24
1	G	442	GLU	C-O	-5.63	1.16	1.24
1	D	366	LYS	N-CA	5.57	1.52	1.46
1	H	154	GLN	CA-C	5.50	1.59	1.52
1	D	22	GLU	N-CA	5.48	1.53	1.46
1	C	19	LYS	CA-CB	5.35	1.61	1.53
1	G	365	LYS	CA-C	5.34	1.58	1.53
1	F	166	ILE	N-CA	-5.33	1.39	1.46
1	F	264	VAL	CA-CB	5.32	1.57	1.53
1	D	22	GLU	CA-CB	5.27	1.62	1.53
1	H	392	ILE	C-O	-5.26	1.18	1.24
1	C	272	LYS	CA-CB	5.24	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	242	MET	SD-CE	-5.23	1.66	1.79
1	H	242	MET	SD-CE	-5.15	1.66	1.79
1	D	306	THR	C-O	-5.14	1.18	1.24
1	C	396	LYS	C-O	-5.14	1.18	1.24
1	E	46	MET	CG-SD	-5.12	1.68	1.80
1	D	158	ASN	CA-CB	5.09	1.62	1.53
1	B	128	ILE	CA-CB	5.08	1.60	1.54
1	F	33	PRO	CA-C	5.07	1.57	1.52
1	C	158	ASN	N-CA	5.06	1.52	1.46
1	E	333	ARG	CD-NE	-5.06	1.39	1.46
1	H	446	LYS	CA-CB	5.04	1.61	1.53
1	E	37	PRO	C-O	-5.03	1.17	1.24
1	G	23	HIS	N-CA	5.01	1.52	1.46

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	88	VAL	N-CA-C	18.31	128.00	110.42
1	B	277	ARG	CB-CA-C	11.16	122.57	109.85
1	H	103	SER	N-CA-C	10.67	133.53	110.80
1	G	130	ILE	CA-CB-CG2	10.01	127.52	110.50
1	H	151	GLU	CA-C-O	-9.93	110.64	119.97
1	F	166	ILE	N-CA-CB	-9.67	99.39	110.99
1	B	48	GLN	CB-CG-CD	9.57	128.87	112.60
1	H	90	LYS	CB-CG-CD	9.57	133.31	111.30
1	H	102	GLY	N-CA-C	9.40	135.46	113.18
1	H	18	PHE	N-CA-C	9.38	122.70	111.82
1	H	66	LEU	N-CA-C	9.34	124.00	109.52
1	A	221	GLN	N-CA-CB	-9.12	97.82	110.95
1	D	22	GLU	N-CA-C	8.96	129.88	110.80
1	G	367	ASP	CA-C-N	-8.86	109.80	119.19
1	G	367	ASP	C-N-CA	-8.86	109.80	119.19
1	H	391	ARG	CA-CB-CG	8.67	131.44	114.10
1	C	23	HIS	N-CA-C	8.65	123.94	109.76
1	B	277	ARG	CA-C-N	8.15	130.03	119.84
1	B	277	ARG	C-N-CA	8.15	130.03	119.84
1	D	358	GLY	N-CA-C	7.93	122.51	112.83
1	D	366	LYS	N-CA-C	-7.93	102.33	110.97
1	H	104	TRP	N-CA-C	7.88	127.59	110.80
1	E	303	ARG	CG-CD-NE	-7.88	94.66	112.00
1	H	150	LEU	N-CA-C	7.85	121.29	112.97
1	G	54	LEU	N-CA-C	7.83	121.64	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	22	GLU	N-CA-C	7.80	122.14	112.47
1	G	325	ARG	CG-CD-NE	7.79	129.15	112.00
1	H	68	ARG	N-CA-C	7.78	121.91	108.76
1	E	153	LYS	N-CA-CB	7.73	121.48	110.12
1	H	448	ALA	N-CA-C	7.58	119.55	111.28
1	G	270	ILE	CA-CB-CG1	7.40	122.98	110.40
1	B	274	THR	CB-CA-C	-7.26	99.26	111.02
1	C	22	GLU	N-CA-C	7.14	126.00	110.80
1	H	46	MET	N-CA-C	7.11	119.89	111.71
1	D	388	ARG	N-CA-CB	7.09	120.30	110.01
1	H	46	MET	CB-CG-SD	7.08	133.93	112.70
1	E	365	LYS	CD-CE-NZ	-7.07	89.27	111.90
1	F	130	ILE	N-CA-C	7.02	119.87	111.09
1	D	427	LEU	CB-CA-C	-7.00	99.61	110.81
1	C	92	VAL	N-CA-CB	-6.96	101.50	112.07
1	D	46	MET	N-CA-C	6.95	119.70	111.71
1	H	57	ILE	CA-CB-CG2	6.94	122.30	110.50
1	D	365	LYS	CA-C-N	6.93	129.81	120.65
1	D	365	LYS	C-N-CA	6.93	129.81	120.65
1	D	10	ILE	CA-CB-CG2	6.92	122.27	110.50
1	F	131	GLU	CB-CA-C	6.91	122.26	111.13
1	D	270	ILE	CA-CB-CG1	6.91	122.15	110.40
1	G	293	MET	CB-CA-C	-6.89	100.06	110.88
1	H	115	CYS	CA-C-O	-6.89	112.05	119.97
1	F	46	MET	N-CA-C	6.88	119.63	111.71
1	C	149	ASP	CA-CB-CG	-6.82	105.78	112.60
1	E	379	GLU	N-CA-CB	6.81	119.95	110.07
1	C	36	ASP	C-N-CD	-6.80	105.64	120.60
1	F	130	ILE	CA-C-N	-6.78	112.49	122.86
1	F	130	ILE	C-N-CA	-6.78	112.49	122.86
1	G	22	GLU	N-CA-C	6.75	125.18	110.80
1	H	150	LEU	CB-CA-C	-6.74	100.86	111.17
1	D	390	ARG	CD-NE-CZ	6.73	133.82	124.40
1	B	157	GLN	N-CA-CB	6.73	120.01	110.12
1	F	39	LEU	N-CA-C	6.68	119.80	108.90
1	H	152	CYS	N-CA-C	-6.66	104.09	111.82
1	D	92	VAL	N-CA-CB	-6.65	101.96	112.07
1	B	92	VAL	N-CA-CB	-6.64	101.98	112.07
1	H	118	ALA	N-CA-C	-6.64	104.90	112.87
1	D	124	GLN	N-CA-CB	6.63	120.46	110.19
1	H	391	ARG	CB-CA-C	-6.62	99.60	110.85
1	C	439	ASP	N-CA-CB	6.52	119.70	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	153	LYS	CG-CD-CE	6.42	126.07	111.30
1	H	117	MET	CA-CB-CG	6.39	126.88	114.10
1	B	236	LYS	N-CA-CB	-6.38	100.55	110.57
1	G	329	ARG	CD-NE-CZ	6.38	133.33	124.40
1	C	47	ASN	N-CA-C	6.34	118.19	111.28
1	G	37	PRO	N-CA-C	6.32	125.49	112.47
1	G	365	LYS	N-CA-CB	-6.27	103.33	110.35
1	C	64	ALA	N-CA-C	-6.26	104.74	112.38
1	H	395	ARG	N-CA-CB	6.25	119.97	110.28
1	C	46	MET	N-CA-C	6.23	118.88	111.71
1	G	223	ASN	N-CA-CB	-6.22	100.04	110.80
1	E	92	VAL	N-CA-CB	-6.21	102.62	112.07
1	E	58	ASP	CA-C-N	6.17	125.85	119.56
1	E	58	ASP	C-N-CA	6.17	125.85	119.56
1	A	445	ARG	CG-CD-NE	6.16	125.55	112.00
1	H	151	GLU	O-C-N	6.12	128.61	122.30
1	C	21	ASN	CA-C-N	6.12	133.23	121.54
1	C	21	ASN	C-N-CA	6.12	133.23	121.54
1	D	270	ILE	CB-CA-C	-6.10	104.17	111.97
1	H	246	ARG	N-CA-CB	-6.10	101.14	110.16
1	H	121	LEU	N-CA-C	-6.09	104.56	111.14
1	B	291	ILE	N-CA-C	6.08	116.86	110.72
1	B	277	ARG	N-CA-C	6.04	118.21	109.04
1	D	157	GLN	N-CA-C	6.03	117.54	110.97
1	C	47	ASN	CA-CB-CG	-5.99	106.61	112.60
1	A	154	GLN	CA-CB-CG	5.97	126.03	114.10
1	A	303	ARG	NE-CZ-NH2	5.95	124.56	119.20
1	E	155	ILE	CB-CG1-CD1	5.93	126.26	113.80
1	G	23	HIS	N-CA-C	5.91	119.54	110.20
1	E	46	MET	N-CA-C	5.91	118.50	111.71
1	G	21	ASN	N-CA-C	-5.91	103.21	110.65
1	A	46	MET	N-CA-C	5.87	118.46	111.71
1	H	358	GLY	N-CA-C	5.81	119.70	112.73
1	C	157	GLN	N-CA-CB	5.80	118.39	109.98
1	C	390	ARG	CD-NE-CZ	5.80	132.52	124.40
1	E	303	ARG	CB-CA-C	5.79	120.69	110.85
1	B	236	LYS	CA-CB-CG	5.78	125.67	114.10
1	E	233	LEU	CB-CA-C	5.77	116.66	108.76
1	B	242	MET	CG-SD-CE	5.76	113.57	100.90
1	H	242	MET	CG-SD-CE	5.71	113.47	100.90
1	D	370	MET	CB-CG-SD	5.71	129.82	112.70
1	C	18	PHE	N-CA-C	5.66	119.44	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	THR	N-CA-CB	5.61	119.83	110.85
1	D	226	ALA	N-CA-C	5.57	117.35	111.28
1	F	189	GLU	CA-CB-CG	5.57	125.25	114.10
1	C	149	ASP	OD1-CG-OD2	-5.57	109.53	122.90
1	D	366	LYS	CA-C-O	5.52	126.80	121.00
1	C	55	ASN	CA-C-O	5.51	126.49	119.16
1	C	21	ASN	N-CA-C	-5.51	99.07	110.80
1	F	303	ARG	CG-CD-NE	5.47	124.05	112.00
1	E	230	LEU	CB-CG-CD1	5.45	127.06	110.70
1	C	68	ARG	CB-CA-C	5.44	119.17	109.65
1	H	103	SER	CB-CA-C	-5.44	99.60	110.42
1	H	117	MET	N-CA-C	5.44	119.11	108.18
1	G	231	LYS	CB-CA-C	5.43	116.91	108.61
1	H	68	ARG	N-CA-CB	-5.42	101.42	110.80
1	H	55	ASN	CB-CA-C	5.42	120.19	111.36
1	H	58	ASP	CA-C-N	5.41	125.08	119.56
1	H	58	ASP	C-N-CA	5.41	125.08	119.56
1	D	18	PHE	N-CA-C	5.41	119.14	112.54
1	H	116	LYS	CB-CG-CD	5.40	123.73	111.30
1	H	320	ARG	CD-NE-CZ	-5.39	116.86	124.40
1	D	113	LEU	N-CA-C	5.38	119.95	112.90
1	H	57	ILE	CB-CA-C	-5.37	104.31	111.13
1	C	272	LYS	CA-CB-CG	-5.37	103.37	114.10
1	C	318	THR	CA-CB-CG2	5.35	119.59	110.50
1	F	153	LYS	CA-CB-CG	-5.34	103.41	114.10
1	D	444	GLU	N-CA-CB	5.33	118.33	110.33
1	A	170	ASN	N-CA-CB	-5.32	103.10	110.38
1	C	19	LYS	CB-CG-CD	5.31	123.52	111.30
1	E	449	GLN	N-CA-C	5.30	117.06	111.28
1	B	410	THR	N-CA-CB	5.29	117.99	110.16
1	D	20	ARG	N-CA-C	-5.28	105.64	111.71
1	F	422	VAL	CB-CA-C	-5.27	103.72	112.26
1	G	46	MET	N-CA-C	5.26	117.76	111.71
1	C	65	LYS	CA-CB-CG	5.23	124.57	114.10
1	F	128	ILE	CB-CA-C	-5.23	105.24	110.89
1	A	452	SER	N-CA-C	-5.23	106.74	113.01
1	D	146	LEU	CB-CG-CD1	5.22	126.35	110.70
1	C	55	ASN	N-CA-CB	-5.21	105.99	113.65
1	D	58	ASP	CA-C-N	5.20	124.87	119.56
1	D	58	ASP	C-N-CA	5.20	124.87	119.56
1	G	226	ALA	N-CA-C	5.20	117.62	111.33
1	F	410	THR	N-CA-CB	5.20	117.85	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	303	ARG	CD-NE-CZ	5.19	131.67	124.40
1	H	110	PHE	CB-CA-C	5.19	120.75	110.42
1	D	113	LEU	N-CA-CB	-5.19	102.55	110.33
1	C	149	ASP	CB-CG-OD1	5.18	130.31	118.40
1	B	230	LEU	CA-CB-CG	-5.17	98.22	116.30
1	H	55	ASN	N-CA-CB	-5.16	104.41	112.41
1	C	410	THR	N-CA-CB	5.15	117.69	110.12
1	D	171	MET	CG-SD-CE	5.15	112.23	100.90
1	C	320	ARG	CG-CD-NE	-5.12	100.75	112.00
1	G	132	ARG	CB-CG-CD	5.11	123.05	111.30
1	E	402	ASP	CB-CG-OD2	-5.09	106.70	118.40
1	D	56	THR	N-CA-C	-5.06	106.88	113.16
1	D	23	HIS	N-CA-C	5.06	117.49	109.24
1	C	422	VAL	CB-CA-C	-5.05	104.07	112.26
1	G	293	MET	CA-CB-CG	5.04	124.19	114.10
1	G	277	ARG	CG-CD-NE	-5.03	100.94	112.00
1	A	395	ARG	N-CA-CB	5.02	118.06	110.28
1	D	422	VAL	CB-CA-C	-5.01	104.14	112.26
1	H	10	ILE	N-CA-CB	-5.00	103.74	110.54

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	61	1
1	B	3560	0	3499	94	0
1	C	3514	0	3449	136	0
1	D	3536	0	3473	87	1
1	E	3560	0	3499	85	2
1	F	3551	0	3491	90	2
1	G	3551	0	3491	96	1
1	H	3528	0	3462	122	1
2	A	28	0	19	1	0
2	B	28	0	19	1	0
2	C	28	0	19	2	0
2	D	28	0	19	2	0
2	E	28	0	19	2	0
2	F	28	0	19	1	0
2	G	28	0	19	0	0
2	H	28	0	19	0	0
All	All	28584	0	28015	748	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 13.

All (748) 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:100:MET:HE2	2:C:500:A5A:H5'2	1.46	0.98
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:10:ILE:CD1	1:H:251:LEU:HD12	2.06	0.80
1:H:113:LEU:HA	1:H:116:LYS:HB2	1.62	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
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:C:242:MET:CE	1:C:247:LEU:HD12	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD21	1:C:323:VAL:HG21	1.67	0.76
1:C:279:TYR:HB2	1:C:295:TYR:CD2	2.21	0.76
1:G:113:LEU:HD23	1:G:117:MET:HE2	1.68	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:C:137:TYR:C	1:C:174:ASN:HD22	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:146:LEU:HD12	1:F:171:MET:HE1	1.75	0.69
1:A:337:GLU:OE1	1:A:390:ARG:NH1	2.26	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:33:PRO:HB2	1:C:36:ASP:OD2	1.93	0.68
1:C:279:TYR:HB2	1:C:295:TYR:CE2	2.28	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:C:19:LYS:HG2	1:C:23:HIS:C	2.18	0.67
1:H:19:LYS:HB2	1:H:23:HIS:O	1.95	0.67
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:E:173:ASP:CG	1:E:205:ASN:HD21	2.04	0.66
1:G:85:LEU:HD11	1:G:330:ARG:NH1	2.11	0.66
1:G:85:LEU:HD11	1:G:330:ARG:HH12	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:173:ASP:CG	1:C:205:ASN:HD21	2.05	0.65
1:H:40:LEU:O	1:H:320:ARG:CZ	2.44	0.65
1:C:19:LYS:HG2	1:C:23:HIS:O	1.97	0.65
1:C:113:LEU:O	1:C:117:MET:HG2	1.96	0.65
1:G:68:ARG:NH1	1:G:68:ARG:HB2	2.12	0.65
1:A:277:ARG:HH22	1:A:289:ASP:CG	2.05	0.65
1:G:133:LEU:O	1:G:165:LYS:NZ	2.20	0.65
1:E:221:GLN:HG3	1:E:221:GLN:O	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:HB2	1:G:68:ARG:HH11	1.62	0.64
1:C:385:THR:HG21	1:C:418:TYR:C	2.22	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:N	1:A:289:ASP:OD1	2.30	0.64
1:B:100:MET:HE2	2:B:500:A5A:H5'1	1.80	0.64
1:B:119:LEU:O	1:B:123:THR:OG1	2.15	0.64
1:D:100:MET:HE2	2:D:500:A5A:H5'1	1.78	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:C:351:ASP:OD2	1:E:232:PRO:CD	2.47	0.63
1:D:19:LYS:HB2	1:D:23:HIS:O	1.99	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
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:F:189:GLU:CD	1:F:216:ASN:HD22	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:173:ASP:CG	1:A:205:ASN:HD21	2.08	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: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:HG3	1:D:444:GLU:O	2.01	0.60
1:H:111:LYS:NZ	1:H:149:ASP:OD1	2.34	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:C:214:ILE:HG22	1:C:242:MET:HE3	1.83	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:HD22	1:D:47:ASN:H	1.48	0.60
1:C:277:ARG:HH21	1:C:280:THR:CG2	2.15	0.59
1:F:122:LEU:C	1:F:128:ILE:HG22	2.26	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:HA	1.83	0.59
1:A:326:ARG:NE	1:A:423:ASP:OD2	2.35	0.59
1:H:19:LYS:HA	1:H:23:HIS:N	2.17	0.59
1:H:102:GLY:O	1:H:104:TRP:CE3	2.55	0.59
1:H:227:ASP:OD2	1:H:229:ILE:HD12	2.01	0.59
1:A:317:ASN:OD1	1:A:325:ARG:NH2	2.35	0.59
1:E:214:ILE:HG22	1:E:242:MET:HE3	1.84	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:F:173:ASP:CG	1:F:205:ASN:HD21	2.10	0.58
1:C:15:ILE:HG13	1:C:16:ASP:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:214:ILE:HG22	1:F:242:MET:HE3	1.84	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:C:242:MET:HE2	1:C:247:LEU:HD12	1.85	0.57
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:D:46:MET:HE3	1:D:176:TRP:CZ3	2.40	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:D:214:ILE:HG22	1:D:242:MET:HE3	1.86	0.57
1:C:323:VAL:HG22	1:C:326:ARG:HH21	1.69	0.57
1:E:444:GLU:OE1	1:E:444:GLU:C	2.48	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:G:214:ILE:HG22	1:G:242:MET:HE3	1.86	0.56
1:C:122:LEU:HD21	1:C:242:MET:HE1	1.86	0.56
1:A:333:ARG:HD3	1:A:424:LEU:HD11	1.86	0.56
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:E:214:ILE:CG2	1:E:242:MET:HE3	2.36	0.56
1:F:326:ARG:NE	1:F:423:ASP:OD2	2.38	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:61:HIS:HA	1:G:340:ASN:ND2	2.18	0.56
1:E:362:PRO:HA	1:E:365:LYS:NZ	2.21	0.56
1:F:214:ILE:CG2	1:F:242:MET:HE3	2.36	0.56
1:G:424:LEU:HA	1:G:427:LEU:HG	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:GLU:HB2	1:D:68:ARG:HD2	1.88	0.56
1:C:214:ILE:CG2	1:C:242:MET:HE3	2.35	0.56
1:F:46:MET:HE3	1:F:176:TRP:CZ3	2.41	0.56
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:B:122:LEU:C	1:B:128:ILE:HG13	2.31	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:A:46:MET:HE3	1:A:176:TRP:CZ3	2.41	0.55
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:C:22:GLU:C	1:C:68:ARG:HD2	2.31	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:D:122:LEU:HD21	1:D:242:MET:HE1	1.88	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: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:46:MET:HG3	1:D:47:ASN:N	2.23	0.54
1:D:333:ARG:NH1	1:D:337:GLU:OE1	2.40	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:F:122:LEU:HD21	1:F:242:MET:HE1	1.88	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:A:110:PHE:C	1:A:238:ILE:HD11	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:214:ILE:CG2	1:G:242:MET:HE3	2.38	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
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:153:LYS:HD2	1:H:153:LYS:C	2.33	0.53
1:H:409:ASP:OD1	1:H:444:GLU:CG	2.54	0.53
1:B:55:ASN:ND2	1:E:158:ASN:OD1	2.41	0.53
1:D:214:ILE:CG2	1:D:242:MET:HE3	2.37	0.53
1:D:328:LEU:CD2	1:D:378:GLU:HB3	2.39	0.53
1:B:422:VAL:HG11	1:B:438:MET:HE1	1.90	0.53
1:D:110:PHE:HD2	1:D:111:LYS:HG2	1.74	0.53
1:E:122:LEU:HD21	1:E:242:MET:HE1	1.88	0.53
1:F:153:LYS:HZ2	1:F:156:TRP:CD1	2.27	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:D:246:ARG:O	1:D:249:SER:OG	2.18	0.53
1:H:86:ASP:O	1:H:90:LYS:HD3	2.08	0.53
1:H:117:MET:C	1:H:119:LEU:H	2.16	0.53
1:F:22:GLU:OE1	1:F:68:ARG:NH1	2.42	0.53
1:F:172:LYS:HG3	1:F:173:ASP:N	2.23	0.53
1:G:122:LEU:HD21	1:G:242:MET:HE1	1.90	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:61:HIS:CA	1:H:340:ASN:HD21	2.23	0.52
1:F:105:SER:HB2	1:F:109:TYR:CE2	2.45	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:A:173:ASP:OD2	1:A:205:ASN:ND2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:G:46:MET:CE	1:G:178:MET:HE2	2.41	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:F:61:HIS:HA	1:H:340:ASN:ND2	2.24	0.51
1:H:117:MET:HB3	1:H:120:GLU:CB	2.38	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:H:102:GLY:C	1:H:104:TRP:CZ3	2.88	0.51
1:C:413:LEU:O	1:C:417:THR:OG1	2.28	0.51
1:G:236:LYS:HD3	1:G:236:LYS:N	2.26	0.50
1:A:422:VAL:HG11	1:A:438:MET:HE1	1.93	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:HD3	1:D:236:LYS:N	2.25	0.50
1:F:222:TYR:C	1:F:233:LEU:HD13	2.35	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:G:132:ARG:HH21	1:G:196:GLY:HA3	1.77	0.50
1:H:413:LEU:O	1:H:417:THR:OG1	2.29	0.50
1:E:412:TRP:CG	1:E:444:GLU:OE1	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:GLY:O	1:F:314:ARG:NH1	2.43	0.50
1:G:403:SER:C	1:G:404:LYS:HD3	2.37	0.50
1:C:12:GLN:O	1:C:15:ILE:HG13	2.11	0.50
1:C:223:ASN:CG	1:C:233:LEU:HD21	2.37	0.50
1:D:45:GLY:HA2	1:D:73:GLN:HG2	1.94	0.50
1:D:222:TYR:CD1	1:D:230:LEU:HD13	2.46	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:E:446:LYS:HZ2	1:E:450:LEU:HD11	1.76	0.50
1:G:413:LEU:O	1:G:417:THR:OG1	2.30	0.50
1:H:33:PRO:HD2	1:H:320:ARG:CZ	2.41	0.50
1:F:110:PHE:C	1:F:238:ILE:HD11	2.37	0.50
1:G:110:PHE:C	1:G:238:ILE:HD11	2.36	0.50
1:C:47:ASN:OD1	1:C:178:MET:SD	2.70	0.50
1:G:46:MET:SD	1:G:178:MET:HE2	2.52	0.50
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: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:A:46:MET:HG3	1:A:47:ASN:N	2.26	0.49
1:B:110:PHE:C	1:B:238:ILE:HD11	2.37	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:HD13	1:G:128:ILE:HA	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:H:422:VAL:HG11	1:H:438:MET:HE1	1.95	0.49
1:A:214:ILE:O	1:A:242:MET:HG3	2.13	0.48
1:B:128:ILE:HD12	1:B:128:ILE:C	2.38	0.48
1:A:61:HIS:ND1	1:A:62:PRO:HD2	2.28	0.48
1:D:171:MET:HE3	1:D:175:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:61:HIS:CA	1:D:340:ASN:HD21	2.23	0.48
1:B:104:TRP:CD1	1:B:239:ASP:HA	2.47	0.48
1:H:102:GLY:O	1:H:104:TRP:CE2	2.66	0.48
1:H:146:LEU:HD12	1:H:146:LEU:C	2.39	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:D:122:LEU:CD2	1:D:242:MET:HE1	2.44	0.48
1:F:422:VAL:HG11	1:F:438:MET:HE1	1.95	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:C:337:GLU:CD	1:C:390:ARG:HH11	2.22	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
1:E:122:LEU:CD2	1:E:242:MET:HE1	2.44	0.48
1:G:85:LEU:CG	1:G:330:ARG:HH12	2.27	0.48
1:H:117:MET:C	1:H:119:LEU:N	2.71	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:C:422:VAL:HG11	1:C:438:MET:HE1	1.95	0.48
1:D:27:HIS:CD2	1:D:28:SER:H	2.32	0.48
1:F:35:ASP:CG	1:H:278:PRO:HD2	2.39	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:E:110:PHE:C	1:E:238:ILE:HD11	2.39	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:F:122:LEU:CD2	1:F:242:MET:HE1	2.44	0.47
1:A:381:GLN:OE1	1:A:384:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:422:VAL:HG11	1:D:438:MET:HE1	1.96	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:A:444:GLU:HA	1:A:447:LEU:HG	1.97	0.47
1:B:162:ASP:OD2	1:B:164:THR:OG1	2.24	0.47
1:B:223:ASN:HB3	1:B:231:LYS:HG2	1.96	0.47
1:C:122:LEU:CD2	1:C:242:MET:HE1	2.44	0.47
1:C:318:THR:HG23	1:C:318:THR:O	2.15	0.47
1:C:437:ASP:OD1	1:C:439:ASP:OD1	2.32	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: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: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: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
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:C:63:MET:C	1:C:65:LYS:N	2.71	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:C:316:ASP:CG	1:C:318:THR:HG22	2.41	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:61:HIS:ND1	1:C:62:PRO:HD2	2.31	0.46
1:C:384:LYS:O	1:C:388:ARG:NH1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:THR:O	1:C:385:THR:CG2	2.64	0.46
1:C:390:ARG:HA	1:C:390:ARG:HD2	1.62	0.46
1:G:80:GLY:HA2	1:G:81:LYS:C	2.40	0.46
1:G:169:GLY:HA3	1:G:174:ASN:ND2	2.30	0.46
1:H:23:HIS:CE1	1:H:68:ARG:HD2	2.50	0.46
1:H:214:ILE:O	1:H:242:MET:HG3	2.15	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:23:HIS:HA	1:H:68:ARG:HG2	1.97	0.46
1:H:138:PHE:CZ	1:H:146:LEU:HD22	2.50	0.46
1:E:35:ASP:CG	1:G:278:PRO:HD2	2.40	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:A:85:LEU:HD23	1:A:326:ARG:NH2	2.30	0.46
1:B:316:ASP:OD1	1:B:317:ASN:N	2.48	0.46
1:C:15:ILE:HG13	1:C:16:ASP:H	1.79	0.46
1:C:23:HIS:CE1	1:C:109:TYR:OH	2.69	0.46
1:G:326:ARG:HH21	1:G:330:ARG:HH22	1.63	0.46
1:G:330:ARG:HH21	1:G:423:ASP:HB2	1.81	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: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:G:122:LEU:CD2	1:G:242:MET:HE1	2.45	0.45
1:H:249:SER:OG	1:H:257:ASN:HA	2.16	0.45
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:C:277:ARG:HH12	1:C:289:ASP:CG	2.24	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:61:HIS:ND1	1:F:62:PRO:HD2	2.31	0.45
1:F:289:ASP:OD1	1:F:289:ASP:N	2.49	0.45
1:B:136:THR:OG1	1:B:189:GLU:HG3	2.15	0.45
1:C:111:LYS:NZ	1:C:149:ASP:CG	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:MET:CG	1:H:120:GLU:HB2	2.47	0.45
1:E:45:GLY:HA2	1:E:73:GLN:HG2	1.98	0.45
1:E:333:ARG:CD	1:E:424:LEU:HD11	2.46	0.45
1:H:444:GLU:O	1:H:448:ALA:N	2.48	0.45
1:F:138:PHE:HZ	1:F:171:MET:HE3	1.82	0.45
1:G:46:MET:HE1	1:G:178:MET:HE2	1.99	0.45
1:C:23:HIS:HD2	1:C:104:TRP:H	1.65	0.45
1:C:300:ASP:OD1	1:C:300:ASP:C	2.60	0.45
1:E:444:GLU:O	1:E:447:LEU:HB3	2.17	0.45
1:H:141:ASP:C	1:H:146:LEU:HD11	2.42	0.45
1:B:274:THR:O	1:B:274:THR:OG1	2.29	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:122:LEU:C	1:A:128:ILE:HG22	2.42	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: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:393:LEU:HD11	1:D:425:THR:HG23	1.99	0.44
1:D:422:VAL:HG21	1:D:441:PHE:CE2	2.52	0.44
1:G:277:ARG:NH2	1:G:292:ASP:CG	2.75	0.44
1:A:46:MET:HE3	1:A:176:TRP:HZ3	1.81	0.44
1:B:28:SER:CB	1:B:73:GLN:HA	2.48	0.44
1:B:289:ASP:OD1	1:B:289:ASP:N	2.48	0.44
1:C:14:PHE:CE2	1:C:101:LEU:HB3	2.53	0.44
1:F:135:VAL:HG23	1:F:153:LYS:HZ1	1.82	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:F:36:ASP:C	1:F:38:THR:H	2.15	0.44
1:C:277:ARG:NH1	1:C:289:ASP:CG	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:MET:HE3	1:D:176:TRP:HZ3	1.80	0.44
1:D:92:VAL:HG13	1:D:256:SER:HA	2.00	0.44
1:D:191:HIS:CD2	1:D:204:VAL:HG13	2.53	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: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: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:C:117:MET:HE2	1:C:117:MET:HB3	1.91	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:C:111:LYS:HZ3	1:C:149:ASP:CG	2.24	0.43
1:E:112:GLU:HG3	1:E:155:ILE:CD1	2.48	0.43
1:B:31:THR:HG21	1:B:308:ALA:HA	2.00	0.43
1:B:223:ASN:HD22	1:B:231:LYS:HE3	1.82	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:92:VAL:CG1	1:B:256:SER:HA	2.48	0.43
1:B:105:SER:HB2	1:B:109:TYR:CE2	2.52	0.43
1:F:45:GLY:HA2	1:F:73:GLN:HG2	2.00	0.43
1:F:46:MET:HE3	1:F:176:TRP:HZ3	1.79	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
1:E:40:LEU:HD12	1:E:40:LEU:HA	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:D:27:HIS:HD2	1:D:28:SER:H	1.64	0.43
1:E:370:MET:HE2	1:E:370:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:ASP:OD2	1:H:277:ARG:HA	2.18	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: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:A:111:LYS:NZ	1:A:149:ASP:OD1	2.52	0.42
1:A:451:LYS:C	1:A:453:GLN:H	2.27	0.42
1:C:22:GLU:H	1:C:22:GLU:HG3	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: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: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:H:150:LEU:HA	1:H:153:LYS:HB3	1.99	0.42
1:B:35:ASP:HB2	1:C:277:ARG:HB2	2.00	0.42
1:B:92:VAL:HG13	1:B:256:SER:HA	2.01	0.42
1:B:231:LYS:HD2	1:B:233:LEU:HD23	2.01	0.42
1:C:113:LEU:HD21	1:C:117:MET:HE1	2.00	0.42
1:F:131:GLU:HB3	1:F:165:LYS:HZ2	1.84	0.42
1:F:225:GLU:OE2	1:F:231:LYS:HB2	2.19	0.42
1:H:46:MET:HE3	1:H:183:PRO:HG2	2.01	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:36:ASP:C	1:H:38:THR:H	2.16	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
1:B:48:GLN:H	1:B:48:GLN:HG3	1.66	0.42
1:B:390:ARG:HH12	1:B:394:ASP:CG	2.22	0.42
1:C:204:VAL:O	1:C:205:ASN:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:LYS:NZ	1:E:450:LEU:HD11	2.35	0.42
1:G:22:GLU:C	1:G:68:ARG:NH1	2.78	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: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: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:E:242:MET:HE2	1:E:247:LEU:HD13	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:F:62:PRO:HD3	1:H:340: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: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: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:G:19:LYS:HD3	1:G:24:THR:HA	2.02	0.41
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:C:23:HIS:HB3	1:C:69:ALA:C	2.45	0.41
1:C:92:VAL:HG13	1:C:256:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:59:PRO:HG2	1:E:150:LEU:HB2	2.02	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:B:363:GLU:H	1:B:363:GLU:CD	2.29	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:E:85:LEU:HD23	1:E:326:ARG:NH2	2.36	0.41
1:F:131:GLU:HB3	1:F:165:LYS:NZ	2.35	0.41
1:G:242:MET:HE2	1:G:247:LEU:HD13	2.03	0.41
1:H:52:ILE:HD11	1:H:63:MET:HG2	2.02	0.41
1:A:109:TYR:CE1	1:A:238:ILE:HD12	2.56	0.41
1:C:381:GLN:OE1	1:C:384:LYS:NZ	2.49	0.41
1:F:100:MET:HE2	2:F:500:A5A:H5'1	2.01	0.41
1:F:113:LEU:O	1:F:117:MET:HG3	2.21	0.41
1:F:242:MET:HE2	1:F:247:LEU:HD13	2.02	0.41
1:A:113:LEU:O	1:A:117:MET:HG3	2.22	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:HH11	1:G:330:ARG:HD2	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:E:58:ASP:CG	1:E:60:SER:HG	2.29	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:97:PHE:CB	1:C:304:THR:HG22	2.52	0.40
1:C:301:HIS:O	1:C:304:THR:OG1	2.40	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:F:363:GLU:CD	1:F:363:GLU:H	2.28	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	43	65
1	B	448/450 (100%)	431 (96%)	12 (3%)	5 (1%)	11	26
1	C	442/450 (98%)	426 (96%)	12 (3%)	4 (1%)	14	31
1	D	445/450 (99%)	431 (97%)	14 (3%)	0	100	100
1	E	448/450 (100%)	436 (97%)	11 (2%)	1 (0%)	43	65
1	F	447/450 (99%)	434 (97%)	11 (2%)	2 (0%)	30	51
1	G	447/450 (99%)	429 (96%)	15 (3%)	3 (1%)	18	37
1	H	444/450 (99%)	421 (95%)	18 (4%)	5 (1%)	11	26
All	All	3569/3600 (99%)	3444 (96%)	104 (3%)	21 (1%)	21	41

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/379 (100%)	357 (94%)	22 (6%)	18	39
1	B	379/379 (100%)	354 (93%)	25 (7%)	15	33
1	C	374/379 (99%)	349 (93%)	25 (7%)	15	32
1	D	376/379 (99%)	349 (93%)	27 (7%)	13	29
1	E	379/379 (100%)	360 (95%)	19 (5%)	22	45
1	F	378/379 (100%)	359 (95%)	19 (5%)	22	45
1	G	378/379 (100%)	359 (95%)	19 (5%)	22	45
1	H	375/379 (99%)	347 (92%)	28 (8%)	12	28
All	All	3018/3032 (100%)	2834 (94%)	184 (6%)	17	37

All (184) 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	123	THR
1	A	131	GLU
1	A	147	GLU
1	A	178	MET
1	A	181	THR
1	A	283	VAL
1	A	355	GLN
1	A	395	ARG
1	A	402	ASP
1	A	403	SER
1	A	422	VAL
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	157	GLN
1	B	159	LEU
1	B	178	MET
1	B	181	THR
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	370	MET
1	B	399	SER
1	B	413	LEU
1	B	422	VAL

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Mol	Chain	Res	Type
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
1	C	66	LEU
1	C	81	LYS
1	C	88	VAL
1	C	92	VAL
1	C	113	LEU
1	C	125	GLU
1	C	150	LEU
1	C	154	GLN
1	C	178	MET
1	C	181	THR
1	C	227	ASP
1	C	240	THR
1	C	303	ARG
1	C	363	GLU
1	C	369	ASP
1	C	390	ARG
1	C	399	SER
1	C	422	VAL
1	C	423	ASP
1	C	443	GLU
1	D	4	THR
1	D	5	LEU
1	D	9	GLU
1	D	10	ILE
1	D	15	ILE
1	D	22	GLU
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

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Mol	Chain	Res	Type
1	D	181	THR
1	D	240	THR
1	D	282	LYS
1	D	283	VAL
1	D	303	ARG
1	D	306	THR
1	D	333	ARG
1	D	374	ILE
1	D	390	ARG
1	D	399	SER
1	D	422	VAL
1	D	423	ASP
1	E	4	THR
1	E	29	SER
1	E	46	MET
1	E	88	VAL
1	E	92	VAL
1	E	123	THR
1	E	150	LEU
1	E	151	GLU
1	E	155	ILE
1	E	178	MET
1	E	221	GLN
1	E	233	LEU
1	E	283	VAL
1	E	303	ARG
1	E	328	LEU
1	E	399	SER
1	E	422	VAL
1	E	423	ASP
1	E	445	ARG
1	F	39	LEU
1	F	46	MET
1	F	60	SER
1	F	88	VAL
1	F	108	ASP
1	F	131	GLU
1	F	150	LEU
1	F	178	MET
1	F	189	GLU
1	F	207	ASP
1	F	227	ASP

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Mol	Chain	Res	Type
1	F	233	LEU
1	F	240	THR
1	F	283	VAL
1	F	328	LEU
1	F	403	SER
1	F	422	VAL
1	F	423	ASP
1	F	443	GLU
1	G	10	ILE
1	G	19	LYS
1	G	29	SER
1	G	31	THR
1	G	55	ASN
1	G	66	LEU
1	G	74	LYS
1	G	131	GLU
1	G	178	MET
1	G	198	ARG
1	G	233	LEU
1	G	240	THR
1	G	293	MET
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
1	H	40	LEU
1	H	46	MET
1	H	57	ILE
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	178	MET
1	H	181	THR

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Mol	Chain	Res	Type
1	H	230	LEU
1	H	233	LEU
1	H	236	LYS
1	H	240	THR
1	H	249	SER
1	H	326	ARG
1	H	328	LEU
1	H	370	MET
1	H	386	LEU
1	H	422	VAL
1	H	423	ASP
1	H	439	ASP
1	H	442	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	221	GLN
1	B	47	ASN
1	B	48	GLN
1	B	221	GLN
1	B	257	ASN
1	C	174	ASN
1	C	205	ASN
1	C	223	ASN
1	C	336	HIS
1	D	27	HIS
1	D	157	GLN
1	D	174	ASN
1	D	191	HIS
1	D	210	ASN
1	D	257	ASN
1	D	340	ASN
1	E	94	HIS
1	E	154	GLN
1	E	210	ASN
1	E	257	ASN
1	E	301	HIS
1	F	221	GLN
1	F	223	ASN
1	F	257	ASN

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Mol	Chain	Res	Type
1	G	21	ASN
1	G	47	ASN
1	G	174	ASN
1	G	210	ASN
1	G	223	ASN
1	G	340	ASN
1	G	355	GLN
1	H	157	GLN
1	H	210	ASN
1	H	257	ASN
1	H	336	HIS
1	H	340	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	500	-	29,30,30	2.02	8 (27%)	42,45,45	2.37	13 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A5A	B	500	-	29,30,30	1.86	7 (24%)	42,45,45	2.86	16 (38%)
2	A5A	D	500	-	29,30,30	1.63	7 (24%)	42,45,45	2.86	19 (45%)
2	A5A	F	500	-	29,30,30	2.29	9 (31%)	42,45,45	2.58	16 (38%)
2	A5A	G	500	-	29,30,30	1.64	7 (24%)	42,45,45	2.40	13 (30%)
2	A5A	H	500	-	29,30,30	1.58	7 (24%)	42,45,45	2.28	11 (26%)
2	A5A	E	500	-	29,30,30	1.70	6 (20%)	42,45,45	2.80	13 (30%)
2	A5A	A	500	-	29,30,30	1.73	5 (17%)	42,45,45	3.28	16 (38%)

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	C	500	-	-	7/18/35/35	0/3/3/3
2	A5A	B	500	-	-	5/18/35/35	0/3/3/3
2	A5A	D	500	-	-	3/18/35/35	0/3/3/3
2	A5A	F	500	-	-	5/18/35/35	0/3/3/3
2	A5A	G	500	-	-	4/18/35/35	0/3/3/3
2	A5A	H	500	-	-	0/18/35/35	0/3/3/3
2	A5A	E	500	-	-	4/18/35/35	0/3/3/3
2	A5A	A	500	-	-	4/18/35/35	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	A5A	O1S-S	5.82	1.47	1.42
2	F	500	A5A	C5-C4	5.31	1.48	1.39
2	C	500	A5A	C5-C4	5.03	1.48	1.39
2	C	500	A5A	O5'-S	-4.75	1.50	1.60
2	F	500	A5A	O2S-S	4.67	1.46	1.42
2	B	500	A5A	O2S-S	4.61	1.46	1.42
2	A	500	A5A	O2S-S	4.59	1.46	1.42
2	B	500	A5A	O5'-S	-4.25	1.51	1.60
2	D	500	A5A	C5-C4	4.24	1.46	1.39
2	G	500	A5A	C5-C4	4.18	1.46	1.39
2	H	500	A5A	C5-C4	4.11	1.46	1.39
2	A	500	A5A	O5'-S	-4.08	1.51	1.60
2	E	500	A5A	C5-C4	3.95	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	A5A	C5-C4	3.81	1.45	1.39
2	F	500	A5A	O5'-S	-3.78	1.52	1.60
2	E	500	A5A	O2S-S	3.74	1.45	1.42
2	A	500	A5A	C5-C4	3.63	1.45	1.39
2	E	500	A5A	C5-C6	3.57	1.50	1.41
2	D	500	A5A	C5-C6	3.52	1.50	1.41
2	C	500	A5A	O1S-S	3.47	1.45	1.42
2	E	500	A5A	C4-N9	-3.42	1.30	1.37
2	C	500	A5A	O2S-S	3.11	1.45	1.42
2	G	500	A5A	C4-N9	-3.10	1.31	1.37
2	F	500	A5A	C8-N9	-3.05	1.32	1.37
2	D	500	A5A	O2S-S	3.04	1.45	1.42
2	C	500	A5A	C5-N7	-2.99	1.33	1.39
2	B	500	A5A	C5-C6	2.99	1.49	1.41
2	F	500	A5A	C5-N7	-2.88	1.33	1.39
2	C	500	A5A	S-N3S	2.81	1.64	1.59
2	A	500	A5A	C8-N7	2.72	1.36	1.31
2	H	500	A5A	C5-C6	2.72	1.48	1.41
2	G	500	A5A	O5'-S	-2.71	1.54	1.60
2	H	500	A5A	O5'-S	-2.70	1.54	1.60
2	E	500	A5A	O5'-S	-2.64	1.54	1.60
2	G	500	A5A	O2S-S	2.63	1.44	1.42
2	D	500	A5A	O5'-S	-2.58	1.54	1.60
2	G	500	A5A	C5-C6	2.55	1.48	1.41
2	A	500	A5A	C5-C6	2.55	1.48	1.41
2	B	500	A5A	C4-N9	-2.53	1.32	1.37
2	F	500	A5A	S-N3S	2.45	1.63	1.59
2	D	500	A5A	C4-N9	-2.42	1.32	1.37
2	H	500	A5A	O2S-S	2.38	1.44	1.42
2	G	500	A5A	C5-N7	-2.38	1.34	1.39
2	G	500	A5A	C8-N9	-2.37	1.33	1.37
2	H	500	A5A	C4-N9	-2.36	1.32	1.37
2	C	500	A5A	O5'-C5'	-2.32	1.37	1.46
2	H	500	A5A	C8-N9	-2.29	1.33	1.37
2	C	500	A5A	C5-C6	2.29	1.47	1.41
2	F	500	A5A	C4-N9	-2.28	1.32	1.37
2	D	500	A5A	S-N3S	2.14	1.63	1.59
2	E	500	A5A	O1S-S	2.12	1.44	1.42
2	H	500	A5A	C5-N7	-2.12	1.35	1.39
2	B	500	A5A	S-N3S	2.09	1.63	1.59
2	D	500	A5A	C8-N9	-2.07	1.34	1.37
2	B	500	A5A	C5-N7	-2.03	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	A5A	C5-C6	2.01	1.46	1.41

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	A5A	O2S-S-O1S	-14.09	99.75	120.85
2	E	500	A5A	O2S-S-O1S	-10.01	105.87	120.85
2	B	500	A5A	O2S-S-O1S	-9.42	106.74	120.85
2	D	500	A5A	O2S-S-O1S	-9.16	107.13	120.85
2	G	500	A5A	O2S-S-O1S	-8.26	108.48	120.85
2	C	500	A5A	O2S-S-O1S	-7.78	109.21	120.85
2	F	500	A5A	O2S-S-O1S	-6.47	111.16	120.85
2	A	500	A5A	C5-C4-N3	-6.41	117.90	126.72
2	H	500	A5A	O2S-S-O1S	-6.39	111.28	120.85
2	E	500	A5A	C5-C4-N3	-6.39	117.92	126.72
2	H	500	A5A	C5-C4-N3	-5.77	118.78	126.72
2	G	500	A5A	C5-C4-N3	-5.76	118.78	126.72
2	E	500	A5A	N3-C4-N9	5.72	136.89	127.17
2	A	500	A5A	N3-C4-N9	5.67	136.80	127.17
2	F	500	A5A	C5-C4-N3	-5.60	119.01	126.72
2	E	500	A5A	C4-N9-C8	5.45	111.46	105.74
2	C	500	A5A	C5-C4-N3	-5.40	119.28	126.72
2	D	500	A5A	C4-N9-C8	5.38	111.39	105.74
2	F	500	A5A	N3-C4-N9	5.38	136.32	127.17
2	B	500	A5A	C4-N9-C8	5.33	111.34	105.74
2	B	500	A5A	N3-C4-N9	5.27	136.13	127.17
2	B	500	A5A	C5-C4-N3	-5.20	119.55	126.72
2	D	500	A5A	C5-C4-N3	-5.18	119.58	126.72
2	G	500	A5A	N3-C4-N9	5.13	135.89	127.17
2	A	500	A5A	N3-C2-N1	-5.09	120.88	128.58
2	B	500	A5A	C2'-C1'-N9	-4.95	101.01	113.30
2	H	500	A5A	N3-C4-N9	4.89	135.48	127.17
2	F	500	A5A	C4-N9-C8	4.89	110.87	105.74
2	A	500	A5A	C4-N9-C8	4.83	110.81	105.74
2	D	500	A5A	N3-C4-N9	4.82	135.36	127.17
2	D	500	A5A	N3-C2-N1	-4.79	121.34	128.58
2	A	500	A5A	C2-N3-C4	4.74	123.41	111.83
2	C	500	A5A	N3-C4-N9	4.65	135.08	127.17
2	B	500	A5A	N3-C2-N1	-4.56	121.67	128.58
2	E	500	A5A	C2-N3-C4	4.46	122.73	111.83
2	D	500	A5A	C2-N3-C4	4.37	122.49	111.83
2	H	500	A5A	C4-N9-C8	4.34	110.29	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	A5A	C2'-C1'-N9	-4.26	102.72	113.30
2	B	500	A5A	C2-N3-C4	4.23	122.17	111.83
2	C	500	A5A	CA-C-N3S	4.22	123.63	114.46
2	F	500	A5A	C4-C5-N7	-4.16	105.82	110.58
2	F	500	A5A	C2'-C1'-N9	-4.16	102.98	113.30
2	H	500	A5A	C4-C5-N7	-4.12	105.87	110.58
2	D	500	A5A	C4-C5-N7	-3.94	106.08	110.58
2	D	500	A5A	C6-C5-N7	3.84	139.49	132.09
2	B	500	A5A	C2'-C3'-C4'	3.83	110.01	102.61
2	G	500	A5A	C4-N9-C8	3.74	109.66	105.74
2	H	500	A5A	C2-N3-C4	3.73	120.93	111.83
2	A	500	A5A	N9-C8-N7	-3.70	108.69	113.94
2	F	500	A5A	N3-C2-N1	-3.67	123.02	128.58
2	E	500	A5A	N9-C8-N7	-3.63	108.79	113.94
2	C	500	A5A	C4-C5-N7	-3.60	106.46	110.58
2	F	500	A5A	C2-N3-C4	3.56	120.53	111.83
2	A	500	A5A	C4-C5-N7	-3.52	106.56	110.58
2	F	500	A5A	C2'-C3'-C4'	3.52	109.41	102.61
2	D	500	A5A	CA-C-N3S	3.48	122.01	114.46
2	E	500	A5A	C4-C5-N7	-3.44	106.65	110.58
2	G	500	A5A	C2-N3-C4	3.44	120.23	111.83
2	B	500	A5A	N9-C8-N7	-3.43	109.06	113.94
2	F	500	A5A	C5-N7-C8	3.43	108.84	103.45
2	D	500	A5A	C2'-C1'-N9	-3.42	104.81	113.30
2	D	500	A5A	N9-C8-N7	-3.41	109.10	113.94
2	G	500	A5A	C4-C5-N7	-3.38	106.71	110.58
2	H	500	A5A	N3-C2-N1	-3.31	123.56	128.58
2	A	500	A5A	C5-N7-C8	3.30	108.64	103.45
2	H	500	A5A	C5-N7-C8	3.26	108.57	103.45
2	C	500	A5A	N3-C2-N1	-3.25	123.66	128.58
2	A	500	A5A	O5'-S-O1S	3.21	115.18	105.48
2	G	500	A5A	N3-C2-N1	-3.19	123.76	128.58
2	C	500	A5A	C5-N7-C8	3.18	108.45	103.45
2	G	500	A5A	C2'-C1'-N9	-3.17	105.44	113.30
2	B	500	A5A	C6-C5-N7	3.14	138.13	132.09
2	D	500	A5A	C5-N7-C8	3.13	108.38	103.45
2	B	500	A5A	C4-C5-N7	-3.13	107.01	110.58
2	C	500	A5A	C2-N3-C4	3.12	119.44	111.83
2	E	500	A5A	N3-C2-N1	-3.12	123.86	128.58
2	B	500	A5A	O-C-N3S	-3.10	117.36	122.98
2	H	500	A5A	N9-C8-N7	-3.09	109.55	113.94
2	B	500	A5A	C5-N7-C8	3.08	108.28	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	A5A	C6-C5-N7	3.07	138.01	132.09
2	C	500	A5A	C2-N1-C6	3.06	123.76	118.73
2	F	500	A5A	N9-C8-N7	-2.92	109.79	113.94
2	H	500	A5A	C6-C5-N7	2.92	137.72	132.09
2	H	500	A5A	C2'-C1'-N9	-2.90	106.11	113.30
2	E	500	A5A	C5-N7-C8	2.82	107.88	103.45
2	C	500	A5A	O5'-S-O1S	2.75	113.79	105.48
2	B	500	A5A	O5'-S-O2S	2.72	113.69	105.48
2	G	500	A5A	C6-C5-N7	2.64	137.19	132.09
2	F	500	A5A	C6-C5-N7	2.62	137.13	132.09
2	E	500	A5A	C6-C5-N7	2.60	137.10	132.09
2	D	500	A5A	O4'-C1'-N9	2.60	113.08	108.09
2	C	500	A5A	C4-N9-C8	2.51	108.38	105.74
2	F	500	A5A	O4'-C1'-C2'	2.50	111.96	106.62
2	G	500	A5A	O5'-S-O1S	2.49	113.02	105.48
2	D	500	A5A	O5'-S-N3S	2.48	112.12	105.69
2	D	500	A5A	C2-N1-C6	2.47	122.79	118.73
2	D	500	A5A	O5'-C5'-C4'	2.47	111.97	107.57
2	A	500	A5A	C2-N1-C6	2.46	122.78	118.73
2	D	500	A5A	C4-N9-C1'	-2.45	120.91	126.63
2	A	500	A5A	C2'-C3'-C4'	2.34	107.13	102.61
2	A	500	A5A	O4'-C4'-C3'	-2.32	100.54	105.15
2	A	500	A5A	O3'-C3'-C2'	-2.31	104.42	111.82
2	G	500	A5A	C5-N7-C8	2.30	107.06	103.45
2	B	500	A5A	O4'-C1'-C2'	2.19	111.29	106.62
2	E	500	A5A	O4'-C1'-N9	2.18	112.28	108.09
2	F	500	A5A	CA-C-N3S	2.16	119.15	114.46
2	G	500	A5A	CA-C-N3S	2.14	119.10	114.46
2	A	500	A5A	O5'-S-N3S	2.13	111.20	105.69
2	G	500	A5A	C5'-O5'-S	2.13	121.44	116.97
2	B	500	A5A	O-C-CA	2.07	125.13	120.56
2	C	500	A5A	O-C-CA	-2.06	116.02	120.56
2	E	500	A5A	C2'-C3'-C4'	2.04	106.55	102.61
2	D	500	A5A	C6-C5-C4	-2.04	114.39	117.18
2	D	500	A5A	O4'-C1'-C2'	2.03	110.97	106.62
2	C	500	A5A	N9-C8-N7	-2.02	111.07	113.94
2	F	500	A5A	C2-N1-C6	2.01	122.04	118.73
2	F	500	A5A	O-C-N3S	-2.01	119.33	122.98

There are no chirality outliers.

All (32) torsion outliers are listed below:

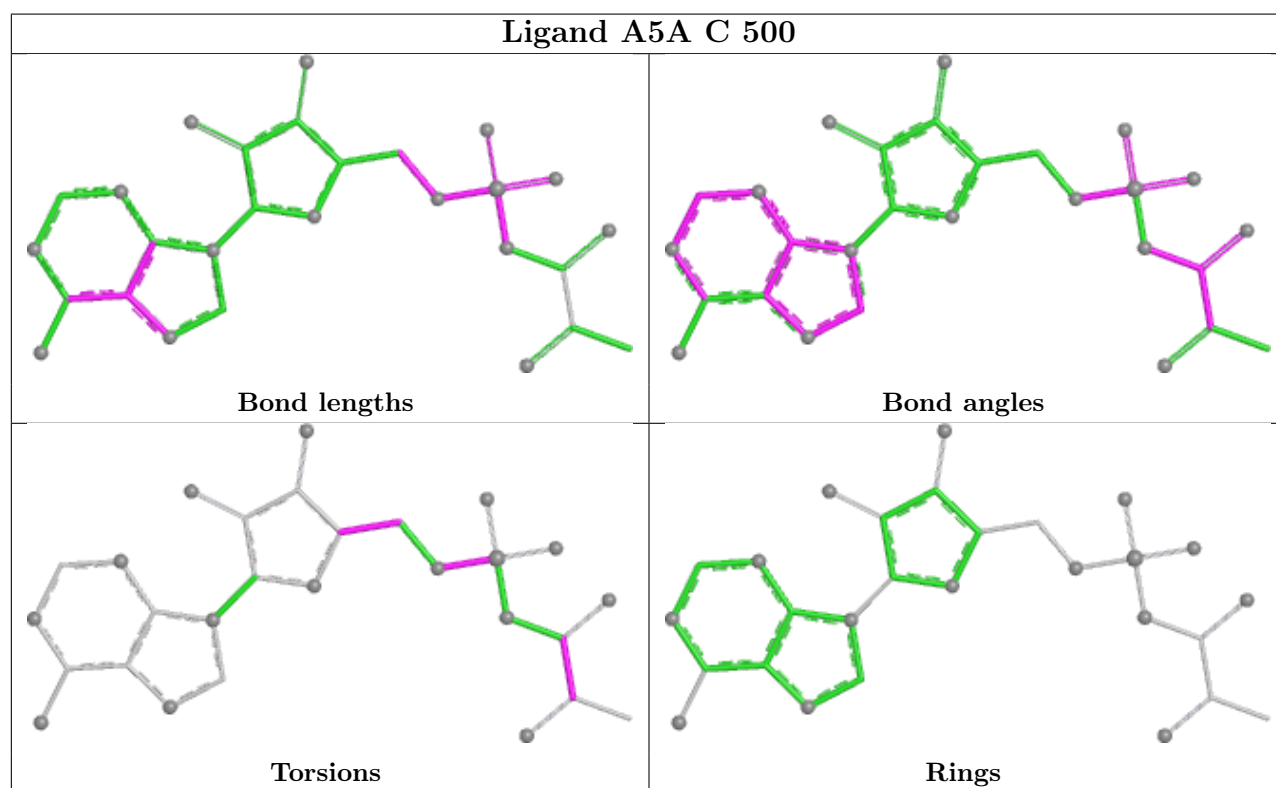
Mol	Chain	Res	Type	Atoms
2	A	500	A5A	C5'-O5'-S-N3S
2	A	500	A5A	C5'-O5'-S-O2S
2	B	500	A5A	C5'-O5'-S-N3S
2	C	500	A5A	C5'-O5'-S-N3S
2	C	500	A5A	C5'-O5'-S-O2S
2	C	500	A5A	O4'-C4'-C5'-O5'
2	C	500	A5A	C3'-C4'-C5'-O5'
2	D	500	A5A	O4'-C4'-C5'-O5'
2	D	500	A5A	C3'-C4'-C5'-O5'
2	E	500	A5A	C5'-O5'-S-N3S
2	F	500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

There are no ring outliers.

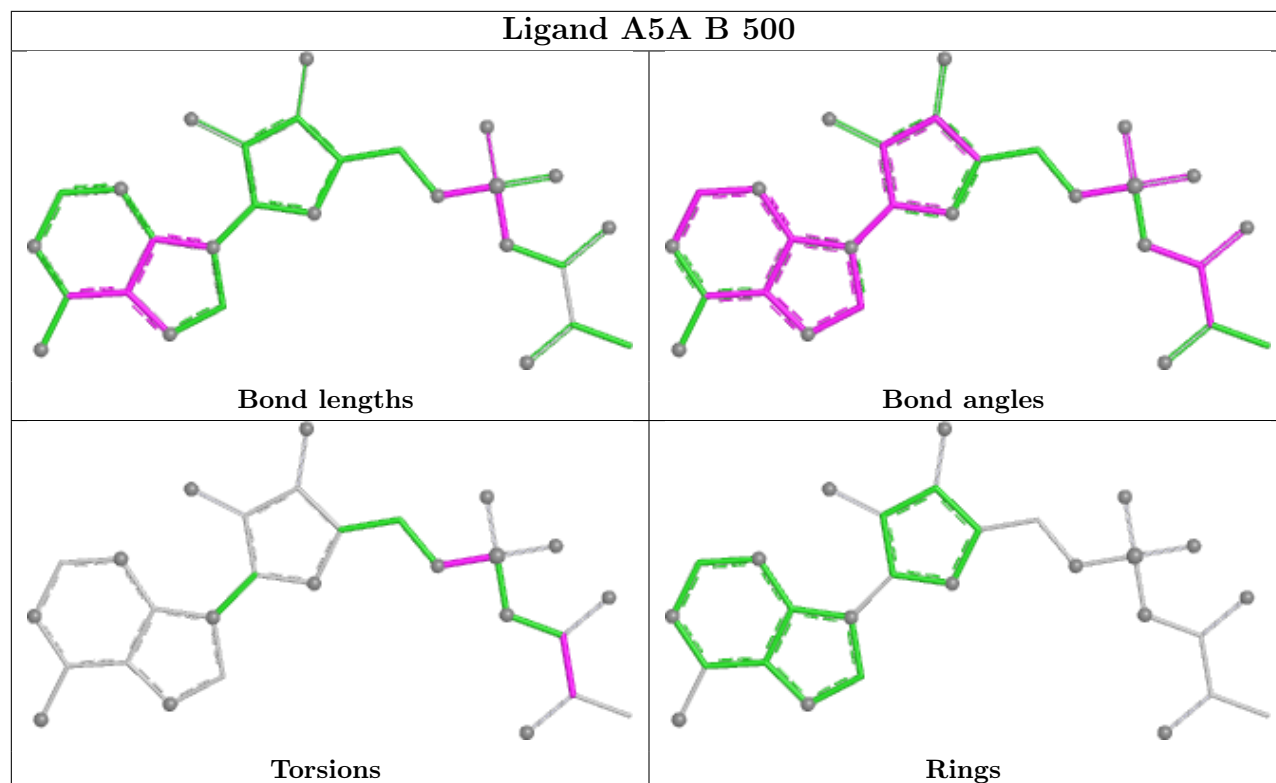
6 monomers are involved in 9 short contacts:

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

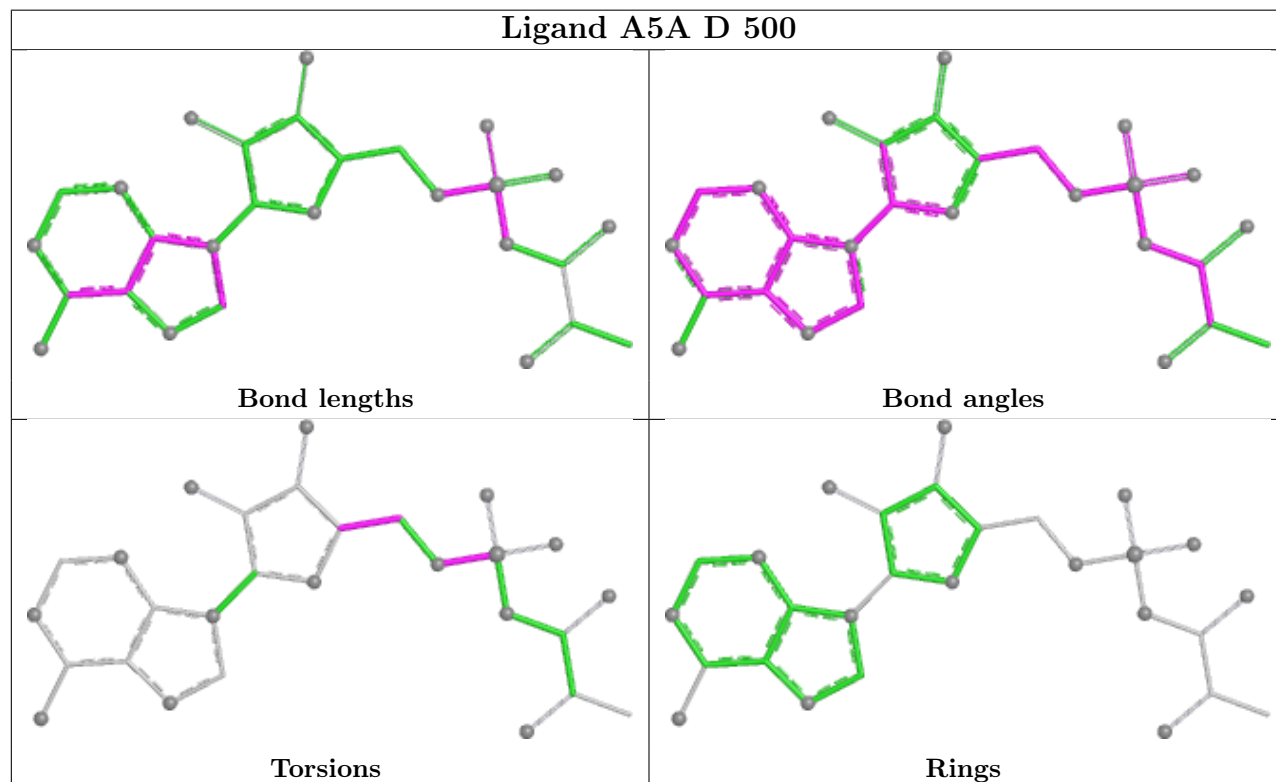
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



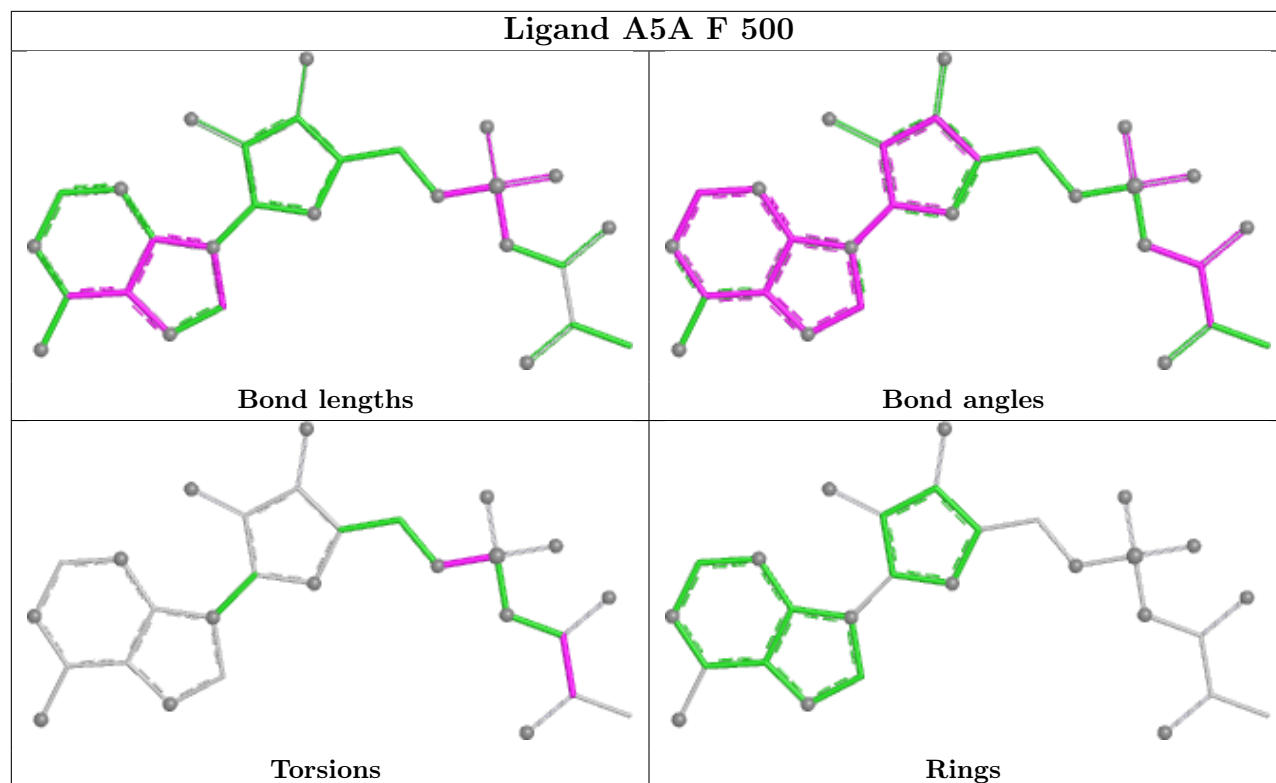
Ligand A5A B 500



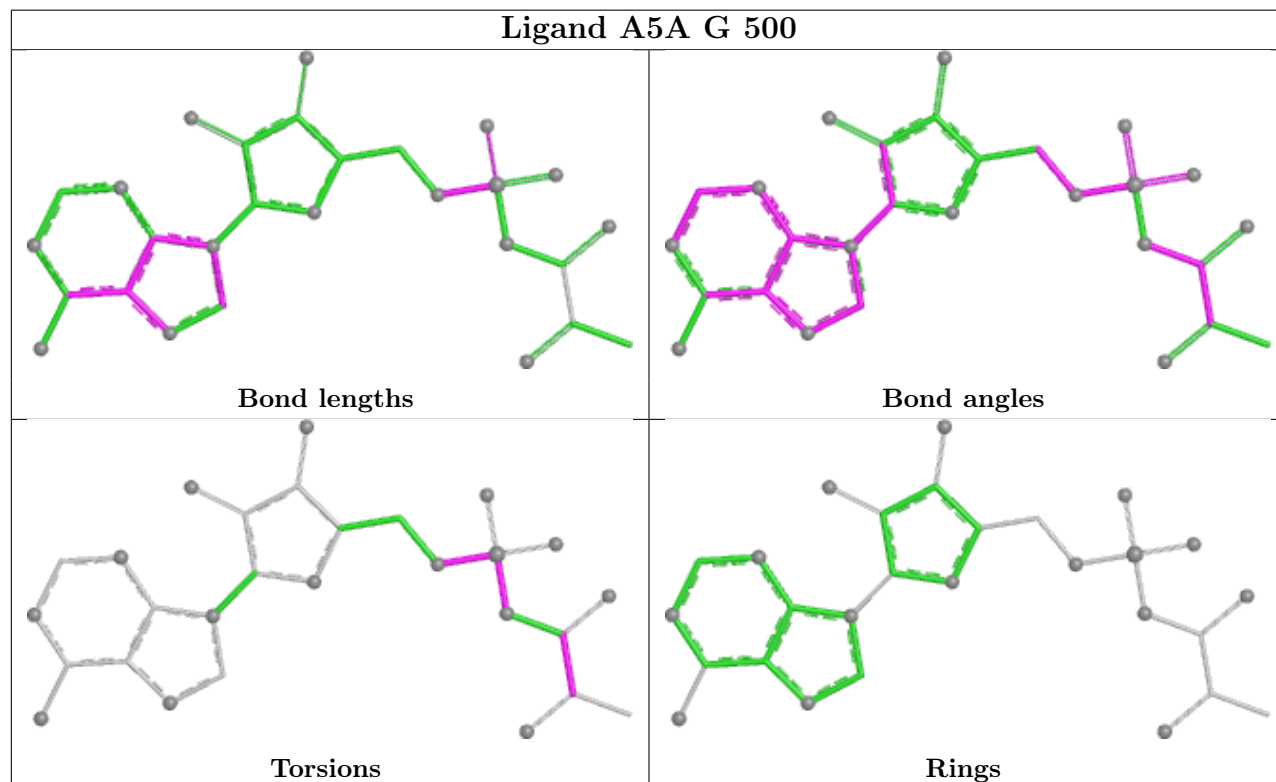
Ligand A5A D 500

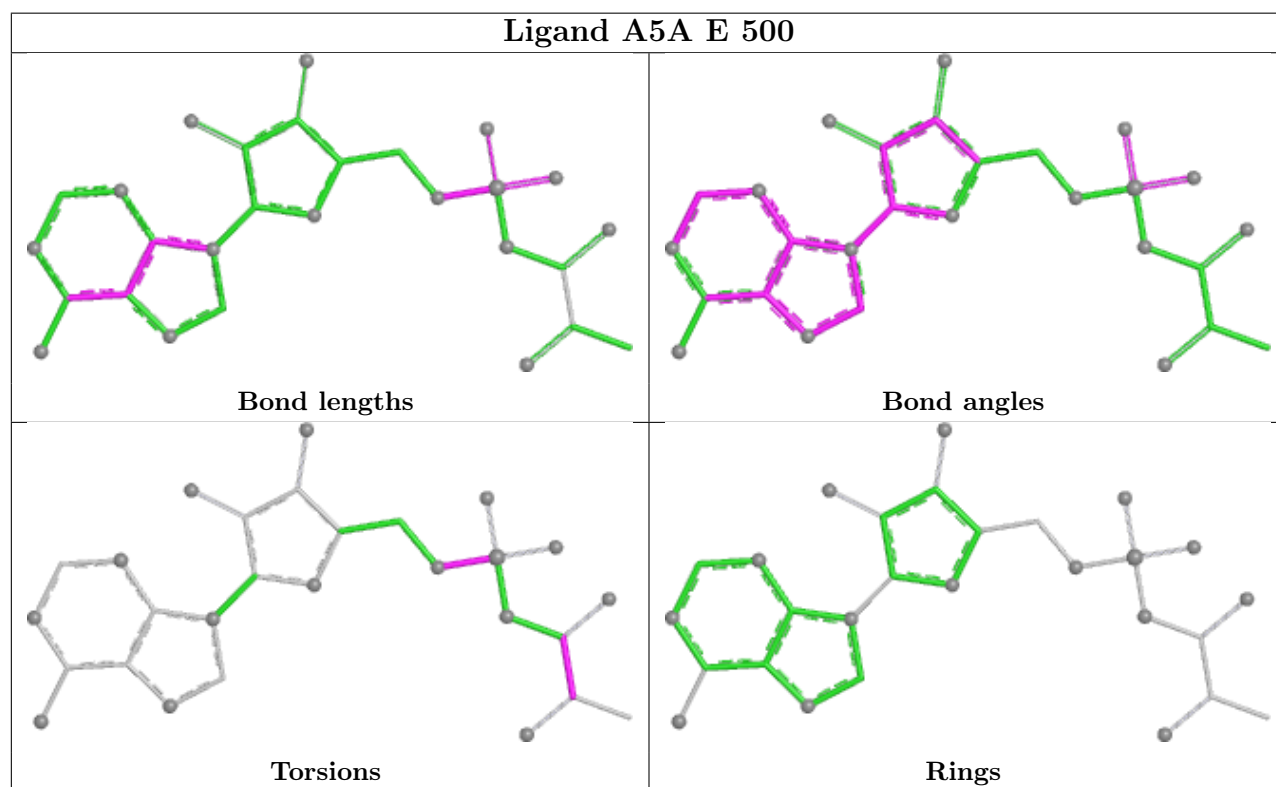
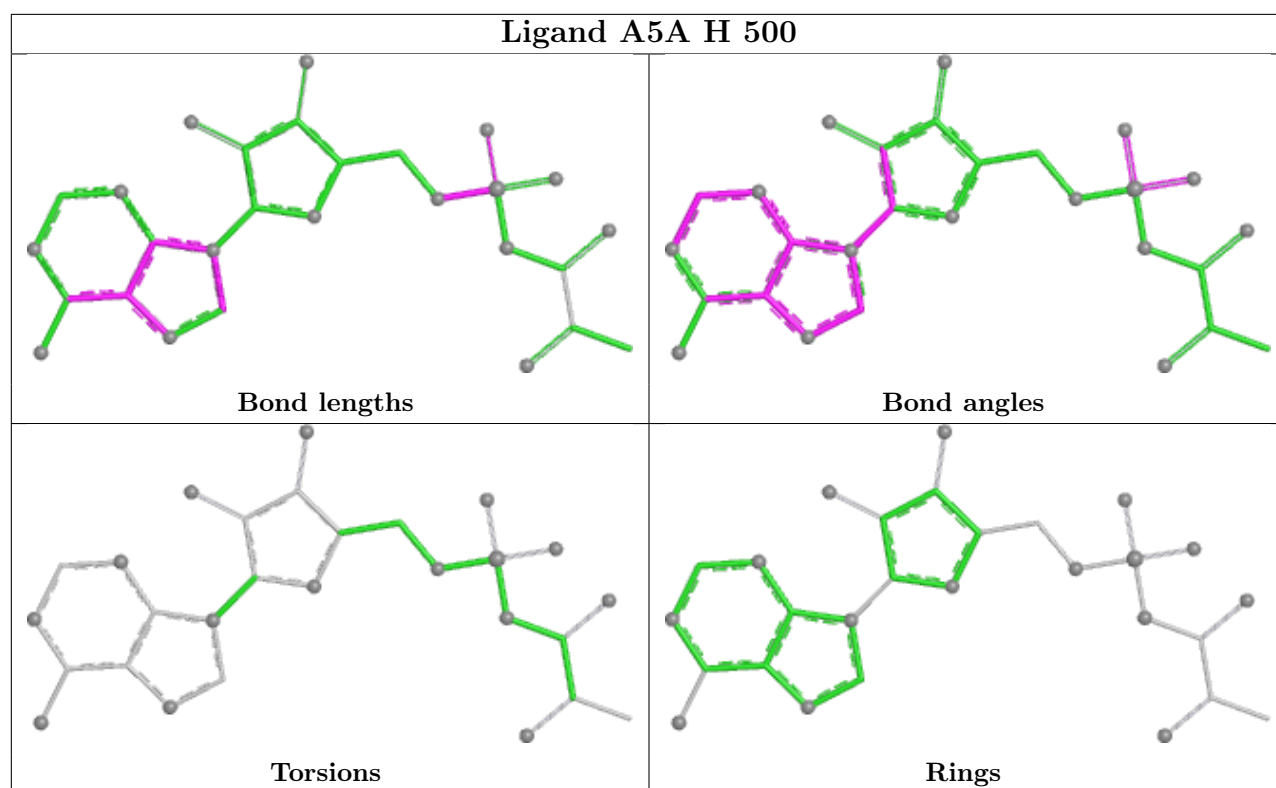


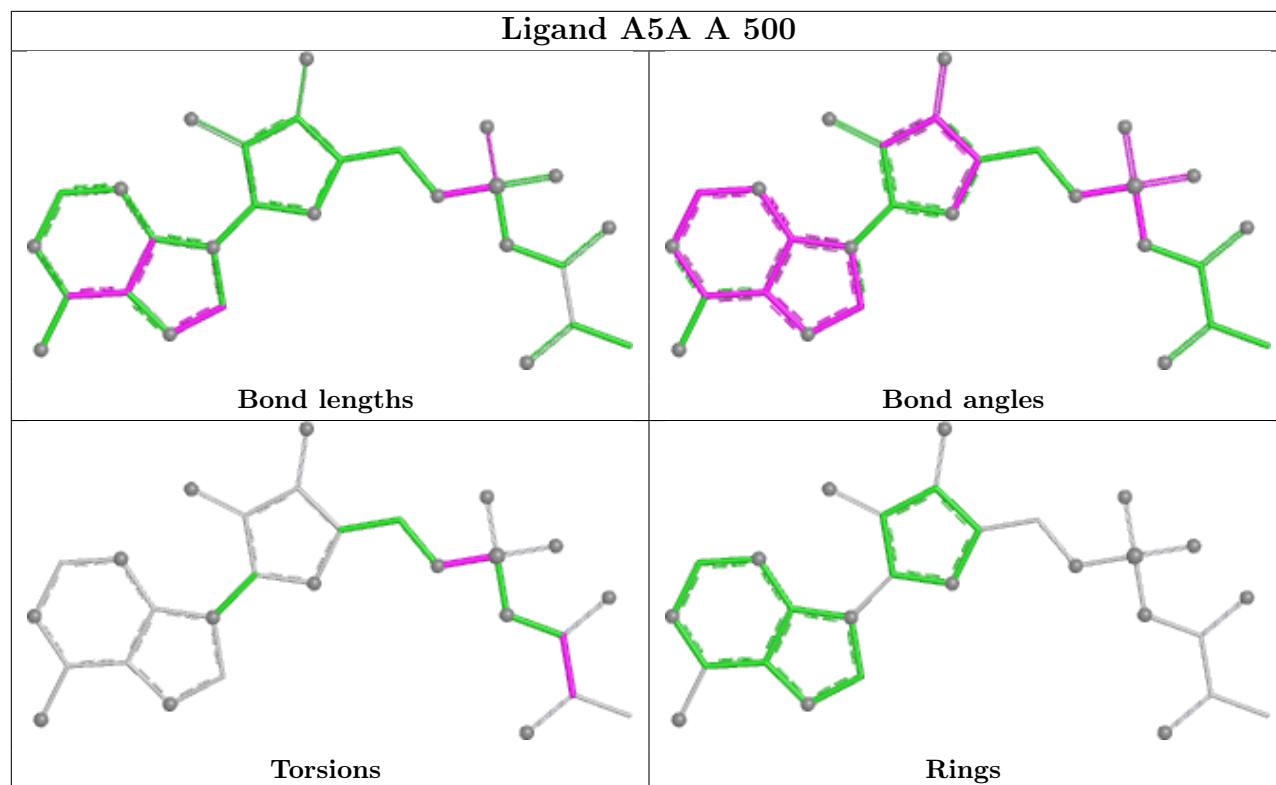
Ligand A5A F 500



Ligand A5A G 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

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	450/450 (100%)	-0.86	0 100 100	19, 47, 69, 87	0
1	B	450/450 (100%)	-0.74	2 (0%) 88 87	22, 48, 86, 113	0
1	C	444/450 (98%)	-0.64	3 (0%) 84 82	34, 63, 92, 124	0
1	D	447/450 (99%)	-0.62	4 (0%) 81 79	19, 61, 89, 127	0
1	E	450/450 (100%)	-0.81	2 (0%) 88 87	21, 48, 75, 90	0
1	F	449/450 (99%)	-0.85	0 100 100	19, 46, 81, 100	0
1	G	449/450 (99%)	-0.69	4 (0%) 81 79	31, 59, 85, 109	0
1	H	446/450 (99%)	-0.67	1 (0%) 91 90	29, 60, 101, 122	0
All	All	3585/3600 (99%)	-0.73	16 (0%) 88 87	19, 54, 88, 127	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	THR	4.6
1	E	288	ALA	3.3
1	H	30	ALA	3.0
1	C	172	LYS	3.0
1	G	122	LEU	2.7
1	D	48	GLN	2.6
1	B	169	GLY	2.5
1	D	243	GLY	2.5
1	D	89	GLY	2.4
1	G	299	ALA	2.3
1	C	29	SER	2.3
1	G	160	GLY	2.3
1	G	185	GLY	2.1
1	E	175	PHE	2.1
1	C	299	ALA	2.1
1	B	397	ILE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

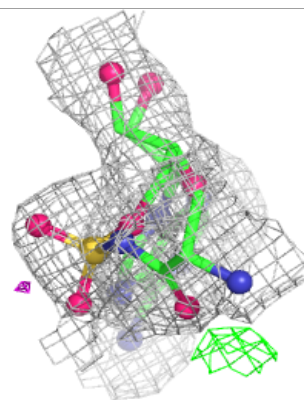
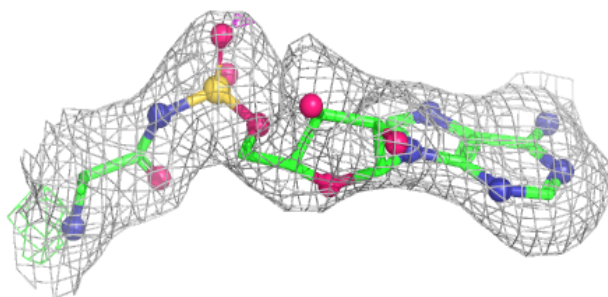
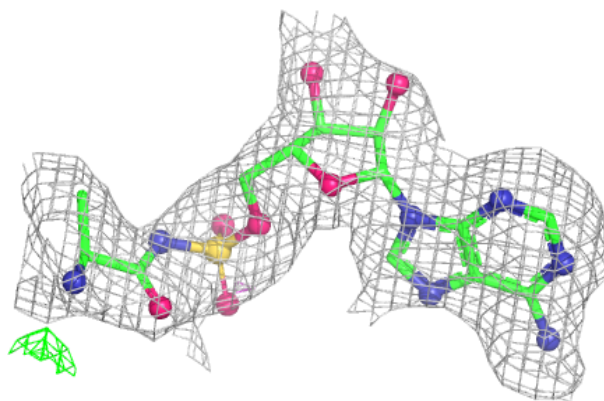
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A5A	A	500	28/28	0.98	0.06	28,34,43,47	0
2	A5A	B	500	28/28	0.98	0.06	24,36,49,53	0
2	A5A	D	500	28/28	0.98	0.05	41,52,59,62	0
2	A5A	E	500	28/28	0.98	0.06	20,24,46,63	0
2	A5A	F	500	28/28	0.98	0.05	26,32,35,39	0
2	A5A	G	500	28/28	0.98	0.05	22,53,68,75	0
2	A5A	C	500	28/28	0.99	0.04	43,52,63,65	0
2	A5A	H	500	28/28	0.99	0.05	35,48,53,58	0

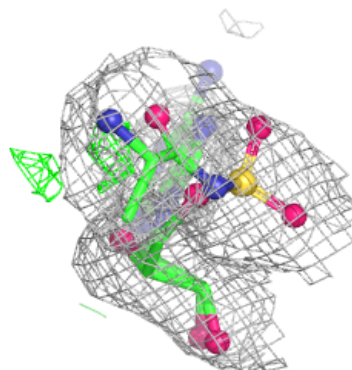
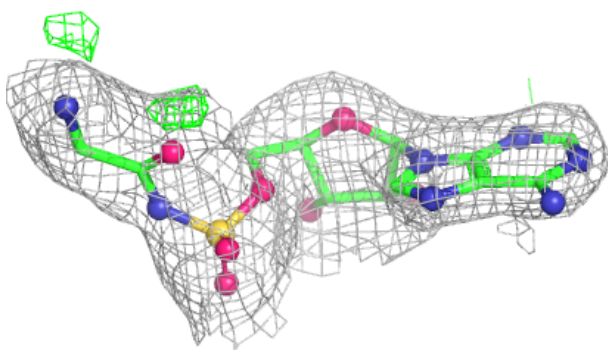
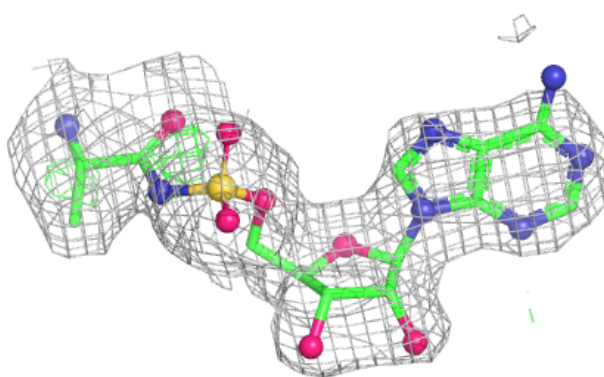
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

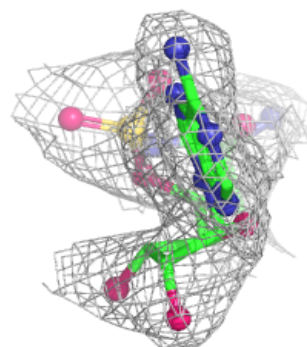
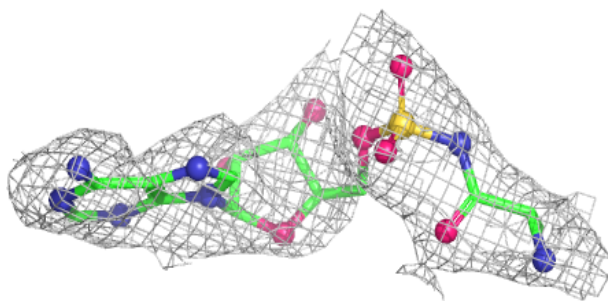
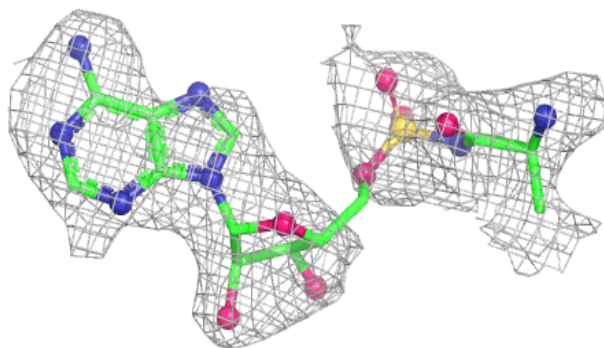
**Electron density around A5A B 500:**

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

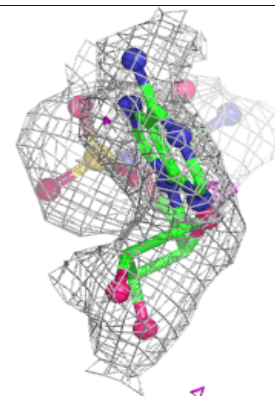
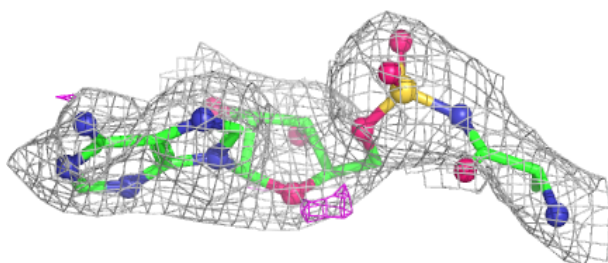
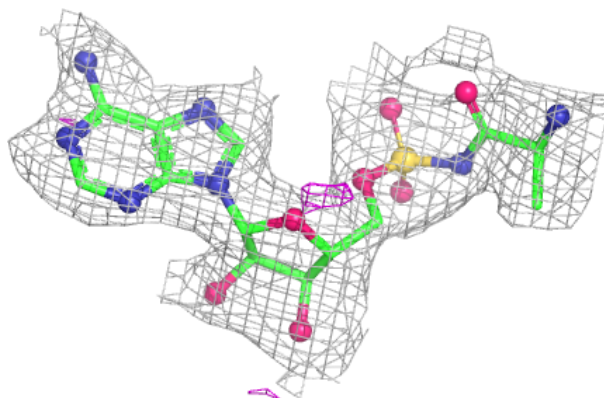


Electron density around A5A D 500:

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

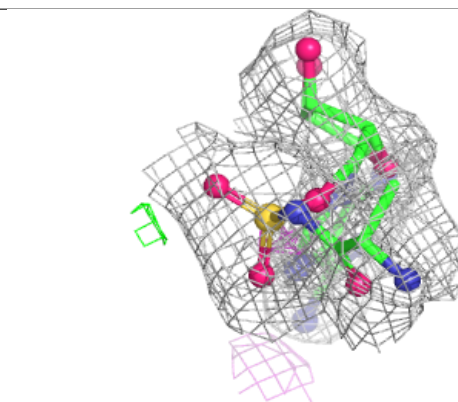
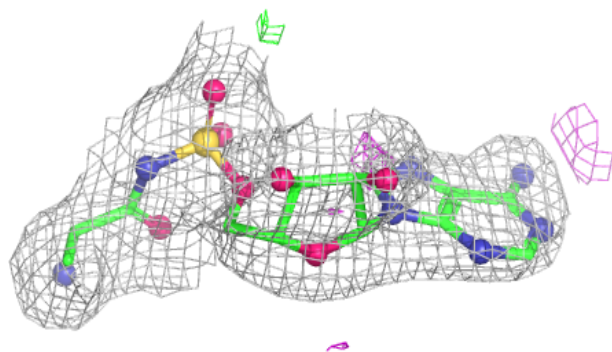
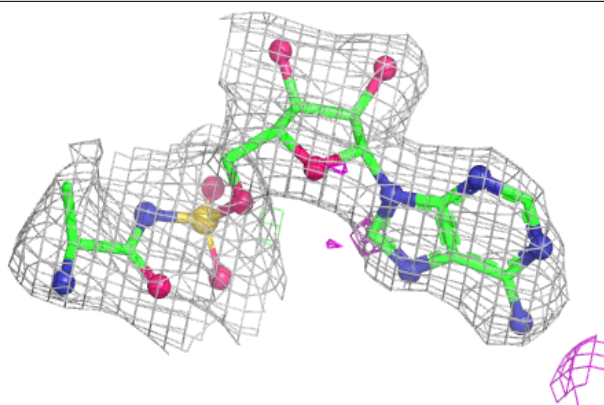
**Electron density around A5A E 500:**

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

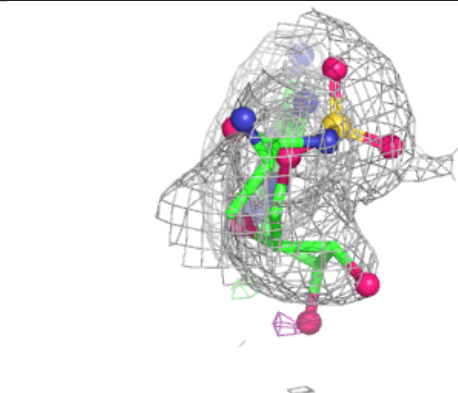
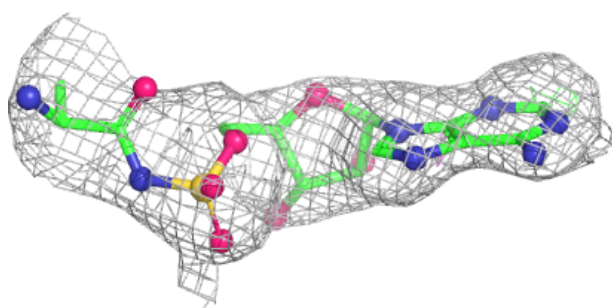
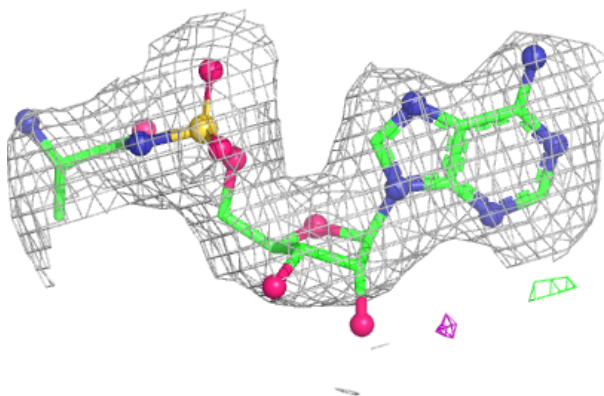


Electron density around A5A F 500:

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

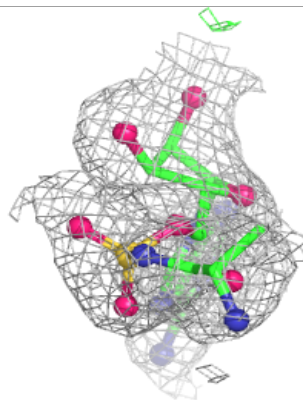
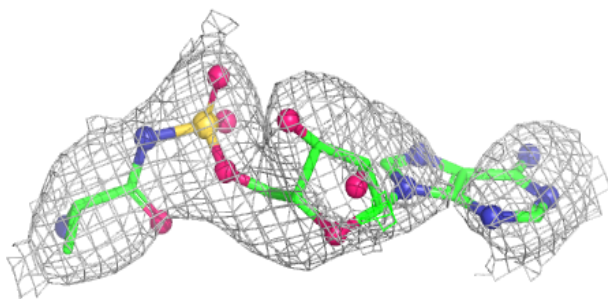
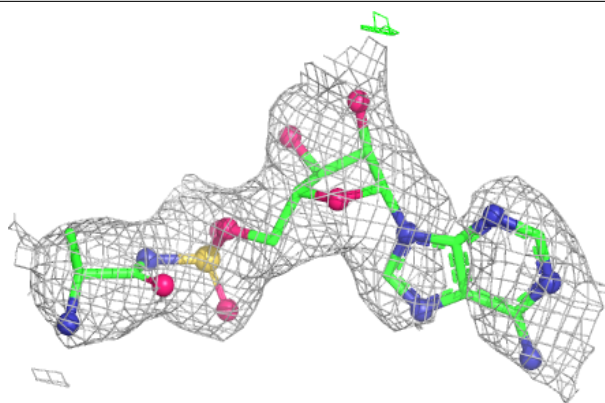
**Electron density around A5A G 500:**

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

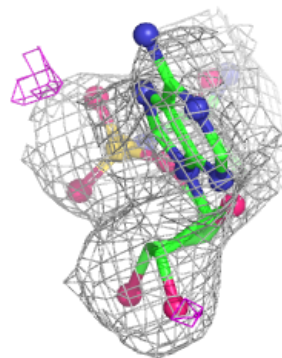
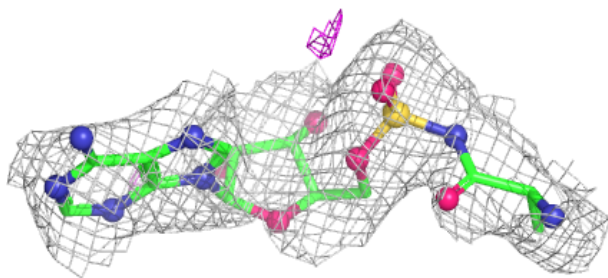
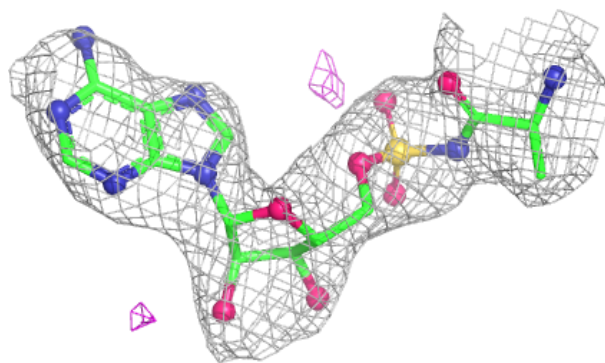


Electron density around A5A C 500:

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

**Electron density around A5A H 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](#)

There are no such residues in this entry.