



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:45 am BST

PDB ID : 2EL9
Title : Crystal structure of E.coli Histidyl-tRNA synthetase complexed with a histidyl-adenylate analogue
Authors : Yanagisawa, T.; Si, S.Y.; Matsuno, M.; Ishii, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-27
Resolution : 2.70 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

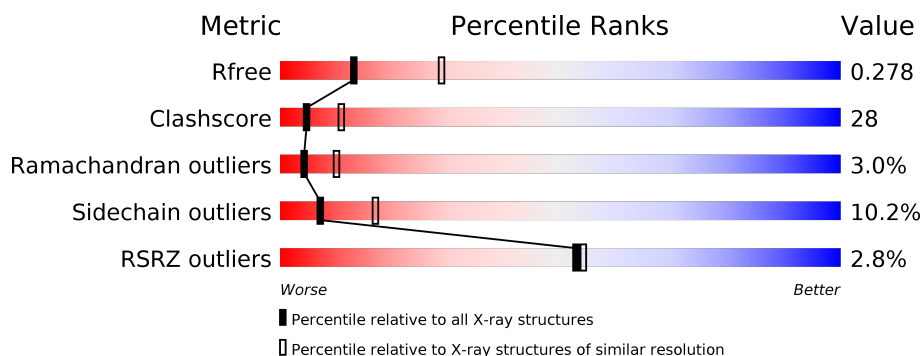
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	431	<div> <div>5%</div> <div> <div>41%</div> <div>39%</div> <div>6%</div> <div>14%</div> </div> </div>
1	B	431	<div> <div>52%</div> <div>30%</div> <div>5%</div> <div>13%</div> </div>
1	C	431	<div> <div>4%</div> <div> <div>44%</div> <div>36%</div> <div>6%</div> <div>14%</div> </div> </div>
1	D	431	<div> <div>48%</div> <div>35%</div> <div>6%</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HSS	C	710	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12050 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 Histidyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2903	1826	521	545	11			
1	B	376	Total	C	N	O	S	0	0	0
			2923	1837	525	550	11			
1	C	372	Total	C	N	O	S	0	0	0
			2899	1822	521	545	11			
1	D	385	Total	C	N	O	S	0	0	0
			2993	1883	535	564	11			

There are 28 discrepancies between the modelled and reference sequences:

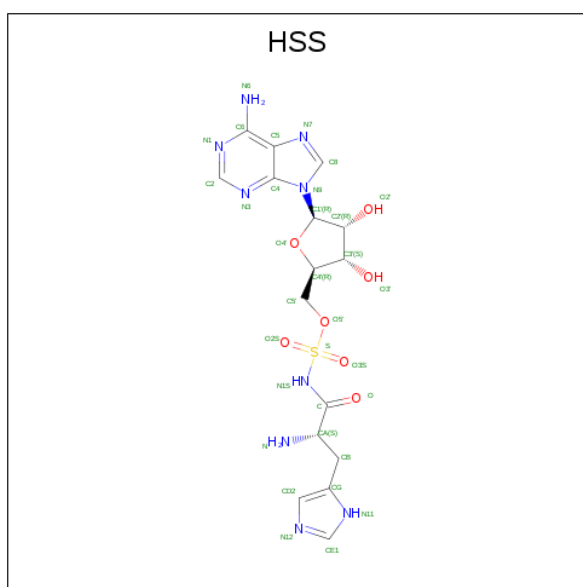
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P60906
A	-5	PRO	-	EXPRESSION TAG	UNP P60906
A	-4	GLY	-	EXPRESSION TAG	UNP P60906
A	-3	TYR	-	EXPRESSION TAG	UNP P60906
A	-2	GLN	-	EXPRESSION TAG	UNP P60906
A	-1	ASP	-	EXPRESSION TAG	UNP P60906
A	0	PRO	-	EXPRESSION TAG	UNP P60906
B	-6	GLY	-	EXPRESSION TAG	UNP P60906
B	-5	PRO	-	EXPRESSION TAG	UNP P60906
B	-4	GLY	-	EXPRESSION TAG	UNP P60906
B	-3	TYR	-	EXPRESSION TAG	UNP P60906
B	-2	GLN	-	EXPRESSION TAG	UNP P60906
B	-1	ASP	-	EXPRESSION TAG	UNP P60906
B	0	PRO	-	EXPRESSION TAG	UNP P60906
C	-6	GLY	-	EXPRESSION TAG	UNP P60906
C	-5	PRO	-	EXPRESSION TAG	UNP P60906
C	-4	GLY	-	EXPRESSION TAG	UNP P60906
C	-3	TYR	-	EXPRESSION TAG	UNP P60906
C	-2	GLN	-	EXPRESSION TAG	UNP P60906
C	-1	ASP	-	EXPRESSION TAG	UNP P60906
C	0	PRO	-	EXPRESSION TAG	UNP P60906

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	EXPRESSION TAG	UNP P60906
D	-5	PRO	-	EXPRESSION TAG	UNP P60906
D	-4	GLY	-	EXPRESSION TAG	UNP P60906
D	-3	TYR	-	EXPRESSION TAG	UNP P60906
D	-2	GLN	-	EXPRESSION TAG	UNP P60906
D	-1	ASP	-	EXPRESSION TAG	UNP P60906
D	0	PRO	-	EXPRESSION TAG	UNP P60906

- Molecule 2 is 5'-O-[(L-HISTIDYLAMINO)SULFONYL]ADENOSINE (three-letter code: HSS) (formula: C₁₆H₂₁N₉O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	16	9	7	1		
2	B	1	Total	C	N	O	S	0	0
			33	16	9	7	1		
2	C	1	Total	C	N	O	S	0	0
			33	16	9	7	1		
2	D	1	Total	C	N	O	S	0	0
			33	16	9	7	1		

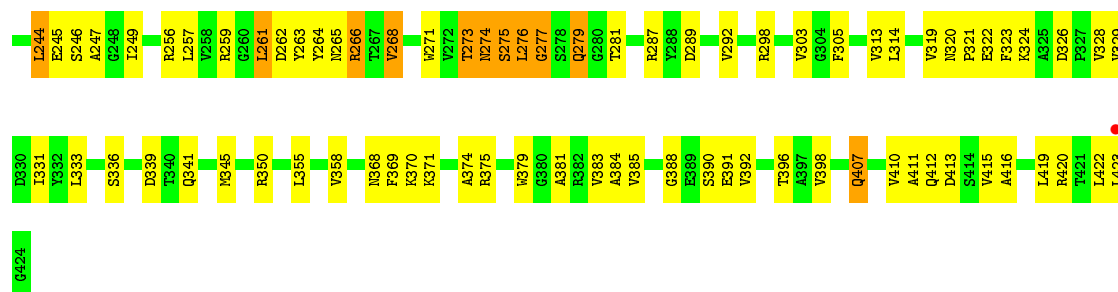
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		

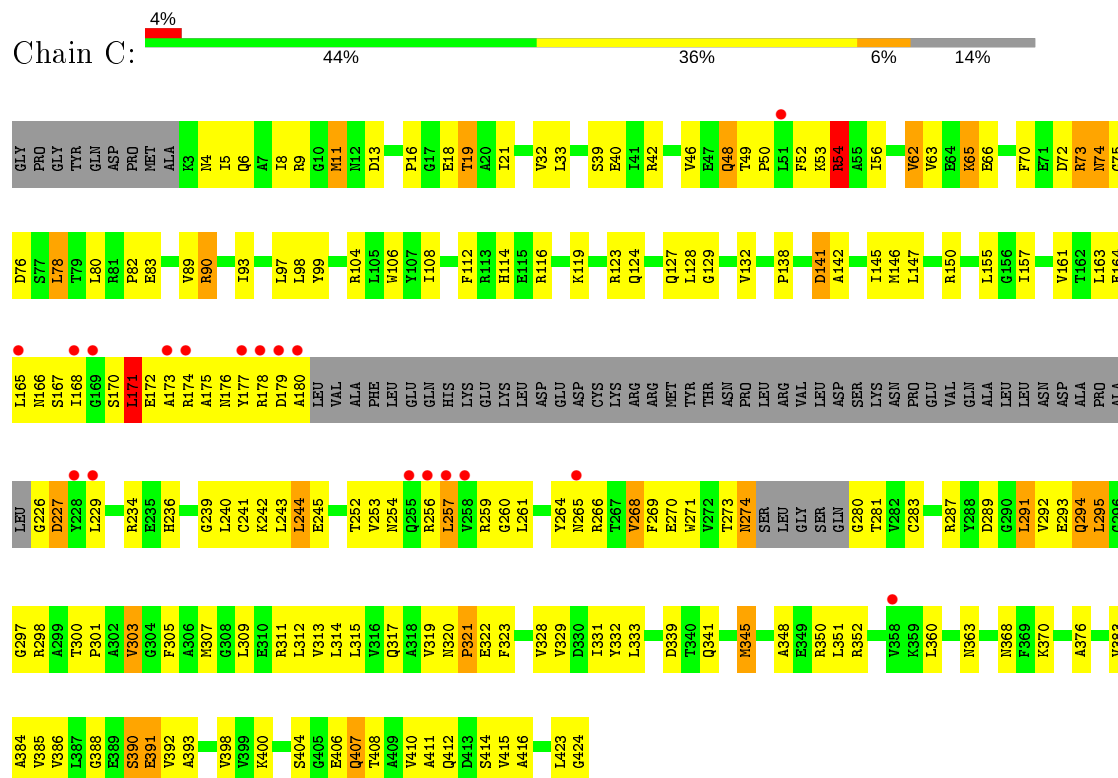
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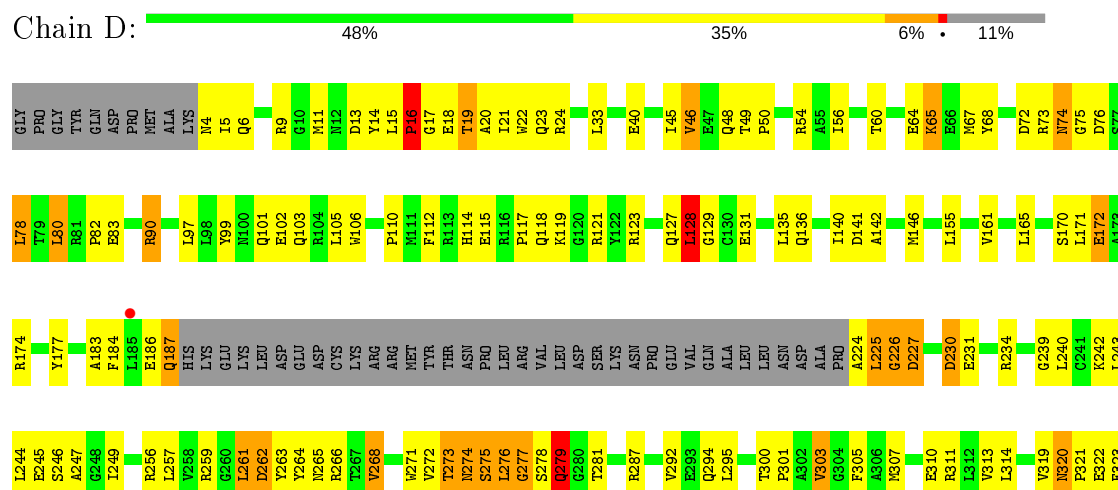
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	49	Total 49	O 49	0	0
3	C	45	Total 45	O 45	0	0
3	D	66	Total 66	O 66	0	0



• Molecule 1: Histidyl-tRNA synthetase



• Molecule 1: Histidyl-tRNA synthetase



WORLDWIDE
PDB
PROTEIN DATA BANK

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.11Å 108.34Å 193.65Å 90.00° 98.21° 90.00°	Depositor
Resolution (Å)	48.80 – 2.70 48.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.80-2.70) 95.4 (48.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.285 0.220 , 0.278	Depositor DCC
R_{free} test set	6521 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12050	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8788e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HSS

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	0.48	0/2955	0.74	0/3995
1	B	0.50	1/2976 (0.0%)	0.74	0/4025
1	C	0.45	0/2951	0.71	2/3989 (0.1%)
1	D	0.50	0/3047	0.75	1/4122 (0.0%)
All	All	0.48	1/11929 (0.0%)	0.74	3/16131 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	CYS	CB-SG	-5.18	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	171	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	128	LEU	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2903	0	2869	198	0
1	B	2923	0	2888	144	0
1	C	2899	0	2861	191	0
1	D	2993	0	2956	177	0
2	A	33	0	21	4	0
2	B	33	0	21	2	0
2	C	33	0	21	9	0
2	D	33	0	21	5	0
3	A	40	0	0	2	0
3	B	49	0	0	2	0
3	C	45	0	0	1	0
3	D	66	0	0	4	0
All	All	12050	0	11658	659	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (659) 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:287:ARG:HG2	1:A:303:VAL:HG13	1.32	1.06
1:C:127:GLN:HE22	2:C:710:HSS:H5'2	1.25	1.01
1:A:320:ASN:HD22	1:A:320:ASN:N	1.55	1.00
1:C:127:GLN:NE2	2:C:710:HSS:H5'2	1.79	0.97
1:C:74:ASN:ND2	1:C:76:ASP:H	1.60	0.97
1:A:4:ASN:HD22	1:A:4:ASN:H	0.99	0.96
1:A:4:ASN:ND2	1:A:4:ASN:H	1.59	0.95
1:C:259:ARG:NH2	2:C:710:HSS:HN1S	1.64	0.94
1:A:168:ILE:HD12	1:A:174:ARG:NH2	1.83	0.94
1:C:40:GLU:O	1:D:19:THR:HG21	1.69	0.93
1:C:311:ARG:NH1	2:C:710:HSS:H2'	1.84	0.93
1:D:127:GLN:NE2	2:D:810:HSS:H5'2	1.83	0.92
1:A:8:ILE:HD12	1:B:46:VAL:HG23	1.48	0.91
1:D:274:ASN:HD22	1:D:276:LEU:HD21	1.34	0.91
1:C:74:ASN:HD21	1:C:76:ASP:H	1.21	0.89
1:C:170:SER:O	1:C:174:ARG:HG3	1.72	0.89
1:B:171:LEU:HA	1:B:174:ARG:HH12	1.39	0.88
1:C:287:ARG:HG2	1:C:303:VAL:HG13	1.57	0.87
1:D:127:GLN:HE21	2:D:810:HSS:H5'2	1.38	0.86
1:C:93:ILE:HD12	1:C:297:GLY:HA3	1.57	0.86
1:B:171:LEU:HA	1:B:174:ARG:NH1	1.91	0.85
1:A:320:ASN:H	1:A:320:ASN:HD22	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HG2	1:A:179:ASP:N	1.94	0.82
1:D:97:LEU:HB3	1:D:103:GLN:HE21	1.45	0.81
1:A:320:ASN:ND2	1:A:320:ASN:N	2.28	0.80
1:C:333:LEU:HG	1:C:385:VAL:HG23	1.64	0.79
1:C:171:LEU:HD13	1:C:172:GLU:H	1.48	0.79
1:A:176:ASN:HB3	1:A:228:TYR:CZ	2.17	0.78
1:C:259:ARG:HH22	2:C:710:HSS:HN1S	1.28	0.78
1:B:171:LEU:H	1:B:171:LEU:HD22	1.49	0.77
1:B:388:GLY:O	1:B:392:VAL:HG23	1.85	0.77
1:D:287:ARG:HG2	1:D:303:VAL:CG1	2.15	0.77
1:B:99:TYR:O	1:B:101:GLN:HG3	1.83	0.77
1:C:328:VAL:HG23	1:C:329:VAL:HG23	1.67	0.76
1:A:40:GLU:O	1:B:19:THR:HG21	1.85	0.76
1:A:333:LEU:HG	1:A:385:VAL:CG2	2.16	0.76
2:D:810:HSS:H5'1	2:D:810:HSS:H8	1.67	0.75
1:C:168:ILE:HG13	1:C:265:ASN:O	1.86	0.75
1:C:259:ARG:NH2	2:C:710:HSS:N1S	2.35	0.75
1:D:368:ASN:OD1	1:D:370:LYS:HB3	1.86	0.75
1:D:5:ILE:H	1:D:5:ILE:HD12	1.52	0.75
1:C:74:ASN:HD22	1:C:75:GLY:N	1.84	0.74
1:B:355:LEU:O	1:B:358:VAL:HG22	1.88	0.74
1:A:404:SER:OG	1:A:406:GLU:HG2	1.87	0.74
1:B:319:VAL:C	1:B:320:ASN:HD22	1.91	0.74
1:D:310:GLU:O	1:D:314:LEU:HD13	1.87	0.74
1:A:161:VAL:HG12	1:A:271:TRP:CE3	2.24	0.73
1:A:328:VAL:HG23	1:A:329:VAL:HG23	1.69	0.73
1:C:119:LYS:HE2	1:C:314:LEU:HD21	1.71	0.73
1:C:171:LEU:HD22	1:C:172:GLU:N	2.03	0.73
1:A:46:VAL:HG12	1:A:80:LEU:HD12	1.70	0.73
1:C:72:ASP:HB2	1:C:78:LEU:CD2	2.19	0.72
1:D:172:GLU:H	1:D:172:GLU:CD	1.90	0.72
1:C:142:ALA:HB1	1:C:146:MET:HE3	1.71	0.72
1:C:309:LEU:O	1:C:313:VAL:HG23	1.88	0.72
1:A:293:GLU:HA	1:A:297:GLY:O	1.90	0.72
1:D:102:GLU:OE1	1:D:135:LEU:HD21	1.89	0.72
1:D:412:GLN:O	1:D:415:VAL:HG22	1.89	0.72
1:D:273:THR:HG23	1:D:276:LEU:HD23	1.71	0.72
1:A:264:TYR:HA	1:A:287:ARG:O	1.89	0.71
1:D:319:VAL:C	1:D:320:ASN:HD22	1.93	0.71
1:C:127:GLN:NE2	2:C:710:HSS:C5'	2.52	0.71
1:B:117:PRO:O	1:B:118:GLN:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ILE:HD12	1:C:21:ILE:H	1.55	0.71
1:D:230:ASP:O	1:D:234:ARG:HG3	1.91	0.71
1:B:412:GLN:O	1:B:415:VAL:HG22	1.90	0.71
1:D:265:ASN:O	1:D:287:ARG:HB2	1.91	0.70
1:A:391:GLU:H	1:A:391:GLU:CD	1.94	0.70
1:C:49:THR:N	1:C:50:PRO:HD2	2.07	0.70
1:A:13:ASP:CG	1:B:90:ARG:HH22	1.95	0.70
1:A:46:VAL:HG23	1:B:8:ILE:HD12	1.73	0.70
1:A:54:ARG:HH22	1:B:4:ASN:HA	1.55	0.70
1:B:16:PRO:O	1:B:19:THR:HG22	1.92	0.70
1:C:264:TYR:HA	1:C:287:ARG:O	1.91	0.70
1:C:175:ALA:O	1:C:178:ARG:HG2	1.92	0.69
1:C:404:SER:OG	1:C:406:GLU:HG2	1.93	0.68
1:A:168:ILE:HD12	1:A:174:ARG:HH21	1.58	0.68
1:C:21:ILE:N	1:C:21:ILE:HD12	2.07	0.68
1:A:388:GLY:O	1:A:392:VAL:HG23	1.93	0.68
1:A:161:VAL:HG12	1:A:271:TRP:HE3	1.56	0.68
1:A:391:GLU:OE1	1:A:391:GLU:N	2.24	0.68
1:A:4:ASN:HD22	1:A:4:ASN:N	1.83	0.67
1:C:391:GLU:N	1:C:391:GLU:OE1	2.26	0.67
1:B:40:GLU:HB2	1:B:106:TRP:CZ2	2.30	0.67
1:C:273:THR:HG22	1:C:280:GLY:O	1.94	0.67
1:B:319:VAL:HG12	1:B:320:ASN:ND2	2.09	0.67
1:D:264:TYR:HA	1:D:287:ARG:O	1.95	0.67
1:D:287:ARG:HG2	1:D:303:VAL:HG13	1.75	0.66
1:A:333:LEU:HG	1:A:385:VAL:HG23	1.75	0.66
1:C:239:GLY:O	1:C:243:LEU:HD13	1.96	0.66
1:C:333:LEU:HG	1:C:385:VAL:CG2	2.25	0.66
1:D:355:LEU:O	1:D:358:VAL:HG22	1.95	0.66
1:C:46:VAL:HG12	1:C:80:LEU:HD12	1.76	0.66
1:A:336:SER:HG	1:A:369:PHE:HZ	1.44	0.65
1:C:9:ARG:HH21	1:C:123:ARG:NH2	1.94	0.65
1:D:350:ARG:NH2	1:D:413:ASP:HA	2.11	0.65
1:C:13:ASP:CG	1:D:90:ARG:HH22	1.99	0.65
1:C:259:ARG:HH11	1:C:259:ARG:HG3	1.62	0.65
1:D:273:THR:CG2	1:D:276:LEU:HD23	2.26	0.65
1:A:97:LEU:C	1:A:98:LEU:HD23	2.17	0.65
1:C:72:ASP:HB2	1:C:78:LEU:HD22	1.78	0.65
1:C:226:GLY:O	1:C:229:LEU:HG	1.97	0.64
1:D:5:ILE:HG22	1:D:6:GLN:N	2.12	0.64
1:C:127:GLN:HE22	2:C:710:HSS:C5'	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:HB2	1:A:299:ALA:HB2	1.79	0.64
1:C:19:THR:HG21	1:D:40:GLU:O	1.97	0.64
1:C:260:GLY:C	1:C:261:LEU:HD22	2.18	0.63
1:A:49:THR:N	1:A:50:PRO:HD2	2.12	0.63
1:A:287:ARG:HG2	1:A:303:VAL:CG1	2.17	0.63
1:A:97:LEU:HD11	1:B:15:LEU:HD13	1.80	0.63
1:C:165:LEU:HD11	1:C:244:LEU:CD2	2.28	0.63
1:C:54:ARG:HH22	1:D:4:ASN:HA	1.61	0.63
1:D:19:THR:O	1:D:23:GLN:HG3	1.97	0.63
1:B:165:LEU:O	1:B:166:ASN:HB2	1.99	0.63
1:B:333:LEU:HG	1:B:385:VAL:HG22	1.81	0.63
1:B:171:LEU:CD2	1:B:171:LEU:H	2.11	0.63
1:B:60:THR:O	1:B:64:GLU:HB2	1.99	0.63
1:D:74:ASN:C	1:D:74:ASN:HD22	2.02	0.63
1:A:141:ASP:HB2	1:A:240:LEU:HD13	1.80	0.63
1:A:336:SER:O	1:A:340:THR:HG21	1.99	0.62
1:C:5:ILE:HG22	1:C:6:GLN:N	2.14	0.62
1:A:353:ASP:OD1	1:B:153:ARG:NH1	2.32	0.62
1:B:391:GLU:CD	1:B:391:GLU:H	2.02	0.62
1:A:138:PRO:HB2	1:A:240:LEU:HB2	1.81	0.62
1:B:22:TRP:CE2	1:B:313:VAL:HG21	2.34	0.62
1:C:256:ARG:HH11	1:C:256:ARG:HG2	1.65	0.62
1:C:128:LEU:HB2	1:C:309:LEU:HD21	1.81	0.62
1:C:40:GLU:HB2	1:C:106:TRP:CZ2	2.35	0.61
1:D:117:PRO:O	1:D:118:GLN:HG2	1.99	0.61
1:A:68:TYR:HB2	1:A:80:LEU:HB2	1.82	0.61
1:C:345:MET:HE3	1:D:146:MET:HE3	1.83	0.61
1:C:46:VAL:CG2	1:D:11:MET:SD	2.89	0.61
1:A:33:LEU:HD11	1:A:128:LEU:HD11	1.81	0.61
1:C:241:CYS:O	1:C:245:GLU:HG3	2.00	0.61
1:D:350:ARG:HH22	1:D:413:ASP:HA	1.66	0.61
1:A:241:CYS:O	1:A:245:GLU:HG3	2.00	0.61
1:B:172:GLU:H	1:B:172:GLU:CD	2.03	0.61
1:B:74:ASN:HD22	1:B:74:ASN:C	2.03	0.61
1:A:13:ASP:OD2	1:B:90:ARG:NH2	2.34	0.61
1:C:33:LEU:HD13	1:C:106:TRP:CG	2.36	0.61
1:C:311:ARG:HH12	2:C:710:HSS:H2'	1.66	0.61
2:A:510:HSS:O3S	2:A:510:HSS:O	2.13	0.60
1:B:277:GLY:HA2	3:B:650:HOH:O	2.01	0.60
1:B:89:VAL:HG13	1:B:292:VAL:HG22	1.84	0.60
1:D:74:ASN:ND2	1:D:76:ASP:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:GLY:O	1:D:242:LYS:HG2	2.01	0.60
1:C:141:ASP:HB2	1:C:240:LEU:HD13	1.84	0.60
1:D:320:ASN:N	1:D:320:ASN:HD22	1.99	0.60
1:A:54:ARG:NH2	1:B:4:ASN:HA	2.16	0.60
1:C:147:LEU:C	1:C:147:LEU:HD23	2.22	0.60
1:D:274:ASN:HB2	1:D:276:LEU:CD2	2.31	0.60
1:A:19:THR:HG21	1:B:40:GLU:O	2.02	0.60
1:A:319:VAL:C	1:A:321:PRO:HD3	2.22	0.60
1:D:261:LEU:N	1:D:261:LEU:HD22	2.16	0.60
1:C:33:LEU:HD23	1:C:147:LEU:HD11	1.84	0.59
1:A:239:GLY:O	1:A:242:LYS:HG2	2.03	0.59
1:D:161:VAL:HG12	1:D:271:TRP:HE3	1.66	0.59
1:A:136:GLN:O	1:A:236:HIS:HE1	1.85	0.59
1:B:21:ILE:H	1:B:21:ILE:HD12	1.68	0.59
1:D:351:LEU:HD21	1:D:415:VAL:HG23	1.84	0.59
1:A:242:LYS:HG3	1:A:243:LEU:N	2.18	0.59
1:A:4:ASN:ND2	1:A:4:ASN:N	2.38	0.59
1:C:72:ASP:HB2	1:C:78:LEU:HD21	1.84	0.59
1:C:56:ILE:HG23	1:C:261:LEU:HD12	1.84	0.59
1:A:313:VAL:O	1:A:317:GLN:HG3	2.02	0.58
1:C:348:ALA:O	1:C:352:ARG:HG3	2.03	0.58
1:A:74:ASN:ND2	1:A:74:ASN:C	2.55	0.58
1:B:165:LEU:HD11	1:B:244:LEU:HD23	1.85	0.58
1:A:166:ASN:OD1	1:A:255:GLN:HA	2.04	0.58
1:C:332:TYR:CE2	1:C:363:ASN:HB2	2.38	0.58
1:C:74:ASN:ND2	1:C:74:ASN:C	2.54	0.58
1:D:401:ASP:OD1	1:D:403:ARG:HB2	2.03	0.58
1:A:178:ARG:CG	1:A:179:ASP:N	2.67	0.58
1:A:412:GLN:O	1:A:415:VAL:HG22	2.04	0.58
1:B:120:GLY:H	1:B:279:GLN:HE21	1.52	0.58
1:A:176:ASN:HB3	1:A:228:TYR:CE1	2.39	0.58
1:C:170:SER:H	1:C:173:ALA:HB3	1.68	0.58
1:C:388:GLY:O	1:C:392:VAL:HG23	2.04	0.58
1:D:259:ARG:CG	1:D:268:VAL:HG22	2.34	0.58
1:B:74:ASN:ND2	1:B:76:ASP:H	2.02	0.58
1:C:21:ILE:CD1	1:C:21:ILE:H	2.16	0.58
1:B:171:LEU:CA	1:B:174:ARG:HH12	2.13	0.57
1:A:74:ASN:C	1:A:74:ASN:HD22	2.06	0.57
1:B:168:ILE:HD12	1:B:174:ARG:HE	1.68	0.57
1:B:171:LEU:N	1:B:171:LEU:HD22	2.19	0.57
1:B:391:GLU:HB3	1:B:396:THR:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:VAL:C	1:C:321:PRO:HD3	2.24	0.57
1:D:165:LEU:HD11	1:D:244:LEU:CD2	2.33	0.57
1:C:175:ALA:O	1:C:177:TYR:N	2.38	0.57
1:D:99:TYR:O	1:D:101:GLN:HG3	2.03	0.57
1:A:139:ASP:HA	1:A:243:LEU:HD23	1.87	0.57
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.70	0.57
1:C:171:LEU:HD22	1:C:172:GLU:HG2	1.86	0.57
1:C:411:ALA:O	1:C:414:SER:N	2.34	0.57
1:D:391:GLU:H	1:D:391:GLU:CD	2.08	0.57
1:D:410:VAL:CG1	1:D:415:VAL:HG12	2.34	0.57
1:A:108:ILE:HD12	1:A:128:LEU:HD23	1.87	0.57
1:A:139:ASP:O	1:A:142:ALA:HB3	2.04	0.57
1:A:74:ASN:ND2	1:A:76:ASP:H	2.02	0.57
1:A:115:GLU:OE1	1:A:121:ARG:HD3	2.05	0.57
1:D:419:LEU:HA	1:D:422:LEU:HD11	1.87	0.57
1:A:74:ASN:HD22	1:A:75:GLY:N	2.03	0.56
1:C:331:ILE:HD11	1:C:423:LEU:HD11	1.88	0.56
1:A:55:ALA:HB2	1:A:295:LEU:HD11	1.86	0.56
1:B:174:ARG:HH21	1:B:265:ASN:HA	1.69	0.56
1:B:5:ILE:HG22	1:B:6:GLN:N	2.18	0.56
1:D:46:VAL:CG1	1:D:80:LEU:HD12	2.36	0.56
1:A:242:LYS:HG3	1:A:243:LEU:HD13	1.86	0.56
1:C:257:LEU:HD12	1:C:268:VAL:CG1	2.35	0.56
1:A:345:MET:HE3	1:B:146:MET:HE3	1.87	0.56
1:C:97:LEU:HD21	1:D:15:LEU:HD13	1.86	0.56
1:B:331:ILE:HD11	1:B:423:LEU:HD11	1.87	0.56
1:D:272:VAL:HG12	1:D:273:THR:N	2.21	0.56
1:B:19:THR:O	1:B:23:GLN:HG3	2.05	0.56
1:D:334:VAL:HG21	1:D:373:PHE:CE1	2.41	0.56
1:A:5:ILE:HD11	1:B:54:ARG:HH21	1.71	0.56
1:C:400:LYS:HE2	1:C:407:GLN:NE2	2.20	0.56
1:B:21:ILE:N	1:B:21:ILE:HD12	2.22	0.55
1:C:138:PRO:HD3	1:C:236:HIS:CD2	2.41	0.55
1:C:70:PHE:CE2	1:C:78:LEU:HD23	2.41	0.55
1:D:46:VAL:HG13	1:D:80:LEU:HD12	1.88	0.55
1:B:411:ALA:O	1:B:415:VAL:HG13	2.06	0.55
1:D:225:LEU:O	1:D:227:ASP:N	2.39	0.55
1:A:82:PRO:HA	1:A:112:PHE:O	2.06	0.55
1:A:8:ILE:HD12	1:B:46:VAL:CG2	2.30	0.55
1:C:63:VAL:HG12	1:C:63:VAL:O	2.06	0.55
1:D:415:VAL:HG23	1:D:416:ALA:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:VAL:HB	1:A:398:VAL:HB	1.87	0.55
1:C:138:PRO:HD3	1:C:236:HIS:HD2	1.72	0.55
1:D:183:ALA:HB3	3:D:837:HOH:O	2.07	0.55
1:A:353:ASP:CG	1:B:153:ARG:HH12	2.09	0.55
1:C:391:GLU:H	1:C:391:GLU:CD	2.10	0.55
1:D:16:PRO:O	1:D:19:THR:HG22	2.07	0.55
1:A:52:PHE:CE1	1:A:82:PRO:HD2	2.42	0.55
1:C:239:GLY:O	1:C:242:LYS:HG2	2.07	0.55
1:A:309:LEU:O	1:A:313:VAL:HG23	2.07	0.54
1:C:62:VAL:HA	1:C:66:GLU:HB2	1.90	0.54
1:D:72:ASP:HB2	1:D:78:LEU:HD22	1.90	0.54
1:A:33:LEU:HD13	1:A:106:TRP:CG	2.41	0.54
1:B:261:LEU:HD22	1:B:261:LEU:N	2.21	0.54
1:B:410:VAL:HB	1:B:415:VAL:HG12	1.89	0.54
1:D:334:VAL:HG21	1:D:373:PHE:HE1	1.73	0.54
1:C:114:HIS:ND1	1:D:73:ARG:HD2	2.22	0.54
1:C:179:ASP:O	1:C:180:ALA:HB2	2.08	0.54
1:D:278:SER:O	1:D:279:GLN:NE2	2.41	0.54
1:C:383:VAL:HG12	1:C:384:ALA:N	2.21	0.54
1:B:273:THR:HG23	1:B:274:ASN:N	2.22	0.54
1:B:136:GLN:O	1:B:236:HIS:HE1	1.91	0.54
1:C:142:ALA:HB3	1:D:345:MET:HE3	1.90	0.54
1:A:401:ASP:OD1	1:A:403:ARG:HB2	2.08	0.54
1:D:172:GLU:N	1:D:172:GLU:OE2	2.41	0.54
1:D:333:LEU:CD1	1:D:348:ALA:HB2	2.38	0.54
1:A:11:MET:SD	1:B:46:VAL:HG22	2.48	0.53
1:C:147:LEU:HD23	1:C:147:LEU:O	2.08	0.53
1:A:72:ASP:HB2	1:A:78:LEU:HD22	1.90	0.53
1:B:273:THR:O	1:B:275:SER:N	2.41	0.53
1:C:307:MET:SD	1:C:312:LEU:HD22	2.48	0.53
1:D:388:GLY:O	1:D:392:VAL:HG23	2.09	0.53
1:C:90:ARG:NH2	1:D:13:ASP:OD2	2.39	0.53
1:D:121:ARG:HG2	1:D:311:ARG:HH21	1.72	0.53
1:A:225:LEU:N	1:A:225:LEU:HD12	2.23	0.53
1:D:161:VAL:HG12	1:D:271:TRP:CE3	2.43	0.53
1:D:5:ILE:CG2	1:D:6:GLN:N	2.71	0.53
1:A:11:MET:HG2	1:A:124:GLN:HB2	1.91	0.53
1:C:400:LYS:HE2	1:C:407:GLN:HE22	1.74	0.53
1:A:410:VAL:HG12	1:A:411:ALA:O	2.09	0.53
1:C:97:LEU:HD11	1:D:15:LEU:HD22	1.91	0.53
1:C:9:ARG:HH21	1:C:123:ARG:HH22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:CG2	1:C:6:GLN:N	2.71	0.53
1:C:73:ARG:NH2	1:D:67:MET:O	2.42	0.53
1:A:5:ILE:HD11	1:B:54:ARG:NH2	2.24	0.53
1:C:40:GLU:HB2	1:C:106:TRP:CE2	2.45	0.52
1:C:74:ASN:HD22	1:C:74:ASN:C	2.06	0.52
1:A:131:GLU:OE1	2:A:510:HSS:N12	2.42	0.52
1:C:163:LEU:HB2	1:C:271:TRP:CZ3	2.45	0.52
1:B:108:ILE:HD12	1:B:128:LEU:CD2	2.39	0.52
1:B:256:ARG:HH11	1:B:256:ARG:HG2	1.74	0.52
1:B:40:GLU:HB2	1:B:106:TRP:CE2	2.45	0.52
1:C:171:LEU:CD2	1:C:172:GLU:HG2	2.39	0.52
1:A:32:VAL:HG13	1:A:150:ARG:HD2	1.91	0.52
1:C:54:ARG:NH2	1:D:4:ASN:HA	2.23	0.52
1:A:272:VAL:HG12	1:A:273:THR:N	2.25	0.52
1:A:329:VAL:HG21	1:A:361:MET:HE3	1.92	0.52
1:A:3:LYS:HB2	1:A:4:ASN:HD22	1.75	0.52
1:D:259:ARG:HG3	1:D:268:VAL:HG22	1.91	0.52
1:A:285:GLY:HA3	1:A:305:PHE:HA	1.92	0.52
1:C:56:ILE:HG23	1:C:261:LEU:CD1	2.40	0.52
1:C:313:VAL:O	1:C:317:GLN:HG3	2.08	0.52
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.25	0.52
1:A:21:ILE:N	1:A:21:ILE:HD12	2.25	0.52
1:B:371:LYS:O	1:B:375:ARG:HG3	2.09	0.52
1:C:171:LEU:HD22	1:C:172:GLU:H	1.74	0.51
1:C:175:ALA:C	1:C:177:TYR:H	2.12	0.51
1:C:320:ASN:O	1:C:322:GLU:N	2.43	0.51
1:C:259:ARG:NH1	1:C:259:ARG:HG3	2.24	0.51
1:C:411:ALA:O	1:C:414:SER:HB2	2.10	0.51
1:C:46:VAL:HG23	1:D:11:MET:SD	2.50	0.51
1:B:350:ARG:NH2	1:B:413:ASP:HA	2.26	0.51
1:C:74:ASN:HD21	1:C:76:ASP:N	2.01	0.51
1:B:287:ARG:HD3	1:B:289:ASP:OD2	2.11	0.51
1:D:273:THR:HG23	1:D:274:ASN:N	2.26	0.51
1:D:274:ASN:ND2	1:D:276:LEU:HD21	2.16	0.51
1:C:74:ASN:ND2	1:C:75:GLY:N	2.55	0.51
1:A:104:ARG:HG2	1:A:132:VAL:HG13	1.93	0.51
1:A:229:LEU:O	1:A:234:ARG:NH1	2.43	0.51
1:A:257:LEU:HD11	1:A:270:GLU:HG3	1.93	0.51
1:C:320:ASN:C	1:C:322:GLU:H	2.13	0.51
1:D:305:PHE:C	1:D:305:PHE:CD1	2.83	0.51
1:A:112:PHE:CE2	1:A:124:GLN:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:N	1:C:5:ILE:HD12	2.26	0.51
1:D:239:GLY:O	1:D:243:LEU:HD13	2.11	0.51
1:D:22:TRP:CE2	1:D:313:VAL:HG21	2.46	0.51
1:C:52:PHE:CE1	1:C:82:PRO:HD2	2.46	0.51
1:D:275:SER:OG	1:D:276:LEU:N	2.44	0.51
1:D:74:ASN:C	1:D:74:ASN:ND2	2.65	0.51
1:B:331:ILE:HD13	1:B:419:LEU:HD13	1.93	0.50
1:D:172:GLU:N	1:D:172:GLU:CD	2.62	0.50
1:B:161:VAL:HG12	1:B:271:TRP:HE3	1.76	0.50
1:B:74:ASN:ND2	1:B:74:ASN:C	2.65	0.50
1:A:319:VAL:O	1:A:321:PRO:HD3	2.12	0.50
1:B:117:PRO:C	1:B:118:GLN:HG2	2.32	0.50
1:B:264:TYR:HA	1:B:287:ARG:O	2.11	0.50
1:B:33:LEU:HD11	1:B:128:LEU:HD11	1.94	0.50
1:D:410:VAL:HG12	1:D:411:ALA:O	2.11	0.50
1:A:28:THR:HG21	1:A:155:LEU:HD13	1.94	0.50
1:B:396:THR:HG22	1:B:411:ALA:HA	1.93	0.50
1:A:102:GLU:HA	1:A:133:PHE:O	2.12	0.49
1:B:15:LEU:HB3	1:B:16:PRO:HD2	1.93	0.49
1:B:355:LEU:HD21	1:B:420:ARG:HB2	1.93	0.49
1:C:150:ARG:HG3	1:C:150:ARG:HH11	1.77	0.49
1:D:231:GLU:OE2	1:D:234:ARG:HD3	2.12	0.49
1:D:146:MET:HG2	1:D:249:ILE:HD11	1.94	0.49
1:A:345:MET:SD	1:A:364:HIS:HE1	2.35	0.49
1:A:383:VAL:HG12	1:A:384:ALA:N	2.26	0.49
1:B:161:VAL:HG12	1:B:271:TRP:CE3	2.48	0.49
1:C:236:HIS:HD1	1:C:266:ARG:HD2	1.77	0.49
1:D:103:GLN:HB3	1:D:105:LEU:HD21	1.93	0.49
1:C:141:ASP:O	1:C:145:ILE:HG13	2.12	0.49
1:C:292:VAL:HG11	1:C:300:THR:HG22	1.94	0.49
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.95	0.49
1:C:73:ARG:HG3	1:D:114:HIS:CE1	2.48	0.49
1:D:18:GLU:HA	1:D:21:ILE:HD13	1.95	0.49
1:D:351:LEU:HD13	1:D:419:LEU:HD11	1.94	0.49
1:A:390:SER:O	1:A:393:ALA:N	2.44	0.49
1:C:150:ARG:HG3	1:C:150:ARG:NH1	2.28	0.49
1:D:385:VAL:O	1:D:385:VAL:HG23	2.12	0.49
1:D:259:ARG:HH22	2:D:810:HSS:HN1S	1.58	0.49
1:B:319:VAL:HG12	1:B:320:ASN:HD21	1.77	0.49
1:C:39:SER:OG	1:D:328:VAL:HG11	2.13	0.49
1:B:5:ILE:CG2	1:B:6:GLN:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:LEU:HD21	1:C:415:VAL:HG23	1.93	0.49
1:D:225:LEU:O	1:D:226:GLY:C	2.51	0.49
1:D:24:ARG:HD3	1:D:323:PHE:CE2	2.48	0.49
1:C:13:ASP:OD2	1:D:90:ARG:NH2	2.42	0.49
1:A:322:GLU:HB2	3:A:524:HOH:O	2.12	0.49
1:C:242:LYS:HG3	1:C:243:LEU:N	2.28	0.48
1:D:333:LEU:HG	1:D:385:VAL:CG2	2.43	0.48
1:A:69:THR:HA	1:A:78:LEU:O	2.13	0.48
1:C:146:MET:HE3	1:D:345:MET:HE3	1.95	0.48
1:C:48:GLN:C	1:C:50:PRO:HD2	2.34	0.48
1:D:259:ARG:NH1	1:D:264:TYR:CZ	2.81	0.48
1:A:118:GLN:HG3	1:A:121:ARG:NE	2.27	0.48
1:B:18:GLU:HA	1:B:21:ILE:HD13	1.95	0.48
1:B:33:LEU:HD13	1:B:106:TRP:CG	2.48	0.48
1:B:54:ARG:HD2	3:B:612:HOH:O	2.14	0.48
1:A:232:GLU:HA	1:A:235:GLU:HB3	1.96	0.48
1:C:274:ASN:N	1:C:274:ASN:HD22	2.11	0.48
1:C:274:ASN:H	1:C:274:ASN:ND2	2.10	0.48
1:D:33:LEU:HD11	1:D:128:LEU:HD11	1.95	0.48
1:D:245:GLU:C	1:D:247:ALA:H	2.17	0.48
1:D:274:ASN:HB2	1:D:276:LEU:HD22	1.95	0.48
1:B:100:ASN:C	1:B:101:GLN:HG3	2.32	0.48
1:B:165:LEU:HD11	1:B:244:LEU:CD2	2.44	0.48
1:B:274:ASN:ND2	1:B:276:LEU:HD22	2.29	0.48
1:D:245:GLU:C	1:D:247:ALA:N	2.67	0.48
1:A:332:TYR:CE2	1:A:363:ASN:HB2	2.49	0.48
1:D:332:TYR:CD2	1:D:376:ALA:HB2	2.49	0.48
1:A:411:ALA:O	1:A:414:SER:HB2	2.14	0.48
1:B:322:GLU:O	1:B:323:PHE:C	2.52	0.48
1:B:5:ILE:HD12	1:B:5:ILE:H	1.79	0.48
1:C:167:SER:HA	1:C:266:ARG:O	2.14	0.48
1:D:351:LEU:HD21	1:D:415:VAL:CG2	2.44	0.48
1:A:118:GLN:HG3	1:A:121:ARG:HE	1.79	0.47
1:A:178:ARG:HG2	1:A:179:ASP:H	1.73	0.47
1:A:65:LYS:O	1:B:73:ARG:NH1	2.38	0.47
1:B:166:ASN:O	1:B:268:VAL:HG12	2.14	0.47
1:B:305:PHE:C	1:B:305:PHE:CD1	2.86	0.47
1:C:383:VAL:CG1	1:C:384:ALA:N	2.77	0.47
1:D:278:SER:C	1:D:279:GLN:HG2	2.33	0.47
1:A:229:LEU:CD1	1:A:233:SER:HB3	2.44	0.47
1:A:5:ILE:HD12	1:A:5:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:VAL:HG23	1:C:416:ALA:N	2.28	0.47
1:A:237:PHE:CE2	1:A:241:CYS:SG	3.07	0.47
1:A:311:ARG:NH1	2:A:510:HSS:H2'	2.29	0.47
1:C:164:GLU:HA	1:C:252:THR:O	2.14	0.47
1:C:390:SER:HB2	1:C:391:GLU:OE1	2.14	0.47
1:C:97:LEU:C	1:C:98:LEU:HD23	2.34	0.47
1:D:245:GLU:O	1:D:247:ALA:N	2.47	0.47
1:A:63:VAL:HA	1:A:67:MET:HG3	1.97	0.47
1:C:320:ASN:N	1:C:321:PRO:HD3	2.29	0.47
1:C:114:HIS:CE1	1:D:73:ARG:HD2	2.49	0.47
1:A:345:MET:HE2	1:B:146:MET:HE1	1.95	0.47
1:A:331:ILE:HD11	1:A:423:LEU:HD11	1.96	0.47
1:C:49:THR:N	1:C:50:PRO:CD	2.76	0.47
1:A:177:TYR:O	1:A:177:TYR:CG	2.67	0.47
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.80	0.47
1:D:5:ILE:N	1:D:5:ILE:HD12	2.25	0.47
1:C:368:ASN:OD1	1:C:370:LYS:HB3	2.14	0.47
1:A:229:LEU:HG	1:A:233:SER:HB2	1.95	0.47
1:B:49:THR:N	1:B:50:PRO:HD2	2.30	0.47
1:D:240:LEU:O	1:D:244:LEU:HD13	2.15	0.47
1:D:127:GLN:HA	1:D:307:MET:O	2.14	0.47
1:D:411:ALA:O	1:D:415:VAL:HG13	2.14	0.47
1:B:333:LEU:HG	1:B:385:VAL:CG2	2.43	0.47
1:D:385:VAL:O	1:D:385:VAL:CG2	2.63	0.47
1:B:383:VAL:HG12	1:B:384:ALA:N	2.30	0.47
1:C:108:ILE:HD12	1:C:128:LEU:HD23	1.96	0.47
1:C:171:LEU:CD1	1:C:172:GLU:H	2.22	0.47
1:C:99:TYR:CE1	1:C:298:ARG:NH1	2.83	0.47
1:C:65:LYS:H	1:C:65:LYS:HG3	1.58	0.46
1:A:96:GLY:O	1:A:97:LEU:HD23	2.14	0.46
1:C:165:LEU:O	1:C:166:ASN:HB2	2.15	0.46
1:C:93:ILE:CD1	1:C:297:GLY:HA3	2.38	0.46
1:A:228:TYR:O	1:A:229:LEU:C	2.53	0.46
1:A:229:LEU:HG	1:A:233:SER:CB	2.45	0.46
1:C:293:GLU:HA	1:C:297:GLY:O	2.15	0.46
1:C:287:ARG:CZ	1:C:303:VAL:HG22	2.45	0.46
1:C:423:LEU:O	1:C:424:GLY:C	2.53	0.46
1:D:398:VAL:CG1	1:D:407:GLN:HB2	2.45	0.46
1:D:410:VAL:HB	1:D:415:VAL:HG12	1.97	0.46
1:A:125:PHE:HA	1:A:310:GLU:OE2	2.16	0.46
1:B:319:VAL:C	1:B:320:ASN:ND2	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:GLU:HB2	1:D:106:TRP:CZ2	2.50	0.46
1:D:171:LEU:HB3	1:D:172:GLU:OE2	2.15	0.46
1:D:224:ALA:HB3	3:D:841:HOH:O	2.14	0.46
1:D:404:SER:OG	1:D:406:GLU:HG2	2.16	0.46
1:B:36:TYR:HE1	1:B:150:ARG:HD2	1.79	0.46
1:B:174:ARG:O	1:B:177:TYR:HB3	2.15	0.46
1:B:368:ASN:OD1	1:B:370:LYS:HB3	2.15	0.46
1:D:256:ARG:HG2	1:D:256:ARG:HH11	1.80	0.46
1:A:254:ASN:ND2	1:A:257:LEU:HB2	2.31	0.46
1:D:56:ILE:O	1:D:262:ASP:HB2	2.16	0.46
1:A:350:ARG:HD3	1:A:354:GLU:OE2	2.16	0.46
1:C:112:PHE:CE2	1:C:124:GLN:HG3	2.50	0.46
1:D:170:SER:O	1:D:174:ARG:HB2	2.16	0.46
1:D:355:LEU:HB3	1:D:358:VAL:CG2	2.46	0.46
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.98	0.46
1:C:291:LEU:HD12	1:C:291:LEU:O	2.15	0.46
1:D:45:ILE:HD12	1:D:110:PRO:HG2	1.97	0.46
1:A:229:LEU:HD11	1:A:233:SER:HB3	1.98	0.45
1:A:291:LEU:O	1:A:291:LEU:HD12	2.16	0.45
1:A:293:GLU:C	1:A:295:LEU:H	2.20	0.45
1:B:132:VAL:HG11	1:B:140:ILE:HG12	1.98	0.45
1:B:350:ARG:HH22	1:B:413:ASP:HA	1.81	0.45
1:A:15:LEU:HD22	1:B:97:LEU:HD11	1.98	0.45
1:C:104:ARG:HG2	1:C:132:VAL:HG13	1.98	0.45
1:D:115:GLU:O	1:D:117:PRO:HD3	2.15	0.45
1:D:331:ILE:HD11	1:D:423:LEU:HD11	1.97	0.45
1:B:163:LEU:HD21	1:B:165:LEU:HD21	1.98	0.45
1:D:230:ASP:N	1:D:230:ASP:OD1	2.46	0.45
1:A:142:ALA:HB3	1:B:345:MET:HE3	1.98	0.45
1:B:298:ARG:HB3	1:B:298:ARG:HE	1.61	0.45
1:C:259:ARG:NH1	1:C:264:TYR:CZ	2.84	0.45
1:A:283:CYS:SG	1:A:305:PHE:CD1	3.09	0.45
1:A:44:PRO:HD3	1:B:13:ASP:OD1	2.15	0.45
1:C:274:ASN:N	1:C:274:ASN:ND2	2.63	0.45
1:D:15:LEU:HB3	1:D:16:PRO:HD2	1.98	0.45
1:D:277:GLY:O	1:D:278:SER:HB3	2.16	0.45
1:D:131:GLU:OE1	2:D:810:HSS:N12	2.49	0.45
1:A:267:THR:HG22	1:A:268:VAL:N	2.32	0.45
1:B:385:VAL:CG2	1:B:385:VAL:O	2.65	0.45
1:B:90:ARG:NH2	1:B:91:ALA:HB2	2.32	0.45
1:C:229:LEU:HB2	1:C:234:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:PHE:C	1:C:305:PHE:CD1	2.90	0.45
1:A:230:ASP:O	1:A:233:SER:HB2	2.17	0.45
1:A:385:VAL:HG23	1:A:385:VAL:O	2.16	0.45
1:C:141:ASP:CB	1:C:240:LEU:HD13	2.46	0.45
1:C:390:SER:O	1:C:393:ALA:N	2.49	0.45
1:D:186:GLU:O	1:D:187:GLN:C	2.54	0.45
1:A:138:PRO:O	1:A:240:LEU:HD13	2.17	0.45
1:C:322:GLU:O	1:C:323:PHE:C	2.55	0.45
1:A:288:TYR:CD2	1:A:288:TYR:O	2.70	0.45
1:D:97:LEU:HB3	1:D:103:GLN:NE2	2.22	0.45
1:A:115:GLU:OE1	1:A:121:ARG:CD	2.64	0.45
1:A:245:GLU:C	1:A:247:ALA:H	2.20	0.45
1:C:256:ARG:NH1	1:C:256:ARG:HG2	2.31	0.45
1:D:117:PRO:C	1:D:118:GLN:HG2	2.37	0.45
1:D:333:LEU:HG	1:D:385:VAL:HG22	1.99	0.45
1:D:60:THR:O	1:D:64:GLU:HB2	2.17	0.45
1:D:68:TYR:OH	1:D:123:ARG:HD3	2.17	0.45
1:A:139:ASP:HA	1:A:243:LEU:CD2	2.47	0.44
1:A:407:GLN:C	1:A:408:THR:HG22	2.36	0.44
1:A:172:GLU:O	1:A:176:ASN:HB2	2.17	0.44
1:A:146:MET:SD	1:B:345:MET:HG2	2.58	0.44
1:A:274:ASN:ND2	1:A:274:ASN:N	2.64	0.44
1:A:289:ASP:OD1	1:A:301:PRO:HA	2.17	0.44
1:D:278:SER:HB3	1:D:279:GLN:HE21	1.82	0.44
1:A:174:ARG:C	1:A:176:ASN:H	2.20	0.44
1:B:146:MET:HG2	1:B:249:ILE:HD11	1.99	0.44
1:C:21:ILE:N	1:C:21:ILE:CD1	2.75	0.44
1:D:165:LEU:HD11	1:D:244:LEU:HD22	1.98	0.44
1:D:49:THR:N	1:D:50:PRO:HD2	2.33	0.44
1:A:245:GLU:C	1:A:247:ALA:N	2.69	0.44
1:D:320:ASN:O	1:D:322:GLU:N	2.51	0.44
1:A:146:MET:O	1:A:149:ALA:HB3	2.17	0.44
1:B:62:VAL:HA	1:B:66:GLU:HB2	1.99	0.44
1:C:320:ASN:C	1:C:322:GLU:N	2.71	0.44
1:C:93:ILE:HD12	1:C:297:GLY:CA	2.38	0.44
1:A:274:ASN:ND2	1:A:274:ASN:H	2.16	0.44
1:C:116:ARG:N	3:C:732:HOH:O	2.50	0.44
1:D:33:LEU:HD13	1:D:106:TRP:CG	2.53	0.44
1:D:259:ARG:CZ	1:D:259:ARG:HB3	2.48	0.44
1:A:38:TYR:N	1:A:38:TYR:CD1	2.86	0.44
1:B:274:ASN:HD22	1:B:276:LEU:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:VAL:HG12	1:C:411:ALA:N	2.31	0.44
1:A:178:ARG:CG	1:A:179:ASP:H	2.30	0.44
1:C:385:VAL:O	1:C:385:VAL:HG23	2.18	0.44
1:D:33:LEU:HD13	1:D:106:TRP:CD2	2.52	0.44
1:D:320:ASN:N	1:D:320:ASN:ND2	2.65	0.43
1:A:269:PHE:CZ	1:A:305:PHE:HB3	2.53	0.43
1:A:307:MET:SD	1:A:312:LEU:HD13	2.57	0.43
1:B:264:TYR:OH	2:B:610:HSS:N11	2.39	0.43
1:C:293:GLU:C	1:C:295:LEU:H	2.22	0.43
1:A:345:MET:HE3	1:B:146:MET:CE	2.48	0.43
1:A:259:ARG:HH22	2:A:510:HSS:HN1S	1.66	0.43
1:A:56:ILE:HG23	1:A:261:LEU:CD1	2.49	0.43
1:B:336:SER:OG	1:B:369:PHE:CZ	2.70	0.43
1:B:68:TYR:HB2	1:B:80:LEU:HB2	1.99	0.43
1:D:74:ASN:ND2	1:D:76:ASP:OD2	2.51	0.43
1:A:293:GLU:HB2	1:A:299:ALA:CB	2.47	0.43
1:B:274:ASN:O	1:B:275:SER:HB3	2.18	0.43
1:C:106:TRP:HA	1:C:129:GLY:O	2.17	0.43
1:C:259:ARG:C	1:C:261:LEU:H	2.20	0.43
1:D:373:PHE:O	1:D:376:ALA:HB3	2.18	0.43
1:D:5:ILE:CD1	1:D:5:ILE:H	2.26	0.43
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.80	0.43
1:B:106:TRP:HA	1:B:129:GLY:O	2.18	0.43
1:D:277:GLY:O	1:D:278:SER:CB	2.67	0.43
1:D:65:LYS:NZ	1:D:65:LYS:HB3	2.33	0.43
1:A:253:VAL:HG12	1:A:254:ASN:N	2.33	0.43
1:A:69:THR:HG23	1:A:78:LEU:O	2.18	0.43
1:C:175:ALA:C	1:C:177:TYR:N	2.72	0.43
1:C:259:ARG:O	1:C:261:LEU:N	2.49	0.43
1:C:157:ILE:HD12	1:C:315:LEU:HD23	2.01	0.43
1:A:168:ILE:CD1	1:A:174:ARG:HH21	2.30	0.43
1:A:176:ASN:HB3	1:A:228:TYR:CE2	2.54	0.43
1:A:167:SER:HA	1:A:266:ARG:O	2.19	0.43
1:C:293:GLU:O	1:C:295:LEU:N	2.51	0.43
1:C:386:VAL:HB	1:C:398:VAL:HB	2.01	0.43
1:C:48:GLN:HB3	1:C:50:PRO:HG2	2.01	0.43
1:A:298:ARG:HA	1:A:298:ARG:HD3	1.88	0.43
1:A:105:LEU:HD22	1:B:16:PRO:HG3	2.00	0.43
1:A:138:PRO:CB	1:A:240:LEU:HB2	2.46	0.43
1:D:142:ALA:HB1	1:D:146:MET:HE3	2.00	0.43
1:D:273:THR:O	1:D:274:ASN:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:LEU:HB3	1:D:358:VAL:HG22	2.00	0.43
1:A:118:GLN:HB2	1:A:121:ARG:HB2	2.01	0.42
1:A:264:TYR:HD1	1:A:287:ARG:O	2.02	0.42
1:B:276:LEU:O	1:B:277:GLY:C	2.56	0.42
1:D:135:LEU:HD12	1:D:140:ILE:HD13	2.01	0.42
1:D:225:LEU:HG	1:D:226:GLY:N	2.34	0.42
1:B:56:ILE:O	1:B:262:ASP:HB2	2.20	0.42
1:B:43:LEU:HD11	1:B:88:CYS:HA	2.00	0.42
1:C:283:CYS:SG	1:C:305:PHE:CD1	3.13	0.42
1:C:410:VAL:CG1	1:C:411:ALA:N	2.81	0.42
1:B:371:LYS:O	1:B:374:ALA:HB3	2.20	0.42
1:D:21:ILE:H	1:D:21:ILE:HD12	1.84	0.42
1:A:17:GLY:O	1:A:21:ILE:HD13	2.19	0.42
1:A:296:GLY:HA3	1:B:4:ASN:HB3	2.02	0.42
1:A:48:GLN:C	1:A:50:PRO:HD2	2.38	0.42
1:B:40:GLU:HA	1:B:106:TRP:O	2.20	0.42
1:D:82:PRO:HA	1:D:112:PHE:O	2.20	0.42
1:A:294:GLN:HG2	1:A:294:GLN:O	2.19	0.42
1:A:412:GLN:C	1:A:414:SER:N	2.73	0.42
1:A:73:ARG:HG3	3:A:550:HOH:O	2.20	0.42
1:A:10:GLY:C	1:A:11:MET:HG3	2.40	0.42
1:A:114:HIS:CE1	1:A:123:ARG:NH1	2.87	0.42
1:B:245:GLU:C	1:B:247:ALA:H	2.23	0.42
1:D:419:LEU:O	1:D:422:LEU:HD12	2.19	0.42
1:A:259:ARG:HG3	1:A:264:TYR:CE2	2.54	0.42
1:C:33:LEU:HD11	1:C:128:LEU:HD11	2.01	0.42
1:C:415:VAL:O	1:C:416:ALA:C	2.58	0.42
1:A:15:LEU:HB3	1:A:16:PRO:HD2	2.01	0.42
1:A:336:SER:O	1:A:340:THR:CG2	2.68	0.42
1:B:233:SER:OG	1:B:266:ARG:HD3	2.20	0.42
1:B:274:ASN:O	1:B:275:SER:CB	2.68	0.42
1:C:259:ARG:NH1	1:C:264:TYR:CE2	2.87	0.42
1:C:332:TYR:CD2	1:C:376:ALA:HB2	2.55	0.42
1:C:8:ILE:O	1:C:11:MET:HG3	2.20	0.42
1:D:174:ARG:O	1:D:177:TYR:HB3	2.19	0.42
1:A:260:GLY:C	1:A:261:LEU:HD22	2.40	0.42
1:A:274:ASN:HD22	1:A:274:ASN:N	2.16	0.42
1:A:46:VAL:HG22	1:B:11:MET:SD	2.60	0.42
1:B:320:ASN:O	1:B:322:GLU:N	2.53	0.42
1:A:351:LEU:HD21	1:A:415:VAL:HG23	2.02	0.42
1:D:106:TRP:HA	1:D:129:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HB	1:A:174:ARG:HH21	1.85	0.41
1:A:269:PHE:HZ	1:A:305:PHE:HB3	1.85	0.41
1:C:165:LEU:HD23	1:C:269:PHE:HB3	2.02	0.41
1:C:171:LEU:HD13	1:C:172:GLU:N	2.26	0.41
1:D:350:ARG:NH1	1:D:412:GLN:HB3	2.35	0.41
1:D:415:VAL:CG2	1:D:416:ALA:N	2.83	0.41
1:A:345:MET:CE	1:B:146:MET:HE1	2.50	0.41
1:D:17:GLY:O	1:D:21:ILE:HD12	2.21	0.41
1:D:24:ARG:HD2	1:D:324:LYS:O	2.20	0.41
1:A:108:ILE:HB	1:A:128:LEU:HD22	2.03	0.41
1:C:270:GLU:OE1	1:C:281:THR:HG21	2.21	0.41
1:D:9:ARG:HG2	1:D:117:PRO:HG2	2.03	0.41
1:A:412:GLN:C	1:A:414:SER:H	2.23	0.41
1:A:49:THR:O	1:A:50:PRO:C	2.57	0.41
1:D:292:VAL:HG21	1:D:300:THR:HG22	2.02	0.41
1:A:291:LEU:HD11	1:A:295:LEU:HD22	2.02	0.41
1:A:5:ILE:CD1	1:B:54:ARG:NH2	2.84	0.41
1:B:175:ALA:C	1:B:177:TYR:H	2.23	0.41
1:B:415:VAL:HG23	1:B:416:ALA:N	2.36	0.41
1:B:419:LEU:O	1:B:422:LEU:N	2.49	0.41
1:D:20:ALA:HB1	1:D:325:ALA:HB1	2.02	0.41
1:B:329:VAL:HB	1:B:379:TRP:HB3	2.02	0.41
1:C:90:ARG:HH22	1:D:13:ASP:CG	2.22	0.41
1:C:89:VAL:O	1:C:93:ILE:HG12	2.20	0.41
1:D:54:ARG:CD	3:D:870:HOH:O	2.68	0.41
1:D:54:ARG:O	1:D:294:GLN:NE2	2.53	0.41
1:D:74:ASN:HD22	1:D:75:GLY:N	2.18	0.41
1:A:242:LYS:HG3	1:A:243:LEU:CD1	2.49	0.41
1:B:259:ARG:HH22	2:B:610:HSS:HN1S	1.69	0.41
1:A:3:LYS:O	1:B:54:ARG:NH2	2.54	0.41
1:D:333:LEU:HD12	1:D:348:ALA:HB2	2.02	0.41
1:D:371:LYS:O	1:D:374:ALA:N	2.53	0.41
1:B:259:ARG:CG	1:B:268:VAL:HG22	2.50	0.41
1:B:257:LEU:HD12	1:B:268:VAL:HG13	2.03	0.41
1:B:320:ASN:N	1:B:320:ASN:HD22	2.15	0.41
1:C:289:ASP:OD1	1:C:301:PRO:HB3	2.21	0.41
1:C:170:SER:O	1:C:171:LEU:C	2.59	0.41
1:C:253:VAL:HG12	1:C:254:ASN:N	2.35	0.41
1:C:56:ILE:O	1:C:56:ILE:HG22	2.19	0.41
1:D:345:MET:O	1:D:348:ALA:HB3	2.21	0.41
1:D:383:VAL:HG21	1:D:422:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLU:O	1:A:392:VAL:HB	2.21	0.41
1:A:73:ARG:HG3	1:B:114:HIS:CE1	2.56	0.41
1:B:17:GLY:O	1:B:21:ILE:CD1	2.69	0.41
1:C:161:VAL:HG12	1:C:271:TRP:CE3	2.56	0.41
1:D:274:ASN:HD22	1:D:276:LEU:CD2	2.19	0.41
1:B:320:ASN:ND2	1:B:320:ASN:N	2.69	0.41
1:B:329:VAL:O	1:B:381:ALA:HA	2.21	0.41
1:C:294:GLN:HG2	1:C:294:GLN:O	2.21	0.41
1:D:340:THR:O	1:D:343:ALA:HB3	2.21	0.41
1:A:18:GLU:O	1:A:22:TRP:HD1	2.04	0.40
1:C:412:GLN:C	1:C:414:SER:H	2.24	0.40
1:D:136:GLN:HB2	1:D:301:PRO:HG2	2.04	0.40
1:C:54:ARG:NH2	1:D:5:ILE:HD12	2.36	0.40
1:C:32:VAL:HG13	1:C:150:ARG:HD2	2.03	0.40
1:D:54:ARG:HD3	3:D:870:HOH:O	2.22	0.40
1:A:165:LEU:HD22	1:A:269:PHE:HB3	2.04	0.40
1:A:368:ASN:OD1	1:A:368:ASN:C	2.59	0.40
1:B:259:ARG:HG2	1:B:268:VAL:CG2	2.52	0.40
1:B:333:LEU:C	1:B:333:LEU:HD23	2.41	0.40
1:B:398:VAL:CG1	1:B:407:GLN:HB2	2.51	0.40
1:C:53:LYS:HA	1:C:63:VAL:HG11	2.04	0.40
1:D:242:LYS:HG3	1:D:243:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/431 (85%)	324 (88%)	31 (8%)	11 (3%)	4	10
1	B	372/431 (86%)	343 (92%)	18 (5%)	11 (3%)	4	10
1	C	366/431 (85%)	329 (90%)	26 (7%)	11 (3%)	4	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	381/431 (88%)	330 (87%)	39 (10%)	12 (3%)	4	9
All	All	1485/1724 (86%)	1326 (89%)	114 (8%)	45 (3%)	4	10

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	A	266	ARG
1	B	274	ASN
1	B	275	SER
1	C	4	ASN
1	C	54	ARG
1	D	279	GLN
1	A	169	GLY
1	B	137	GLY
1	B	277	GLY
1	B	341	GLN
1	C	176	ASN
1	C	291	LEU
1	C	341	GLN
1	C	390	SER
1	D	226	GLY
1	D	274	ASN
1	D	275	SER
1	D	277	GLY
1	D	341	GLN
1	A	294	GLN
1	A	397	ALA
1	B	166	ASN
1	B	390	SER
1	C	294	GLN
1	D	119	LYS
1	D	246	SER
1	D	276	LEU
1	A	16	PRO
1	A	137	GLY
1	B	321	PRO
1	C	321	PRO
1	A	54	ARG
1	A	228	TYR
1	B	246	SER
1	C	227	ASP

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Mol	Chain	Res	Type
1	C	391	GLU
1	D	16	PRO
1	D	225	LEU
1	D	321	PRO
1	A	170	SER
1	A	321	PRO
1	B	16	PRO
1	C	16	PRO
1	B	157	ILE

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	297/347 (86%)	267 (90%)	30 (10%)	7	17
1	B	299/347 (86%)	267 (89%)	32 (11%)	6	15
1	C	296/347 (85%)	269 (91%)	27 (9%)	9	21
1	D	306/347 (88%)	273 (89%)	33 (11%)	6	15
All	All	1198/1388 (86%)	1076 (90%)	122 (10%)	7	17

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	18	GLU
1	A	19	THR
1	A	65	LYS
1	A	74	ASN
1	A	78	LEU
1	A	83	GLU
1	A	90	ARG
1	A	98	LEU
1	A	141	ASP
1	A	152	TRP
1	A	155	LEU

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Mol	Chain	Res	Type
1	A	172	GLU
1	A	178	ARG
1	A	225	LEU
1	A	228	TYR
1	A	244	LEU
1	A	274	ASN
1	A	281	THR
1	A	295	LEU
1	A	303	VAL
1	A	314	LEU
1	A	320	ASN
1	A	324	LYS
1	A	326	ASP
1	A	339	ASP
1	A	345	MET
1	A	350	ARG
1	A	407	GLN
1	A	408	THR
1	B	16	PRO
1	B	19	THR
1	B	46	VAL
1	B	74	ASN
1	B	78	LEU
1	B	80	LEU
1	B	83	GLU
1	B	90	ARG
1	B	128	LEU
1	B	136	GLN
1	B	141	ASP
1	B	171	LEU
1	B	174	ARG
1	B	178	ARG
1	B	229	LEU
1	B	230	ASP
1	B	244	LEU
1	B	261	LEU
1	B	263	TYR
1	B	266	ARG
1	B	268	VAL
1	B	273	THR
1	B	276	LEU
1	B	279	GLN

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Mol	Chain	Res	Type
1	B	281	THR
1	B	303	VAL
1	B	314	LEU
1	B	324	LYS
1	B	326	ASP
1	B	328	VAL
1	B	339	ASP
1	B	407	GLN
1	C	11	MET
1	C	18	GLU
1	C	19	THR
1	C	48	GLN
1	C	54	ARG
1	C	62	VAL
1	C	65	LYS
1	C	73	ARG
1	C	74	ASN
1	C	78	LEU
1	C	83	GLU
1	C	90	ARG
1	C	141	ASP
1	C	155	LEU
1	C	171	LEU
1	C	227	ASP
1	C	244	LEU
1	C	257	LEU
1	C	268	VAL
1	C	274	ASN
1	C	295	LEU
1	C	303	VAL
1	C	339	ASP
1	C	345	MET
1	C	350	ARG
1	C	407	GLN
1	C	408	THR
1	D	16	PRO
1	D	19	THR
1	D	46	VAL
1	D	48	GLN
1	D	65	LYS
1	D	74	ASN
1	D	78	LEU

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Mol	Chain	Res	Type
1	D	80	LEU
1	D	83	GLU
1	D	90	ARG
1	D	128	LEU
1	D	141	ASP
1	D	155	LEU
1	D	172	GLU
1	D	184	PHE
1	D	187	GLN
1	D	227	ASP
1	D	230	ASP
1	D	257	LEU
1	D	261	LEU
1	D	262	ASP
1	D	263	TYR
1	D	266	ARG
1	D	268	VAL
1	D	273	THR
1	D	279	GLN
1	D	281	THR
1	D	295	LEU
1	D	303	VAL
1	D	320	ASN
1	D	326	ASP
1	D	362	THR
1	D	422	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	6	GLN
1	A	74	ASN
1	A	236	HIS
1	A	274	ASN
1	A	320	ASN
1	A	341	GLN
1	A	407	GLN
1	B	6	GLN
1	B	12	ASN
1	B	74	ASN
1	B	114	HIS

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	236	HIS
1	B	274	ASN
1	B	279	GLN
1	B	320	ASN
1	C	74	ASN
1	C	127	GLN
1	C	254	ASN
1	C	274	ASN
1	C	317	GLN
1	C	364	HIS
1	C	407	GLN
1	D	6	GLN
1	D	12	ASN
1	D	74	ASN
1	D	103	GLN
1	D	114	HIS
1	D	127	GLN
1	D	236	HIS
1	D	274	ASN
1	D	320	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	HSS	A	510	-	29,36,36	2.99	6 (20%)	31,53,53	2.38	5 (16%)
2	HSS	B	610	-	29,36,36	3.01	6 (20%)	31,53,53	1.69	6 (19%)
2	HSS	C	710	-	29,36,36	3.01	6 (20%)	31,53,53	2.07	5 (16%)
2	HSS	D	810	-	29,36,36	3.00	6 (20%)	31,53,53	1.87	7 (22%)

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	HSS	A	510	-	-	2/18/39/39	0/4/4/4
2	HSS	B	610	-	-	4/18/39/39	0/4/4/4
2	HSS	C	710	-	-	7/18/39/39	0/4/4/4
2	HSS	D	810	-	-	5/18/39/39	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	HSS	O2S-S	9.72	1.50	1.42
2	C	710	HSS	O2S-S	9.54	1.50	1.42
2	D	810	HSS	O2S-S	9.53	1.50	1.42
2	A	510	HSS	O3S-S	9.50	1.50	1.42
2	C	710	HSS	O3S-S	9.34	1.50	1.42
2	A	510	HSS	O2S-S	9.32	1.50	1.42
2	D	810	HSS	O3S-S	9.28	1.50	1.42
2	B	610	HSS	O3S-S	9.16	1.50	1.42
2	C	710	HSS	O5'-S	-7.81	1.43	1.59
2	D	810	HSS	O5'-S	-7.76	1.43	1.59
2	A	510	HSS	O5'-S	-7.74	1.43	1.59
2	B	610	HSS	O5'-S	-7.68	1.43	1.59
2	B	610	HSS	O4'-C1'	2.54	1.44	1.41
2	C	710	HSS	O4'-C1'	2.34	1.44	1.41
2	A	510	HSS	O4'-C1'	2.31	1.44	1.41
2	B	610	HSS	S-N1S	2.29	1.63	1.59
2	D	810	HSS	O4'-C1'	2.26	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	810	HSS	S-N1S	2.22	1.63	1.59
2	C	710	HSS	C-N1S	-2.16	1.33	1.37
2	C	710	HSS	S-N1S	2.11	1.63	1.59
2	A	510	HSS	C-N1S	-2.10	1.33	1.37
2	A	510	HSS	S-N1S	2.06	1.63	1.59
2	B	610	HSS	C-N1S	-2.02	1.33	1.37
2	D	810	HSS	C-N1S	-2.02	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	710	HSS	C-N1S-S	-8.66	110.59	124.61
2	A	510	HSS	C-N1S-S	-7.96	111.73	124.61
2	A	510	HSS	O3S-S-O2S	-7.38	109.26	120.76
2	D	810	HSS	C-N1S-S	-6.29	114.43	124.61
2	B	610	HSS	C-N1S-S	-4.91	116.66	124.61
2	D	810	HSS	N3-C2-N1	-4.73	121.29	128.68
2	C	710	HSS	N3-C2-N1	-4.55	121.57	128.68
2	A	510	HSS	N3-C2-N1	-4.52	121.61	128.68
2	B	610	HSS	N3-C2-N1	-4.46	121.71	128.68
2	B	610	HSS	O5'-C5'-C4'	3.15	113.51	107.62
2	D	810	HSS	C5'-O5'-S	2.55	122.64	117.37
2	D	810	HSS	O5'-S-O3S	-2.51	97.92	105.59
2	C	710	HSS	O5'-C5'-C4'	2.35	112.01	107.62
2	B	610	HSS	O5'-S-O3S	-2.26	98.68	105.59
2	A	510	HSS	O5'-C5'-C4'	2.25	111.82	107.62
2	D	810	HSS	O5'-S-N1S	-2.24	99.36	105.60
2	C	710	HSS	O5'-S-O3S	-2.23	98.76	105.59
2	D	810	HSS	C4-C5-N7	-2.18	107.13	109.40
2	C	710	HSS	C4-C5-N7	-2.15	107.16	109.40
2	D	810	HSS	O5'-C5'-C4'	2.11	111.56	107.62
2	B	610	HSS	C4-C5-N7	-2.10	107.21	109.40
2	B	610	HSS	C2'-C3'-C4'	-2.07	98.62	102.64
2	A	510	HSS	O4'-C4'-C3'	-2.01	101.13	105.11

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	510	HSS	C-N1S-S-O2S
2	A	510	HSS	C-N1S-S-O3S
2	B	610	HSS	N1S-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	C	710	HSS	CA-CB-CG-N11
2	D	810	HSS	C5'-O5'-S-N1S
2	D	810	HSS	C5'-O5'-S-O3S
2	D	810	HSS	C3'-C4'-C5'-O5'
2	C	710	HSS	C5'-O5'-S-O3S
2	D	810	HSS	C5'-O5'-S-O2S
2	B	610	HSS	O-C-CA-N
2	B	610	HSS	N1S-C-CA-N
2	C	710	HSS	O-C-CA-N
2	C	710	HSS	N1S-C-CA-N
2	B	610	HSS	O-C-CA-CB
2	C	710	HSS	O-C-CA-CB
2	C	710	HSS	C5'-O5'-S-O2S
2	C	710	HSS	N1S-C-CA-CB
2	D	810	HSS	O4'-C4'-C5'-O5'

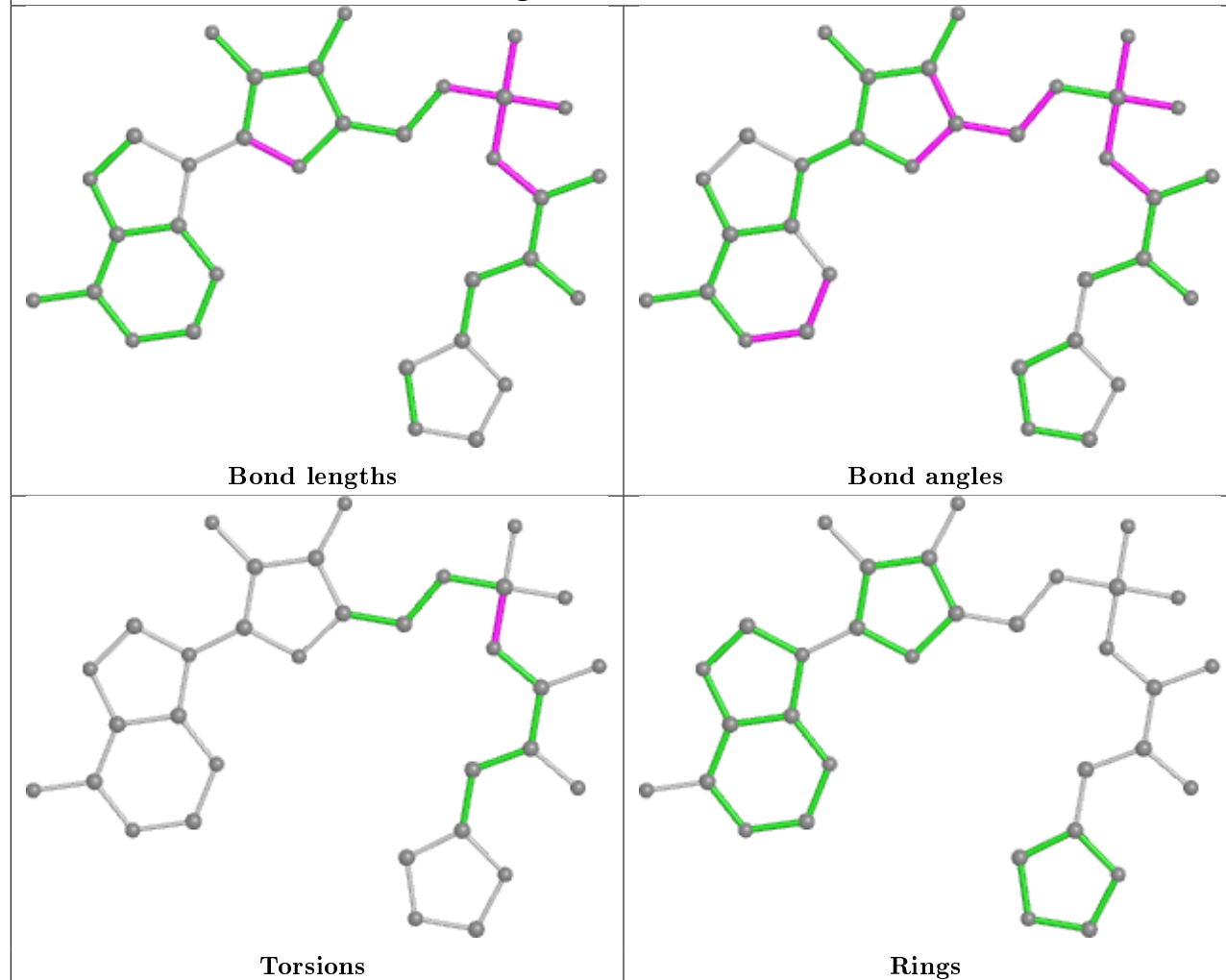
There are no ring outliers.

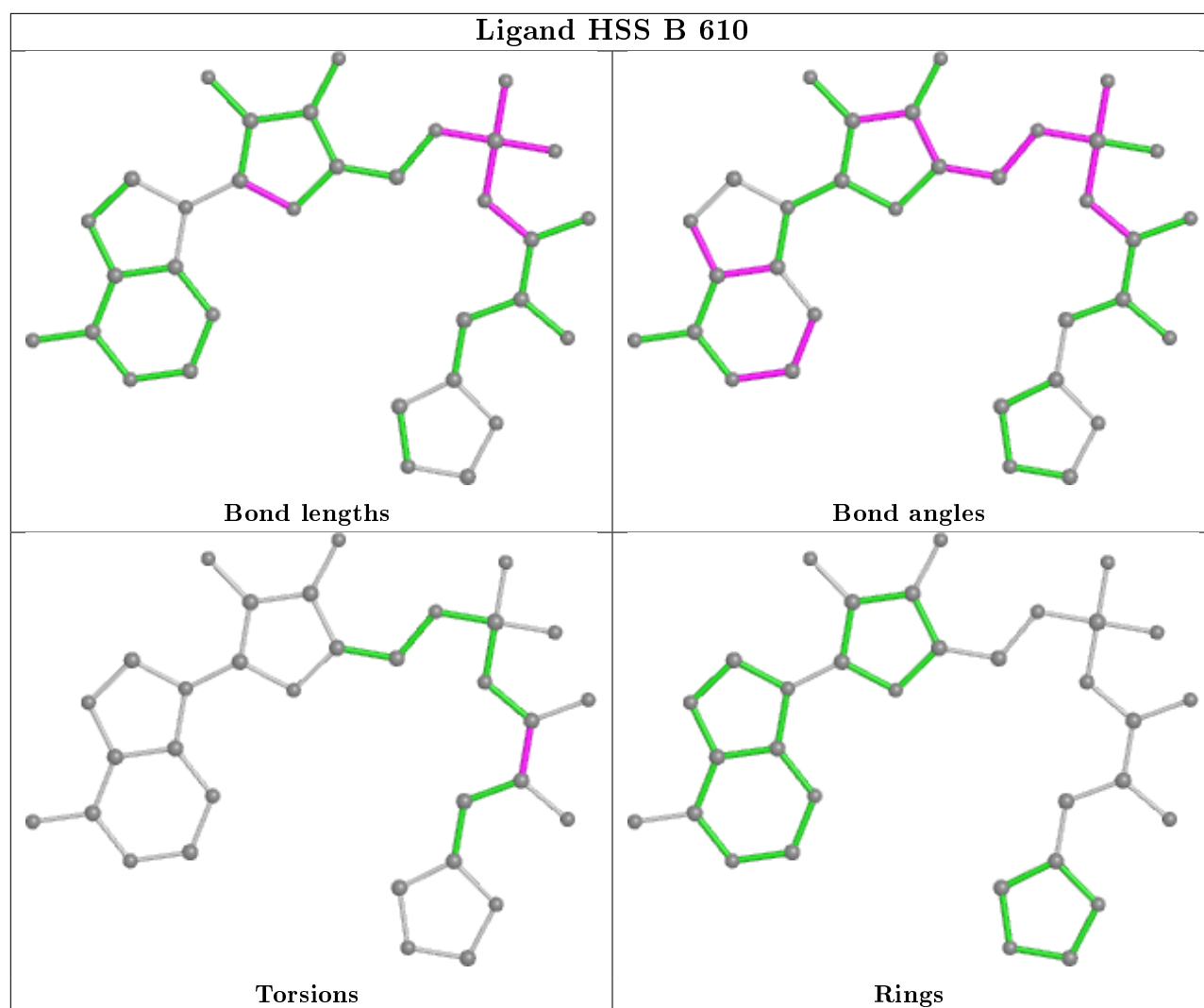
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	510	HSS	4	0
2	B	610	HSS	2	0
2	C	710	HSS	9	0
2	D	810	HSS	5	0

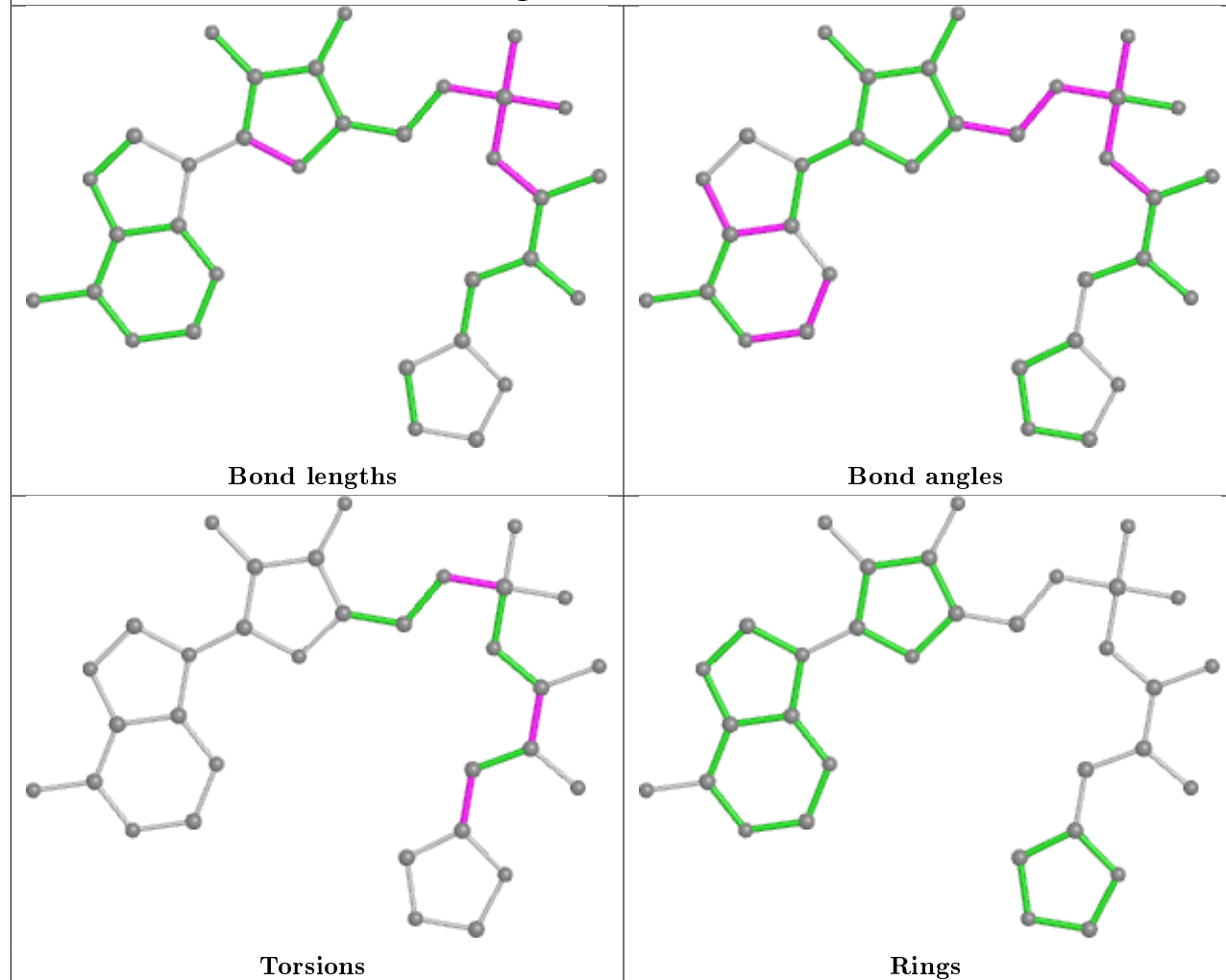
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

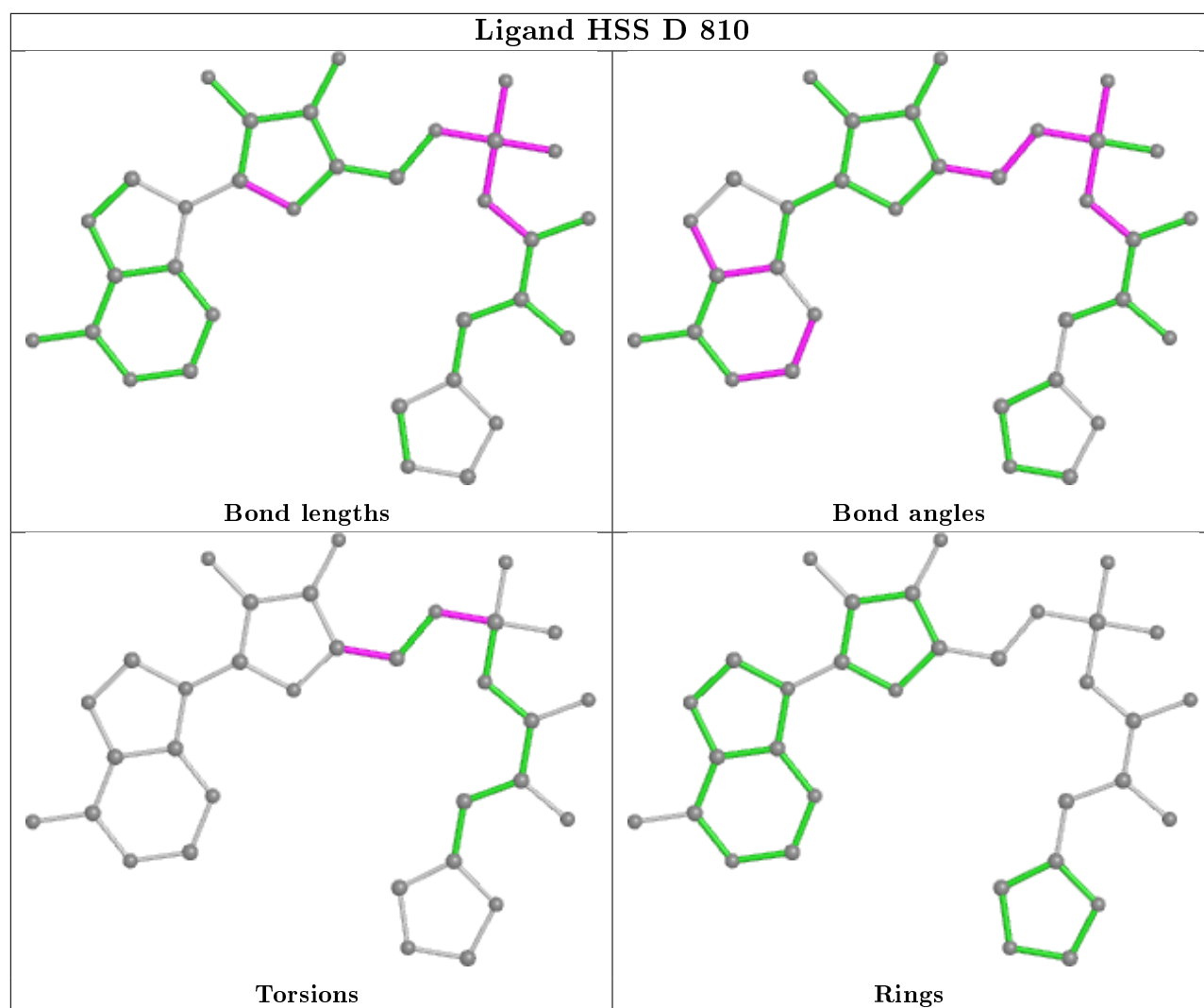
Ligand HSS A 510





Ligand HSS C 710





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	372/431 (86%)	0.15	22 (5%) 22 21	27, 57, 113, 140	0
1	B	376/431 (87%)	-0.14	1 (0%) 94 95	21, 50, 90, 109	0
1	C	372/431 (86%)	0.12	18 (4%) 30 28	27, 56, 111, 129	0
1	D	385/431 (89%)	-0.09	1 (0%) 94 95	19, 51, 97, 136	0
All	All	1505/1724 (87%)	0.01	42 (2%) 53 54	19, 54, 104, 140	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	LEU	6.1
1	A	225	LEU	5.4
1	A	175	ALA	5.2
1	A	228	TYR	4.7
1	C	173	ALA	4.6
1	A	257	LEU	4.3
1	C	168	ILE	3.5
1	C	180	ALA	3.5
1	C	228	TYR	3.4
1	D	185	LEU	3.4
1	A	249	ILE	3.4
1	C	178	ARG	3.4
1	C	179	ASP	3.4
1	C	255	GLN	3.2
1	A	253	VAL	3.1
1	A	258	VAL	2.9
1	C	177	TYR	2.9
1	C	169	GLY	2.7
1	A	169	GLY	2.7
1	A	266	ARG	2.7
1	C	256	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	165	LEU	2.7
1	A	165	LEU	2.6
1	C	229	LEU	2.6
1	A	229	LEU	2.6
1	A	56	ILE	2.5
1	C	51	LEU	2.5
1	A	173	ALA	2.5
1	A	174	ARG	2.4
1	B	423	LEU	2.4
1	A	163	LEU	2.3
1	A	424	GLY	2.3
1	C	265	ASN	2.2
1	A	256	ARG	2.2
1	A	339	ASP	2.2
1	A	244	LEU	2.2
1	A	167	SER	2.2
1	A	176	ASN	2.2
1	A	178	ARG	2.2
1	C	358	VAL	2.1
1	C	174	ARG	2.1
1	C	258	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
2	HSS	A	510	33/33	0.97	0.15	23,48,71,77	0
2	HSS	C	710	33/33	0.97	0.16	39,49,66,71	0

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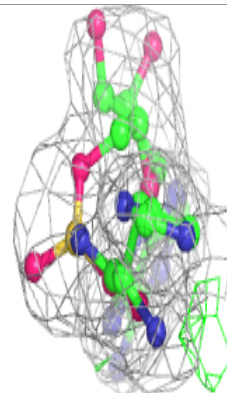
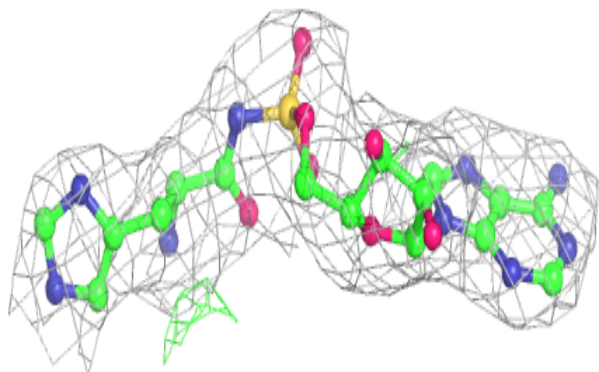
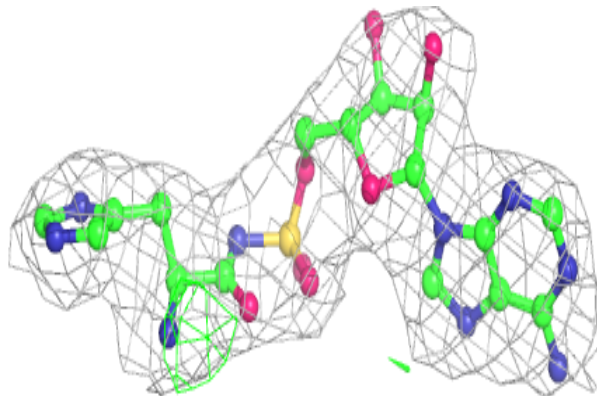
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HSS	B	610	33/33	0.98	0.17	17,31,38,49	0
2	HSS	D	810	33/33	0.98	0.15	15,30,37,44	0

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.

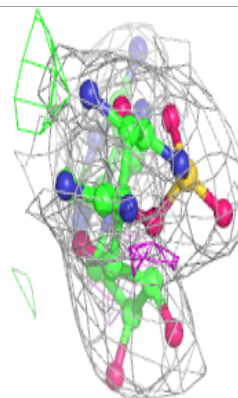
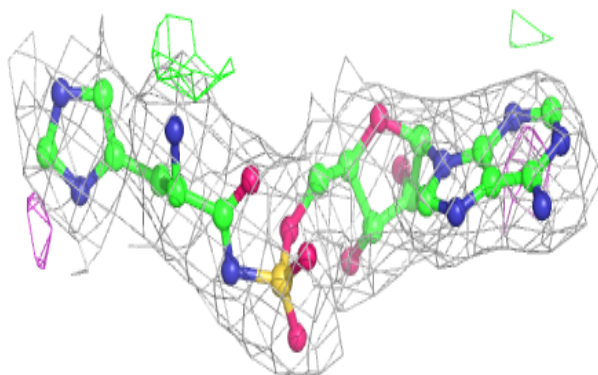
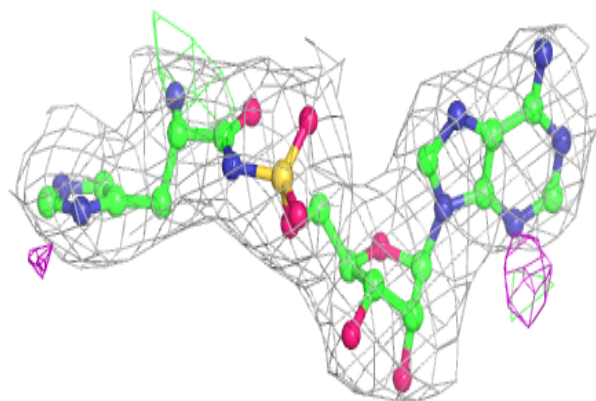
Electron density around HSS A 510:

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

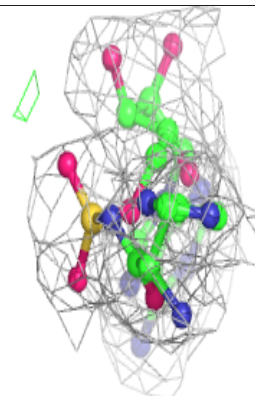
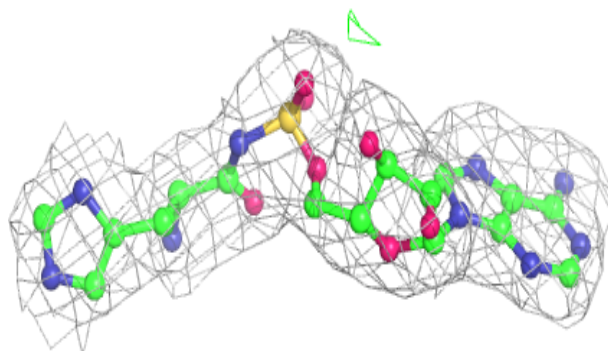
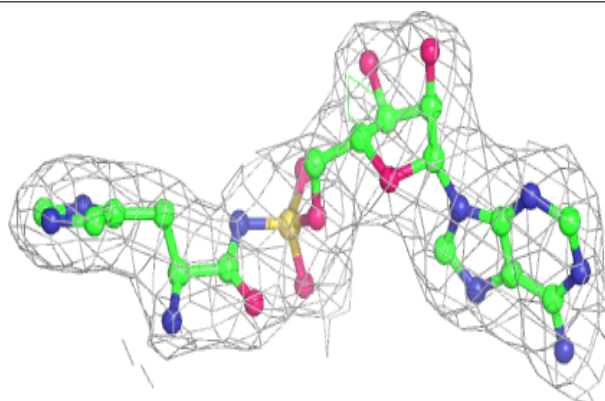


Electron density around HSS C 710:

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

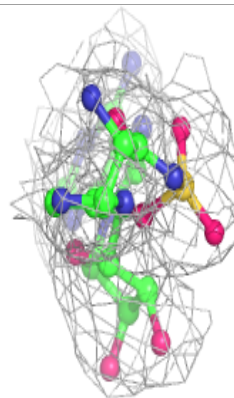
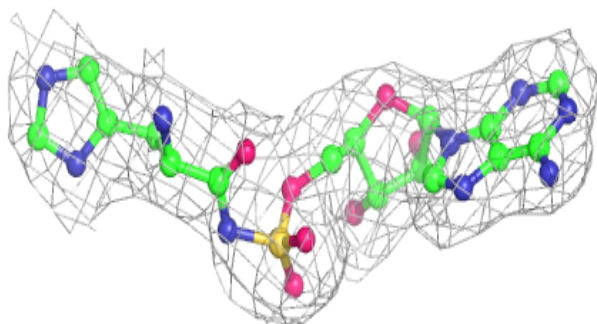
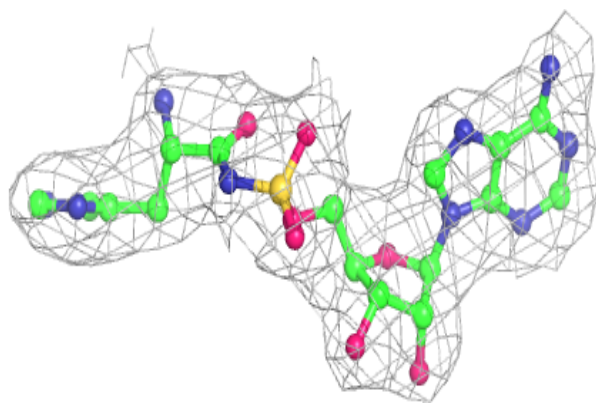
**Electron density around HSS B 610:**

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



Electron density around HSS D 810:

$2mF_o-DF_c$ (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.