



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:02 AM UTC

PDB ID : 6LG0 / pdb_00006lg0
Title : Crystal structure of SbCGTa in complex with UDP
Authors : Gao, H.M.; Yun, C.H.
Deposited on : 2019-12-04
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

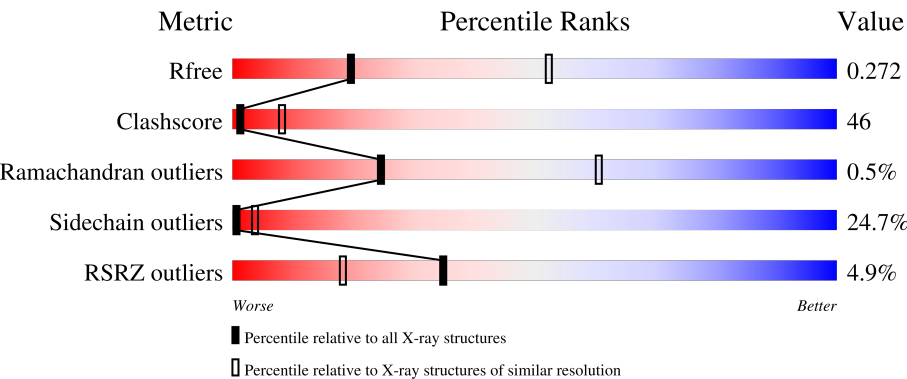
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	
1	B	460	
1	C	460	
1	D	460	
1	E	460	

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Mol	Chain	Length	Quality of chain
1	F	460	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UDP	C	500	-	-	X	-
2	UDP	E	500	-	-	X	-

2 Entry composition [i](#)

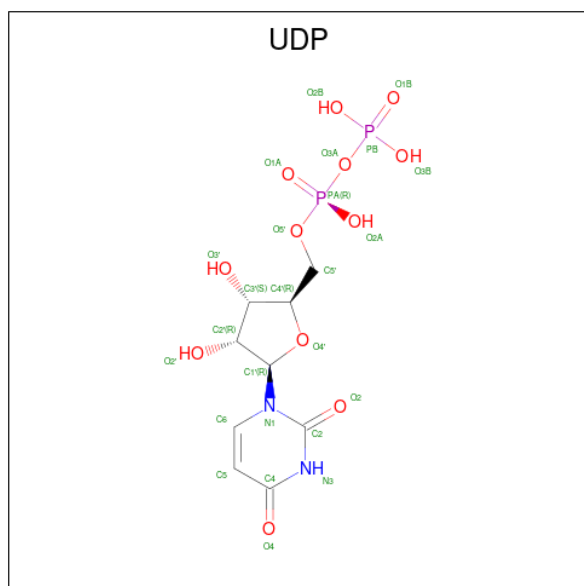
There are 3 unique types of molecules in this entry. The entry contains 19522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SbCGTa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3204	2056	539	597	12			
1	B	445	Total	C	N	O	S	0	0	1
			3198	2053	544	589	12			
1	C	439	Total	C	N	O	S	0	0	0
			3257	2091	548	603	15			
1	D	437	Total	C	N	O	S	0	0	0
			3129	2005	522	589	13			
1	E	443	Total	C	N	O	S	0	0	0
			3255	2085	547	608	15			
1	F	444	Total	C	N	O	S	0	0	0
			3319	2124	561	620	14			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

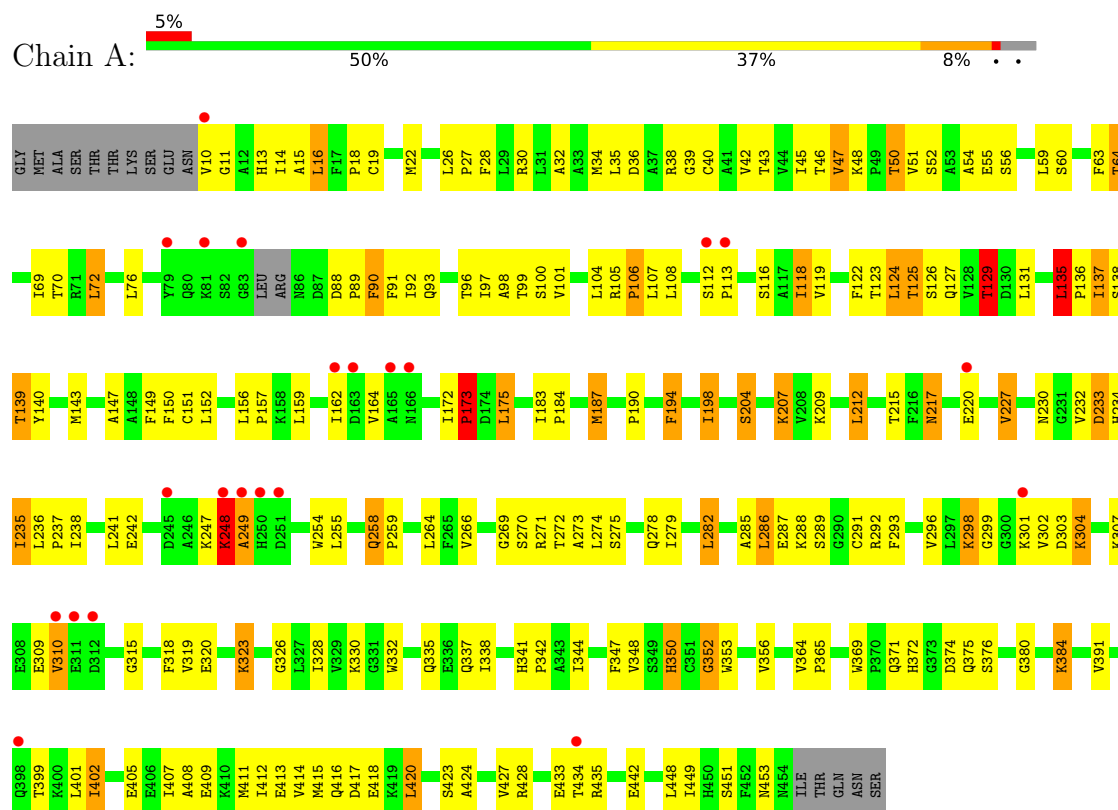
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		
3	E	1	Total	O	0	0
			1	1		

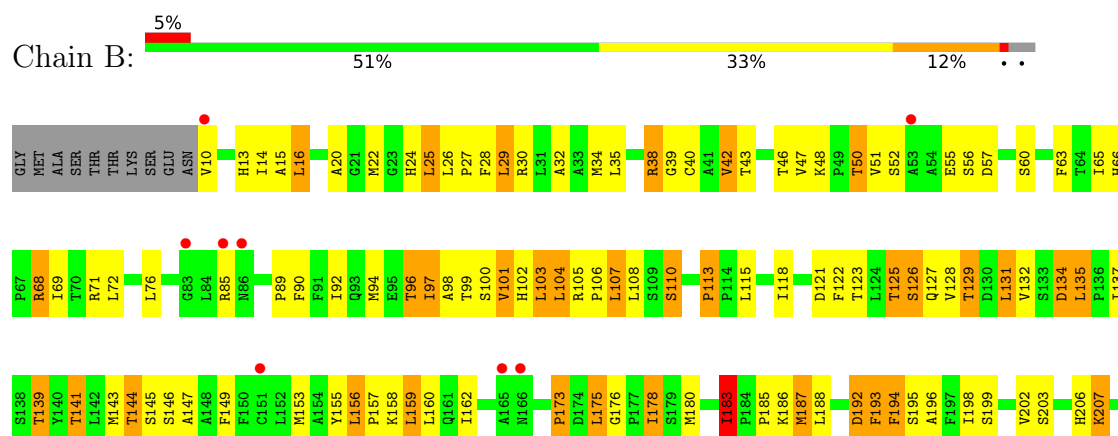
3 Residue-property plots

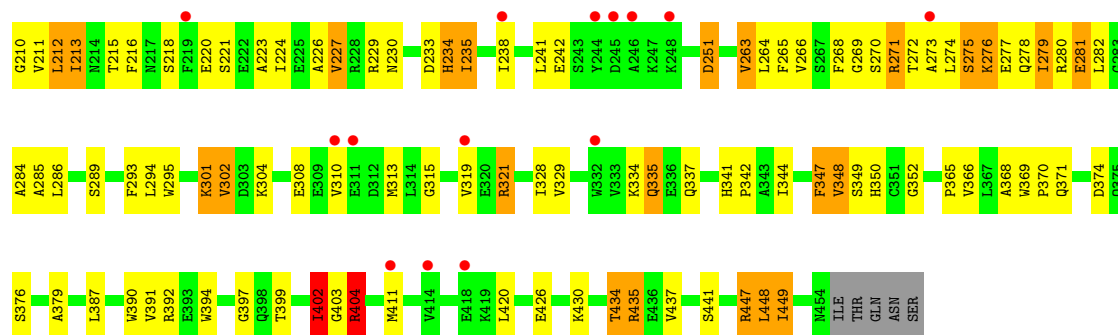
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: SbCGTa

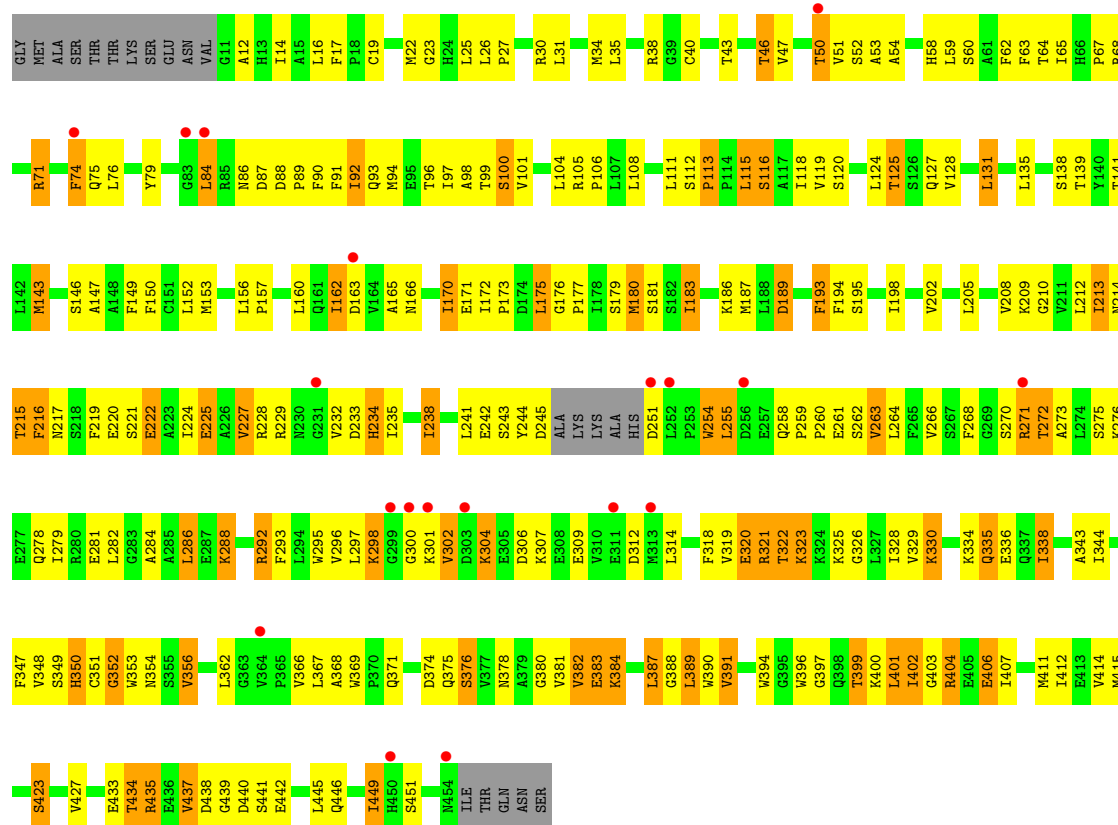


• Molecule 1: SbCGTa

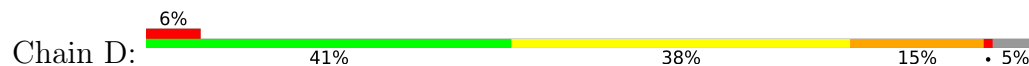


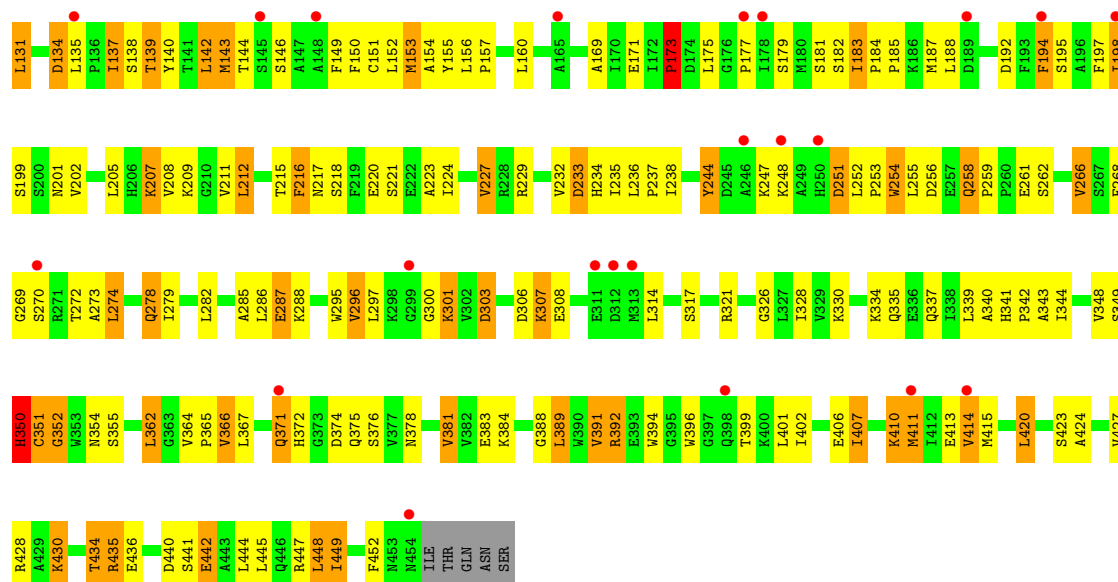


• Molecule 1: SbCGTa

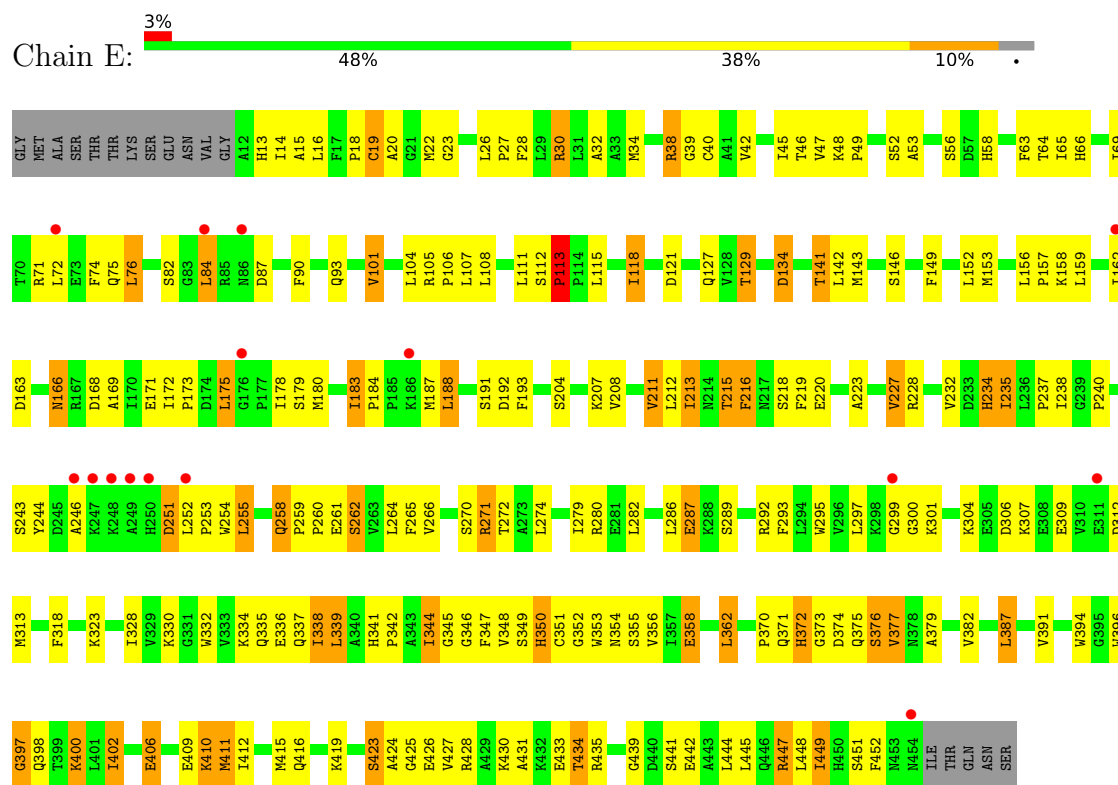


• Molecule 1: SbCGTa

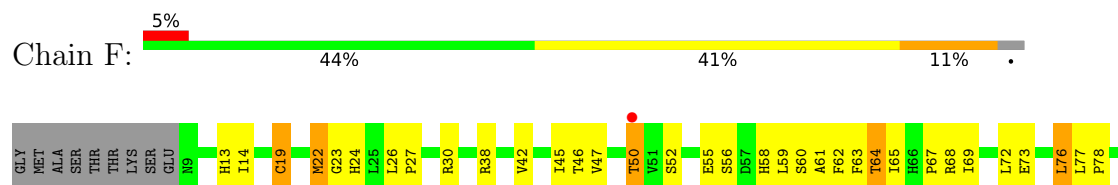


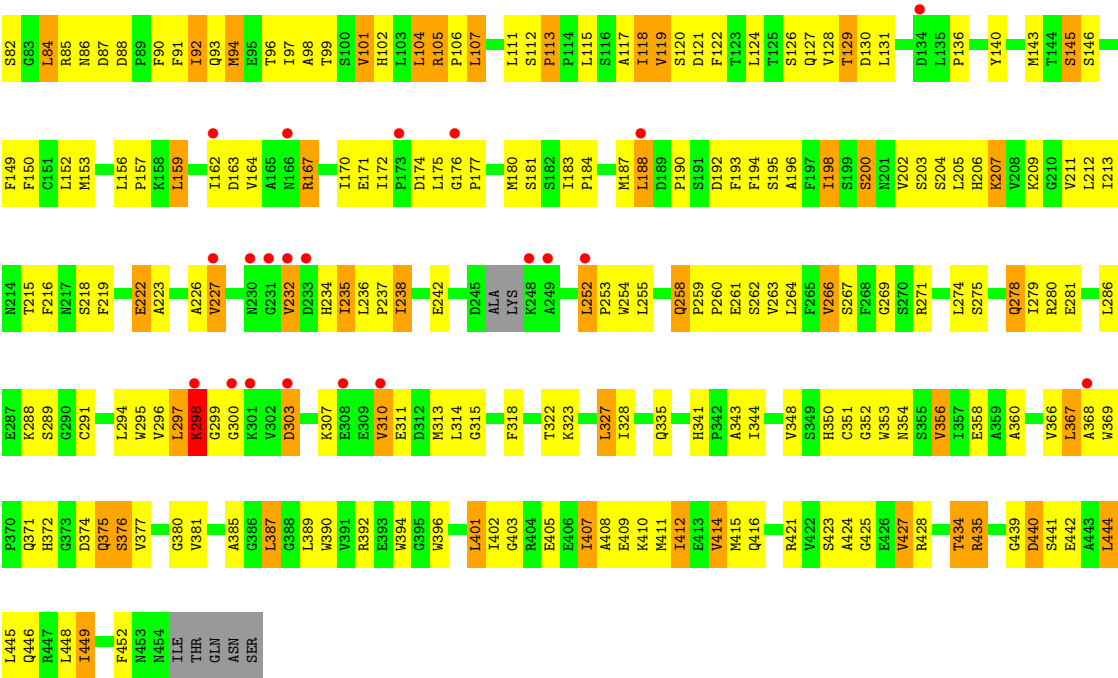


• Molecule 1: SbCGTa



• Molecule 1: SbCGTa





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.32Å 171.59Å 179.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 3.00 46.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.96-3.00) 97.7 (46.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.242 , 0.271 0.244 , 0.272	Depositor DCC
R_{free} test set	2946 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19522	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.28% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	7/3268 (0.2%)	1.31	17/4441 (0.4%)
1	B	0.96	0/3263	1.38	30/4438 (0.7%)
1	C	0.90	0/3328	1.13	12/4522 (0.3%)
1	D	0.86	1/3191 (0.0%)	1.19	17/4345 (0.4%)
1	E	0.99	1/3329 (0.0%)	1.28	15/4532 (0.3%)
1	F	0.90	0/3392	1.10	11/4614 (0.2%)
All	All	0.97	9/19771 (0.0%)	1.23	102/26892 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	PRO	C-O	-8.53	1.17	1.24
1	A	236	LEU	C-O	-6.78	1.19	1.25
1	A	259	PRO	C-O	-6.15	1.17	1.24
1	A	184	PRO	C-O	-6.05	1.17	1.24
1	D	254	TRP	C-O	-5.83	1.16	1.24
1	E	372	HIS	C-O	-5.31	1.17	1.23
1	A	106	PRO	C-O	-5.20	1.17	1.24
1	A	104	LEU	C-O	-5.13	1.17	1.24
1	A	90	PHE	C-O	-5.09	1.17	1.24

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ILE	CA-C-N	9.81	129.34	119.92
1	B	402	ILE	C-N-CA	9.81	129.34	119.92
1	D	253	PRO	N-CA-C	-9.16	101.94	113.84
1	F	298	LYS	N-CA-C	-9.10	102.74	112.93
1	B	113	PRO	N-CA-C	-9.04	99.67	110.70
1	E	352	GLY	N-CA-C	-8.07	101.91	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	ASP	N-CA-C	-7.73	103.58	113.16
1	A	352	GLY	N-CA-C	-7.67	102.39	111.36
1	B	403	GLY	N-CA-C	7.64	120.29	111.36
1	F	113	PRO	N-CA-C	-7.56	101.48	110.70
1	E	113	PRO	N-CA-C	-7.29	101.81	110.70
1	A	125	THR	CB-CA-C	7.25	122.82	110.79
1	C	399	THR	N-CA-C	-7.02	103.85	113.18
1	C	254	TRP	N-CA-C	-6.96	103.63	111.07
1	D	350	HIS	N-CA-C	-6.83	104.81	113.01
1	A	113	PRO	N-CA-C	-6.80	102.41	110.70
1	D	94	MET	N-CA-C	-6.78	103.89	111.28
1	A	11	GLY	N-CA-C	6.71	120.79	112.73
1	B	173	PRO	N-CA-C	6.70	124.64	113.78
1	B	135	LEU	N-CA-C	-6.70	99.93	109.24
1	D	19	CYS	N-CA-C	6.65	118.32	111.14
1	F	162	ILE	CB-CA-C	-6.64	106.06	111.71
1	A	129	THR	CB-CA-C	-6.58	100.29	110.81
1	B	25	LEU	N-CA-C	6.45	118.39	111.36
1	E	173	PRO	N-CA-C	6.41	122.44	113.53
1	D	22	MET	N-CA-C	-6.30	105.59	113.28
1	B	194	PHE	N-CA-C	-6.30	104.41	111.28
1	D	352	GLY	N-CA-C	-6.27	104.02	111.36
1	D	307	LYS	CB-CA-C	-6.20	100.96	110.88
1	B	183	ILE	N-CA-C	6.18	114.77	109.02
1	B	251	ASP	CA-C-N	-6.18	115.97	122.89
1	B	251	ASP	C-N-CA	-6.18	115.97	122.89
1	D	270	SER	N-CA-C	-6.16	103.19	111.87
1	E	287	GLU	CB-CA-C	-6.14	101.20	110.90
1	B	188	LEU	N-CA-C	6.08	117.99	111.36
1	E	350	HIS	N-CA-C	-6.03	105.90	113.20
1	B	89	PRO	N-CA-C	6.00	121.75	113.65
1	C	46	THR	CA-C-N	5.99	131.44	122.58
1	C	46	THR	C-N-CA	5.99	131.44	122.58
1	A	139	THR	CA-CB-OG1	-5.97	100.65	109.60
1	C	292	ARG	N-CA-C	-5.96	101.58	110.23
1	B	29	LEU	N-CA-C	-5.94	104.80	111.28
1	C	46	THR	CB-CA-C	5.93	121.72	110.51
1	E	39	GLY	N-CA-C	5.92	123.61	115.27
1	A	350	HIS	N-CA-C	-5.89	105.86	113.16
1	A	315	GLY	CA-C-O	-5.84	118.20	122.23
1	A	248	LYS	CA-C-N	5.82	132.65	121.54
1	A	248	LYS	C-N-CA	5.82	132.65	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	355	SER	CB-CA-C	-5.79	101.75	110.90
1	C	440	ASP	N-CA-C	5.76	117.56	111.28
1	C	350	HIS	N-CA-C	-5.71	106.16	113.01
1	D	244	TYR	CA-C-N	-5.67	113.03	122.21
1	D	244	TYR	C-N-CA	-5.67	113.03	122.21
1	A	135	LEU	CA-C-O	-5.65	115.13	119.71
1	E	251	ASP	N-CA-C	-5.64	105.60	112.88
1	E	397	GLY	N-CA-C	-5.64	103.87	111.54
1	E	312	ASP	N-CA-C	-5.61	105.02	112.94
1	B	115	LEU	CA-C-N	5.55	128.17	120.29
1	B	115	LEU	C-N-CA	5.55	128.17	120.29
1	F	188	LEU	N-CA-C	5.55	117.41	111.36
1	F	94	MET	N-CA-C	-5.53	105.25	111.28
1	D	270	SER	CA-C-N	5.49	133.05	121.91
1	D	270	SER	C-N-CA	5.49	133.05	121.91
1	B	301	LYS	CA-C-N	-5.48	117.55	123.08
1	B	301	LYS	C-N-CA	-5.48	117.55	123.08
1	A	173	PRO	N-CA-CB	-5.46	97.51	103.25
1	B	173	PRO	CA-C-N	-5.38	115.15	123.17
1	B	173	PRO	C-N-CA	-5.38	115.15	123.17
1	B	42	VAL	N-CA-C	5.37	116.22	108.48
1	A	418	GLU	N-CA-C	5.36	117.20	111.36
1	A	172	ILE	CA-C-N	5.35	126.53	119.84
1	A	172	ILE	C-N-CA	5.35	126.53	119.84
1	A	173	PRO	N-CA-C	5.33	123.45	112.47
1	F	136	PRO	CA-C-N	-5.29	115.63	122.99
1	F	136	PRO	C-N-CA	-5.29	115.63	122.99
1	D	173	PRO	N-CA-C	5.29	123.36	112.47
1	B	352	GLY	N-CA-C	-5.24	104.41	111.54
1	E	172	ILE	N-CA-C	-5.22	104.17	109.02
1	F	315	GLY	CA-C-O	-5.21	117.78	122.57
1	C	352	GLY	N-CA-C	-5.19	105.29	111.36
1	E	244	TYR	CB-CA-C	5.18	119.94	110.36
1	D	330	LYS	CA-C-N	-5.18	117.30	122.63
1	D	330	LYS	C-N-CA	-5.18	117.30	122.63
1	F	238	ILE	CB-CA-C	-5.16	105.26	110.93
1	C	116	SER	N-CA-C	-5.15	105.29	112.45
1	F	107	LEU	N-CA-C	5.13	116.87	111.28
1	A	151	CYS	CB-CA-C	-5.12	102.84	110.88
1	B	397	GLY	O-C-N	5.09	126.23	122.62
1	E	355	SER	N-CA-C	-5.06	105.68	111.14
1	B	347	PHE	CA-C-N	-5.05	116.55	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	PHE	C-N-CA	-5.05	116.55	123.12
1	C	183	ILE	CB-CA-C	-5.05	105.18	110.53
1	B	404	ARG	N-CA-C	-5.04	105.47	110.97
1	B	403	GLY	CA-C-N	5.02	127.28	120.65
1	B	403	GLY	C-N-CA	5.02	127.28	120.65
1	D	244	TYR	CA-C-O	-5.02	114.98	120.36
1	B	103	LEU	N-CA-C	-5.02	106.26	112.38
1	F	375	GLN	N-CA-C	5.02	116.75	111.28
1	E	66	HIS	CA-C-N	5.01	124.32	118.85
1	E	66	HIS	C-N-CA	5.01	124.32	118.85
1	B	315	GLY	CA-C-O	-5.01	118.96	122.22
1	D	371	GLN	N-CA-C	5.01	116.82	111.36

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	3204	0	3037	214	0
1	B	3198	0	3010	311	0
1	C	3257	0	3129	359	0
1	D	3129	0	2923	345	0
1	E	3255	0	3076	243	0
1	F	3319	0	3177	292	0
2	A	25	0	11	6	0
2	B	25	0	11	2	0
2	C	25	0	11	7	0
2	D	25	0	11	4	0
2	E	25	0	11	15	0
2	F	25	0	11	1	0
3	A	7	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	19522	0	18418	1761	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 46.

All (1761) 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:B:47:VAL:HG11	1:B:97:ILE:CD1	1.35	1.50
1:D:211:VAL:C	1:D:212:LEU:HD23	1.39	1.43
1:A:47:VAL:CG1	1:A:76:LEU:HD21	1.57	1.34
1:C:434:THR:CG2	1:C:441:SER:HB2	1.60	1.31
1:C:401:LEU:C	1:C:401:LEU:HD12	1.53	1.31
1:C:401:LEU:HD12	1:C:402:ILE:N	1.43	1.30
1:D:341:HIS:ND1	1:D:342:PRO:HD2	1.42	1.28
1:C:300:GLY:CA	1:C:307:LYS:HG2	1.63	1.26
1:C:27:PRO:HG3	1:C:354:ASN:ND2	1.47	1.25
1:F:401:LEU:HD23	1:F:401:LEU:C	1.50	1.25
1:B:212:LEU:HB3	1:B:238:ILE:CD1	1.65	1.25
1:C:27:PRO:CG	1:C:354:ASN:HD21	1.49	1.24
1:D:448:LEU:HD12	1:D:448:LEU:O	1.36	1.24
1:A:34:MET:CE	1:A:241:LEU:HD23	1.66	1.23
1:C:175:LEU:C	1:C:175:LEU:HD12	1.61	1.22
1:D:394:TRP:NE1	1:D:402:ILE:HD11	1.53	1.21
1:E:286:LEU:CD2	1:E:411:MET:HE2	1.67	1.21
1:B:212:LEU:CB	1:B:238:ILE:HD12	1.72	1.19
1:B:47:VAL:CG2	1:B:76:LEU:HD21	1.70	1.19
1:B:156:LEU:CD1	1:B:160:LEU:HG	1.72	1.19
1:B:223:ALA:O	1:B:227:VAL:HG22	1.43	1.19
1:A:407:ILE:HG22	1:A:411:MET:CE	1.73	1.18
1:D:350:HIS:CE1	1:D:352:GLY:H	1.60	1.17
1:B:211:VAL:C	1:B:212:LEU:HD12	1.69	1.17
1:E:286:LEU:CD2	1:E:411:MET:CE	2.23	1.16
1:B:47:VAL:CG1	1:B:97:ILE:CD1	2.23	1.16
1:C:138:SER:OG	1:C:209:LYS:HG3	1.44	1.15
1:D:391:VAL:HG11	1:D:394:TRP:CD1	1.82	1.15
1:C:53:ALA:HB3	1:C:304:LYS:HD3	1.24	1.15
1:B:34:MET:HE2	1:B:242:GLU:H	0.98	1.14
1:D:394:TRP:CD1	1:D:402:ILE:CD1	2.30	1.14
1:A:54:ALA:HB2	1:A:304:LYS:HE2	1.17	1.14
1:F:88:ASP:O	1:F:92:ILE:HG13	1.44	1.14
1:F:159:LEU:C	1:F:159:LEU:HD12	1.73	1.14
1:E:38:ARG:HH11	1:E:38:ARG:HG3	1.07	1.14
1:F:254:TRP:CD2	1:F:327:LEU:HD22	1.82	1.13
1:C:300:GLY:N	1:C:307:LYS:HG2	1.61	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:PRO:HD2	1:D:187:MET:HE3	1.20	1.13
1:B:212:LEU:HD23	1:B:238:ILE:HD11	1.30	1.13
1:C:149:PHE:CD2	1:C:153:MET:HE2	1.84	1.13
1:A:47:VAL:CG1	1:A:76:LEU:CD2	2.28	1.12
1:C:227:VAL:HG11	1:C:235:ILE:HD12	1.20	1.12
1:E:169:ALA:HB1	1:E:178:ILE:O	1.48	1.11
1:B:22:MET:HE1	1:B:25:LEU:HD23	1.31	1.11
1:F:434:THR:CG2	1:F:441:SER:HB2	1.79	1.11
1:F:434:THR:HG22	1:F:441:SER:HB2	1.31	1.11
1:B:90:PHE:O	1:B:94:MET:HG3	1.48	1.09
1:C:88:ASP:O	1:C:92:ILE:HG13	1.52	1.09
1:D:115:LEU:HB2	1:D:137:ILE:HD11	1.14	1.09
1:B:156:LEU:HD11	1:B:160:LEU:HG	1.12	1.09
1:C:213:ILE:HG23	1:C:215:THR:HG22	1.29	1.09
1:E:335:GLN:OE1	2:E:500:UDP:H2'	1.52	1.09
1:F:318:PHE:O	1:F:322:THR:HG23	1.53	1.09
1:C:175:LEU:HD12	1:C:175:LEU:O	1.51	1.09
1:C:300:GLY:HA3	1:C:307:LYS:HG2	1.26	1.09
1:A:407:ILE:CG2	1:A:411:MET:CE	2.30	1.08
1:D:389:LEU:HD21	1:D:420:LEU:CD2	1.83	1.08
1:A:407:ILE:HG22	1:A:411:MET:HE1	1.12	1.08
1:C:63:PHE:CZ	1:C:71:ARG:HB2	1.88	1.08
1:B:271:ARG:HB3	1:B:301:LYS:O	1.52	1.08
1:E:286:LEU:HD23	1:E:411:MET:HE2	1.31	1.08
1:E:447:ARG:HH11	1:E:447:ARG:CG	1.62	1.08
1:C:268:PHE:O	1:C:272:THR:HG23	1.53	1.08
1:F:278:GLN:HE21	1:F:278:GLN:CA	1.58	1.08
1:B:229:ARG:O	1:B:229:ARG:HG3	1.50	1.07
1:C:434:THR:HG22	1:C:441:SER:CB	1.85	1.07
1:C:434:THR:HG22	1:C:441:SER:HB2	1.08	1.06
1:D:448:LEU:HD12	1:D:448:LEU:C	1.75	1.06
1:A:407:ILE:CG2	1:A:411:MET:HE1	1.83	1.06
1:E:38:ARG:HH11	1:E:38:ARG:CG	1.68	1.06
1:B:47:VAL:CG2	1:B:76:LEU:CD2	2.33	1.05
1:D:424:ALA:O	1:D:427:VAL:HG12	1.54	1.05
1:C:63:PHE:CE1	1:C:71:ARG:HB2	1.91	1.05
1:C:434:THR:CG2	1:C:441:SER:CB	2.35	1.05
1:B:47:VAL:HG21	1:B:76:LEU:CD2	1.84	1.05
1:B:224:ILE:O	1:B:227:VAL:HG23	1.56	1.04
1:D:394:TRP:CE2	1:D:402:ILE:HD11	1.92	1.04
1:D:76:LEU:HD13	1:D:96:THR:HG21	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:VAL:C	1:D:212:LEU:CD2	2.30	1.04
1:A:173:PRO:HB2	1:A:230:ASN:HD21	1.19	1.04
1:B:47:VAL:HG11	1:B:97:ILE:HD13	1.09	1.04
1:C:162:ILE:HD12	1:C:163:ASP:H	1.22	1.04
1:F:401:LEU:C	1:F:401:LEU:CD2	2.30	1.03
1:C:54:ALA:H	1:C:304:LYS:HD2	1.23	1.03
1:C:175:LEU:C	1:C:175:LEU:CD1	2.30	1.03
1:F:149:PHE:HE2	1:F:153:MET:HE3	1.19	1.03
1:B:76:LEU:HD13	1:B:96:THR:HG22	1.39	1.03
1:C:298:LYS:HB2	1:C:298:LYS:NZ	1.72	1.03
1:C:401:LEU:C	1:C:401:LEU:CD1	2.30	1.03
1:C:387:LEU:HD23	1:C:387:LEU:O	1.58	1.03
1:E:16:LEU:HD22	1:E:32:ALA:HB2	1.37	1.03
1:A:60:SER:O	1:A:64:THR:HG23	1.57	1.02
1:B:34:MET:HE2	1:B:242:GLU:N	1.74	1.02
1:D:115:LEU:HB2	1:D:137:ILE:CD1	1.89	1.02
1:D:212:LEU:HD23	1:D:212:LEU:N	1.65	1.02
1:F:348:VAL:HG22	1:F:367:LEU:HD23	1.41	1.02
1:C:84:LEU:HD22	1:C:84:LEU:H	1.22	1.02
1:E:286:LEU:HD21	1:E:411:MET:CE	1.88	1.02
1:F:235:ILE:O	1:F:236:LEU:HD23	1.59	1.02
1:A:424:ALA:O	1:A:427:VAL:HG12	1.59	1.02
1:D:378:ASN:O	1:D:381:VAL:HG23	1.60	1.02
1:B:34:MET:HE1	1:B:241:LEU:HA	1.41	1.02
1:C:50:THR:HG21	1:C:52:SER:O	1.59	1.02
1:C:74:PHE:CZ	1:C:104:LEU:HG	1.95	1.02
1:D:184:PRO:HD2	1:D:187:MET:CE	1.88	1.02
1:E:49:PRO:HD2	1:E:76:LEU:HD21	1.42	1.01
1:A:47:VAL:HG11	1:A:76:LEU:CD2	1.89	1.01
1:A:411:MET:O	1:A:414:VAL:HG12	1.61	1.01
1:C:101:VAL:HG21	1:C:127:GLN:HB3	1.41	1.01
1:E:286:LEU:HD23	1:E:411:MET:CE	1.90	1.01
1:B:76:LEU:HD13	1:B:96:THR:CG2	1.90	1.01
1:C:138:SER:HG	1:C:209:LYS:HG3	1.25	1.01
1:E:447:ARG:HH11	1:E:447:ARG:HG2	0.87	1.01
1:F:286:LEU:HD23	1:F:411:MET:SD	2.00	1.01
1:A:16:LEU:CD1	1:A:32:ALA:HB2	1.90	1.00
1:F:235:ILE:C	1:F:236:LEU:HD23	1.85	1.00
1:E:169:ALA:HB2	1:E:179:SER:HA	1.40	0.99
1:B:42:VAL:CG1	1:B:69:ILE:HG12	1.91	0.99
1:F:112:SER:HB3	1:F:113:PRO:HD3	1.38	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:HIS:ND1	1:A:342:PRO:HD2	1.77	0.99
1:D:341:HIS:CG	1:D:342:PRO:HD2	1.97	0.99
1:D:350:HIS:CE1	1:D:352:GLY:N	2.30	0.99
1:B:22:MET:CE	1:B:25:LEU:HD23	1.92	0.99
1:F:278:GLN:HA	1:F:278:GLN:NE2	1.74	0.99
1:A:16:LEU:HD11	1:A:32:ALA:CB	1.92	0.99
1:B:271:ARG:HG2	1:B:271:ARG:HH11	1.22	0.99
1:B:126:SER:O	1:B:129:THR:HG22	1.62	0.99
1:F:61:ALA:O	1:F:64:THR:HG22	1.63	0.99
1:B:47:VAL:HG11	1:B:97:ILE:HD11	1.40	0.99
1:F:159:LEU:HD12	1:F:159:LEU:O	1.61	0.99
1:F:171:GLU:CG	1:F:177:PRO:HB3	1.91	0.99
1:E:286:LEU:HD21	1:E:411:MET:HE2	1.42	0.98
1:C:300:GLY:HA3	1:C:307:LYS:CG	1.93	0.98
1:D:394:TRP:CD1	1:D:402:ILE:HD12	1.96	0.98
1:B:47:VAL:HG21	1:B:76:LEU:HD21	0.98	0.98
1:F:120:SER:OG	1:F:128:VAL:HG11	1.62	0.98
1:C:278:GLN:NE2	1:C:369:TRP:CH2	2.31	0.98
1:F:149:PHE:CE2	1:F:153:MET:HE3	1.98	0.97
1:F:401:LEU:HD23	1:F:402:ILE:N	1.79	0.97
1:F:434:THR:CG2	1:F:441:SER:CB	2.41	0.97
1:B:263:VAL:HG22	1:B:344:ILE:HD12	1.42	0.97
1:C:353:TRP:HA	1:C:356:VAL:CG2	1.95	0.97
1:D:105:ARG:HG2	1:D:131:LEU:HD11	1.47	0.96
1:A:47:VAL:HG11	1:A:76:LEU:HD21	0.97	0.96
1:F:403:GLY:O	1:F:407:ILE:HG13	1.66	0.96
1:D:389:LEU:CD2	1:D:420:LEU:CD2	2.42	0.96
1:F:254:TRP:CE3	1:F:327:LEU:CD2	2.48	0.96
1:D:202:VAL:O	1:D:205:LEU:HB2	1.65	0.96
1:E:424:ALA:O	1:E:427:VAL:HG12	1.66	0.96
1:A:254:TRP:O	1:A:258:GLN:HG2	1.66	0.95
1:B:156:LEU:HD11	1:B:160:LEU:CG	1.95	0.95
1:B:212:LEU:HD12	1:B:212:LEU:N	1.75	0.95
1:E:354:ASN:O	1:E:358:GLU:HG3	1.65	0.95
1:B:276:LYS:NZ	1:B:280:ARG:HH21	1.65	0.95
1:A:341:HIS:ND1	1:A:342:PRO:CD	2.30	0.95
1:B:213:ILE:HG23	1:B:215:THR:HG22	1.46	0.95
1:B:289:SER:HB3	1:B:411:MET:CE	1.95	0.95
1:F:278:GLN:HE21	1:F:278:GLN:HA	1.26	0.95
1:D:394:TRP:NE1	1:D:402:ILE:CD1	2.30	0.95
1:A:16:LEU:HD11	1:A:32:ALA:HB2	0.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:N	1:B:212:LEU:CD1	2.30	0.95
1:D:295:TRP:HB3	1:D:328:ILE:HD12	1.46	0.95
1:B:47:VAL:CG1	1:B:97:ILE:HD11	1.90	0.95
1:D:391:VAL:HG11	1:D:394:TRP:NE1	1.81	0.94
1:C:401:LEU:CD1	1:C:402:ILE:N	2.30	0.94
1:D:126:SER:O	1:D:129:THR:HG22	1.67	0.94
1:E:447:ARG:HG2	1:E:447:ARG:NH1	1.66	0.94
1:F:434:THR:CG2	1:F:441:SER:H	1.81	0.94
1:C:213:ILE:CG2	1:C:215:THR:HG22	1.97	0.94
1:D:184:PRO:CD	1:D:187:MET:CE	2.46	0.94
1:E:358:GLU:O	1:E:362:LEU:HD12	1.68	0.93
1:B:434:THR:CG2	1:B:441:SER:HB2	1.97	0.93
1:F:278:GLN:HE21	1:F:278:GLN:C	1.75	0.93
1:C:300:GLY:H	1:C:307:LYS:CG	1.82	0.92
1:F:159:LEU:C	1:F:159:LEU:CD1	2.42	0.92
1:A:407:ILE:HG23	1:A:411:MET:HE2	1.51	0.92
1:D:184:PRO:CD	1:D:187:MET:HE3	1.99	0.92
1:D:184:PRO:HG2	1:D:187:MET:HE2	1.52	0.92
1:D:367:LEU:HD12	1:D:389:LEU:O	1.69	0.92
1:F:254:TRP:CD2	1:F:327:LEU:CD2	2.52	0.92
1:A:350:HIS:CD2	1:A:352:GLY:H	1.87	0.92
1:F:26:LEU:O	1:F:30:ARG:HG3	1.69	0.92
1:A:54:ALA:CB	1:A:304:LYS:HE2	2.00	0.92
1:F:242:GLU:OE1	1:F:435:ARG:HD2	1.70	0.92
1:F:238:ILE:O	1:F:238:ILE:HG22	1.70	0.91
1:C:50:THR:HG23	1:C:52:SER:H	1.31	0.91
1:F:222:GLU:CD	1:F:222:GLU:H	1.78	0.91
1:C:403:GLY:O	1:C:407:ILE:HG13	1.71	0.91
1:F:434:THR:HG21	1:F:441:SER:CB	1.99	0.91
1:B:52:SER:OG	1:B:55:GLU:HG3	1.69	0.91
1:D:76:LEU:HD13	1:D:96:THR:CG2	2.00	0.91
1:E:90:PHE:CE2	1:E:271:ARG:HB3	2.07	0.90
1:D:24:HIS:O	1:D:27:PRO:HG2	1.72	0.90
1:F:86:ASN:ND2	1:F:92:ILE:HG12	1.86	0.89
1:B:155:TYR:CE1	1:B:159:LEU:HB2	2.07	0.89
1:D:341:HIS:ND1	1:D:342:PRO:CD	2.32	0.89
1:C:105:ARG:HB3	1:C:106:PRO:HD3	1.54	0.89
1:C:353:TRP:O	1:C:356:VAL:HG23	1.72	0.89
1:E:42:VAL:HG12	1:E:69:ILE:HG23	1.54	0.89
1:A:47:VAL:HG12	1:A:76:LEU:CD2	2.02	0.89
1:B:212:LEU:CD2	1:B:238:ILE:HD11	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LYS:CB	1:C:298:LYS:HZ3	1.85	0.89
1:C:162:ILE:HD12	1:C:163:ASP:N	1.88	0.89
1:D:52:SER:OG	1:D:55:GLU:HB2	1.74	0.88
1:C:434:THR:HG21	1:C:441:SER:HB2	1.55	0.88
1:C:298:LYS:NZ	1:C:298:LYS:CB	2.30	0.88
1:D:391:VAL:CG1	1:D:394:TRP:CD1	2.56	0.88
1:D:366:VAL:HG12	1:D:388:GLY:HA3	1.55	0.88
1:D:389:LEU:HD21	1:D:420:LEU:HD23	1.53	0.88
1:D:153:MET:HA	1:D:198:ILE:HD11	1.53	0.88
1:A:407:ILE:O	1:A:411:MET:HE3	1.73	0.88
1:C:26:LEU:O	1:C:30:ARG:HG3	1.73	0.88
1:D:341:HIS:CG	1:D:342:PRO:CD	2.56	0.88
1:A:34:MET:HE1	1:A:241:LEU:HD23	1.53	0.88
1:D:26:LEU:O	1:D:30:ARG:HG3	1.74	0.88
1:D:194:PHE:O	1:D:194:PHE:HD1	1.57	0.88
1:F:112:SER:CB	1:F:113:PRO:HD3	2.04	0.88
1:C:16:LEU:HD21	1:C:31:LEU:HD23	1.55	0.88
1:C:149:PHE:HD2	1:C:153:MET:HE2	1.34	0.87
1:D:22:MET:HE3	1:D:25:LEU:HD23	1.56	0.87
1:D:26:LEU:N	1:D:27:PRO:HD2	1.89	0.87
1:D:38:ARG:HB3	1:D:449:ILE:HD12	1.55	0.87
1:F:434:THR:HG22	1:F:441:SER:CB	2.04	0.87
1:B:22:MET:HE2	1:B:22:MET:HA	1.57	0.87
1:D:266:VAL:HB	1:D:295:TRP:CD1	2.09	0.87
1:A:54:ALA:HB2	1:A:304:LYS:CE	2.03	0.87
1:F:434:THR:HG21	1:F:441:SER:OG	1.73	0.87
1:B:218:SER:OG	1:B:430:LYS:HD3	1.73	0.87
1:C:278:GLN:HE21	1:C:369:TRP:HH2	1.16	0.87
1:C:383:GLU:HG2	1:C:384:LYS:NZ	1.88	0.87
1:C:434:THR:CG2	1:C:441:SER:H	1.86	0.87
1:B:16:LEU:HD11	1:B:32:ALA:HB2	1.56	0.86
1:C:278:GLN:NE2	1:C:369:TRP:CZ2	2.43	0.86
1:F:90:PHE:HB2	1:F:271:ARG:HH12	1.37	0.86
1:B:198:ILE:O	1:B:202:VAL:HG23	1.76	0.86
1:D:394:TRP:CD1	1:D:402:ILE:HD11	2.06	0.86
1:E:65:ILE:HG13	1:E:246:ALA:HB1	1.57	0.86
1:D:394:TRP:CE2	1:D:402:ILE:CD1	2.59	0.86
1:B:34:MET:CE	1:B:241:LEU:HA	2.05	0.86
1:A:34:MET:CE	1:A:241:LEU:CD2	2.51	0.86
1:C:124:LEU:O	1:C:128:VAL:HG23	1.76	0.85
1:F:223:ALA:O	1:F:227:VAL:HG23	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:LEU:CD2	1:E:411:MET:HE1	2.05	0.85
1:C:183:ILE:HG23	1:C:187:MET:CE	2.05	0.85
1:C:300:GLY:H	1:C:307:LYS:HG2	1.29	0.85
1:F:297:LEU:HD13	1:F:297:LEU:N	1.91	0.85
1:D:63:PHE:CZ	1:D:71:ARG:HB2	2.12	0.85
1:D:394:TRP:CG	1:D:402:ILE:CD1	2.60	0.84
1:A:285:ALA:HB1	1:A:407:ILE:HG22	1.56	0.84
1:A:272:THR:CB	1:A:301:LYS:HA	2.08	0.84
1:E:335:GLN:OE1	2:E:500:UDP:C2'	2.24	0.84
1:F:143:MET:HE1	1:F:145:SER:C	2.03	0.84
1:F:298:LYS:HB3	1:F:298:LYS:HZ3	1.43	0.84
1:A:43:THR:HA	1:A:70:THR:HG22	1.59	0.84
1:B:203:SER:O	1:B:206:HIS:CG	2.30	0.84
1:C:112:SER:HB2	1:C:113:PRO:HD3	1.57	0.84
1:F:171:GLU:HA	1:F:177:PRO:HA	1.57	0.84
1:C:213:ILE:CG2	1:C:215:THR:CG2	2.57	0.83
1:D:218:SER:OG	1:D:430:LYS:HE2	1.78	0.83
1:D:448:LEU:C	1:D:448:LEU:CD1	2.51	0.83
1:F:143:MET:CE	1:F:145:SER:N	2.41	0.83
1:C:84:LEU:HD22	1:C:84:LEU:N	1.94	0.83
1:C:238:ILE:H	1:C:238:ILE:HD13	1.42	0.83
1:A:299:GLY:H	1:A:330:LYS:NZ	1.77	0.83
1:D:211:VAL:O	1:D:212:LEU:HD23	1.78	0.83
1:B:276:LYS:HZ2	1:B:280:ARG:HH21	1.24	0.83
1:C:225:GLU:OE1	1:C:225:GLU:HA	1.77	0.83
1:E:346:GLY:HA3	1:E:415:MET:CE	2.08	0.83
1:C:314:LEU:HD12	1:C:328:ILE:HD12	1.60	0.82
1:B:107:LEU:HD12	1:B:107:LEU:O	1.79	0.82
1:C:401:LEU:HD12	1:C:402:ILE:CA	2.08	0.82
1:F:143:MET:CE	1:F:145:SER:CA	2.56	0.82
1:B:263:VAL:CG2	1:B:344:ILE:HD12	2.09	0.82
1:C:298:LYS:HB2	1:C:298:LYS:HZ2	1.44	0.82
1:C:298:LYS:HB2	1:C:298:LYS:HZ3	1.39	0.82
1:C:171:GLU:HA	1:C:177:PRO:HB3	1.62	0.82
1:C:268:PHE:O	1:C:272:THR:CG2	2.27	0.82
1:D:151:CYS:HA	1:D:154:ALA:HB3	1.61	0.82
1:F:90:PHE:HB2	1:F:271:ARG:NH1	1.92	0.82
1:B:34:MET:CE	1:B:242:GLU:H	1.87	0.81
1:B:156:LEU:HD13	1:B:156:LEU:O	1.79	0.81
1:A:272:THR:CB	1:A:301:LYS:HG2	2.10	0.81
1:D:212:LEU:CD2	1:D:212:LEU:N	2.41	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:TRP:O	1:E:400:LYS:HD2	1.81	0.81
1:C:295:TRP:CE2	1:C:297:LEU:CD1	2.64	0.81
1:A:173:PRO:CB	1:A:230:ASN:HD21	1.94	0.81
1:F:143:MET:CE	1:F:145:SER:H	1.94	0.81
1:F:401:LEU:HD23	1:F:401:LEU:O	1.79	0.81
1:C:149:PHE:CE2	1:C:153:MET:HE2	2.16	0.81
1:D:273:ALA:HB1	1:D:371:GLN:CG	2.10	0.81
1:B:218:SER:OG	1:B:430:LYS:CD	2.29	0.81
1:B:434:THR:HG22	1:B:441:SER:HB2	1.63	0.81
1:A:278:GLN:HE22	1:A:402:ILE:H	1.26	0.80
1:C:84:LEU:H	1:C:84:LEU:CD2	1.94	0.80
1:C:353:TRP:HA	1:C:356:VAL:HG23	1.61	0.80
1:C:334:LYS:O	1:C:338:ILE:HG13	1.82	0.80
1:C:394:TRP:CE2	1:C:402:ILE:CD1	2.65	0.80
1:F:159:LEU:O	1:F:159:LEU:CD1	2.30	0.80
1:A:34:MET:HE2	1:A:241:LEU:HD23	1.63	0.80
1:D:350:HIS:HE1	1:D:352:GLY:CA	1.94	0.80
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.47	0.80
1:C:175:LEU:CD1	1:C:176:GLY:O	2.30	0.80
1:D:278:GLN:O	1:D:278:GLN:NE2	2.15	0.80
1:D:220:GLU:O	1:D:224:ILE:CG1	2.30	0.80
1:B:34:MET:CE	1:B:241:LEU:HD23	2.11	0.80
1:F:198:ILE:O	1:F:202:VAL:HG23	1.80	0.80
1:A:88:ASP:OD1	1:A:89:PRO:HD2	1.81	0.80
1:B:156:LEU:CD1	1:B:156:LEU:O	2.30	0.80
1:B:85:ARG:CB	1:B:193:PHE:CE1	2.64	0.80
1:C:434:THR:HG21	1:C:441:SER:CB	2.07	0.79
1:F:424:ALA:O	1:F:427:VAL:HG23	1.82	0.79
1:B:271:ARG:HG2	1:B:271:ARG:NH1	1.88	0.79
1:E:38:ARG:CG	1:E:38:ARG:NH1	2.39	0.79
1:F:50:THR:CG2	1:F:52:SER:O	2.30	0.79
1:A:173:PRO:HB2	1:A:230:ASN:ND2	1.97	0.79
1:D:10:VAL:O	1:D:10:VAL:CG1	2.30	0.79
1:E:354:ASN:O	1:E:358:GLU:CG	2.29	0.79
1:F:314:LEU:HD12	1:F:328:ILE:HD13	1.65	0.79
1:C:210:GLY:HA2	1:C:234:HIS:HB2	1.65	0.79
1:F:372:HIS:O	1:F:375:GLN:HG3	1.83	0.79
1:A:282:LEU:HD13	1:A:369:TRP:HZ3	1.48	0.79
1:C:300:GLY:N	1:C:307:LYS:CG	2.41	0.79
1:D:410:LYS:CE	1:D:413:GLU:OE1	2.30	0.79
1:E:168:ASP:O	1:E:180:MET:HB2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:LEU:CD2	1:F:411:MET:SD	2.70	0.79
1:D:149:PHE:CD2	1:D:153:MET:HE3	2.17	0.79
1:D:350:HIS:HE1	1:D:352:GLY:HA3	1.46	0.79
1:B:42:VAL:HG13	1:B:69:ILE:HG23	1.65	0.79
1:C:50:THR:CG2	1:C:52:SER:O	2.30	0.79
1:D:391:VAL:O	1:D:391:VAL:HG12	1.83	0.79
1:B:126:SER:O	1:B:129:THR:CG2	2.30	0.78
1:B:223:ALA:O	1:B:227:VAL:CG2	2.30	0.78
1:B:102:HIS:O	1:B:105:ARG:HG3	1.82	0.78
1:D:378:ASN:O	1:D:381:VAL:CG2	2.30	0.78
1:B:90:PHE:O	1:B:94:MET:CG	2.30	0.78
1:F:254:TRP:CG	1:F:327:LEU:HD22	2.18	0.78
1:B:16:LEU:HD13	1:B:28:PHE:O	1.83	0.78
1:F:184:PRO:HD2	1:F:187:MET:HE3	1.63	0.78
1:C:353:TRP:C	1:C:356:VAL:HG23	2.09	0.78
1:D:269:GLY:HA2	1:D:350:HIS:CD2	2.19	0.78
1:B:289:SER:CB	1:B:411:MET:HE3	2.14	0.78
1:E:175:LEU:HD12	1:E:175:LEU:N	1.98	0.78
1:D:10:VAL:O	1:D:10:VAL:HG13	1.83	0.78
1:A:407:ILE:CG2	1:A:411:MET:HE2	2.06	0.77
1:C:278:GLN:NE2	1:C:369:TRP:HH2	1.74	0.77
1:E:166:ASN:OD1	1:E:166:ASN:N	2.18	0.77
1:F:434:THR:HG23	1:F:441:SER:H	1.49	0.77
1:C:183:ILE:HG23	1:C:187:MET:HE1	1.66	0.77
1:D:47:VAL:HG11	1:D:97:ILE:HD11	1.67	0.77
1:D:278:GLN:C	1:D:278:GLN:HE21	1.92	0.77
1:E:346:GLY:HA3	1:E:415:MET:HE3	1.66	0.77
1:B:224:ILE:C	1:B:227:VAL:HG23	2.08	0.77
1:E:279:ILE:HD12	1:E:313:MET:HE2	1.65	0.77
1:F:424:ALA:C	1:F:427:VAL:HG23	2.10	0.77
1:C:387:LEU:O	1:C:387:LEU:CD2	2.31	0.77
1:D:152:LEU:HD21	1:D:183:ILE:HG12	1.66	0.77
1:B:159:LEU:O	1:B:159:LEU:HD12	1.85	0.77
1:C:227:VAL:HG11	1:C:235:ILE:CD1	2.07	0.77
1:D:211:VAL:O	1:D:212:LEU:CD2	2.32	0.77
1:E:14:ILE:HD11	1:E:452:PHE:CD2	2.20	0.77
1:E:434:THR:HG23	1:E:441:SER:HB2	1.65	0.77
1:B:212:LEU:HD23	1:B:238:ILE:CD1	2.11	0.77
1:C:434:THR:HG23	1:C:441:SER:H	1.50	0.77
1:F:143:MET:HE3	1:F:145:SER:H	1.48	0.77
1:C:50:THR:CG2	1:C:52:SER:H	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PHE:CE2	1:B:153:MET:HE2	2.19	0.76
1:E:38:ARG:HG3	1:E:38:ARG:NH1	1.88	0.76
1:C:149:PHE:CD2	1:C:153:MET:CE	2.66	0.76
1:D:194:PHE:HD1	1:D:194:PHE:C	1.92	0.76
1:C:295:TRP:CZ2	1:C:297:LEU:CD1	2.67	0.76
1:C:435:ARG:NE	1:C:435:ARG:HA	2.00	0.76
1:A:93:GLN:HA	1:A:96:THR:HG22	1.65	0.76
1:B:284:ALA:CB	1:B:404:ARG:NH1	2.49	0.76
1:A:50:THR:HG22	1:A:52:SER:O	1.85	0.76
1:C:53:ALA:CB	1:C:304:LYS:HD3	2.13	0.76
1:A:47:VAL:HG12	1:A:76:LEU:CG	2.16	0.76
1:C:366:VAL:HG13	1:C:388:GLY:HA3	1.66	0.76
1:C:394:TRP:CD2	1:C:402:ILE:HD13	2.21	0.76
1:D:350:HIS:CE1	1:D:352:GLY:CA	2.68	0.76
1:D:354:ASN:CB	2:D:500:UDP:H5'1	2.15	0.76
1:A:19:CYS:HB3	1:A:97:ILE:HD12	1.67	0.76
1:C:27:PRO:HG3	1:C:354:ASN:HD21	0.63	0.76
1:C:389:LEU:HD12	1:C:414:VAL:HG22	1.67	0.76
1:A:13:HIS:C	1:A:14:ILE:HD13	2.10	0.75
1:A:255:LEU:HD23	1:A:341:HIS:HD2	1.51	0.75
1:D:266:VAL:HG13	1:D:348:VAL:HB	1.68	0.75
1:B:212:LEU:CB	1:B:238:ILE:CD1	2.44	0.75
1:C:141:THR:CG2	1:C:208:VAL:HG11	2.16	0.75
1:E:424:ALA:O	1:E:427:VAL:CG1	2.35	0.75
1:F:105:ARG:HB2	1:F:105:ARG:HH11	1.50	0.75
1:F:143:MET:CE	1:F:145:SER:C	2.60	0.75
1:A:149:PHE:CE2	1:A:374:ASP:HA	2.22	0.75
1:E:84:LEU:HD13	1:E:84:LEU:N	2.00	0.75
1:C:318:PHE:O	1:C:322:THR:HG23	1.87	0.75
1:F:297:LEU:N	1:F:297:LEU:CD1	2.50	0.75
1:A:13:HIS:O	1:A:14:ILE:HD13	1.87	0.75
1:D:391:VAL:CG1	1:D:394:TRP:CG	2.69	0.75
1:B:27:PRO:HA	1:B:30:ARG:HG3	1.69	0.75
1:F:143:MET:HE2	1:F:145:SER:N	2.01	0.74
1:C:295:TRP:CZ2	1:C:297:LEU:HD11	2.23	0.74
1:E:169:ALA:CB	1:E:178:ILE:O	2.32	0.74
1:E:426:GLU:O	1:E:430:LYS:HG3	1.87	0.74
1:F:124:LEU:O	1:F:128:VAL:HG23	1.87	0.74
1:C:105:ARG:HE	1:C:135:LEU:HD11	1.53	0.74
1:F:296:VAL:C	1:F:297:LEU:HD13	2.12	0.74
1:C:367:LEU:HB2	1:C:414:VAL:HG21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LEU:CD2	1:D:420:LEU:HD22	2.18	0.74
1:C:378:ASN:O	1:C:381:VAL:HG12	1.87	0.74
1:D:22:MET:HE1	1:D:58:HIS:CG	2.23	0.74
1:D:194:PHE:C	1:D:194:PHE:CD1	2.66	0.74
1:F:149:PHE:HE2	1:F:153:MET:CE	2.00	0.74
1:B:47:VAL:HG11	1:B:97:ILE:HD12	1.65	0.73
1:C:54:ALA:HB2	1:C:304:LYS:HE3	1.70	0.73
1:B:156:LEU:CD1	1:B:156:LEU:C	2.61	0.73
1:D:149:PHE:HD2	1:D:153:MET:HE3	1.52	0.73
1:B:192:ASP:OD1	1:B:192:ASP:C	2.31	0.73
1:E:13:HIS:HB3	1:E:115:LEU:HA	1.70	0.73
1:A:47:VAL:HG12	1:A:76:LEU:HG	1.70	0.73
1:B:16:LEU:CD1	1:B:28:PHE:O	2.36	0.73
1:C:189:ASP:C	1:C:189:ASP:OD1	2.30	0.73
1:A:407:ILE:O	1:A:411:MET:CE	2.36	0.73
1:D:350:HIS:CE1	1:D:352:GLY:HA3	2.23	0.73
1:B:434:THR:CG2	1:B:441:SER:CB	2.65	0.73
1:C:300:GLY:CA	1:C:307:LYS:CG	2.52	0.73
1:D:218:SER:OG	1:D:430:LYS:CE	2.36	0.73
1:E:15:ALA:HB2	1:E:115:LEU:HD22	1.70	0.73
1:A:320:GLU:O	1:A:323:LYS:HB3	1.88	0.73
1:B:213:ILE:CG2	1:B:215:THR:HG22	2.17	0.73
1:C:54:ALA:H	1:C:304:LYS:CD	2.00	0.73
1:C:175:LEU:HD13	1:C:176:GLY:O	1.89	0.73
1:F:143:MET:HE3	1:F:145:SER:CB	2.19	0.73
1:A:341:HIS:CE1	1:A:342:PRO:HG2	2.24	0.72
1:C:88:ASP:O	1:C:92:ILE:CG1	2.34	0.72
1:D:16:LEU:HD22	1:D:32:ALA:HB2	1.71	0.72
1:D:274:LEU:HD22	1:D:278:GLN:HG2	1.71	0.72
1:A:105:ARG:HB2	1:A:106:PRO:HD3	1.71	0.72
1:F:298:LYS:HA	1:F:298:LYS:HE2	1.71	0.72
1:A:30:ARG:HG2	1:A:242:GLU:O	1.89	0.72
1:B:47:VAL:CG1	1:B:97:ILE:HD13	2.01	0.72
1:E:19:CYS:HB2	1:E:121:ASP:OD2	1.89	0.72
1:B:146:SER:OG	1:B:149:PHE:CB	2.37	0.72
1:F:13:HIS:C	1:F:14:ILE:HD13	2.14	0.72
1:B:276:LYS:NZ	1:B:280:ARG:NH2	2.37	0.72
1:D:24:HIS:HA	1:D:144:THR:HG21	1.71	0.72
1:D:153:MET:CA	1:D:198:ILE:HD11	2.19	0.72
1:C:183:ILE:CG2	1:C:187:MET:CE	2.67	0.72
1:C:378:ASN:O	1:C:381:VAL:CG1	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:VAL:HG12	1:E:69:ILE:CG2	2.19	0.72
1:F:50:THR:HG22	1:F:52:SER:H	1.55	0.72
1:A:98:ALA:HB1	1:A:127:GLN:HG3	1.72	0.72
1:A:299:GLY:H	1:A:330:LYS:HZ3	1.36	0.72
1:B:34:MET:HE3	1:B:241:LEU:HD23	1.71	0.72
1:D:215:THR:HG22	1:D:216:PHE:N	2.03	0.72
1:F:143:MET:CE	1:F:145:SER:CB	2.67	0.72
1:A:212:LEU:N	1:A:212:LEU:HD12	2.05	0.72
1:B:226:ALA:O	1:B:230:ASN:HB2	1.90	0.72
1:C:352:GLY:O	1:C:356:VAL:HG22	1.89	0.72
1:E:18:PRO:HG3	1:E:28:PHE:CB	2.20	0.72
1:C:50:THR:HG23	1:C:52:SER:N	2.05	0.71
1:F:50:THR:HG22	1:F:52:SER:O	1.90	0.71
1:A:72:LEU:HG	1:A:107:LEU:HD11	1.72	0.71
1:B:141:THR:CG2	1:B:211:VAL:HG13	2.20	0.71
1:B:289:SER:HB3	1:B:411:MET:HE3	1.72	0.71
1:D:15:ALA:HA	1:D:43:THR:O	1.88	0.71
1:D:113:PRO:N	1:D:113:PRO:O	2.23	0.71
1:E:76:LEU:CD2	1:E:76:LEU:H	2.03	0.71
1:C:149:PHE:HD2	1:C:153:MET:CE	2.01	0.71
1:D:350:HIS:C	1:D:350:HIS:ND1	2.48	0.71
1:E:159:LEU:HD23	1:E:159:LEU:C	2.16	0.71
1:F:238:ILE:O	1:F:238:ILE:CG2	2.36	0.71
1:E:90:PHE:CE2	1:E:271:ARG:CB	2.74	0.71
1:E:112:SER:HB3	1:E:113:PRO:HD3	1.70	0.71
1:C:232:VAL:HG13	1:C:234:HIS:CE1	2.25	0.71
1:C:353:TRP:CA	1:C:356:VAL:HG23	2.19	0.71
1:F:50:THR:HG21	1:F:55:GLU:HB2	1.71	0.71
1:C:387:LEU:HD23	1:C:387:LEU:C	2.13	0.71
1:D:394:TRP:CD2	1:D:402:ILE:HD13	2.25	0.71
1:D:251:ASP:OD1	1:D:251:ASP:N	2.24	0.70
1:C:300:GLY:HA3	1:C:307:LYS:CB	2.21	0.70
1:D:317:SER:O	1:D:321:ARG:HG3	1.90	0.70
1:D:389:LEU:HD21	1:D:420:LEU:HD22	1.68	0.70
1:C:383:GLU:CG	1:C:384:LYS:NZ	2.54	0.70
1:F:187:MET:O	1:F:195:SER:HB2	1.91	0.70
1:B:34:MET:HE3	1:B:241:LEU:CD2	2.21	0.70
1:F:299:GLY:HA3	1:F:313:MET:HE1	1.72	0.70
1:B:266:VAL:HB	1:B:295:TRP:CD1	2.27	0.70
1:D:350:HIS:HE1	1:D:352:GLY:N	1.88	0.70
1:E:243:SER:CB	1:E:336:GLU:OE1	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD13	1:B:96:THR:HG21	1.71	0.70
1:A:285:ALA:HB1	1:A:407:ILE:CG2	2.21	0.70
1:B:22:MET:HE3	1:B:55:GLU:HG2	1.71	0.70
1:D:339:LEU:CB	1:D:362:LEU:HD12	2.22	0.70
1:B:155:TYR:CD2	1:B:173:PRO:HD3	2.26	0.70
1:D:152:LEU:HD21	1:D:183:ILE:CG1	2.22	0.70
1:D:194:PHE:O	1:D:194:PHE:CD1	2.44	0.70
1:C:222:GLU:CD	1:C:222:GLU:H	2.00	0.70
1:C:383:GLU:HG2	1:C:384:LYS:HZ1	1.55	0.70
1:E:175:LEU:HD12	1:E:175:LEU:H	1.56	0.70
1:F:50:THR:HG22	1:F:52:SER:N	2.07	0.70
1:F:412:ILE:HG23	1:F:416:GLN:HG3	1.73	0.70
1:D:354:ASN:HB3	2:D:500:UDP:H5'1	1.74	0.69
1:E:65:ILE:HG13	1:E:246:ALA:CB	2.22	0.69
1:F:50:THR:HG21	1:F:52:SER:O	1.92	0.69
1:C:27:PRO:CG	1:C:354:ASN:ND2	2.28	0.69
1:C:353:TRP:HA	1:C:356:VAL:HG21	1.72	0.69
1:D:16:LEU:CD2	1:D:28:PHE:O	2.40	0.69
1:C:187:MET:O	1:C:195:SER:HB2	1.92	0.69
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.56	0.69
1:D:26:LEU:N	1:D:27:PRO:CD	2.55	0.69
1:D:391:VAL:HG12	1:D:394:TRP:CG	2.25	0.69
1:E:90:PHE:HE2	1:E:271:ARG:HB3	1.56	0.69
1:C:445:LEU:O	1:C:449:ILE:HG12	1.93	0.69
1:E:76:LEU:H	1:E:76:LEU:HD23	1.56	0.69
1:F:424:ALA:HA	1:F:427:VAL:CG2	2.22	0.69
1:C:387:LEU:CD2	1:C:387:LEU:C	2.64	0.69
1:D:153:MET:HB3	1:D:198:ILE:HD11	1.74	0.69
1:D:215:THR:CG2	1:D:216:PHE:N	2.55	0.69
1:F:232:VAL:O	1:F:232:VAL:HG22	1.92	0.69
1:F:286:LEU:HD21	1:F:411:MET:CE	2.22	0.69
1:A:47:VAL:HG12	1:A:76:LEU:HD21	1.61	0.69
1:C:54:ALA:N	1:C:304:LYS:HD2	2.04	0.69
1:E:252:LEU:N	1:E:253:PRO:CD	2.55	0.69
1:E:260:PRO:O	1:E:261:GLU:HB3	1.93	0.69
1:A:227:VAL:HG11	1:A:235:ILE:HD12	1.75	0.69
1:C:335:GLN:HB2	2:C:500:UDP:O2	1.93	0.69
1:C:50:THR:CG2	1:C:52:SER:N	2.55	0.68
1:D:410:LYS:HE3	1:D:413:GLU:OE1	1.93	0.68
1:E:152:LEU:HD21	1:E:183:ILE:HG13	1.75	0.68
1:D:184:PRO:CG	1:D:187:MET:HE2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:LEU:HD13	1:E:84:LEU:H	1.57	0.68
1:E:188:LEU:N	1:E:188:LEU:HD23	2.07	0.68
1:F:88:ASP:O	1:F:92:ILE:CG1	2.33	0.68
1:D:350:HIS:ND1	1:D:352:GLY:N	2.36	0.68
1:D:394:TRP:CD2	1:D:402:ILE:CD1	2.76	0.68
1:B:156:LEU:CD1	1:B:160:LEU:CG	2.61	0.68
1:A:254:TRP:CE2	1:A:258:GLN:OE1	2.46	0.68
1:D:14:ILE:HG13	1:D:40:CYS:SG	2.33	0.68
1:E:280:ARG:NE	1:E:280:ARG:HA	2.07	0.68
1:D:50:THR:HG21	1:D:55:GLU:HB3	1.75	0.68
1:E:49:PRO:CD	1:E:76:LEU:HD21	2.21	0.68
1:A:258:GLN:HA	1:A:258:GLN:HE21	1.57	0.68
1:B:35:LEU:O	1:B:40:CYS:HB2	1.94	0.68
1:C:64:THR:HG22	1:E:82:SER:CA	2.23	0.68
1:C:141:THR:HG23	1:C:208:VAL:HG11	1.76	0.68
1:D:268:PHE:O	1:D:350:HIS:CD2	2.47	0.67
1:E:72:LEU:HD11	1:E:111:LEU:HD11	1.76	0.67
1:E:215:THR:HG21	1:E:220:GLU:HG3	1.75	0.67
1:E:346:GLY:CA	1:E:415:MET:HE1	2.24	0.67
1:B:289:SER:HB3	1:B:411:MET:HE2	1.75	0.67
1:D:434:THR:HG22	1:D:441:SER:H	1.60	0.67
1:E:394:TRP:O	1:E:400:LYS:CD	2.42	0.67
1:F:206:HIS:CD2	1:F:207:LYS:HG2	2.30	0.67
1:B:289:SER:CB	1:B:411:MET:CE	2.69	0.67
1:C:300:GLY:H	1:C:307:LYS:CD	2.08	0.67
1:B:100:SER:O	1:B:103:LEU:HB2	1.94	0.67
1:E:23:GLY:O	1:E:27:PRO:HG2	1.94	0.67
1:F:42:VAL:HB	1:F:69:ILE:HG23	1.75	0.67
1:E:347:PHE:CD1	1:E:348:VAL:N	2.63	0.67
1:C:244:TYR:O	1:C:245:ASP:HB2	1.95	0.67
1:B:141:THR:HG22	1:B:211:VAL:HG13	1.75	0.67
1:D:424:ALA:O	1:D:427:VAL:CG1	2.36	0.67
1:E:26:LEU:HD12	2:E:500:UDP:H4'	1.77	0.67
1:F:101:VAL:HG13	1:F:131:LEU:HD21	1.77	0.67
1:F:271:ARG:HD2	1:F:271:ARG:O	1.95	0.67
1:B:146:SER:OG	1:B:149:PHE:HB3	1.95	0.67
1:B:158:LYS:O	1:B:162:ILE:HG13	1.94	0.67
1:D:153:MET:HB3	1:D:198:ILE:CD1	2.25	0.67
1:C:314:LEU:HD12	1:C:328:ILE:CD1	2.24	0.67
1:B:26:LEU:N	1:B:27:PRO:HD2	2.09	0.66
1:C:46:THR:HG21	1:C:59:LEU:CD2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:VAL:CG1	1:C:388:GLY:HA3	2.25	0.66
1:B:50:THR:CG2	1:B:52:SER:O	2.43	0.66
1:C:86:ASN:HD21	1:C:91:PHE:HB3	1.59	0.66
1:E:307:LYS:CG	1:E:330:LYS:NZ	2.58	0.66
1:F:101:VAL:O	1:F:131:LEU:HD21	1.96	0.66
1:D:24:HIS:O	1:D:27:PRO:CG	2.42	0.66
1:B:212:LEU:HB3	1:B:238:ILE:HD12	0.78	0.66
1:C:156:LEU:HB3	1:C:157:PRO:HD3	1.77	0.66
1:F:188:LEU:O	1:F:190:PRO:HD3	1.95	0.66
1:A:273:ALA:O	1:A:301:LYS:HE3	1.96	0.66
1:C:260:PRO:O	1:C:261:GLU:HB2	1.95	0.66
1:C:295:TRP:CE2	1:C:297:LEU:HD13	2.30	0.66
1:D:317:SER:O	1:D:321:ARG:CG	2.43	0.66
1:B:50:THR:HG21	1:B:55:GLU:HB2	1.78	0.66
1:C:243:SER:CB	1:C:336:GLU:OE2	2.44	0.66
1:E:346:GLY:N	1:E:415:MET:HE1	2.10	0.66
1:F:203:SER:O	1:F:206:HIS:CE1	2.48	0.66
1:F:390:TRP:CH2	1:F:392:ARG:HD3	2.31	0.66
1:B:104:LEU:HD13	1:B:108:LEU:HD11	1.77	0.66
1:C:25:LEU:HD12	1:C:25:LEU:O	1.96	0.66
1:C:407:ILE:O	1:C:411:MET:HG3	1.96	0.66
1:C:60:SER:O	1:C:64:THR:HG23	1.96	0.66
1:C:284:ALA:CB	1:C:404:ARG:HD3	2.26	0.66
1:D:391:VAL:HG11	1:D:394:TRP:CE2	2.30	0.66
1:E:227:VAL:HG13	1:E:232:VAL:HB	1.78	0.66
1:A:34:MET:HE3	1:A:241:LEU:HD23	1.69	0.66
1:C:366:VAL:HG12	1:C:387:LEU:HD22	1.78	0.66
1:F:434:THR:CG2	1:F:441:SER:N	2.56	0.66
1:A:282:LEU:HD13	1:A:369:TRP:CZ3	2.29	0.66
1:B:101:VAL:O	1:B:104:LEU:HB2	1.96	0.65
1:C:16:LEU:CD2	1:C:31:LEU:HD23	2.26	0.65
1:D:445:LEU:O	1:D:449:ILE:HG13	1.96	0.65
1:E:183:ILE:HG23	1:E:187:MET:HE2	1.79	0.65
1:F:278:GLN:CA	1:F:278:GLN:NE2	2.30	0.65
1:B:13:HIS:HD2	1:B:113:PRO:O	1.78	0.65
1:E:397:GLY:O	1:E:398:GLN:CB	2.44	0.65
1:B:212:LEU:CG	1:B:238:ILE:HD11	2.25	0.65
1:C:260:PRO:HA	1:C:343:ALA:HA	1.79	0.65
1:E:279:ILE:CD1	1:E:313:MET:HE2	2.27	0.65
1:B:25:LEU:HD12	1:B:25:LEU:O	1.96	0.65
1:C:264:LEU:HB2	1:C:415:MET:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:TRP:O	1:E:258:GLN:NE2	2.30	0.65
1:E:338:ILE:O	1:E:344:ILE:HG13	1.96	0.65
1:A:278:GLN:HE22	1:A:402:ILE:N	1.94	0.65
1:B:263:VAL:HG22	1:B:344:ILE:CD1	2.22	0.65
1:D:43:THR:HA	1:D:70:THR:HG22	1.79	0.65
1:C:286:LEU:HD23	1:C:411:MET:SD	2.36	0.65
1:C:350:HIS:O	1:C:351:CYS:HB2	1.96	0.65
1:D:410:LYS:NZ	1:D:413:GLU:OE1	2.30	0.65
1:F:152:LEU:HD21	1:F:183:ILE:HG12	1.79	0.65
1:A:233:ASP:N	1:A:233:ASP:OD1	2.29	0.65
1:B:145:SER:HG	1:B:149:PHE:HD2	1.44	0.65
1:B:276:LYS:HD2	1:B:313:MET:HA	1.78	0.65
1:D:194:PHE:O	1:D:198:ILE:HG22	1.96	0.65
1:D:339:LEU:HB2	1:D:362:LEU:HD12	1.77	0.65
1:E:16:LEU:CD2	1:E:32:ALA:HB2	2.20	0.65
1:F:146:SER:HB3	1:F:353:TRP:CE3	2.32	0.65
1:C:238:ILE:HD13	1:C:238:ILE:N	2.12	0.65
1:C:434:THR:HG22	1:C:441:SER:H	1.60	0.65
1:D:127:GLN:OE1	1:D:127:GLN:N	2.30	0.65
1:A:285:ALA:CB	1:A:407:ILE:CG2	2.75	0.65
1:B:394:TRP:CD2	1:B:402:ILE:HD12	2.32	0.65
1:D:51:VAL:HG11	1:D:90:PHE:CE1	2.32	0.65
1:D:171:GLU:HB2	1:D:177:PRO:HG3	1.79	0.65
1:E:350:HIS:HE1	2:E:500:UDP:O1B	1.80	0.65
1:F:408:ALA:O	1:F:412:ILE:HD12	1.97	0.65
1:A:50:THR:CG2	1:A:52:SER:O	2.45	0.65
1:D:269:GLY:O	2:D:500:UDP:H5	1.79	0.65
1:F:254:TRP:O	1:F:258:GLN:NE2	2.29	0.65
1:B:192:ASP:OD1	1:B:194:PHE:N	2.30	0.64
1:C:284:ALA:HB1	1:C:404:ARG:HD3	1.79	0.64
1:A:278:GLN:NE2	1:A:402:ILE:H	1.95	0.64
1:B:269:GLY:CA	1:B:350:HIS:CE1	2.81	0.64
1:F:50:THR:CG2	1:F:52:SER:H	2.10	0.64
1:B:284:ALA:HB1	1:B:404:ARG:HH11	1.62	0.64
1:E:307:LYS:CG	1:E:330:LYS:HZ2	2.10	0.64
1:F:286:LEU:HD21	1:F:411:MET:HE1	1.77	0.64
1:A:36:ASP:OD1	1:A:36:ASP:C	2.41	0.64
1:A:402:ILE:HG22	1:A:407:ILE:CD1	2.28	0.64
1:D:197:PHE:O	1:D:201:ASN:ND2	2.30	0.64
1:D:224:ILE:O	1:D:227:VAL:HG23	1.97	0.64
1:C:138:SER:OG	1:C:209:LYS:CG	2.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ILE:HD13	1:C:180:MET:CE	2.28	0.64
1:C:215:THR:OG1	1:C:220:GLU:HG3	1.97	0.64
1:D:155:TYR:C	1:D:157:PRO:HD2	2.23	0.64
1:F:104:LEU:N	1:F:104:LEU:HD23	2.12	0.64
1:F:303:ASP:OD1	1:F:303:ASP:N	2.28	0.64
1:A:14:ILE:HG21	1:A:35:LEU:CD1	2.26	0.64
1:B:47:VAL:HG13	1:B:97:ILE:HD11	1.77	0.64
1:B:448:LEU:O	1:B:448:LEU:HD12	1.98	0.64
1:C:105:ARG:HG2	1:C:105:ARG:NH1	2.10	0.64
1:C:434:THR:HG21	1:C:441:SER:OG	1.98	0.64
1:D:269:GLY:CA	1:D:350:HIS:CD2	2.80	0.64
1:E:402:ILE:CG2	1:E:406:GLU:HG2	2.27	0.64
1:F:278:GLN:NE2	1:F:278:GLN:O	2.30	0.64
1:B:34:MET:HE1	1:B:241:LEU:HD23	1.78	0.64
1:B:193:PHE:HD1	1:B:193:PHE:H	1.41	0.64
1:C:374:ASP:OD1	1:C:375:GLN:N	2.30	0.64
1:A:164:VAL:HG11	1:A:190:PRO:HD3	1.80	0.64
1:C:383:GLU:OE2	1:C:384:LYS:NZ	2.30	0.64
1:C:434:THR:CG2	1:C:441:SER:N	2.60	0.64
1:D:424:ALA:C	1:D:427:VAL:HG12	2.23	0.64
1:F:440:ASP:N	1:F:440:ASP:OD1	2.30	0.64
1:A:76:LEU:HD13	1:A:96:THR:HG23	1.80	0.64
1:D:61:ALA:O	1:D:65:ILE:HD12	1.98	0.64
1:E:48:LYS:O	1:E:76:LEU:CD2	2.46	0.64
1:C:170:ILE:CD1	1:C:180:MET:CE	2.76	0.63
1:F:101:VAL:HG12	1:F:131:LEU:HD11	1.80	0.63
1:D:349:SER:OG	1:D:351:CYS:N	2.30	0.63
1:E:159:LEU:O	1:E:163:ASP:CB	2.46	0.63
1:B:275:SER:O	1:B:279:ILE:HG13	1.98	0.63
1:E:169:ALA:HB1	1:E:178:ILE:C	2.22	0.63
1:F:298:LYS:HB3	1:F:298:LYS:NZ	2.13	0.63
1:B:104:LEU:O	1:B:108:LEU:HD12	1.98	0.63
1:F:254:TRP:CE3	1:F:327:LEU:HD21	2.31	0.63
1:C:255:LEU:HD21	1:C:344:ILE:HD11	1.79	0.63
1:F:26:LEU:O	1:F:30:ARG:CG	2.46	0.63
1:F:296:VAL:C	1:F:297:LEU:CD1	2.72	0.63
1:A:272:THR:CB	1:A:301:LYS:CG	2.77	0.63
1:B:224:ILE:HA	1:B:227:VAL:CG2	2.29	0.63
1:C:193:PHE:CD1	1:C:193:PHE:C	2.77	0.63
1:D:184:PRO:HG2	1:D:187:MET:CE	2.27	0.63
1:D:389:LEU:HD23	1:D:420:LEU:CD2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:HD12	1:E:212:LEU:N	2.13	0.63
1:C:320:GLU:OE2	1:C:320:GLU:HA	1.99	0.62
1:E:347:PHE:HD1	1:E:348:VAL:N	1.97	0.62
1:D:212:LEU:HA	1:D:236:LEU:O	1.99	0.62
1:B:146:SER:OG	1:B:149:PHE:N	2.30	0.62
1:C:295:TRP:HB3	1:C:328:ILE:HG22	1.80	0.62
1:D:394:TRP:CG	1:D:402:ILE:HD13	2.32	0.62
1:C:307:LYS:O	1:C:330:LYS:HE3	1.99	0.62
1:C:374:ASP:OD1	1:C:374:ASP:C	2.38	0.62
1:D:47:VAL:CG1	1:D:97:ILE:HD11	2.29	0.62
1:A:271:ARG:HB3	1:A:301:LYS:O	2.00	0.62
1:D:153:MET:CB	1:D:198:ILE:HD11	2.29	0.62
1:D:391:VAL:CG1	1:D:391:VAL:O	2.45	0.62
1:F:219:PHE:HE1	1:F:385:ALA:CB	2.11	0.62
1:A:217:ASN:OD1	1:A:217:ASN:N	2.33	0.62
1:B:218:SER:CB	1:B:430:LYS:HD2	2.29	0.62
1:E:346:GLY:CA	1:E:415:MET:CE	2.78	0.62
1:E:108:LEU:HD22	1:E:115:LEU:HD11	1.82	0.62
1:A:274:LEU:HD22	1:A:278:GLN:HG2	1.80	0.62
1:A:129:THR:HG22	1:A:207:LYS:HD2	1.81	0.62
1:C:23:GLY:O	1:C:27:PRO:HG2	2.00	0.62
1:C:30:ARG:O	1:C:34:MET:HG3	1.98	0.62
1:E:159:LEU:HD23	1:E:159:LEU:O	1.99	0.62
1:F:86:ASN:HD21	1:F:92:ILE:N	1.98	0.62
1:B:286:LEU:HD21	1:B:293:PHE:CD2	2.35	0.61
1:D:341:HIS:CE1	1:D:342:PRO:HD2	2.30	0.61
1:F:19:CYS:HB2	1:F:121:ASP:OD2	2.00	0.61
1:F:90:PHE:O	1:F:94:MET:HG3	1.99	0.61
1:D:402:ILE:O	1:D:402:ILE:HG23	2.00	0.61
1:E:235:ILE:HD12	1:E:235:ILE:O	2.00	0.61
1:B:275:SER:O	1:B:279:ILE:CG1	2.48	0.61
1:B:341:HIS:ND1	1:B:342:PRO:HD2	2.15	0.61
1:C:320:GLU:OE2	1:C:323:LYS:CE	2.49	0.61
1:D:22:MET:HE2	1:D:26:LEU:HG	1.82	0.61
1:F:129:THR:CG2	1:F:130:ASP:N	2.63	0.61
1:A:285:ALA:HB1	1:A:411:MET:HE1	1.81	0.61
1:D:47:VAL:HB	1:D:97:ILE:CD1	2.31	0.61
1:D:184:PRO:CG	1:D:187:MET:CE	2.78	0.61
1:F:354:ASN:O	1:F:358:GLU:HG3	2.00	0.61
1:B:213:ILE:HG23	1:B:215:THR:CG2	2.28	0.61
1:B:272:THR:CB	1:B:301:LYS:HA	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:THR:HG22	1:C:441:SER:N	2.16	0.61
1:F:369:TRP:O	1:F:371:GLN:NE2	2.30	0.61
1:E:346:GLY:HA3	1:E:415:MET:HE1	1.81	0.61
1:A:341:HIS:ND1	1:A:342:PRO:N	2.49	0.61
1:B:218:SER:HB3	1:B:430:LYS:HD2	1.83	0.61
1:C:198:ILE:O	1:C:202:VAL:HG23	2.01	0.61
1:E:335:GLN:CD	2:E:500:UDP:H2'	2.24	0.61
1:F:85:ARG:HB2	1:F:192:ASP:HA	1.83	0.61
1:C:292:ARG:HA	1:C:325:LYS:O	2.00	0.60
1:F:360:ALA:HB2	1:F:387:LEU:HD11	1.82	0.60
1:A:238:ILE:O	1:A:238:ILE:HG22	2.00	0.60
1:D:411:MET:O	1:D:414:VAL:HG12	2.01	0.60
1:F:389:LEU:HD12	1:F:414:VAL:HB	1.84	0.60
1:B:289:SER:OG	1:B:411:MET:HE3	2.01	0.60
1:C:371:GLN:HE21	1:C:397:GLY:HA3	1.67	0.60
1:C:383:GLU:HG2	1:C:384:LYS:CE	2.31	0.60
1:D:24:HIS:C	1:D:27:PRO:HD2	2.27	0.60
1:E:347:PHE:HD1	1:E:348:VAL:H	1.49	0.60
1:F:424:ALA:CA	1:F:427:VAL:HG23	2.32	0.60
1:C:434:THR:HG22	1:C:441:SER:CA	2.31	0.60
1:D:211:VAL:O	1:D:236:LEU:N	2.28	0.60
1:B:321:ARG:HG2	1:B:321:ARG:NH1	2.14	0.60
1:D:35:LEU:O	1:D:40:CYS:HB2	2.02	0.60
1:F:112:SER:CB	1:F:113:PRO:CD	2.78	0.60
1:F:143:MET:HE1	1:F:145:SER:HB3	1.82	0.60
1:A:108:LEU:HD13	1:A:137:ILE:HD11	1.83	0.60
1:D:278:GLN:OE1	1:D:402:ILE:HG22	2.02	0.60
1:E:42:VAL:CG1	1:E:69:ILE:HG23	2.28	0.60
1:A:51:VAL:HG11	1:A:90:PHE:CE1	2.36	0.60
1:A:298:LYS:NZ	2:A:500:UDP:O4	2.29	0.60
1:D:115:LEU:CB	1:D:137:ILE:CD1	2.75	0.60
1:F:131:LEU:N	1:F:131:LEU:HD12	2.17	0.60
1:A:254:TRP:CD2	1:A:258:GLN:OE1	2.55	0.59
1:D:105:ARG:HB2	1:D:106:PRO:HD3	1.84	0.59
1:D:350:HIS:ND1	1:D:351:CYS:N	2.50	0.59
1:E:76:LEU:HD23	1:E:76:LEU:N	2.16	0.59
1:B:107:LEU:HD12	1:B:107:LEU:C	2.26	0.59
1:A:293:PHE:CE1	1:A:326:GLY:HA3	2.38	0.59
1:B:42:VAL:HG12	1:B:69:ILE:HG12	1.81	0.59
1:D:156:LEU:HD11	1:D:160:LEU:HG	1.83	0.59
1:E:264:LEU:HD12	1:E:346:GLY:HA3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:ARG:HG2	1:F:446:GLN:NE2	2.16	0.59
1:C:353:TRP:CA	1:C:356:VAL:CG2	2.74	0.59
1:C:394:TRP:CE2	1:C:402:ILE:HD12	2.36	0.59
1:E:53:ALA:H	1:E:304:LYS:CG	2.15	0.59
1:E:350:HIS:O	1:E:375:GLN:HB3	2.01	0.59
1:F:289:SER:HA	1:F:412:ILE:HD11	1.83	0.59
1:A:22:MET:HG3	1:A:332:TRP:CH2	2.37	0.59
1:A:59:LEU:O	1:A:63:PHE:CD2	2.54	0.59
1:B:212:LEU:CG	1:B:238:ILE:CD1	2.79	0.59
1:C:335:GLN:HB2	2:C:500:UDP:C2	2.36	0.59
1:F:23:GLY:O	1:F:27:PRO:HG2	2.03	0.59
1:F:143:MET:HE3	1:F:145:SER:N	2.12	0.59
1:D:285:ALA:HB1	1:D:407:ILE:HG22	1.83	0.59
1:E:238:ILE:HG22	1:E:238:ILE:O	2.01	0.59
1:F:401:LEU:C	1:F:402:ILE:HD12	2.28	0.59
1:B:155:TYR:CG	1:B:155:TYR:O	2.56	0.59
1:C:371:GLN:O	1:C:397:GLY:O	2.21	0.59
1:B:26:LEU:O	1:B:30:ARG:HG3	2.02	0.59
1:A:34:MET:HE3	1:A:241:LEU:CD2	2.28	0.59
1:C:309:GLU:O	1:C:330:LYS:HD2	2.03	0.59
1:D:342:PRO:HD2	1:D:343:ALA:H	1.68	0.59
1:F:266:VAL:HG13	1:F:348:VAL:HB	1.85	0.59
1:A:26:LEU:HB3	1:A:30:ARG:NH2	2.17	0.58
1:A:50:THR:HG21	1:A:55:GLU:HB2	1.85	0.58
1:B:263:VAL:CG2	1:B:344:ILE:CD1	2.78	0.58
1:D:125:THR:O	1:D:207:LYS:NZ	2.36	0.58
1:F:311:GLU:HA	1:F:311:GLU:OE1	2.02	0.58
1:A:88:ASP:OD1	1:A:89:PRO:CD	2.50	0.58
1:D:25:LEU:C	1:D:27:PRO:HD2	2.27	0.58
1:B:85:ARG:CB	1:B:193:PHE:HE1	2.14	0.58
1:D:296:VAL:HG12	1:D:296:VAL:O	2.01	0.58
1:D:448:LEU:O	1:D:448:LEU:CD1	2.30	0.58
1:C:54:ALA:HB2	1:C:304:LYS:CE	2.33	0.58
1:C:171:GLU:HA	1:C:177:PRO:CB	2.33	0.58
1:F:105:ARG:HB3	1:F:106:PRO:HD3	1.85	0.58
1:A:10:VAL:HG23	1:A:10:VAL:O	2.02	0.58
1:A:350:HIS:CD2	1:A:352:GLY:N	2.67	0.58
1:B:276:LYS:HZ1	1:B:280:ARG:NH2	1.97	0.58
1:C:165:ALA:O	1:C:166:ASN:CB	2.49	0.58
1:C:383:GLU:CG	1:C:384:LYS:HZ3	2.16	0.58
1:B:156:LEU:C	1:B:156:LEU:HD12	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HB2	1:A:215:THR:HG21	1.86	0.58
1:D:126:SER:O	1:D:129:THR:CG2	2.46	0.58
1:D:130:ASP:OD1	1:D:130:ASP:N	2.29	0.58
1:D:192:ASP:OD1	1:D:194:PHE:N	2.30	0.58
1:F:216:PHE:CE2	1:F:219:PHE:HB2	2.39	0.58
1:D:273:ALA:HB1	1:D:371:GLN:CB	2.33	0.58
1:C:394:TRP:CD2	1:C:402:ILE:CD1	2.85	0.58
1:F:23:GLY:O	1:F:27:PRO:CG	2.51	0.58
1:A:26:LEU:N	1:A:27:PRO:HD2	2.19	0.58
1:E:216:PHE:N	1:E:216:PHE:CD1	2.72	0.58
1:F:105:ARG:HB2	1:F:105:ARG:NH1	2.18	0.58
1:F:269:GLY:O	1:F:298:LYS:HG3	2.04	0.58
1:B:156:LEU:O	1:B:156:LEU:HD12	2.03	0.57
1:B:271:ARG:NH1	1:B:302:VAL:HG12	2.19	0.57
1:C:125:THR:OG1	1:C:141:THR:HG21	2.03	0.57
1:E:447:ARG:CG	1:E:447:ARG:NH1	2.35	0.57
1:C:170:ILE:CD1	1:C:180:MET:HE1	2.34	0.57
1:D:22:MET:CE	1:D:25:LEU:HD23	2.32	0.57
1:F:264:LEU:HD13	1:F:415:MET:SD	2.44	0.57
1:F:434:THR:HA	1:F:439:GLY:HA3	1.86	0.57
1:F:445:LEU:O	1:F:449:ILE:HG13	2.04	0.57
1:A:135:LEU:HG	1:C:87:ASP:HB2	1.84	0.57
1:B:434:THR:HG21	1:B:441:SER:OG	2.04	0.57
1:C:76:LEU:HD22	1:C:96:THR:HG22	1.87	0.57
1:B:38:ARG:HB2	1:B:449:ILE:HD13	1.86	0.57
1:B:271:ARG:CB	1:B:301:LYS:O	2.42	0.57
1:F:215:THR:O	1:F:237:PRO:HB3	2.05	0.57
1:F:328:ILE:O	1:F:328:ILE:HG13	2.04	0.57
1:A:278:GLN:NE2	1:A:401:LEU:HD12	2.19	0.57
1:B:155:TYR:O	1:B:155:TYR:CD1	2.58	0.57
1:D:273:ALA:CB	1:D:371:GLN:CG	2.80	0.57
1:D:341:HIS:CG	1:D:342:PRO:HD3	2.35	0.57
1:F:50:THR:CG2	1:F:55:GLU:HB2	2.35	0.57
1:F:143:MET:CE	1:F:145:SER:HB3	2.34	0.57
1:F:424:ALA:HA	1:F:427:VAL:HG23	1.87	0.57
1:B:10:VAL:HG11	1:B:68:ARG:NH2	2.19	0.57
1:B:16:LEU:HD21	1:B:32:ALA:HB2	1.85	0.57
1:B:26:LEU:O	1:B:30:ARG:CG	2.53	0.57
1:B:175:LEU:HD22	1:B:176:GLY:H	1.70	0.57
1:B:368:ALA:HB3	1:B:390:TRP:HB2	1.87	0.57
1:C:353:TRP:HE3	1:C:378:ASN:ND2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:NE2	2:A:500:UDP:H2'	2.20	0.57
1:B:50:THR:HG21	1:B:52:SER:O	2.05	0.57
1:B:105:ARG:NH2	1:B:134:ASP:OD2	2.37	0.57
1:D:47:VAL:HG23	1:D:76:LEU:HD21	1.85	0.57
1:D:50:THR:CG2	1:D:55:GLU:HB3	2.34	0.56
1:D:334:LYS:HB3	1:D:337:GLN:HB3	1.87	0.56
1:E:16:LEU:HD23	1:E:28:PHE:O	2.05	0.56
1:A:140:TYR:CZ	1:A:448:LEU:HD11	2.40	0.56
1:B:42:VAL:HG13	1:B:69:ILE:HG12	1.81	0.56
1:B:180:MET:HA	1:B:183:ILE:HG13	1.86	0.56
1:F:434:THR:HG21	1:F:441:SER:HB2	1.65	0.56
1:A:435:ARG:NH1	1:A:442:GLU:OE1	2.38	0.56
1:C:89:PRO:HG3	1:C:302:VAL:HG21	1.88	0.56
1:F:390:TRP:CZ2	1:F:392:ARG:HD3	2.41	0.56
1:C:135:LEU:HD12	1:C:135:LEU:N	2.19	0.56
1:D:211:VAL:HG23	1:D:234:HIS:CD2	2.40	0.56
1:D:274:LEU:HD22	1:D:278:GLN:CG	2.34	0.56
1:A:52:SER:OG	1:A:55:GLU:HG3	2.06	0.56
1:C:183:ILE:CG2	1:C:187:MET:HE2	2.34	0.56
1:C:371:GLN:NE2	1:C:397:GLY:HA3	2.21	0.56
1:C:435:ARG:HA	1:C:435:ARG:HE	1.69	0.56
1:D:435:ARG:O	1:D:435:ARG:HD3	2.05	0.56
1:E:299:GLY:HA3	1:E:313:MET:HE1	1.86	0.56
1:F:86:ASN:ND2	1:F:92:ILE:N	2.53	0.56
1:D:115:LEU:CB	1:D:137:ILE:HD11	2.09	0.56
1:E:334:LYS:O	1:E:338:ILE:HD12	2.06	0.56
1:F:120:SER:OG	1:F:128:VAL:CG1	2.45	0.56
1:F:286:LEU:CD2	1:F:411:MET:CE	2.83	0.56
1:B:211:VAL:C	1:B:212:LEU:CD1	2.59	0.56
1:D:124:LEU:O	1:D:128:VAL:HG23	2.06	0.56
1:E:14:ILE:CD1	1:E:452:PHE:CD2	2.88	0.56
1:C:46:THR:HG21	1:C:59:LEU:HD21	1.85	0.56
1:D:16:LEU:HD23	1:D:28:PHE:O	2.05	0.56
1:D:100:SER:O	1:D:103:LEU:HB2	2.06	0.56
1:D:410:LYS:NZ	1:D:410:LYS:HA	2.21	0.56
1:E:168:ASP:O	1:E:180:MET:CB	2.51	0.56
1:F:424:ALA:HA	1:F:427:VAL:HG21	1.88	0.56
1:B:24:HIS:HA	1:B:144:THR:HG21	1.88	0.56
1:C:50:THR:HG23	1:C:51:VAL:N	2.21	0.56
1:F:434:THR:HG22	1:F:441:SER:H	1.69	0.56
1:C:74:PHE:HZ	1:C:104:LEU:HG	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HD13	1:C:115:LEU:HG	1.86	0.56
1:C:394:TRP:CZ2	1:C:402:ILE:CD1	2.88	0.56
1:C:394:TRP:HE1	1:C:406:GLU:CD	2.14	0.56
1:A:350:HIS:HE1	2:A:500:UDP:O2B	1.89	0.55
1:B:284:ALA:HB1	1:B:404:ARG:NH1	2.18	0.55
1:C:286:LEU:HD21	1:C:411:MET:HE1	1.88	0.55
1:D:268:PHE:O	1:D:350:HIS:HD2	1.86	0.55
1:E:158:LYS:O	1:E:162:ILE:HG22	2.06	0.55
1:E:264:LEU:CD1	1:E:415:MET:HE3	2.36	0.55
1:F:260:PRO:O	1:F:261:GLU:HB2	2.06	0.55
1:C:217:ASN:O	1:C:221:SER:HB2	2.06	0.55
1:E:286:LEU:CG	1:E:411:MET:HE1	2.35	0.55
1:B:266:VAL:HG13	1:B:348:VAL:HG22	1.89	0.55
1:C:445:LEU:O	1:C:449:ILE:CG1	2.54	0.55
1:D:47:VAL:CB	1:D:97:ILE:HD11	2.36	0.55
1:E:112:SER:CB	1:E:113:PRO:HD3	2.36	0.55
1:C:170:ILE:CD1	1:C:180:MET:HE3	2.36	0.55
1:D:268:PHE:O	1:D:350:HIS:HB3	2.06	0.55
1:D:354:ASN:HB2	2:D:500:UDP:H5'1	1.87	0.55
1:E:213:ILE:HG22	1:E:237:PRO:HA	1.89	0.55
1:D:156:LEU:N	1:D:157:PRO:CD	2.70	0.55
1:D:389:LEU:HD13	1:D:413:GLU:HG2	1.88	0.55
1:E:374:ASP:O	1:E:377:VAL:CG1	2.54	0.55
1:A:258:GLN:HA	1:A:258:GLN:NE2	2.20	0.55
1:C:293:PHE:CD1	1:C:293:PHE:C	2.84	0.55
1:D:105:ARG:HB2	1:D:106:PRO:CD	2.36	0.55
1:D:23:GLY:O	1:D:354:ASN:ND2	2.40	0.55
1:D:216:PHE:N	1:D:216:PHE:CD1	2.75	0.55
1:B:276:LYS:HZ1	1:B:280:ARG:HH21	1.45	0.55
1:B:268:PHE:HZ	1:B:369:TRP:CE3	2.25	0.55
1:B:269:GLY:HA3	1:B:350:HIS:CE1	2.41	0.55
1:B:65:ILE:HG22	1:B:66:HIS:CE1	2.42	0.55
1:B:341:HIS:CG	1:B:342:PRO:HD2	2.42	0.55
1:D:45:ILE:HA	1:D:72:LEU:O	2.07	0.55
1:D:278:GLN:HE21	1:D:278:GLN:CA	2.18	0.55
1:D:303:ASP:HB3	1:D:306:ASP:HB2	1.88	0.55
1:E:434:THR:HG23	1:E:441:SER:CB	2.37	0.55
1:F:101:VAL:CG1	1:F:131:LEU:HD21	2.37	0.55
1:D:156:LEU:N	1:D:157:PRO:HD2	2.21	0.54
1:E:213:ILE:HG23	1:E:215:THR:H	1.71	0.54
1:F:286:LEU:CD2	1:F:411:MET:HE1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:VAL:HB	1:D:235:ILE:HA	1.90	0.54
1:D:269:GLY:CA	1:D:350:HIS:HD2	2.19	0.54
1:D:389:LEU:CD2	1:D:420:LEU:HD21	2.32	0.54
1:F:368:ALA:HB3	1:F:390:TRP:HB2	1.89	0.54
1:A:173:PRO:CB	1:A:230:ASN:ND2	2.62	0.54
1:B:448:LEU:HD12	1:B:448:LEU:C	2.32	0.54
1:C:170:ILE:HD13	1:C:180:MET:HE1	1.90	0.54
1:C:225:GLU:OE1	1:C:225:GLU:CA	2.53	0.54
1:C:286:LEU:CD2	1:C:411:MET:SD	2.96	0.54
1:C:335:GLN:NE2	2:C:500:UDP:H2'	2.22	0.54
1:B:293:PHE:C	1:B:293:PHE:CD1	2.85	0.54
1:C:214:ASN:OD1	1:C:241:LEU:HG	2.08	0.54
1:E:251:ASP:C	1:E:253:PRO:HD2	2.32	0.54
1:C:74:PHE:HZ	1:C:104:LEU:HA	1.73	0.54
1:C:170:ILE:HD13	1:C:180:MET:HE3	1.89	0.54
1:C:216:PHE:N	1:C:216:PHE:CD1	2.76	0.54
1:F:434:THR:HG22	1:F:441:SER:N	2.22	0.54
1:A:372:HIS:N	1:A:375:GLN:OE1	2.30	0.54
1:D:134:ASP:N	1:D:134:ASP:OD1	2.40	0.54
1:D:150:PHE:O	1:D:154:ALA:N	2.38	0.54
1:D:151:CYS:O	1:D:155:TYR:N	2.31	0.54
1:D:440:ASP:O	1:D:444:LEU:HG	2.07	0.54
1:E:286:LEU:HG	1:E:411:MET:HE1	1.88	0.54
1:F:101:VAL:HG13	1:F:131:LEU:CD2	2.37	0.54
1:F:298:LYS:HE2	1:F:298:LYS:CA	2.38	0.54
1:B:234:HIS:ND1	1:B:234:HIS:N	2.42	0.54
1:B:242:GLU:OE2	1:B:435:ARG:HD3	2.08	0.54
1:B:335:GLN:HB2	2:B:500:UDP:C2	2.43	0.54
1:D:156:LEU:O	1:D:156:LEU:HD12	2.08	0.54
1:E:445:LEU:O	1:E:449:ILE:HG13	2.07	0.54
1:B:105:ARG:HB2	1:B:106:PRO:HD3	1.89	0.54
1:B:156:LEU:HD11	1:B:160:LEU:CD1	2.37	0.54
1:D:60:SER:O	1:D:64:THR:OG1	2.21	0.54
1:C:101:VAL:O	1:C:104:LEU:HB2	2.08	0.54
1:D:339:LEU:HB3	1:D:362:LEU:HD12	1.90	0.54
1:E:18:PRO:HG3	1:E:28:PHE:HB3	1.90	0.54
1:E:227:VAL:HG11	1:E:235:ILE:HG21	1.89	0.54
1:F:295:TRP:CE2	1:F:297:LEU:HD11	2.43	0.54
1:A:59:LEU:HD22	1:A:63:PHE:CE2	2.43	0.54
1:A:97:ILE:HG22	1:A:124:LEU:HD11	1.90	0.54
1:A:341:HIS:ND1	1:A:342:PRO:CG	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:PHE:CE1	1:C:71:ARG:CB	2.80	0.54
1:F:38:ARG:NH2	1:F:442:GLU:OE1	2.41	0.54
1:F:255:LEU:HB3	1:F:341:HIS:CD2	2.43	0.54
1:F:300:GLY:HA3	1:F:307:LYS:CG	2.38	0.54
1:A:38:ARG:HB3	1:A:449:ILE:HD13	1.88	0.53
1:B:34:MET:CE	1:B:241:LEU:CA	2.83	0.53
1:C:105:ARG:NE	1:C:135:LEU:HD11	2.19	0.53
1:D:295:TRP:CE3	1:D:328:ILE:CD1	2.91	0.53
1:C:12:ALA:HB1	1:C:116:SER:OG	2.08	0.53
1:C:351:CYS:SG	1:C:368:ALA:HB1	2.48	0.53
1:D:344:ILE:HD13	1:D:344:ILE:N	2.22	0.53
1:B:155:TYR:CE1	1:B:159:LEU:CB	2.86	0.53
1:D:30:ARG:O	1:D:34:MET:HG3	2.09	0.53
1:E:141:THR:HG23	1:E:211:VAL:HG22	1.89	0.53
1:E:345:GLY:C	1:E:415:MET:HE1	2.32	0.53
1:A:34:MET:O	1:A:38:ARG:HD2	2.08	0.53
1:D:47:VAL:HB	1:D:97:ILE:HD13	1.90	0.53
1:D:342:PRO:CD	1:D:343:ALA:H	2.21	0.53
1:F:112:SER:HB3	1:F:113:PRO:CD	2.26	0.53
1:B:147:ALA:HB2	1:B:215:THR:HG21	1.90	0.53
1:C:262:SER:HB2	1:C:292:ARG:HH11	1.71	0.53
1:D:28:PHE:O	1:D:31:LEU:HB3	2.08	0.53
1:E:149:PHE:HE2	1:E:153:MET:HE3	1.74	0.53
1:B:273:ALA:HB1	1:B:371:GLN:CG	2.38	0.53
1:C:293:PHE:CD1	1:C:293:PHE:O	2.62	0.53
1:C:319:VAL:HG22	1:C:328:ILE:HD11	1.90	0.53
1:E:26:LEU:HB3	1:E:30:ARG:HH11	1.73	0.53
1:E:255:LEU:HD21	1:E:344:ILE:HD11	1.91	0.53
1:E:280:ARG:HE	1:E:280:ARG:CA	2.20	0.53
1:F:167:ARG:NH2	1:F:170:ILE:HD13	2.23	0.53
1:A:299:GLY:N	1:A:330:LYS:NZ	2.54	0.53
1:E:18:PRO:HG3	1:E:28:PHE:CG	2.42	0.53
1:D:427:VAL:HG13	1:D:428:ARG:N	2.24	0.53
1:B:156:LEU:N	1:B:157:PRO:HD2	2.24	0.53
1:C:98:ALA:O	1:C:101:VAL:HG22	2.09	0.53
1:C:335:GLN:NE2	2:C:500:UDP:O2'	2.42	0.53
1:E:309:GLU:O	1:E:330:LYS:HE2	2.09	0.53
1:F:143:MET:HE1	1:F:145:SER:CA	2.36	0.53
1:F:341:HIS:HD2	1:F:343:ALA:HB3	1.72	0.53
1:B:274:LEU:HD22	1:B:278:GLN:HG2	1.90	0.52
1:B:285:ALA:O	1:B:411:MET:HE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ASP:CG	1:C:233:ASP:O	2.52	0.52
1:F:22:MET:CE	1:F:58:HIS:CD2	2.92	0.52
1:B:280:ARG:NE	1:B:313:MET:O	2.42	0.52
1:C:30:ARG:HB3	1:C:242:GLU:O	2.09	0.52
1:C:74:PHE:HZ	1:C:104:LEU:CA	2.22	0.52
1:C:227:VAL:CG1	1:C:228:ARG:N	2.72	0.52
1:F:46:THR:O	1:F:73:GLU:HA	2.09	0.52
1:A:309:GLU:O	1:A:330:LYS:HE3	2.09	0.52
1:B:22:MET:CE	1:B:22:MET:HA	2.34	0.52
1:D:13:HIS:HA	1:D:41:ALA:HB3	1.91	0.52
1:D:101:VAL:O	1:D:104:LEU:HB2	2.10	0.52
1:F:143:MET:HE3	1:F:145:SER:CA	2.40	0.52
1:C:34:MET:O	1:C:38:ARG:HG2	2.09	0.52
1:E:220:GLU:HB3	1:E:223:ALA:HB3	1.90	0.52
1:E:332:TRP:CH2	2:E:500:UDP:C2	2.97	0.52
1:A:255:LEU:HD23	1:A:341:HIS:CD2	2.37	0.52
1:D:233:ASP:N	1:D:233:ASP:OD1	2.42	0.52
1:E:26:LEU:HB2	1:E:27:PRO:CD	2.39	0.52
1:F:402:ILE:N	1:F:402:ILE:HD12	2.24	0.52
1:A:269:GLY:O	1:A:298:LYS:HE2	2.10	0.52
1:C:298:LYS:HZ3	1:C:298:LYS:HB3	1.72	0.52
1:D:149:PHE:CE2	1:D:153:MET:HE3	2.45	0.52
1:E:447:ARG:HH11	1:E:447:ARG:CB	2.22	0.52
1:F:119:VAL:O	1:F:119:VAL:CG2	2.56	0.52
1:B:47:VAL:HG22	1:B:76:LEU:HG	1.91	0.52
1:C:62:PHE:HD1	1:C:244:TYR:CD2	2.28	0.52
1:C:238:ILE:N	1:C:238:ILE:CD1	2.72	0.52
1:C:348:VAL:HG22	1:C:367:LEU:HD23	1.91	0.52
1:D:378:ASN:HA	1:D:381:VAL:CG2	2.39	0.52
1:E:16:LEU:CD2	1:E:28:PHE:O	2.58	0.52
1:C:27:PRO:CD	1:C:354:ASN:ND2	2.73	0.52
1:E:419:LYS:O	1:E:423:SER:HB3	2.10	0.52
1:B:218:SER:OG	1:B:430:LYS:HD2	2.08	0.52
1:D:402:ILE:HG23	1:D:407:ILE:HD11	1.91	0.52
1:F:101:VAL:O	1:F:104:LEU:HG	2.09	0.52
1:A:212:LEU:N	1:A:212:LEU:CD1	2.72	0.52
1:E:65:ILE:HG21	1:E:246:ALA:HB2	1.91	0.52
1:E:84:LEU:N	1:E:84:LEU:CD1	2.73	0.52
1:E:156:LEU:N	1:E:157:PRO:HD2	2.25	0.52
1:E:415:MET:HA	1:E:415:MET:HE2	1.92	0.52
1:F:403:GLY:O	1:F:407:ILE:CG1	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:CG2	1:A:407:ILE:CD1	2.87	0.51
1:B:155:TYR:CE2	1:B:173:PRO:HD3	2.45	0.51
1:D:278:GLN:NE2	1:D:278:GLN:CA	2.73	0.51
1:E:252:LEU:N	1:E:253:PRO:HD2	2.24	0.51
1:E:292:ARG:HG3	1:E:292:ARG:HH21	1.75	0.51
1:F:374:ASP:OD1	1:F:375:GLN:N	2.42	0.51
1:C:437:VAL:HG12	1:C:438:ASP:N	2.24	0.51
1:F:64:THR:CG2	1:F:65:ILE:N	2.72	0.51
1:B:402:ILE:O	1:B:402:ILE:HG12	2.09	0.51
1:C:286:LEU:HD13	1:C:293:PHE:CD2	2.45	0.51
1:D:143:MET:HG2	1:D:212:LEU:O	2.11	0.51
1:E:175:LEU:N	1:E:175:LEU:CD1	2.72	0.51
1:E:282:LEU:O	1:E:282:LEU:HD12	2.10	0.51
1:A:138:SER:HB3	1:A:209:LYS:HG3	1.91	0.51
1:B:155:TYR:HE1	1:B:159:LEU:HB2	1.71	0.51
1:B:321:ARG:NH1	1:B:321:ARG:CG	2.72	0.51
1:B:334:LYS:HB3	1:B:337:GLN:HB3	1.91	0.51
1:C:62:PHE:HD1	1:C:244:TYR:CE2	2.29	0.51
1:C:147:ALA:HB3	1:C:220:GLU:OE2	2.10	0.51
1:D:340:ALA:HA	1:D:362:LEU:HD13	1.92	0.51
1:F:143:MET:HE3	1:F:145:SER:HB2	1.92	0.51
1:C:135:LEU:N	1:C:135:LEU:CD1	2.73	0.51
1:D:349:SER:OG	1:D:351:CYS:HA	2.11	0.51
1:E:234:HIS:ND1	1:E:234:HIS:N	2.59	0.51
1:E:264:LEU:HD12	1:E:415:MET:HE3	1.93	0.51
1:E:292:ARG:HH21	1:E:292:ARG:CG	2.23	0.51
1:E:374:ASP:O	1:E:377:VAL:HG13	2.10	0.51
1:A:16:LEU:HD13	1:A:28:PHE:O	2.11	0.51
1:B:347:PHE:CZ	1:B:349:SER:HB2	2.46	0.51
1:C:175:LEU:CD1	1:C:176:GLY:N	2.74	0.51
1:C:254:TRP:O	1:C:258:GLN:NE2	2.44	0.51
1:F:380:GLY:HA2	1:F:390:TRP:CE3	2.46	0.51
1:B:264:LEU:O	1:B:293:PHE:HA	2.10	0.51
1:F:156:LEU:HB3	1:F:157:PRO:HD3	1.91	0.51
1:B:434:THR:HG23	1:B:441:SER:HB2	1.89	0.51
1:B:50:THR:HG22	1:B:52:SER:O	2.10	0.51
1:C:59:LEU:O	1:C:63:PHE:CD2	2.64	0.51
1:D:48:LYS:HA	1:D:49:PRO:C	2.36	0.51
1:F:99:THR:O	1:F:102:HIS:CD2	2.64	0.51
1:F:129:THR:HG23	1:F:130:ASP:N	2.26	0.51
1:F:402:ILE:HG22	1:F:407:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:421:ARG:CZ	1:F:421:ARG:HB2	2.40	0.51
1:A:126:SER:OG	1:A:204:SER:OG	2.23	0.51
1:B:16:LEU:CD1	1:B:32:ALA:HB2	2.35	0.51
1:C:378:ASN:O	1:C:381:VAL:HG13	2.11	0.51
1:E:341:HIS:CG	1:E:342:PRO:HD2	2.46	0.51
1:F:288:LYS:NZ	1:F:405:GLU:CG	2.74	0.51
1:A:175:LEU:C	1:A:175:LEU:CD1	2.84	0.50
1:A:372:HIS:O	1:A:375:GLN:OE1	2.30	0.50
1:B:42:VAL:HG11	1:B:69:ILE:HG12	1.87	0.50
1:B:268:PHE:CZ	1:B:369:TRP:CE3	2.99	0.50
1:B:434:THR:HG23	1:B:441:SER:H	1.76	0.50
1:C:74:PHE:CZ	1:C:104:LEU:CG	2.83	0.50
1:C:314:LEU:CD1	1:C:328:ILE:HD12	2.36	0.50
1:A:264:LEU:HD11	1:A:348:VAL:HG23	1.93	0.50
1:C:35:LEU:O	1:C:40:CYS:HB2	2.12	0.50
1:C:261:GLU:N	1:C:343:ALA:O	2.45	0.50
1:C:278:GLN:NE2	1:C:369:TRP:HZ2	2.03	0.50
1:D:13:HIS:HD2	1:D:41:ALA:O	1.95	0.50
1:D:218:SER:OG	1:D:430:LYS:HE3	2.12	0.50
1:D:285:ALA:HB1	1:D:407:ILE:CG2	2.42	0.50
1:E:26:LEU:CB	1:E:27:PRO:CD	2.89	0.50
1:E:212:LEU:N	1:E:212:LEU:CD1	2.74	0.50
1:A:402:ILE:HG21	1:A:407:ILE:HG13	1.92	0.50
1:B:65:ILE:HG22	1:B:66:HIS:ND1	2.27	0.50
1:B:185:PRO:HG2	1:B:186:LYS:N	2.27	0.50
1:B:212:LEU:CD2	1:B:238:ILE:CD1	2.81	0.50
1:F:196:ALA:O	1:F:200:SER:OG	2.30	0.50
1:A:98:ALA:HB2	1:A:124:LEU:HD22	1.93	0.50
1:E:211:VAL:O	1:E:211:VAL:HG12	2.12	0.50
1:A:36:ASP:OD1	1:A:36:ASP:O	2.30	0.50
1:D:50:THR:CG2	1:D:52:SER:O	2.59	0.50
1:D:149:PHE:CE2	1:D:153:MET:CE	2.95	0.50
1:F:288:LYS:HZ2	1:F:405:GLU:CG	2.24	0.50
1:A:14:ILE:HG21	1:A:35:LEU:HD13	1.93	0.50
1:A:183:ILE:HG23	1:A:187:MET:HE2	1.94	0.50
1:A:350:HIS:CD2	1:A:350:HIS:C	2.89	0.50
1:C:47:VAL:HG12	1:C:76:LEU:HG	1.93	0.50
1:C:112:SER:CB	1:C:113:PRO:HD3	2.31	0.50
1:C:125:THR:OG1	1:C:141:THR:CG2	2.59	0.50
1:D:16:LEU:HD21	1:D:31:LEU:HB3	1.92	0.50
1:E:259:PRO:O	1:E:262:SER:OG	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ILE:HG23	1:C:118:ILE:O	2.11	0.50
1:D:372:HIS:O	1:D:375:GLN:OE1	2.30	0.50
1:F:121:ASP:OD1	1:F:122:PHE:N	2.45	0.50
1:A:255:LEU:CD2	1:A:341:HIS:CD2	2.95	0.50
1:A:402:ILE:CG2	1:A:407:ILE:HG13	2.42	0.50
1:B:47:VAL:CG2	1:B:76:LEU:CG	2.90	0.50
1:B:224:ILE:CA	1:B:227:VAL:CG2	2.90	0.50
1:D:295:TRP:CE3	1:D:328:ILE:HD11	2.47	0.50
1:E:146:SER:HB3	1:E:353:TRP:CE3	2.47	0.50
1:E:299:GLY:HA3	1:E:313:MET:CE	2.42	0.50
1:E:394:TRP:CG	1:E:402:ILE:HD12	2.47	0.50
1:E:184:PRO:HG3	1:E:373:GLY:O	2.12	0.49
1:F:14:ILE:HD12	1:F:117:ALA:HB3	1.94	0.49
1:F:172:ILE:O	1:F:175:LEU:O	2.30	0.49
1:C:54:ALA:N	1:C:304:LYS:CD	2.69	0.49
1:C:273:ALA:CB	1:C:301:LYS:HA	2.42	0.49
1:D:63:PHE:O	1:D:66:HIS:O	2.30	0.49
1:F:77:LEU:HB3	1:F:78:PRO:CD	2.42	0.49
1:F:153:MET:HE2	1:F:198:ILE:HD13	1.92	0.49
1:F:351:CYS:HA	1:F:356:VAL:HG23	1.93	0.49
1:A:285:ALA:CB	1:A:407:ILE:HG21	2.42	0.49
1:A:402:ILE:HG22	1:A:407:ILE:HD11	1.93	0.49
1:B:47:VAL:CG2	1:B:76:LEU:HD23	2.37	0.49
1:B:85:ARG:CB	1:B:193:PHE:CZ	2.94	0.49
1:B:233:ASP:O	1:B:233:ASP:OD1	2.30	0.49
2:C:500:UDP:O2A	2:C:500:UDP:O1B	2.30	0.49
1:D:235:ILE:O	1:D:235:ILE:HG23	2.12	0.49
1:F:156:LEU:HB3	1:F:157:PRO:CD	2.43	0.49
1:A:26:LEU:HD12	2:A:500:UDP:O4'	2.12	0.49
1:B:134:ASP:N	1:B:134:ASP:OD1	2.45	0.49
1:C:300:GLY:N	1:C:307:LYS:CD	2.72	0.49
1:E:38:ARG:NE	1:E:442:GLU:OE1	2.28	0.49
1:F:163:ASP:O	1:F:164:VAL:C	2.52	0.49
1:A:380:GLY:O	1:A:384:LYS:HG3	2.13	0.49
1:B:141:THR:O	1:B:212:LEU:HD13	2.13	0.49
1:C:89:PRO:CG	1:C:302:VAL:HG21	2.42	0.49
1:C:446:GLN:HA	1:C:449:ILE:HG13	1.94	0.49
1:A:407:ILE:C	1:A:411:MET:HE3	2.34	0.49
1:B:24:HIS:O	1:B:28:PHE:HD1	1.96	0.49
1:C:259:PRO:O	1:C:262:SER:OG	2.30	0.49
1:C:295:TRP:CE2	1:C:297:LEU:HD12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:LEU:HD23	1:F:402:ILE:CA	2.43	0.49
1:A:427:VAL:HG13	1:A:428:ARG:N	2.27	0.49
1:C:17:PHE:CD1	1:C:17:PHE:C	2.91	0.49
1:C:307:LYS:CD	1:C:307:LYS:C	2.86	0.49
1:D:391:VAL:CG1	1:D:394:TRP:CD2	2.96	0.49
1:E:280:ARG:NE	1:E:280:ARG:CA	2.72	0.49
1:E:394:TRP:CD2	1:E:402:ILE:HD12	2.48	0.49
1:F:91:PHE:CG	1:F:193:PHE:CE2	3.00	0.49
1:F:255:LEU:HB3	1:F:341:HIS:NE2	2.28	0.49
1:E:105:ARG:HB3	1:E:106:PRO:HD3	1.93	0.49
1:E:425:GLY:O	1:E:428:ARG:HB3	2.12	0.49
1:E:445:LEU:O	1:E:449:ILE:CG1	2.61	0.49
1:F:254:TRP:CE3	1:F:327:LEU:HD23	2.44	0.49
1:B:13:HIS:CD2	1:B:113:PRO:O	2.63	0.49
1:C:208:VAL:O	1:C:234:HIS:HD2	1.95	0.49
1:D:317:SER:O	1:D:321:ARG:HG2	2.13	0.49
1:D:402:ILE:CG2	1:D:407:ILE:HD11	2.43	0.49
1:F:434:THR:HG22	1:F:441:SER:CA	2.43	0.49
1:A:40:CYS:SG	1:A:449:ILE:HG12	2.53	0.49
1:A:88:ASP:HB3	1:A:91:PHE:HB2	1.94	0.49
1:A:258:GLN:NE2	1:A:258:GLN:CA	2.73	0.49
1:B:63:PHE:CE2	1:B:71:ARG:HB2	2.47	0.49
1:B:269:GLY:HA2	1:B:350:HIS:CE1	2.48	0.49
1:C:234:HIS:ND1	1:C:234:HIS:N	2.59	0.49
1:C:383:GLU:HG2	1:C:384:LYS:HE2	1.94	0.49
1:D:14:ILE:HG22	1:D:15:ALA:N	2.27	0.49
1:D:442:GLU:OE1	1:D:442:GLU:O	2.30	0.49
1:E:15:ALA:HB3	1:E:118:ILE:HD13	1.95	0.49
1:E:20:ALA:HB2	1:E:93:GLN:HG2	1.93	0.48
1:F:91:PHE:HB3	1:F:193:PHE:CE2	2.48	0.48
1:C:383:GLU:HA	1:C:388:GLY:O	2.12	0.48
1:D:340:ALA:CA	1:D:362:LEU:HD13	2.43	0.48
1:E:159:LEU:C	1:E:159:LEU:CD2	2.84	0.48
1:A:255:LEU:CD2	1:A:341:HIS:HD2	2.24	0.48
1:A:414:VAL:HG13	1:A:415:MET:N	2.29	0.48
1:B:40:CYS:SG	1:B:449:ILE:HG12	2.53	0.48
1:C:62:PHE:CD1	1:C:244:TYR:CD2	3.00	0.48
1:C:263:VAL:HG11	1:C:344:ILE:HD13	1.95	0.48
1:D:182:SER:O	1:D:396:TRP:CH2	2.66	0.48
1:D:297:LEU:HD22	1:D:314:LEU:HD11	1.95	0.48
1:E:274:LEU:N	1:E:274:LEU:HD23	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ARG:HB3	1:F:106:PRO:CD	2.42	0.48
1:F:131:LEU:N	1:F:131:LEU:CD1	2.76	0.48
1:F:434:THR:HG21	1:F:441:SER:HG	1.77	0.48
1:C:120:SER:O	1:C:141:THR:HA	2.13	0.48
1:D:127:GLN:O	1:D:130:ASP:OD1	2.30	0.48
1:D:259:PRO:O	1:D:262:SER:OG	2.30	0.48
1:D:449:ILE:O	1:D:452:PHE:HB2	2.14	0.48
1:E:287:GLU:HG3	1:E:318:PHE:CE1	2.48	0.48
1:E:350:HIS:H	1:E:350:HIS:CD2	2.32	0.48
1:E:409:GLU:HG3	1:E:410:LYS:N	2.25	0.48
1:F:170:ILE:HG13	1:F:171:GLU:N	2.28	0.48
1:F:298:LYS:HA	1:F:298:LYS:CE	2.37	0.48
1:A:51:VAL:CG1	1:A:90:PHE:CE1	2.96	0.48
1:B:271:ARG:HH12	1:B:302:VAL:HG12	1.76	0.48
1:D:238:ILE:O	1:D:238:ILE:HG22	2.12	0.48
1:E:228:ARG:CG	1:E:235:ILE:HD11	2.44	0.48
1:F:205:LEU:HD22	1:F:211:VAL:CG2	2.44	0.48
1:F:259:PRO:O	1:F:262:SER:OG	2.30	0.48
1:A:13:HIS:HE1	1:A:43:THR:OG1	1.97	0.48
1:A:254:TRP:O	1:A:258:GLN:CG	2.51	0.48
1:B:156:LEU:HD23	1:B:187:MET:HE2	1.96	0.48
1:B:185:PRO:CG	1:B:186:LYS:N	2.76	0.48
1:B:192:ASP:OD1	1:B:193:PHE:N	2.46	0.48
1:B:310:VAL:N	1:B:310:VAL:C	2.72	0.48
1:C:89:PRO:HG3	1:C:302:VAL:CG2	2.43	0.48
1:C:270:SER:OG	2:C:500:UDP:O3B	2.29	0.48
1:D:146:SER:OG	1:D:378:ASN:OD1	2.29	0.48
1:D:402:ILE:O	1:D:402:ILE:CG2	2.61	0.48
1:E:26:LEU:CD1	2:E:500:UDP:H4'	2.42	0.48
1:E:169:ALA:CB	1:E:179:SER:HA	2.28	0.48
1:E:300:GLY:HA3	1:E:307:LYS:CG	2.44	0.48
1:A:38:ARG:HH21	1:A:442:GLU:CD	2.22	0.48
1:D:113:PRO:N	1:D:113:PRO:C	2.71	0.48
1:E:23:GLY:O	1:E:27:PRO:CG	2.61	0.48
1:A:15:ALA:HA	1:A:43:THR:O	2.13	0.48
1:A:45:ILE:HA	1:A:72:LEU:O	2.14	0.48
1:C:213:ILE:HG21	1:C:215:THR:CG2	2.41	0.48
1:C:278:GLN:HE22	1:C:369:TRP:HZ2	1.60	0.48
1:D:185:PRO:O	1:D:188:LEU:HB2	2.13	0.48
1:F:180:MET:HA	1:F:183:ILE:HD12	1.95	0.48
1:F:238:ILE:O	1:F:435:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:CD2	1:A:374:ASP:HA	2.48	0.48
1:A:341:HIS:ND1	1:A:342:PRO:HG2	2.27	0.48
1:C:46:THR:HG21	1:C:59:LEU:HD22	1.93	0.48
1:C:366:VAL:HG13	1:C:366:VAL:O	2.14	0.48
1:F:143:MET:CE	1:F:145:SER:O	2.62	0.48
1:F:376:SER:HB2	1:F:396:TRP:CH2	2.48	0.48
1:B:145:SER:OG	1:B:149:PHE:HD2	1.97	0.48
1:B:149:PHE:CD2	1:B:153:MET:HE2	2.48	0.48
1:B:213:ILE:CG2	1:B:215:THR:CG2	2.89	0.48
1:D:183:ILE:HG23	1:D:184:PRO:HD2	1.96	0.48
1:E:412:ILE:O	1:E:416:GLN:HG3	2.14	0.48
1:F:13:HIS:O	1:F:14:ILE:HD13	2.14	0.48
1:F:387:LEU:HG	1:F:427:VAL:HG11	1.95	0.48
1:A:274:LEU:CD2	1:A:278:GLN:HG2	2.44	0.47
1:B:47:VAL:HG22	1:B:76:LEU:CG	2.44	0.47
1:B:47:VAL:HG23	1:B:76:LEU:CD2	2.38	0.47
1:D:26:LEU:O	1:D:30:ARG:CG	2.53	0.47
1:E:347:PHE:CE1	1:E:348:VAL:O	2.67	0.47
1:F:86:ASN:HD21	1:F:91:PHE:HB2	1.79	0.47
1:A:414:VAL:CG1	1:A:415:MET:N	2.77	0.47
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.69	0.47
1:B:224:ILE:HA	1:B:227:VAL:HG21	1.94	0.47
1:C:108:LEU:HD23	1:C:111:LEU:HD11	1.95	0.47
1:C:335:GLN:NE2	2:C:500:UDP:C2'	2.76	0.47
1:E:30:ARG:O	1:E:34:MET:HG3	2.13	0.47
1:F:150:PHE:O	1:F:150:PHE:CD1	2.67	0.47
1:B:50:THR:CG2	1:B:55:GLU:HB2	2.43	0.47
1:C:76:LEU:CD1	1:C:93:GLN:NE2	2.77	0.47
1:C:353:TRP:CZ3	1:C:381:VAL:HG11	2.49	0.47
1:D:51:VAL:HG11	1:D:90:PHE:CD1	2.49	0.47
1:D:152:LEU:O	1:D:156:LEU:HB2	2.15	0.47
1:E:280:ARG:HA	1:E:280:ARG:HE	1.77	0.47
1:F:119:VAL:O	1:F:119:VAL:HG22	2.13	0.47
1:C:90:PHE:O	1:C:94:MET:HG3	2.14	0.47
1:D:71:ARG:O	1:D:71:ARG:CG	2.59	0.47
1:D:254:TRP:O	1:D:254:TRP:CE3	2.67	0.47
1:F:59:LEU:O	1:F:63:PHE:HD2	1.98	0.47
1:D:63:PHE:CE2	1:D:71:ARG:HB2	2.50	0.47
1:F:254:TRP:CE2	1:F:327:LEU:HD22	2.44	0.47
1:B:98:ALA:HB1	1:B:127:GLN:HG3	1.95	0.47
1:B:156:LEU:HD13	1:B:156:LEU:C	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASP:OD1	1:B:251:ASP:N	2.45	0.47
1:C:38:ARG:NH2	1:C:442:GLU:OE2	2.47	0.47
1:C:378:ASN:C	1:C:381:VAL:HG12	2.39	0.47
1:D:198:ILE:HG23	1:D:199:SER:N	2.29	0.47
1:D:389:LEU:HD23	1:D:420:LEU:HD22	1.93	0.47
1:E:108:LEU:HD22	1:E:115:LEU:CD1	2.44	0.47
1:E:292:ARG:CG	1:E:292:ARG:NH2	2.76	0.47
1:E:448:LEU:O	1:E:451:SER:OG	2.30	0.47
1:F:263:VAL:CG1	1:F:344:ILE:HD13	2.44	0.47
1:C:76:LEU:HD11	1:C:93:GLN:NE2	2.29	0.47
1:C:286:LEU:HD13	1:C:293:PHE:CG	2.49	0.47
1:D:38:ARG:HB3	1:D:449:ILE:CD1	2.37	0.47
1:F:146:SER:HB3	1:F:353:TRP:CZ3	2.50	0.47
1:A:14:ILE:O	1:A:42:VAL:HA	2.15	0.47
1:C:193:PHE:CD1	1:C:194:PHE:N	2.82	0.47
1:C:213:ILE:CG2	1:C:215:THR:HG23	2.44	0.47
1:C:288:LYS:HD2	1:C:288:LYS:HA	1.64	0.47
1:C:383:GLU:CD	1:C:384:LYS:NZ	2.73	0.47
1:E:307:LYS:CG	1:E:330:LYS:HZ1	2.28	0.47
1:F:167:ARG:HH22	1:F:170:ILE:HD13	1.80	0.47
1:F:236:LEU:HD13	1:F:448:LEU:HD13	1.97	0.47
1:C:47:VAL:HG13	1:C:74:PHE:HB3	1.96	0.47
1:C:394:TRP:CZ2	1:C:402:ILE:HD11	2.50	0.47
1:D:47:VAL:CB	1:D:97:ILE:CD1	2.93	0.47
1:D:51:VAL:CG1	1:D:90:PHE:HE1	2.28	0.47
1:D:252:LEU:C	1:D:254:TRP:N	2.69	0.47
1:E:372:HIS:CD2	1:E:372:HIS:O	2.68	0.47
1:C:347:PHE:HD1	1:C:348:VAL:N	2.14	0.46
1:D:24:HIS:O	1:D:27:PRO:HD2	2.15	0.46
1:E:48:LYS:O	1:E:76:LEU:HD22	2.15	0.46
1:E:105:ARG:N	1:E:106:PRO:CD	2.78	0.46
1:E:149:PHE:CE2	1:E:153:MET:HE3	2.50	0.46
1:F:425:GLY:HA2	1:F:428:ARG:NH2	2.30	0.46
1:A:353:TRP:CZ3	1:A:356:VAL:HG11	2.50	0.46
1:C:79:TYR:C	1:C:79:TYR:CD1	2.92	0.46
1:A:70:THR:HG23	1:A:72:LEU:HD13	1.97	0.46
1:A:118:ILE:HG22	1:A:139:THR:HG22	1.97	0.46
1:C:353:TRP:CE3	1:C:378:ASN:ND2	2.82	0.46
1:D:198:ILE:HG23	1:D:199:SER:H	1.80	0.46
1:F:143:MET:HE2	1:F:145:SER:O	2.15	0.46
1:A:420:LEU:HD23	1:A:420:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HA	1:B:39:GLY:C	2.40	0.46
1:B:212:LEU:N	1:B:212:LEU:HD13	2.25	0.46
1:B:213:ILE:HB	1:B:235:ILE:HD11	1.97	0.46
1:D:142:LEU:HA	1:D:212:LEU:O	2.16	0.46
1:A:34:MET:HE2	1:A:241:LEU:CD2	2.36	0.46
1:A:129:THR:CG2	1:A:207:LYS:HD2	2.45	0.46
1:A:156:LEU:N	1:A:157:PRO:HD2	2.30	0.46
1:B:348:VAL:HG22	1:B:348:VAL:O	2.15	0.46
1:C:233:ASP:O	1:C:233:ASP:OD1	2.33	0.46
1:D:76:LEU:HD13	1:D:96:THR:HG22	1.93	0.46
1:D:150:PHE:HA	1:D:153:MET:HG3	1.98	0.46
1:F:274:LEU:HG	1:F:278:GLN:HB3	1.96	0.46
1:A:143:MET:HE2	1:A:150:PHE:CE1	2.51	0.46
1:A:164:VAL:HG11	1:A:190:PRO:CD	2.45	0.46
1:B:285:ALA:HB2	1:B:404:ARG:HA	1.98	0.46
1:D:14:ILE:N	1:D:41:ALA:O	2.30	0.46
1:D:254:TRP:CH2	1:D:326:GLY:HA2	2.50	0.46
1:E:243:SER:CB	1:E:336:GLU:CD	2.88	0.46
1:E:313:MET:HE2	1:E:313:MET:HB3	1.73	0.46
1:F:27:PRO:HG3	1:F:354:ASN:OD1	2.15	0.46
1:F:131:LEU:CD1	1:F:131:LEU:H	2.28	0.46
1:F:401:LEU:CD2	1:F:401:LEU:O	2.50	0.46
1:B:34:MET:HE3	1:B:241:LEU:HD22	1.97	0.46
1:B:193:PHE:N	1:B:193:PHE:CD1	2.69	0.46
1:D:211:VAL:O	1:D:212:LEU:HD22	2.12	0.46
1:D:254:TRP:O	1:D:258:GLN:NE2	2.49	0.46
1:E:129:THR:HG21	1:E:207:LYS:HD3	1.97	0.46
1:A:307:LYS:CG	1:A:330:LYS:HZ1	2.28	0.46
1:D:268:PHE:O	1:D:350:HIS:CB	2.64	0.46
1:B:30:ARG:O	1:B:34:MET:HG3	2.15	0.46
1:C:59:LEU:O	1:C:63:PHE:HD2	1.99	0.46
1:C:356:VAL:CG1	1:C:382:VAL:CG2	2.94	0.46
1:D:278:GLN:NE2	1:D:278:GLN:HA	2.31	0.46
1:D:367:LEU:CD1	1:D:389:LEU:O	2.53	0.46
1:E:293:PHE:C	1:E:293:PHE:CD1	2.94	0.46
1:F:175:LEU:HG	1:F:176:GLY:N	2.29	0.46
1:A:338:ILE:O	1:A:344:ILE:HG13	2.16	0.46
1:C:65:ILE:C	1:C:67:PRO:HD3	2.41	0.46
1:C:293:PHE:CE1	1:C:326:GLY:HA3	2.50	0.46
1:D:217:ASN:CG	1:D:218:SER:N	2.73	0.46
1:E:409:GLU:CG	1:E:410:LYS:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:GLN:O	1:F:97:ILE:HG13	2.16	0.46
1:A:286:LEU:O	1:A:289:SER:OG	2.30	0.45
1:A:407:ILE:C	1:A:411:MET:CE	2.89	0.45
1:B:26:LEU:N	1:B:27:PRO:CD	2.78	0.45
1:B:276:LYS:O	1:B:280:ARG:HG3	2.16	0.45
1:C:383:GLU:CD	1:C:384:LYS:HZ3	2.24	0.45
1:D:51:VAL:CG1	1:D:90:PHE:CE1	2.99	0.45
1:F:129:THR:CG2	1:F:130:ASP:OD1	2.64	0.45
1:F:380:GLY:HA2	1:F:390:TRP:CZ3	2.51	0.45
1:A:420:LEU:C	1:A:420:LEU:CD2	2.89	0.45
1:B:128:VAL:O	1:B:131:LEU:HB2	2.17	0.45
1:B:159:LEU:HD12	1:B:159:LEU:C	2.42	0.45
1:C:87:ASP:C	1:C:87:ASP:OD1	2.59	0.45
1:C:366:VAL:O	1:C:388:GLY:HA3	2.16	0.45
1:C:394:TRP:CH2	1:C:402:ILE:HD11	2.52	0.45
1:E:332:TRP:CZ2	2:E:500:UDP:O2	2.69	0.45
1:F:310:VAL:O	1:F:313:MET:HG2	2.15	0.45
1:A:149:PHE:CD1	1:A:149:PHE:O	2.69	0.45
1:A:350:HIS:HB2	1:A:371:GLN:CG	2.46	0.45
1:B:146:SER:HG	1:B:149:PHE:H	1.58	0.45
1:B:218:SER:HG	1:B:430:LYS:HD3	1.76	0.45
1:C:433:GLU:O	1:C:439:GLY:HA3	2.16	0.45
1:C:25:LEU:HD12	1:C:25:LEU:C	2.41	0.45
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.81	0.45
1:D:169:ALA:HA	1:D:179:SER:HA	1.98	0.45
1:A:116:SER:OG	1:A:453:ASN:O	2.29	0.45
1:B:50:THR:CG2	1:B:52:SER:H	2.30	0.45
1:B:52:SER:HG	1:B:55:GLU:HG3	1.77	0.45
1:B:275:SER:O	1:B:279:ILE:HG12	2.16	0.45
1:C:352:GLY:O	1:C:356:VAL:CG2	2.63	0.45
1:D:45:ILE:HG12	1:D:72:LEU:HD12	1.99	0.45
1:D:50:THR:HG22	1:D:52:SER:O	2.15	0.45
1:F:203:SER:O	1:F:206:HIS:ND1	2.50	0.45
1:F:412:ILE:O	1:F:416:GLN:HG2	2.17	0.45
1:F:445:LEU:O	1:F:449:ILE:CG1	2.64	0.45
1:C:96:THR:O	1:C:100:SER:OG	2.34	0.45
1:D:14:ILE:O	1:D:42:VAL:HA	2.16	0.45
1:D:105:ARG:CB	1:D:106:PRO:CD	2.95	0.45
1:E:26:LEU:HB2	1:E:27:PRO:HD2	1.98	0.45
1:E:350:HIS:CE1	2:E:500:UDP:O3A	2.70	0.45
1:F:194:PHE:O	1:F:198:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:LEU:HD22	1:F:211:VAL:HG21	1.98	0.45
1:A:282:LEU:O	1:A:286:LEU:N	2.45	0.45
1:B:149:PHE:CD2	1:B:374:ASP:HB2	2.51	0.45
1:C:104:LEU:HB3	1:C:131:LEU:HD11	1.98	0.45
1:C:278:GLN:OE1	1:C:401:LEU:HA	2.17	0.45
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.80	0.45
1:F:298:LYS:CA	1:F:298:LYS:CE	2.94	0.45
1:B:14:ILE:O	1:B:42:VAL:HA	2.16	0.45
1:C:172:ILE:O	1:C:175:LEU:O	2.34	0.45
1:D:47:VAL:O	1:D:48:LYS:HD2	2.16	0.45
1:D:244:TYR:O	1:D:244:TYR:CG	2.70	0.45
1:E:354:ASN:HB2	2:E:500:UDP:H5'1	1.99	0.45
1:F:65:ILE:C	1:F:67:PRO:HD3	2.41	0.45
1:F:124:LEU:O	1:F:128:VAL:CG2	2.62	0.45
1:F:150:PHE:O	1:F:150:PHE:HD1	2.00	0.45
1:B:226:ALA:O	1:B:230:ASN:CB	2.62	0.45
1:C:263:VAL:HG11	1:C:344:ILE:CD1	2.47	0.45
1:F:58:HIS:O	1:F:62:PHE:N	2.39	0.45
1:F:313:MET:HG2	1:F:313:MET:H	1.62	0.45
1:B:434:THR:CG2	1:B:441:SER:OG	2.63	0.45
1:C:26:LEU:HB2	1:C:27:PRO:HD3	1.98	0.45
1:D:149:PHE:HE2	1:D:153:MET:HE2	1.81	0.45
1:F:98:ALA:O	1:F:127:GLN:HG2	2.18	0.45
1:B:125:THR:O	1:B:207:LYS:NZ	2.50	0.44
1:B:135:LEU:HG	1:F:87:ASP:HB2	1.99	0.44
1:B:365:PRO:HB3	1:B:420:LEU:CD2	2.47	0.44
1:D:391:VAL:CG1	1:D:394:TRP:CE2	3.00	0.44
1:E:143:MET:HE3	1:E:143:MET:HB3	1.55	0.44
1:E:295:TRP:CE3	1:E:328:ILE:HD13	2.52	0.44
1:F:86:ASN:HD21	1:F:91:PHE:CB	2.29	0.44
1:F:394:TRP:N	1:F:394:TRP:CD1	2.84	0.44
1:B:155:TYR:CD2	1:B:173:PRO:CD	2.98	0.44
1:B:185:PRO:CD	1:B:186:LYS:H	2.31	0.44
1:C:304:LYS:HB3	1:C:304:LYS:HE2	1.68	0.44
1:C:338:ILE:O	1:C:344:ILE:HG13	2.16	0.44
1:D:52:SER:OG	1:D:55:GLU:OE2	2.30	0.44
1:D:152:LEU:HD11	1:D:183:ILE:HD11	1.98	0.44
1:D:287:GLU:H	1:D:287:GLU:HG3	1.53	0.44
1:E:433:GLU:O	1:E:439:GLY:HA3	2.16	0.44
1:F:280:ARG:HG2	1:F:281:GLU:N	2.31	0.44
1:F:374:ASP:OD1	1:F:374:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLY:N	1:A:330:LYS:HZ3	2.07	0.44
1:B:16:LEU:HD11	1:B:32:ALA:CB	2.38	0.44
1:B:52:SER:HB2	1:B:304:LYS:CG	2.47	0.44
1:B:224:ILE:C	1:B:227:VAL:CG2	2.86	0.44
1:D:27:PRO:HG3	1:D:144:THR:CG2	2.47	0.44
1:B:211:VAL:O	1:B:235:ILE:HA	2.17	0.44
1:B:265:PHE:HE2	1:B:335:GLN:HG2	1.80	0.44
1:C:27:PRO:HD3	1:C:354:ASN:ND2	2.32	0.44
1:D:378:ASN:HA	1:D:381:VAL:HG22	1.99	0.44
1:F:314:LEU:HD13	1:F:318:PHE:CE2	2.52	0.44
1:E:26:LEU:HD12	2:E:500:UDP:C4'	2.46	0.44
1:B:105:ARG:HB2	1:B:106:PRO:CD	2.48	0.44
1:E:215:THR:HG23	1:E:353:TRP:HZ2	1.81	0.44
1:E:350:HIS:HE1	2:E:500:UDP:PB	2.41	0.44
1:F:314:LEU:HD12	1:F:328:ILE:CD1	2.43	0.44
1:B:13:HIS:C	1:B:14:ILE:HG12	2.43	0.44
1:D:272:THR:CB	1:D:301:LYS:HA	2.47	0.44
1:D:389:LEU:HD11	1:D:414:VAL:HA	2.00	0.44
1:D:410:LYS:HA	1:D:410:LYS:HZ2	1.83	0.44
1:E:372:HIS:O	1:E:372:HIS:CG	2.70	0.44
1:E:374:ASP:O	1:E:377:VAL:HG12	2.17	0.44
1:A:105:ARG:HB2	1:A:106:PRO:CD	2.43	0.44
1:A:402:ILE:HG22	1:A:402:ILE:O	2.17	0.44
1:B:24:HIS:O	1:B:28:PHE:CD1	2.70	0.44
1:B:278:GLN:O	1:B:281:GLU:HB2	2.18	0.44
1:D:10:VAL:HA	1:D:39:GLY:C	2.42	0.44
1:D:235:ILE:O	1:D:236:LEU:HD12	2.17	0.44
1:D:328:ILE:O	1:D:328:ILE:HG23	2.18	0.44
1:A:402:ILE:CG2	1:A:407:ILE:HD11	2.47	0.44
1:B:185:PRO:HG2	1:B:186:LYS:H	1.83	0.44
1:B:276:LYS:CG	1:B:313:MET:HB3	2.47	0.44
1:C:376:SER:HB2	1:C:396:TRP:CH2	2.52	0.44
1:B:132:VAL:CB	1:B:139:THR:HG21	2.48	0.43
1:D:274:LEU:CD2	1:D:278:GLN:HG2	2.44	0.43
1:D:300:GLY:H	1:D:307:LYS:HB2	1.83	0.43
1:F:120:SER:HG	1:F:128:VAL:HG11	1.74	0.43
1:A:122:PHE:O	1:A:122:PHE:CG	2.70	0.43
1:B:16:LEU:HD21	1:B:32:ALA:CB	2.49	0.43
1:B:101:VAL:HG11	1:B:127:GLN:HB3	2.00	0.43
1:C:263:VAL:CG1	1:C:344:ILE:HD13	2.48	0.43
1:C:295:TRP:NE1	1:C:297:LEU:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:TRP:HE1	1:C:406:GLU:CG	2.31	0.43
1:D:22:MET:HE2	1:D:26:LEU:CG	2.48	0.43
1:D:391:VAL:HG11	1:D:394:TRP:CG	2.30	0.43
1:E:28:PHE:CZ	1:E:142:LEU:HB3	2.53	0.43
1:E:169:ALA:HB2	1:E:179:SER:CA	2.30	0.43
1:A:59:LEU:HD22	1:A:63:PHE:CZ	2.53	0.43
1:A:227:VAL:HG13	1:A:232:VAL:HB	2.00	0.43
2:A:500:UDP:O1A	2:A:500:UDP:O1B	2.36	0.43
1:C:146:SER:HB3	1:C:353:TRP:CE3	2.53	0.43
1:E:101:VAL:HG22	1:E:127:GLN:HB3	1.99	0.43
1:E:272:THR:HG23	1:E:372:HIS:CE1	2.53	0.43
1:E:447:ARG:NH1	1:E:447:ARG:CB	2.81	0.43
1:F:140:TYR:CE1	1:F:452:PHE:HE1	2.36	0.43
1:B:50:THR:HG23	1:B:52:SER:H	1.83	0.43
1:B:193:PHE:O	1:B:196:ALA:N	2.51	0.43
1:B:276:LYS:HE3	1:B:276:LYS:HB3	1.53	0.43
1:B:321:ARG:HH11	1:B:321:ARG:CG	2.24	0.43
1:C:183:ILE:HG23	1:C:187:MET:HE2	1.90	0.43
1:C:273:ALA:HB3	1:C:301:LYS:HA	2.00	0.43
1:F:59:LEU:O	1:F:63:PHE:CD2	2.71	0.43
1:F:254:TRP:CZ3	1:F:327:LEU:HD23	2.53	0.43
1:A:10:VAL:HG12	1:A:39:GLY:HA2	1.99	0.43
1:A:212:LEU:HD12	1:A:212:LEU:H	1.82	0.43
1:A:273:ALA:O	1:A:301:LYS:CE	2.65	0.43
1:B:110:SER:HB3	1:F:303:ASP:OD2	2.18	0.43
1:E:358:GLU:OE1	2:E:500:UDP:O3'	2.35	0.43
1:F:235:ILE:C	1:F:236:LEU:CD2	2.73	0.43
1:F:341:HIS:HD2	1:F:343:ALA:CB	2.32	0.43
1:A:299:GLY:H	1:A:330:LYS:HZ1	1.64	0.43
1:A:427:VAL:CG1	1:A:428:ARG:N	2.81	0.43
1:B:90:PHE:CE2	1:B:271:ARG:NH1	2.87	0.43
1:C:366:VAL:O	1:C:388:GLY:CA	2.67	0.43
1:A:347:PHE:N	1:A:365:PRO:O	2.50	0.43
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.87	0.43
1:B:149:PHE:CE2	1:B:374:ASP:HB3	2.53	0.43
1:B:411:MET:HE2	1:B:411:MET:HB2	1.67	0.43
1:C:75:GLN:HA	1:C:75:GLN:OE1	2.18	0.43
1:C:353:TRP:HB2	1:C:378:ASN:HD21	1.82	0.43
1:D:66:HIS:CB	1:D:69:ILE:HG13	2.49	0.43
1:D:341:HIS:CE1	1:D:342:PRO:CD	2.97	0.43
1:D:392:ARG:HE	1:D:392:ARG:HB2	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:ASN:HD21	1:F:91:PHE:C	2.26	0.43
1:B:233:ASP:OD1	1:B:233:ASP:C	2.59	0.43
1:C:16:LEU:HG	1:C:119:VAL:HB	2.00	0.43
1:C:156:LEU:HB3	1:C:157:PRO:CD	2.48	0.43
1:C:160:LEU:HD23	1:C:160:LEU:HA	1.68	0.43
1:C:423:SER:O	1:C:427:VAL:HG23	2.19	0.43
1:D:184:PRO:HA	1:D:185:PRO:HD3	1.87	0.43
1:D:340:ALA:N	1:D:362:LEU:HD13	2.34	0.43
1:F:212:LEU:HD12	1:F:212:LEU:N	2.34	0.43
1:E:38:ARG:HH11	1:E:38:ARG:HG2	1.74	0.43
1:B:366:VAL:HG23	1:B:387:LEU:HG	2.01	0.43
1:C:105:ARG:HB3	1:C:106:PRO:CD	2.36	0.43
1:C:150:PHE:O	1:C:150:PHE:CD1	2.72	0.43
1:D:119:VAL:HG13	1:D:140:TYR:HB2	2.00	0.43
1:F:86:ASN:HD22	1:F:92:ILE:HG12	1.77	0.43
1:F:350:HIS:HE1	2:F:500:UDP:O2B	2.02	0.43
1:B:229:ARG:O	1:B:229:ARG:CG	2.38	0.42
1:B:370:PRO:HG3	1:B:379:ALA:HB2	2.00	0.42
1:D:47:VAL:HG23	1:D:76:LEU:CD2	2.47	0.42
1:D:349:SER:OG	1:D:351:CYS:CA	2.67	0.42
1:E:22:MET:CE	1:E:58:HIS:CD2	3.01	0.42
1:E:107:LEU:HA	1:F:190:PRO:HB2	2.01	0.42
1:E:255:LEU:HB3	1:E:341:HIS:CE1	2.53	0.42
1:E:382:VAL:HG13	1:E:387:LEU:HB3	2.00	0.42
1:A:43:THR:CB	1:A:72:LEU:HD22	2.49	0.42
1:A:152:LEU:HD21	1:A:187:MET:HE1	2.00	0.42
1:B:26:LEU:O	1:B:30:ARG:HG2	2.19	0.42
1:B:271:ARG:HH11	1:B:271:ARG:CG	2.04	0.42
1:C:224:ILE:O	1:C:227:VAL:HG12	2.19	0.42
1:E:410:LYS:HD2	1:E:410:LYS:HA	1.62	0.42
1:F:22:MET:HE1	1:F:58:HIS:CD2	2.55	0.42
1:A:18:PRO:HD2	1:A:18:PRO:O	2.18	0.42
1:A:52:SER:HG	1:A:55:GLU:HG3	1.83	0.42
1:A:187:MET:HB3	1:A:187:MET:HE3	1.66	0.42
1:A:350:HIS:HE1	2:A:500:UDP:PB	2.43	0.42
1:B:27:PRO:CA	1:B:30:ARG:HG3	2.43	0.42
1:B:434:THR:HG23	1:B:441:SER:CB	2.48	0.42
1:D:224:ILE:C	1:D:227:VAL:HG23	2.44	0.42
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.67	0.42
1:F:118:ILE:HG13	1:F:119:VAL:N	2.34	0.42
1:A:14:ILE:HG12	1:A:40:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLY:HA2	1:B:234:HIS:HB2	2.01	0.42
1:C:271:ARG:O	1:C:302:VAL:HG12	2.18	0.42
1:D:143:MET:HE2	1:D:150:PHE:CE1	2.55	0.42
1:B:216:PHE:N	1:B:216:PHE:CD1	2.88	0.42
1:C:17:PHE:C	1:C:17:PHE:HD1	2.27	0.42
1:C:380:GLY:HA2	1:C:390:TRP:CE3	2.54	0.42
1:D:24:HIS:O	1:D:27:PRO:CD	2.67	0.42
1:E:162:ILE:HG13	1:E:162:ILE:O	2.19	0.42
1:A:408:ALA:HA	1:A:411:MET:HE3	2.01	0.42
1:B:185:PRO:CG	1:B:186:LYS:H	2.32	0.42
1:C:376:SER:HB2	1:C:396:TRP:CZ3	2.54	0.42
1:D:156:LEU:CD1	1:D:160:LEU:HG	2.49	0.42
1:E:141:THR:HG22	1:E:208:VAL:HG11	2.01	0.42
1:E:265:PHE:CD2	1:E:339:LEU:HD21	2.54	0.42
1:F:62:PHE:CD1	1:F:62:PHE:C	2.97	0.42
1:A:164:VAL:HG11	1:A:190:PRO:CG	2.49	0.42
1:B:27:PRO:O	1:B:30:ARG:HB2	2.20	0.42
1:C:143:MET:HB3	1:C:143:MET:HE3	1.59	0.42
1:D:234:HIS:ND1	1:D:234:HIS:N	2.62	0.42
1:E:105:ARG:HH12	1:E:134:ASP:HB2	1.85	0.42
1:E:376:SER:O	1:E:379:ALA:HB3	2.20	0.42
1:F:76:LEU:HD22	1:F:96:THR:HG22	2.01	0.42
1:F:143:MET:HE1	1:F:145:SER:CB	2.38	0.42
1:A:47:VAL:CG1	1:A:76:LEU:HD23	2.40	0.42
1:A:207:LYS:O	1:A:207:LYS:HG2	2.17	0.42
1:A:428:ARG:O	1:A:428:ARG:HG2	2.17	0.42
1:B:35:LEU:HD23	1:B:449:ILE:HD11	2.01	0.42
1:B:72:LEU:HD22	1:B:107:LEU:HD11	2.02	0.42
1:B:273:ALA:HB1	1:B:371:GLN:CB	2.50	0.42
1:C:135:LEU:CD1	1:C:135:LEU:H	2.32	0.42
1:D:105:ARG:HG2	1:D:131:LEU:CD1	2.34	0.42
1:D:435:ARG:HD3	1:D:435:ARG:C	2.45	0.42
1:F:14:ILE:HD13	1:F:14:ILE:N	2.35	0.42
1:F:318:PHE:O	1:F:322:THR:CG2	2.44	0.42
1:B:121:ASP:OD1	1:B:122:PHE:N	2.53	0.42
1:E:47:VAL:HA	1:E:74:PHE:O	2.20	0.42
1:E:63:PHE:CE1	1:E:71:ARG:HB2	2.54	0.42
1:E:72:LEU:HD23	1:E:72:LEU:HA	1.83	0.42
1:F:183:ILE:HG23	1:F:184:PRO:HD2	2.01	0.42
1:B:276:LYS:HG2	1:B:313:MET:CB	2.49	0.42
1:B:394:TRP:CE3	1:B:402:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:GLY:O	1:C:384:LYS:HE2	2.20	0.42
1:D:149:PHE:CE1	1:D:374:ASP:HA	2.55	0.42
1:F:88:ASP:HB3	1:F:91:PHE:HB2	2.02	0.42
1:F:297:LEU:C	1:F:299:GLY:H	2.26	0.42
1:A:32:ALA:HB1	1:A:42:VAL:HG11	2.03	0.41
1:A:194:PHE:CE1	1:A:198:ILE:HD11	2.55	0.41
1:F:84:LEU:HG	1:F:193:PHE:HA	2.02	0.41
1:F:350:HIS:CD2	1:F:352:GLY:H	2.38	0.41
1:A:42:VAL:HB	1:A:69:ILE:HG12	2.02	0.41
1:B:30:ARG:NH2	2:B:500:UDP:O3'	2.51	0.41
1:B:268:PHE:CE2	1:B:274:LEU:CD1	3.03	0.41
1:C:152:LEU:HD21	1:C:187:MET:HE1	2.03	0.41
1:C:171:GLU:CA	1:C:177:PRO:HB3	2.41	0.41
1:D:220:GLU:HB3	1:D:223:ALA:HB3	2.01	0.41
1:E:193:PHE:CD1	1:E:193:PHE:C	2.97	0.41
1:E:255:LEU:HD12	1:E:255:LEU:HA	1.81	0.41
1:E:297:LEU:HD12	1:E:297:LEU:HA	1.85	0.41
1:F:111:LEU:HD23	1:F:111:LEU:HA	1.83	0.41
1:A:408:ALA:O	1:A:412:ILE:HG13	2.20	0.41
1:C:162:ILE:CD1	1:C:163:ASP:N	2.71	0.41
1:C:172:ILE:HA	1:C:173:PRO:HD3	1.74	0.41
1:C:281:GLU:OE1	1:C:404:ARG:HG2	2.19	0.41
1:C:321:ARG:CG	1:C:321:ARG:HH21	2.34	0.41
1:D:38:ARG:CB	1:D:449:ILE:HD12	2.39	0.41
1:D:105:ARG:CB	1:D:106:PRO:HD3	2.48	0.41
1:E:30:ARG:NH2	1:E:358:GLU:OE2	2.54	0.41
1:E:376:SER:HB2	1:E:396:TRP:CH2	2.55	0.41
1:F:295:TRP:CZ3	1:F:314:LEU:HD11	2.55	0.41
1:B:276:LYS:HD2	1:B:313:MET:CA	2.48	0.41
1:C:46:THR:HB	1:C:59:LEU:HD11	2.03	0.41
1:C:105:ARG:NH1	1:C:105:ARG:CG	2.72	0.41
1:D:192:ASP:OD1	1:D:194:PHE:CB	2.68	0.41
1:D:402:ILE:HG23	1:D:407:ILE:CD1	2.50	0.41
1:F:26:LEU:N	1:F:27:PRO:HD2	2.36	0.41
1:A:173:PRO:HG2	1:A:230:ASN:CG	2.46	0.41
1:B:271:ARG:NH1	1:B:271:ARG:CG	2.65	0.41
1:D:118:ILE:HG22	1:D:139:THR:HB	2.02	0.41
1:D:389:LEU:CD1	1:D:413:GLU:HG2	2.50	0.41
1:E:447:ARG:NH1	1:E:447:ARG:HB3	2.35	0.41
1:F:174:ASP:HB2	1:F:226:ALA:HA	2.01	0.41
1:A:105:ARG:CB	1:A:106:PRO:HD3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HB3	1:A:249:ALA:H	1.46	0.41
1:C:282:LEU:HD12	1:C:282:LEU:O	2.20	0.41
1:D:143:MET:N	1:D:212:LEU:O	2.40	0.41
1:D:223:ALA:O	1:D:227:VAL:CG2	2.68	0.41
1:D:266:VAL:O	1:D:295:TRP:HD1	2.04	0.41
1:D:303:ASP:CB	1:D:306:ASP:HB2	2.49	0.41
1:E:289:SER:O	1:E:412:ILE:HD11	2.20	0.41
1:F:149:PHE:CE2	1:F:153:MET:CE	2.86	0.41
1:B:104:LEU:O	1:B:108:LEU:CD1	2.68	0.41
1:B:215:THR:OG1	1:B:220:GLU:HG3	2.21	0.41
1:C:156:LEU:N	1:C:157:PRO:HD2	2.36	0.41
1:C:175:LEU:HD13	1:C:176:GLY:N	2.35	0.41
1:C:368:ALA:HB3	1:C:390:TRP:HB2	2.01	0.41
1:C:391:VAL:O	1:C:391:VAL:HG22	2.20	0.41
1:D:47:VAL:O	1:D:47:VAL:HG13	2.20	0.41
1:D:107:LEU:HD13	1:D:107:LEU:HA	1.87	0.41
1:D:391:VAL:HG11	1:D:394:TRP:CD2	2.56	0.41
1:E:240:PRO:HG2	1:E:431:ALA:HB1	2.02	0.41
1:F:38:ARG:HG2	1:F:446:GLN:HE22	1.85	0.41
1:F:45:ILE:HA	1:F:72:LEU:O	2.20	0.41
1:F:252:LEU:HA	1:F:253:PRO:HD3	1.87	0.41
1:A:318:PHE:HE2	1:A:328:ILE:HD11	1.85	0.41
1:B:178:ILE:HD12	1:B:178:ILE:HA	1.82	0.41
1:D:247:LYS:HA	1:D:248:LYS:HA	1.78	0.41
1:D:427:VAL:CG1	1:D:428:ARG:N	2.84	0.41
1:E:354:ASN:O	1:E:358:GLU:HG2	2.18	0.41
1:F:294:LEU:HD13	1:F:327:LEU:HD21	2.02	0.41
1:A:402:ILE:HG22	1:A:407:ILE:HD12	2.00	0.41
1:A:413:GLU:O	1:A:417:ASP:HB2	2.19	0.41
1:B:15:ALA:HA	1:B:43:THR:O	2.19	0.41
1:B:25:LEU:HD12	1:B:25:LEU:C	2.45	0.41
1:C:22:MET:HE1	1:C:58:HIS:CG	2.56	0.41
1:C:255:LEU:HA	1:C:255:LEU:HD12	1.78	0.41
1:C:435:ARG:NE	1:C:435:ARG:CA	2.67	0.41
1:D:195:SER:HA	1:D:198:ILE:CG2	2.51	0.41
1:E:13:HIS:ND1	1:E:113:PRO:O	2.53	0.41
1:E:149:PHE:HD1	1:E:377:VAL:HG11	1.86	0.41
1:E:347:PHE:CD1	1:E:347:PHE:C	2.94	0.41
1:E:350:HIS:CE1	2:E:500:UDP:O1B	2.68	0.41
1:E:394:TRP:O	1:E:400:LYS:HD3	2.21	0.41
1:F:216:PHE:CZ	1:F:219:PHE:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:ILE:O	1:F:235:ILE:HG23	2.19	0.41
1:F:440:ASP:O	1:F:444:LEU:HB2	2.21	0.41
1:A:16:LEU:H	1:A:16:LEU:HG	1.72	0.41
1:B:20:ALA:O	1:B:24:HIS:HB2	2.21	0.41
1:D:27:PRO:HG3	1:D:144:THR:HG21	2.03	0.41
1:D:375:GLN:O	1:D:378:ASN:HB2	2.20	0.41
1:E:84:LEU:HA	1:E:191:SER:O	2.21	0.41
1:E:212:LEU:HG	1:E:238:ILE:HD11	2.03	0.41
1:F:101:VAL:CG1	1:F:131:LEU:HD11	2.50	0.41
1:A:254:TRP:CG	1:A:258:GLN:OE1	2.74	0.40
1:A:307:LYS:CG	1:A:330:LYS:NZ	2.84	0.40
1:B:42:VAL:HG13	1:B:69:ILE:CG2	2.44	0.40
1:B:447:ARG:HD3	1:B:447:ARG:HA	1.82	0.40
1:C:26:LEU:CB	1:C:27:PRO:HD3	2.50	0.40
1:C:384:LYS:HD3	1:C:384:LYS:HA	1.69	0.40
1:D:47:VAL:CG2	1:D:76:LEU:HD21	2.50	0.40
1:D:88:ASP:HB3	1:D:91:PHE:HB2	2.03	0.40
1:D:137:ILE:O	1:D:137:ILE:HG22	2.21	0.40
1:D:288:LYS:HB3	1:D:288:LYS:HE3	1.76	0.40
1:E:213:ILE:HD13	1:E:213:ILE:HA	1.77	0.40
1:D:13:HIS:C	1:D:14:ILE:HG12	2.46	0.40
1:D:192:ASP:OD1	1:D:194:PHE:HB3	2.20	0.40
1:E:192:ASP:OD1	1:E:193:PHE:N	2.55	0.40
1:F:24:HIS:CD2	1:F:94:MET:HE1	2.55	0.40
1:F:234:HIS:O	1:F:234:HIS:ND1	2.48	0.40
1:A:341:HIS:CG	1:A:342:PRO:HD2	2.51	0.40
1:B:29:LEU:N	1:B:29:LEU:HD23	2.35	0.40
1:B:218:SER:CB	1:B:430:LYS:CD	2.94	0.40
1:C:87:ASP:O	1:C:87:ASP:CG	2.63	0.40
1:D:90:PHE:O	1:D:94:MET:HG3	2.22	0.40
1:E:334:LYS:HB3	1:E:337:GLN:HG3	2.03	0.40
1:E:370:PRO:HG2	1:E:376:SER:HA	2.03	0.40
1:B:285:ALA:HB2	1:B:404:ARG:O	2.21	0.40
1:D:43:THR:CA	1:D:70:THR:HG22	2.49	0.40
1:F:145:SER:O	1:F:213:ILE:HD11	2.22	0.40
1:A:282:LEU:HA	1:A:285:ALA:HB3	2.02	0.40
1:B:25:LEU:O	1:B:29:LEU:HG	2.21	0.40
1:B:211:VAL:CA	1:B:212:LEU:HD12	2.47	0.40
1:C:118:ILE:O	1:C:118:ILE:CG2	2.70	0.40
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.77	0.40
1:D:227:VAL:O	1:D:232:VAL:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:TRP:CZ2	2:E:500:UDP:C2	3.10	0.40
1:E:351:CYS:HA	1:E:356:VAL:HG23	2.03	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	439/460 (95%)	417 (95%)	15 (3%)	7 (2%)	7	34
1	B	442/460 (96%)	429 (97%)	13 (3%)	0	100	100
1	C	435/460 (95%)	423 (97%)	11 (2%)	1 (0%)	43	76
1	D	432/460 (94%)	417 (96%)	12 (3%)	3 (1%)	18	53
1	E	441/460 (96%)	423 (96%)	16 (4%)	2 (0%)	24	60
1	F	440/460 (96%)	430 (98%)	9 (2%)	1 (0%)	43	76
All	All	2629/2760 (95%)	2539 (97%)	76 (3%)	14 (0%)	24	60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	173	PRO
1	A	249	ALA
1	E	301	LYS
1	A	248	LYS
1	D	173	PRO
1	A	247	LYS
1	A	310	VAL
1	F	310	VAL
1	C	113	PRO

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Mol	Chain	Res	Type
1	D	18	PRO
1	A	136	PRO
1	D	237	PRO
1	E	113	PRO

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	310/390 (80%)	238 (77%)	72 (23%)	1	4
1	B	301/390 (77%)	223 (74%)	78 (26%)	0	3
1	C	328/390 (84%)	244 (74%)	84 (26%)	0	3
1	D	297/390 (76%)	197 (66%)	100 (34%)	0	1
1	E	322/390 (83%)	258 (80%)	64 (20%)	1	7
1	F	335/390 (86%)	266 (79%)	69 (21%)	1	7
All	All	1893/2340 (81%)	1426 (75%)	467 (25%)	1	4

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	46	THR
1	A	47	VAL
1	A	48	LYS
1	A	50	THR
1	A	56	SER
1	A	64	THR
1	A	72	LEU
1	A	92	ILE
1	A	99	THR
1	A	100	SER
1	A	101	VAL
1	A	118	ILE
1	A	119	VAL

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Mol	Chain	Res	Type
1	A	123	THR
1	A	124	LEU
1	A	125	THR
1	A	129	THR
1	A	131	LEU
1	A	135	LEU
1	A	137	ILE
1	A	159	LEU
1	A	162	ILE
1	A	173	PRO
1	A	175	LEU
1	A	187	MET
1	A	194	PHE
1	A	198	ILE
1	A	204	SER
1	A	207	LYS
1	A	212	LEU
1	A	217	ASN
1	A	220	GLU
1	A	227	VAL
1	A	233	ASP
1	A	234	HIS
1	A	235	ILE
1	A	248	LYS
1	A	258	GLN
1	A	266	VAL
1	A	270	SER
1	A	275	SER
1	A	279	ILE
1	A	282	LEU
1	A	286	LEU
1	A	287	GLU
1	A	288	LYS
1	A	291	CYS
1	A	292	ARG
1	A	296	VAL
1	A	298	LYS
1	A	302	VAL
1	A	303	ASP
1	A	304	LYS
1	A	310	VAL
1	A	319	VAL

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Mol	Chain	Res	Type
1	A	323	LYS
1	A	337	GLN
1	A	364	VAL
1	A	376	SER
1	A	384	LYS
1	A	391	VAL
1	A	399	THR
1	A	402	ILE
1	A	405	GLU
1	A	409	GLU
1	A	416	GLN
1	A	420	LEU
1	A	423	SER
1	A	433	GLU
1	A	434	THR
1	A	451	SER
1	B	16	LEU
1	B	38	ARG
1	B	46	THR
1	B	48	LYS
1	B	50	THR
1	B	51	VAL
1	B	56	SER
1	B	57	ASP
1	B	60	SER
1	B	68	ARG
1	B	92	ILE
1	B	96	THR
1	B	97	ILE
1	B	99	THR
1	B	101	VAL
1	B	104	LEU
1	B	107	LEU
1	B	110	SER
1	B	118	ILE
1	B	123	THR
1	B	125	THR
1	B	126	SER
1	B	129	THR
1	B	131	LEU
1	B	134	ASP
1	B	137	ILE

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Mol	Chain	Res	Type
1	B	139	THR
1	B	141	THR
1	B	143	MET
1	B	144	THR
1	B	156	LEU
1	B	159	LEU
1	B	175	LEU
1	B	178	ILE
1	B	183	ILE
1	B	187	MET
1	B	192	ASP
1	B	193	PHE
1	B	195	SER
1	B	199	SER
1	B	207	LYS
1	B	212	LEU
1	B	213	ILE
1	B	221	SER
1	B	227	VAL
1	B	234	HIS
1	B	235	ILE
1	B	263	VAL
1	B	270	SER
1	B	271	ARG
1	B	275	SER
1	B	276	LYS
1	B	277	GLU
1	B	279	ILE
1	B	281	GLU
1	B	282	LEU
1	B	294	LEU
1	B	302	VAL
1	B	308	GLU
1	B	319	VAL
1	B	321	ARG
1	B	328	ILE
1	B	329	VAL
1	B	335	GLN
1	B	348	VAL
1	B	376	SER
1	B	391	VAL
1	B	392	ARG

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Mol	Chain	Res	Type
1	B	399	THR
1	B	402	ILE
1	B	404	ARG
1	B	426	GLU
1	B	434	THR
1	B	435	ARG
1	B	437	VAL
1	B	447	ARG
1	B	448	LEU
1	B	449	ILE
1	C	14	ILE
1	C	19	CYS
1	C	43	THR
1	C	50	THR
1	C	68	ARG
1	C	71	ARG
1	C	74	PHE
1	C	84	LEU
1	C	92	ILE
1	C	97	ILE
1	C	99	THR
1	C	100	SER
1	C	115	LEU
1	C	125	THR
1	C	131	LEU
1	C	139	THR
1	C	143	MET
1	C	162	ILE
1	C	170	ILE
1	C	175	LEU
1	C	179	SER
1	C	180	MET
1	C	181	SER
1	C	186	LYS
1	C	189	ASP
1	C	193	PHE
1	C	212	LEU
1	C	213	ILE
1	C	215	THR
1	C	216	PHE
1	C	219	PHE
1	C	222	GLU

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Mol	Chain	Res	Type
1	C	225	GLU
1	C	227	VAL
1	C	229	ARG
1	C	234	HIS
1	C	238	ILE
1	C	251	ASP
1	C	255	LEU
1	C	263	VAL
1	C	266	VAL
1	C	271	ARG
1	C	272	THR
1	C	275	SER
1	C	276	LYS
1	C	279	ILE
1	C	286	LEU
1	C	288	LYS
1	C	296	VAL
1	C	298	LYS
1	C	302	VAL
1	C	304	LYS
1	C	306	ASP
1	C	320	GLU
1	C	321	ARG
1	C	322	THR
1	C	323	LYS
1	C	329	VAL
1	C	330	LYS
1	C	335	GLN
1	C	338	ILE
1	C	349	SER
1	C	356	VAL
1	C	362	LEU
1	C	376	SER
1	C	382	VAL
1	C	383	GLU
1	C	384	LYS
1	C	387	LEU
1	C	389	LEU
1	C	391	VAL
1	C	399	THR
1	C	400	LYS
1	C	401	LEU

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Mol	Chain	Res	Type
1	C	402	ILE
1	C	404	ARG
1	C	406	GLU
1	C	412	ILE
1	C	423	SER
1	C	434	THR
1	C	435	ARG
1	C	437	VAL
1	C	449	ILE
1	C	451	SER
1	D	10	VAL
1	D	14	ILE
1	D	19	CYS
1	D	22	MET
1	D	40	CYS
1	D	46	THR
1	D	48	LYS
1	D	50	THR
1	D	51	VAL
1	D	57	ASP
1	D	60	SER
1	D	65	ILE
1	D	69	ILE
1	D	70	THR
1	D	72	LEU
1	D	73	GLU
1	D	91	PHE
1	D	92	ILE
1	D	95	GLU
1	D	96	THR
1	D	97	ILE
1	D	99	THR
1	D	118	ILE
1	D	119	VAL
1	D	123	THR
1	D	128	VAL
1	D	129	THR
1	D	130	ASP
1	D	131	LEU
1	D	134	ASP
1	D	135	LEU
1	D	137	ILE

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Mol	Chain	Res	Type
1	D	138	SER
1	D	139	THR
1	D	142	LEU
1	D	143	MET
1	D	153	MET
1	D	173	PRO
1	D	175	LEU
1	D	181	SER
1	D	183	ILE
1	D	194	PHE
1	D	198	ILE
1	D	207	LYS
1	D	208	VAL
1	D	209	LYS
1	D	212	LEU
1	D	216	PHE
1	D	221	SER
1	D	227	VAL
1	D	229	ARG
1	D	233	ASP
1	D	251	ASP
1	D	256	ASP
1	D	258	GLN
1	D	261	GLU
1	D	266	VAL
1	D	274	LEU
1	D	278	GLN
1	D	279	ILE
1	D	282	LEU
1	D	286	LEU
1	D	287	GLU
1	D	296	VAL
1	D	301	LYS
1	D	303	ASP
1	D	308	GLU
1	D	335	GLN
1	D	350	HIS
1	D	351	CYS
1	D	355	SER
1	D	362	LEU
1	D	364	VAL
1	D	365	PRO

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Mol	Chain	Res	Type
1	D	366	VAL
1	D	376	SER
1	D	381	VAL
1	D	383	GLU
1	D	384	LYS
1	D	389	LEU
1	D	391	VAL
1	D	392	ARG
1	D	399	THR
1	D	401	LEU
1	D	406	GLU
1	D	407	ILE
1	D	410	LYS
1	D	411	MET
1	D	414	VAL
1	D	415	MET
1	D	420	LEU
1	D	423	SER
1	D	430	LYS
1	D	434	THR
1	D	435	ARG
1	D	436	GLU
1	D	442	GLU
1	D	447	ARG
1	D	448	LEU
1	D	449	ILE
1	E	19	CYS
1	E	30	ARG
1	E	38	ARG
1	E	40	CYS
1	E	45	ILE
1	E	46	THR
1	E	52	SER
1	E	56	SER
1	E	64	THR
1	E	75	GLN
1	E	76	LEU
1	E	84	LEU
1	E	87	ASP
1	E	101	VAL
1	E	104	LEU
1	E	118	ILE

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Mol	Chain	Res	Type
1	E	129	THR
1	E	134	ASP
1	E	141	THR
1	E	166	ASN
1	E	171	GLU
1	E	175	LEU
1	E	183	ILE
1	E	188	LEU
1	E	204	SER
1	E	211	VAL
1	E	213	ILE
1	E	215	THR
1	E	216	PHE
1	E	218	SER
1	E	219	PHE
1	E	227	VAL
1	E	234	HIS
1	E	235	ILE
1	E	255	LEU
1	E	258	GLN
1	E	262	SER
1	E	266	VAL
1	E	270	SER
1	E	271	ARG
1	E	306	ASP
1	E	323	LYS
1	E	338	ILE
1	E	339	LEU
1	E	344	ILE
1	E	349	SER
1	E	358	GLU
1	E	362	LEU
1	E	371	GLN
1	E	376	SER
1	E	377	VAL
1	E	387	LEU
1	E	391	VAL
1	E	400	LYS
1	E	402	ILE
1	E	406	GLU
1	E	410	LYS
1	E	411	MET

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Mol	Chain	Res	Type
1	E	423	SER
1	E	434	THR
1	E	435	ARG
1	E	444	LEU
1	E	447	ARG
1	E	449	ILE
1	F	19	CYS
1	F	22	MET
1	F	47	VAL
1	F	50	THR
1	F	56	SER
1	F	60	SER
1	F	64	THR
1	F	68	ARG
1	F	76	LEU
1	F	82	SER
1	F	84	LEU
1	F	92	ILE
1	F	101	VAL
1	F	104	LEU
1	F	105	ARG
1	F	107	LEU
1	F	115	LEU
1	F	118	ILE
1	F	119	VAL
1	F	126	SER
1	F	129	THR
1	F	145	SER
1	F	159	LEU
1	F	167	ARG
1	F	181	SER
1	F	198	ILE
1	F	200	SER
1	F	204	SER
1	F	207	LYS
1	F	209	LYS
1	F	218	SER
1	F	222	GLU
1	F	227	VAL
1	F	232	VAL
1	F	235	ILE
1	F	252	LEU

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Mol	Chain	Res	Type
1	F	258	GLN
1	F	266	VAL
1	F	267	SER
1	F	275	SER
1	F	278	GLN
1	F	279	ILE
1	F	291	CYS
1	F	297	LEU
1	F	298	LYS
1	F	303	ASP
1	F	323	LYS
1	F	327	LEU
1	F	335	GLN
1	F	356	VAL
1	F	366	VAL
1	F	367	LEU
1	F	376	SER
1	F	377	VAL
1	F	381	VAL
1	F	387	LEU
1	F	401	LEU
1	F	407	ILE
1	F	409	GLU
1	F	410	LYS
1	F	412	ILE
1	F	414	VAL
1	F	423	SER
1	F	427	VAL
1	F	434	THR
1	F	435	ARG
1	F	440	ASP
1	F	444	LEU
1	F	449	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	127	GLN
1	A	230	ASN
1	A	258	GLN
1	A	278	GLN

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Mol	Chain	Res	Type
1	A	337	GLN
1	A	350	HIS
1	B	13	HIS
1	B	278	GLN
1	B	335	GLN
1	C	66	HIS
1	C	258	GLN
1	C	335	GLN
1	C	354	ASN
1	C	371	GLN
1	D	258	GLN
1	E	371	GLN
1	E	372	HIS
1	E	446	GLN
1	F	9	ASN
1	F	24	HIS
1	F	58	HIS
1	F	86	ASN
1	F	102	HIS
1	F	206	HIS
1	F	258	GLN
1	F	278	GLN
1	F	341	HIS
1	F	350	HIS
1	F	446	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	UDP	B	500	-	25,26,26	0.69	0	38,40,40	0.76	1 (2%)
2	UDP	F	500	-	25,26,26	1.44	5 (20%)	38,40,40	1.64	6 (15%)
2	UDP	A	500	-	25,26,26	1.28	4 (16%)	38,40,40	1.67	7 (18%)
2	UDP	C	500	-	25,26,26	1.38	5 (20%)	38,40,40	1.72	7 (18%)
2	UDP	D	500	-	25,26,26	0.71	0	38,40,40	0.84	1 (2%)
2	UDP	E	500	-	25,26,26	1.31	4 (16%)	38,40,40	1.69	5 (13%)

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	UDP	B	500	-	-	4/16/32/32	0/2/2/2
2	UDP	F	500	-	-	3/16/32/32	0/2/2/2
2	UDP	A	500	-	-	6/16/32/32	0/2/2/2
2	UDP	C	500	-	-	5/16/32/32	0/2/2/2
2	UDP	D	500	-	-	4/16/32/32	0/2/2/2
2	UDP	E	500	-	-	2/16/32/32	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	UDP	C4-N3	-3.10	1.33	1.38
2	A	500	UDP	C4-N3	-3.09	1.33	1.38
2	F	500	UDP	PB-O1B	3.03	1.59	1.50
2	F	500	UDP	C4-N3	-2.96	1.33	1.38
2	C	500	UDP	C4-N3	-2.91	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	UDP	C2-N3	-2.78	1.33	1.38
2	C	500	UDP	PB-O1B	2.77	1.59	1.50
2	E	500	UDP	C5-C4	-2.55	1.38	1.43
2	E	500	UDP	C2-N3	-2.55	1.33	1.38
2	F	500	UDP	C2-N3	-2.54	1.33	1.38
2	C	500	UDP	C5-C4	-2.54	1.38	1.43
2	C	500	UDP	C2-N3	-2.41	1.33	1.38
2	F	500	UDP	C5-C4	-2.39	1.38	1.43
2	C	500	UDP	C6-N1	-2.27	1.32	1.38
2	A	500	UDP	C6-N1	-2.25	1.32	1.38
2	A	500	UDP	C5-C4	-2.22	1.38	1.43
2	E	500	UDP	C6-N1	-2.09	1.33	1.38
2	F	500	UDP	C6-N1	-2.09	1.33	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	UDP	C4-N3-C2	-4.91	120.52	126.61
2	A	500	UDP	C4-N3-C2	-4.88	120.56	126.61
2	C	500	UDP	C4-N3-C2	-4.73	120.74	126.61
2	A	500	UDP	N3-C2-N1	4.64	120.93	114.89
2	F	500	UDP	C4-N3-C2	-4.63	120.86	126.61
2	E	500	UDP	C5-C4-N3	4.19	120.67	114.80
2	F	500	UDP	N3-C2-N1	4.01	120.11	114.89
2	C	500	UDP	N3-C2-N1	3.95	120.04	114.89
2	E	500	UDP	N3-C2-N1	3.85	119.90	114.89
2	F	500	UDP	C5-C4-N3	3.72	120.02	114.80
2	C	500	UDP	C5-C4-N3	3.70	119.98	114.80
2	C	500	UDP	O4-C4-C5	-3.43	119.25	125.16
2	A	500	UDP	C5-C4-N3	3.38	119.54	114.80
2	C	500	UDP	O3B-PB-O2B	3.35	120.37	107.80
2	E	500	UDP	O4-C4-C5	-3.25	119.55	125.16
2	F	500	UDP	O4-C4-C5	-2.89	120.18	125.16
2	F	500	UDP	O2-C2-N1	-2.87	119.06	122.80
2	A	500	UDP	O2-C2-N1	-2.86	119.08	122.80
2	D	500	UDP	C4'-O4'-C1'	-2.75	103.39	109.47
2	A	500	UDP	O4-C4-C5	-2.65	120.59	125.16
2	E	500	UDP	O2-C2-N1	-2.65	119.35	122.80
2	F	500	UDP	O3B-PB-O2B	2.61	117.59	107.80
2	A	500	UDP	O2B-PB-O1B	2.48	120.48	110.83
2	C	500	UDP	O2-C2-N1	-2.32	119.77	122.80
2	B	500	UDP	O4'-C1'-C2'	-2.18	101.95	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	UDP	O3'-C3'-C2'	-2.08	105.15	111.82
2	A	500	UDP	C2'-C3'-C4'	2.04	106.56	102.61

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	UDP	C5'-O5'-PA-O1A
2	A	500	UDP	C5'-O5'-PA-O3A
2	B	500	UDP	C5'-O5'-PA-O1A
2	B	500	UDP	C5'-O5'-PA-O3A
2	C	500	UDP	C5'-O5'-PA-O1A
2	C	500	UDP	C5'-O5'-PA-O2A
2	C	500	UDP	C5'-O5'-PA-O3A
2	D	500	UDP	C5'-O5'-PA-O3A
2	E	500	UDP	C5'-O5'-PA-O2A
2	E	500	UDP	C5'-O5'-PA-O3A
2	F	500	UDP	C5'-O5'-PA-O1A
2	F	500	UDP	C5'-O5'-PA-O2A
2	F	500	UDP	C5'-O5'-PA-O3A
2	A	500	UDP	C3'-C4'-C5'-O5'
2	A	500	UDP	O4'-C4'-C5'-O5'
2	D	500	UDP	O4'-C4'-C5'-O5'
2	D	500	UDP	C3'-C4'-C5'-O5'
2	B	500	UDP	PB-O3A-PA-O5'
2	C	500	UDP	O4'-C4'-C5'-O5'
2	A	500	UDP	C5'-O5'-PA-O2A
2	B	500	UDP	C5'-O5'-PA-O2A
2	D	500	UDP	C5'-O5'-PA-O1A
2	A	500	UDP	C4'-C5'-O5'-PA
2	C	500	UDP	C3'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 35 short contacts:

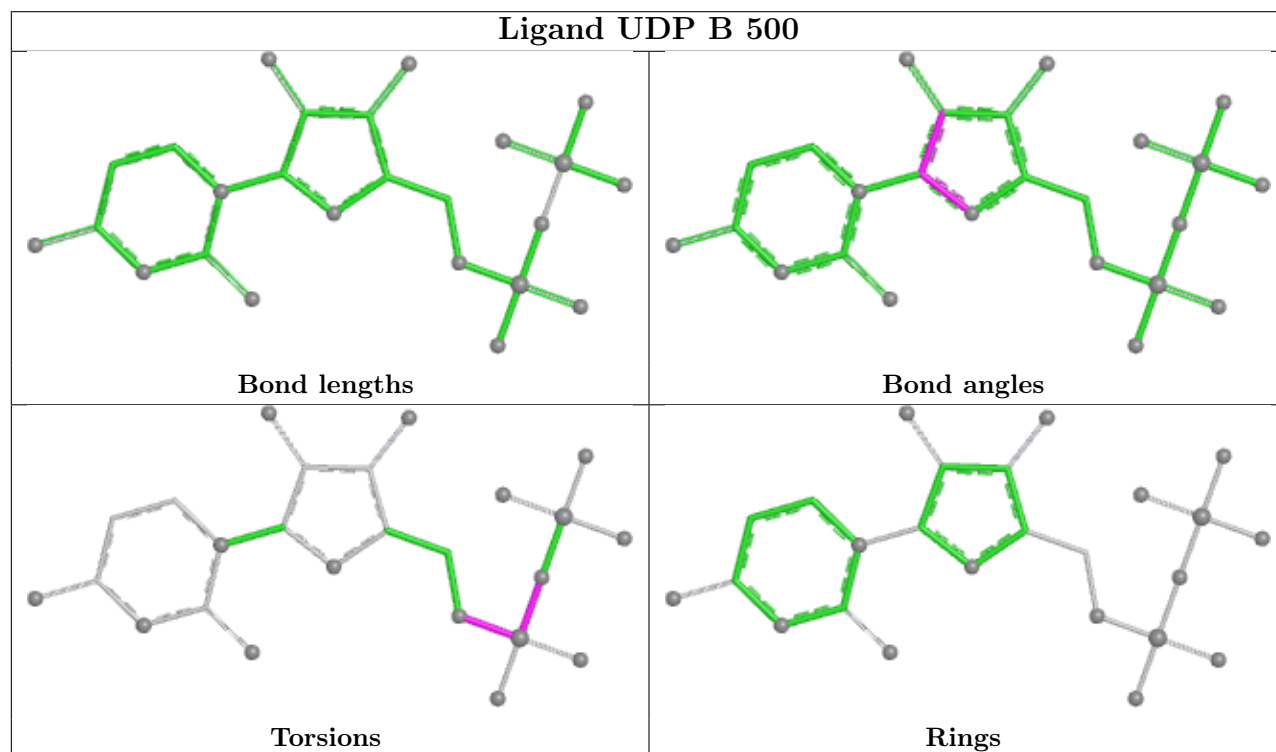
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	UDP	2	0
2	F	500	UDP	1	0
2	A	500	UDP	6	0
2	C	500	UDP	7	0
2	D	500	UDP	4	0

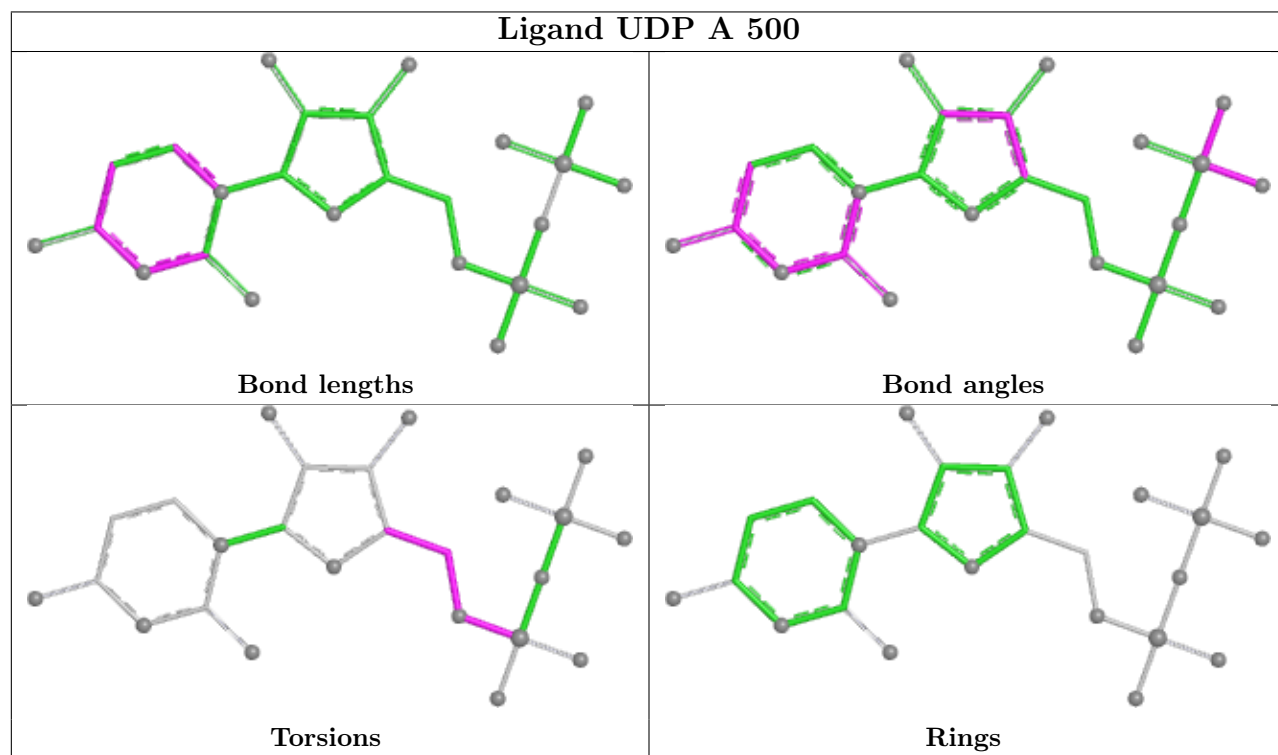
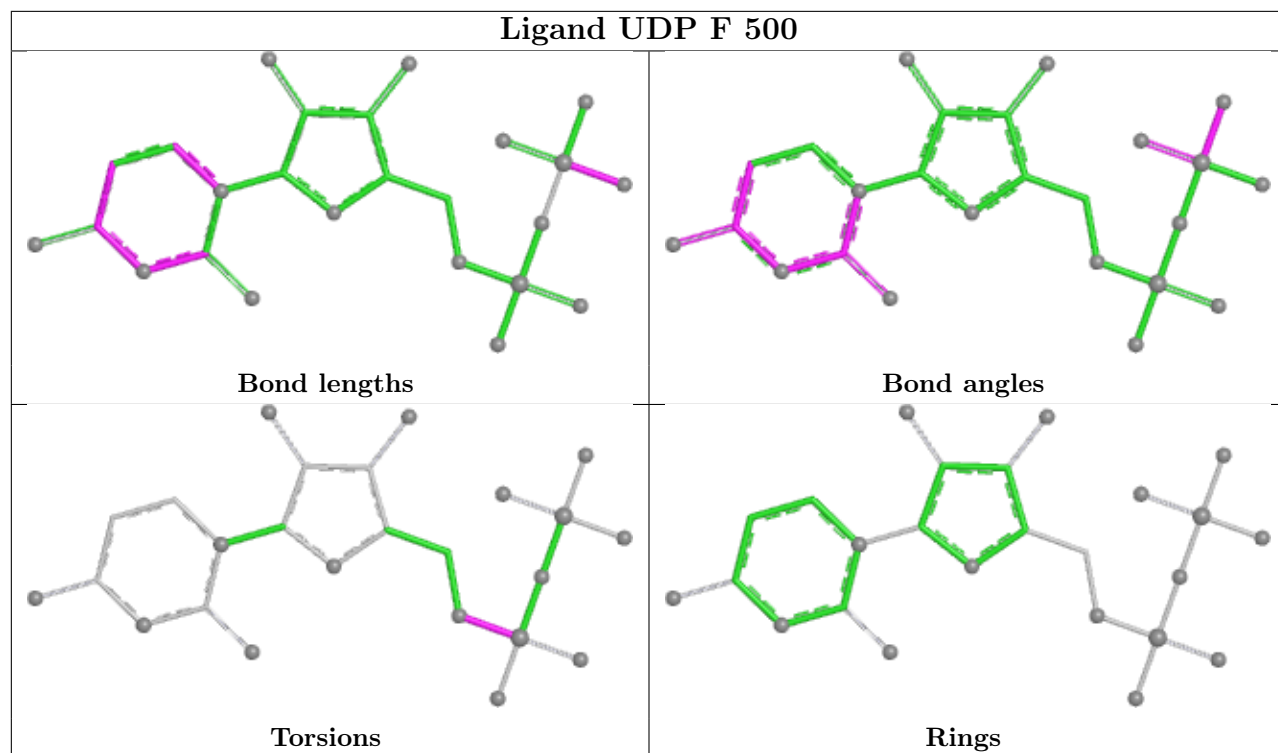
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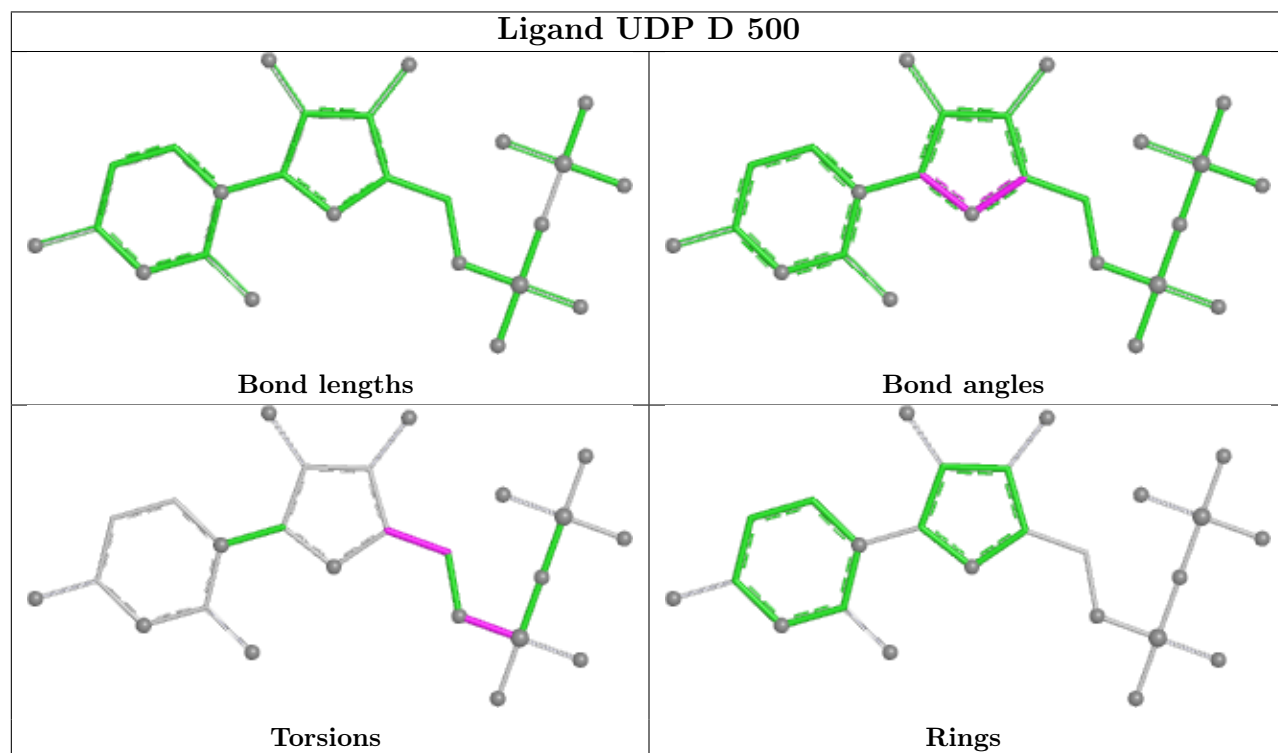
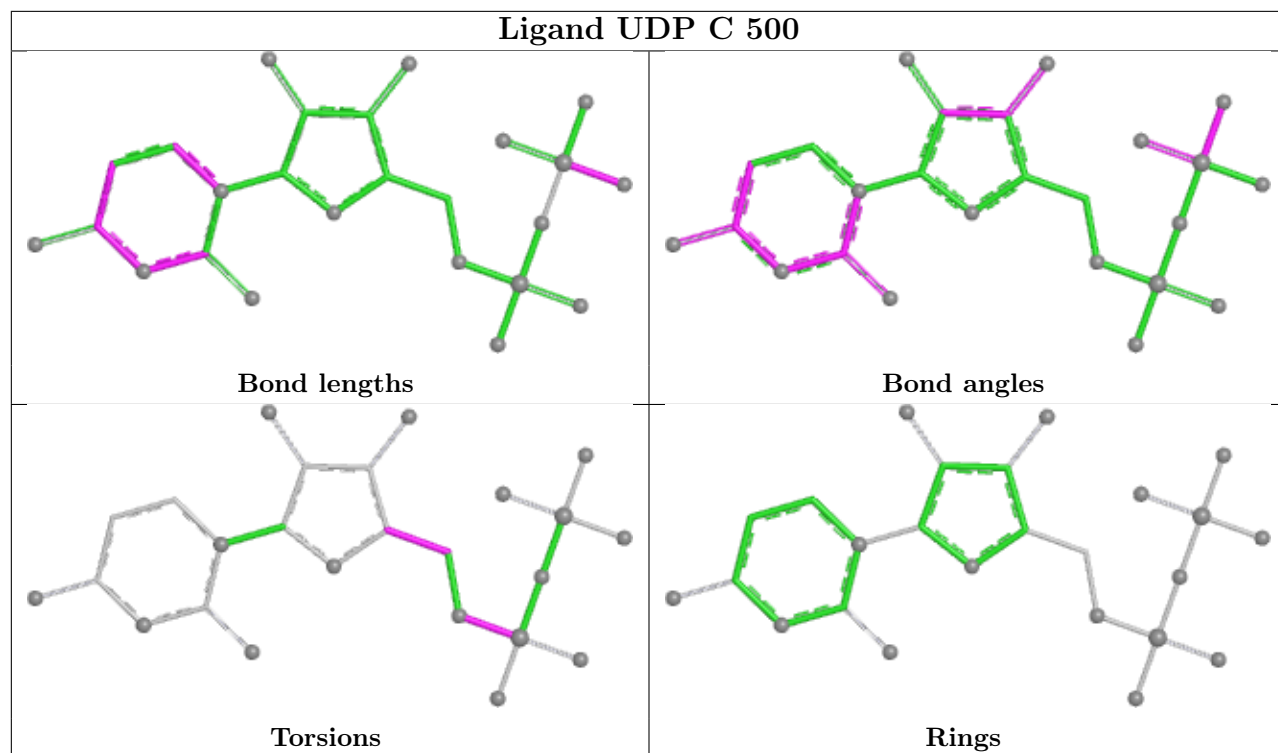
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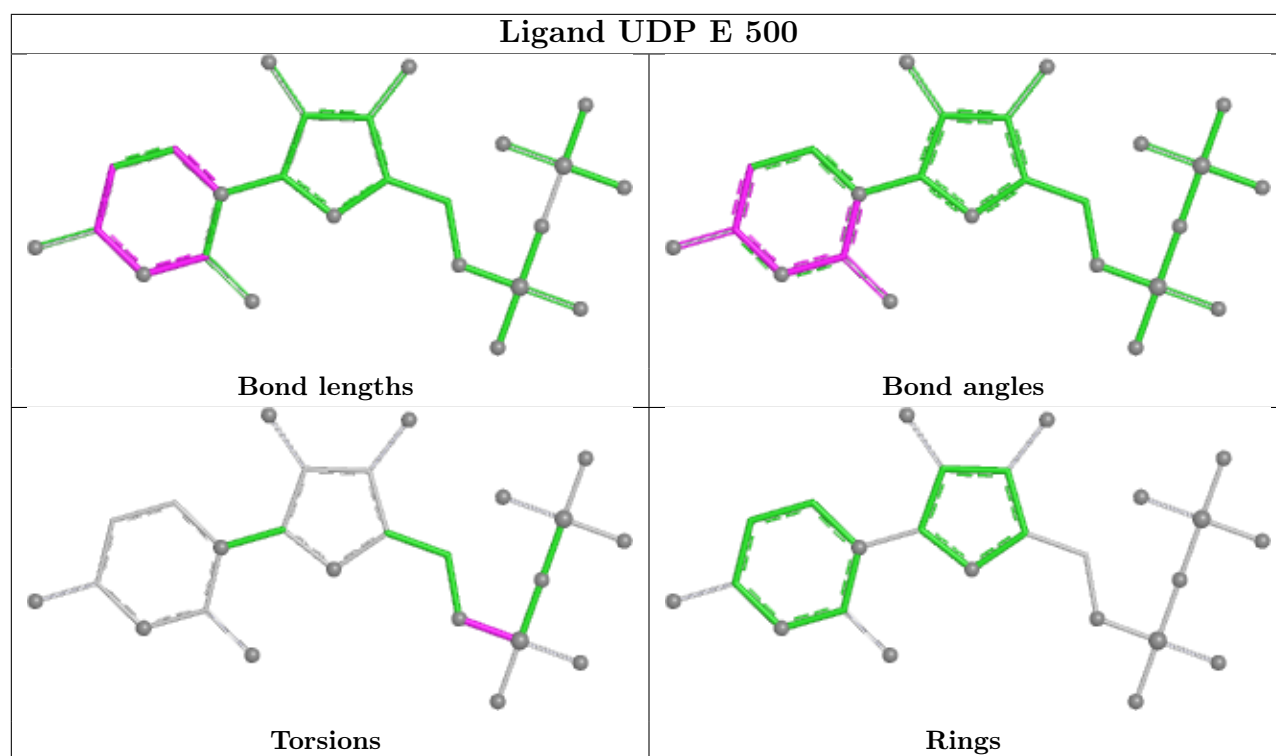
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	UDP	15	0

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.









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	443/460 (96%)	0.35	22 (4%)	34	18	25, 39, 64, 102	0
1	B	445/460 (96%)	0.52	22 (4%)	35	18	28, 48, 75, 116	0
1	C	439/460 (95%)	0.39	19 (4%)	40	21	28, 46, 66, 90	0
1	D	437/460 (95%)	0.67	29 (6%)	24	12	36, 56, 80, 110	0
1	E	443/460 (96%)	0.40	15 (3%)	48	27	30, 45, 68, 108	0
1	F	444/460 (96%)	0.31	22 (4%)	34	18	25, 42, 70, 126	0
All	All	2651/2760 (96%)	0.44	129 (4%)	35	18	25, 46, 73, 126	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	ALA	6.2
1	D	10	VAL	5.8
1	F	249	ALA	5.7
1	E	246	ALA	4.5
1	B	246	ALA	4.4
1	B	166	ASN	4.1
1	C	311	GLU	4.0
1	F	248	LYS	4.0
1	B	310	VAL	3.9
1	E	249	ALA	3.9
1	A	245	ASP	3.9
1	D	113	PRO	3.8
1	F	300	GLY	3.7
1	A	112	SER	3.6
1	F	230	ASN	3.6
1	D	189	ASP	3.5
1	F	310	VAL	3.5
1	B	311	GLU	3.4
1	A	113	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	252	LEU	3.3
1	D	312	ASP	3.3
1	B	85	ARG	3.3
1	C	251	ASP	3.3
1	D	311	GLU	3.3
1	F	301	LYS	3.2
1	E	454	ASN	3.2
1	D	194	PHE	3.2
1	A	79	TYR	3.1
1	F	166	ASN	3.0
1	A	251	ASP	3.0
1	B	86	ASN	3.0
1	A	301	LYS	3.0
1	E	86	ASN	3.0
1	E	84	LEU	3.0
1	D	313	MET	3.0
1	B	10	VAL	2.9
1	D	53	ALA	2.9
1	F	227	VAL	2.9
1	B	165	ALA	2.9
1	D	177	PRO	2.8
1	A	163	ASP	2.8
1	B	219	PHE	2.8
1	A	250	HIS	2.8
1	C	74	PHE	2.7
1	C	84	LEU	2.7
1	E	247	LYS	2.7
1	E	176	GLY	2.6
1	E	299	GLY	2.6
1	C	83	GLY	2.6
1	D	165	ALA	2.6
1	D	178	ILE	2.5
1	E	162	ILE	2.5
1	D	454	ASN	2.5
1	E	250	HIS	2.5
1	D	135	LEU	2.5
1	C	231	GLY	2.5
1	C	301	LYS	2.5
1	D	19	CYS	2.5
1	C	299	GLY	2.4
1	B	244	TYR	2.4
1	A	398	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	2.4
1	F	188	LEU	2.4
1	D	398	GLN	2.4
1	D	411	MET	2.4
1	B	238	ILE	2.4
1	C	300	GLY	2.3
1	F	176	GLY	2.3
1	F	134	ASP	2.3
1	C	50	THR	2.3
1	B	319	VAL	2.3
1	C	454	ASN	2.3
1	A	312	ASP	2.3
1	F	162	ILE	2.3
1	A	248	LYS	2.3
1	A	165	ALA	2.3
1	A	220	GLU	2.3
1	F	308	GLU	2.3
1	D	87	ASP	2.3
1	F	298	LYS	2.3
1	A	310	VAL	2.3
1	C	364	VAL	2.3
1	B	83	GLY	2.3
1	D	11	GLY	2.3
1	D	246	ALA	2.2
1	E	248	LYS	2.2
1	F	233	ASP	2.2
1	A	81	LYS	2.2
1	D	248	LYS	2.2
1	A	434	THR	2.2
1	B	414	VAL	2.2
1	D	414	VAL	2.2
1	D	270	SER	2.2
1	D	250	HIS	2.2
1	A	10	VAL	2.2
1	F	232	VAL	2.2
1	F	368	ALA	2.2
1	B	245	ASP	2.2
1	C	163	ASP	2.2
1	C	303	ASP	2.2
1	D	371	GLN	2.1
1	B	248	LYS	2.1
1	D	299	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	151	CYS	2.1
1	A	311	GLU	2.1
1	D	198	ILE	2.1
1	C	450	HIS	2.1
1	C	256	ASP	2.1
1	D	130	ASP	2.1
1	B	53	ALA	2.1
1	D	148	ALA	2.1
1	D	145	SER	2.1
1	F	252	LEU	2.1
1	A	162	ILE	2.1
1	A	249	ALA	2.1
1	C	313	MET	2.1
1	E	72	LEU	2.1
1	A	83	GLY	2.1
1	C	271	ARG	2.1
1	F	50	THR	2.1
1	F	303	ASP	2.1
1	B	332	TRP	2.1
1	B	411	MET	2.0
1	F	173	PRO	2.0
1	F	231	GLY	2.0
1	A	166	ASN	2.0
1	B	418	GLU	2.0
1	E	186	LYS	2.0
1	E	311	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

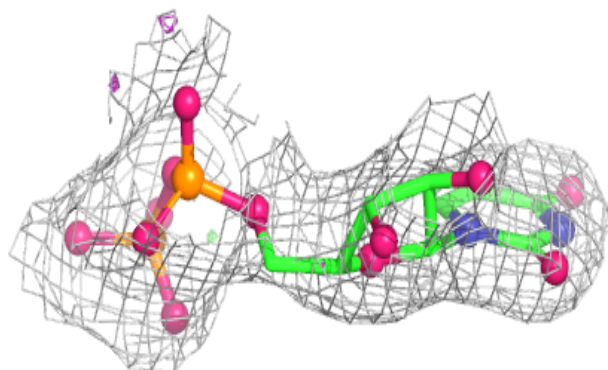
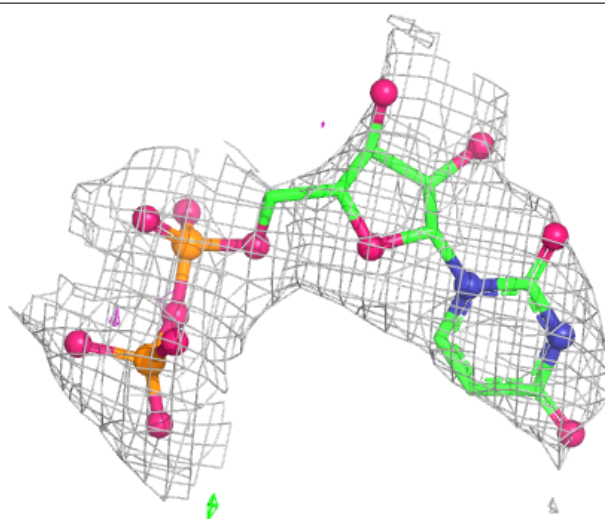
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	UDP	D	500	25/25	0.89	0.10	44,58,68,76	0
2	UDP	C	500	25/25	0.90	0.12	40,46,65,73	0
2	UDP	B	500	25/25	0.92	0.10	43,51,57,70	0
2	UDP	F	500	25/25	0.92	0.12	28,43,56,70	0
2	UDP	E	500	25/25	0.93	0.09	36,47,53,70	0
2	UDP	A	500	25/25	0.93	0.09	33,41,53,70	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.

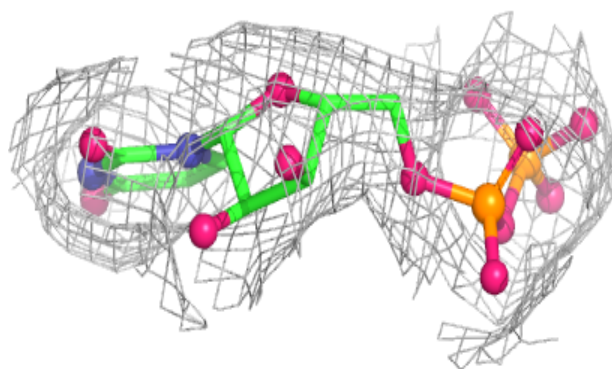
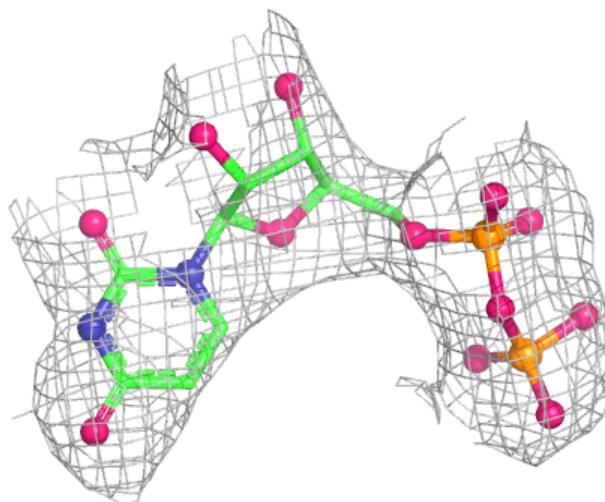
Electron density around UDP D 500:

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



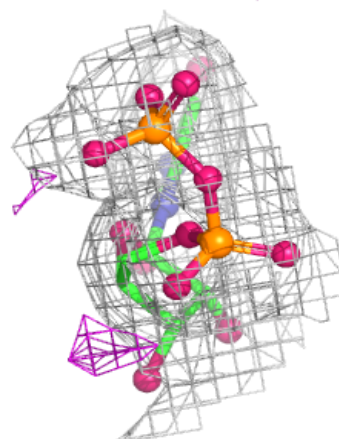
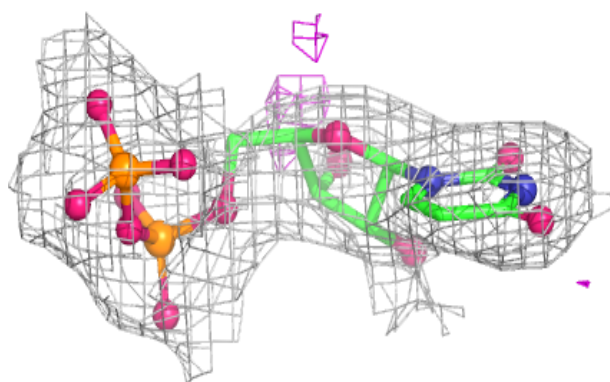
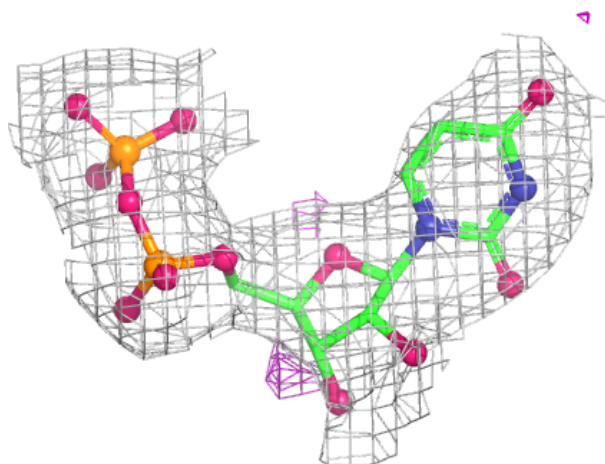
Electron density around UDP C 500:

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



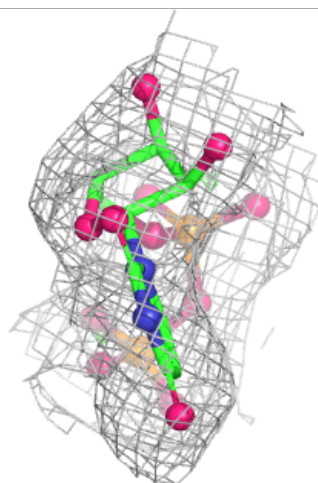
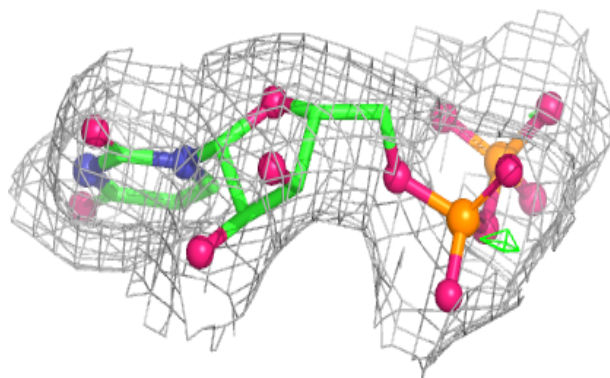
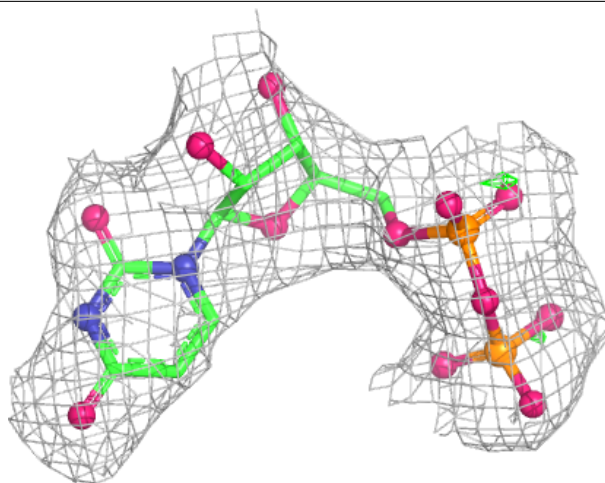
Electron density around UDP B 500:

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



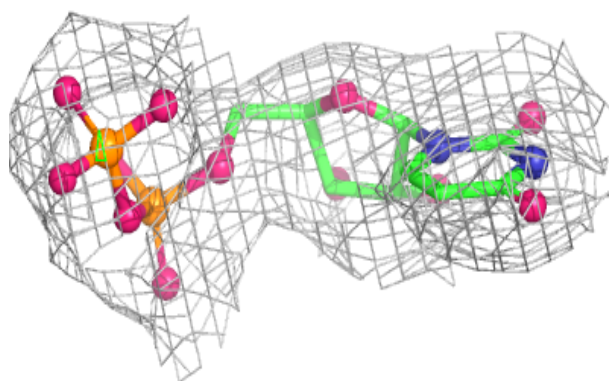
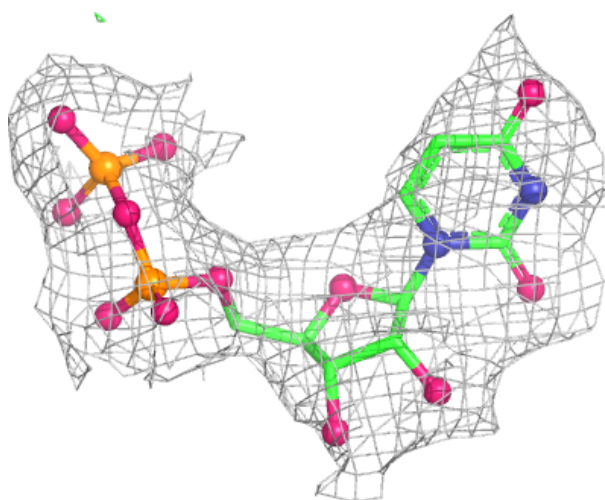
Electron density around UDP F 500:

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and green (positive)



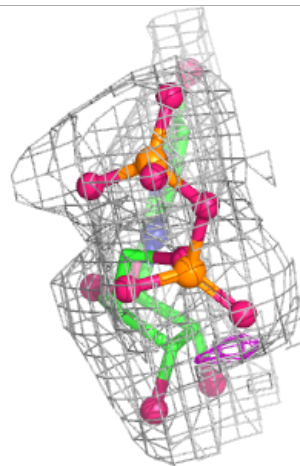
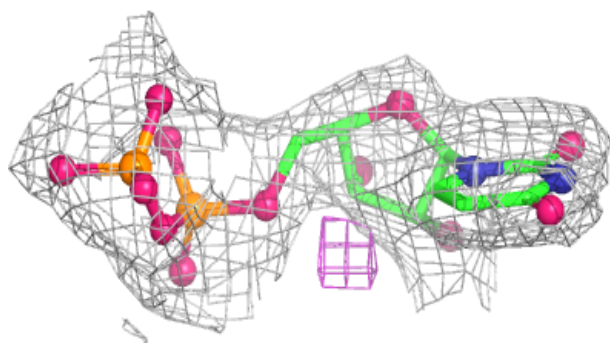
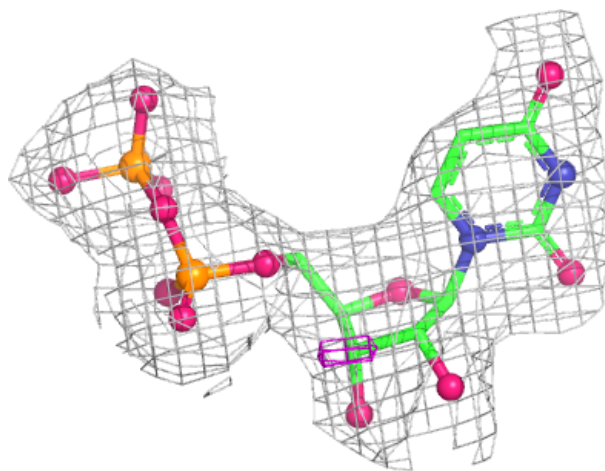
Electron density around UDP E 500:

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



Electron density around UDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.