



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:11 PM UTC

PDB ID : 1C30 / pdb_00001c30
Title : CRYSTAL STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE:
SMALL SUBUNIT MUTATION C269S
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-07-24
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

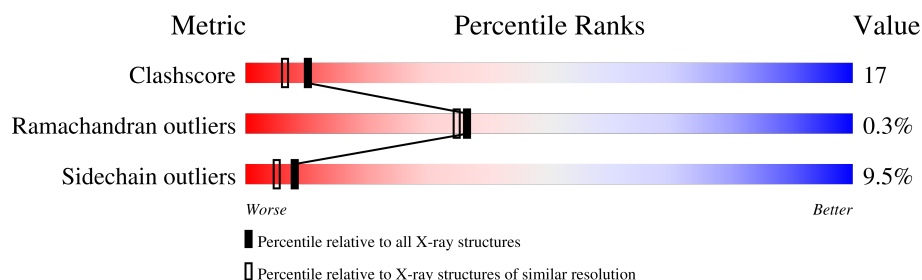
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	64% 29% 5% ..
1	C	1073	64% 28% 6% .
1	E	1073	69% 25% 5% .
1	G	1073	56% 36% 7% ..
2	B	382	60% 34% . ..
2	D	382	60% 34% 5% ..
2	F	382	57% 34% 8% ..
2	H	382	48% 45% 6% ..

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
6	PO4	C	4025	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48668 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 CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	6	0
			8189	5141	1429	1574	45			
1	C	1058	Total	C	N	O	S	0	1	0
			8165	5126	1422	1572	45			
1	E	1058	Total	C	N	O	S	0	6	0
			8188	5141	1426	1575	46			
1	G	1058	Total	C	N	O	S	0	4	0
			8178	5137	1424	1572	45			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	H	379	Total	C	N	O	S	0	1	0
			2900	1828	508	555	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	SER	CYS	engineered mutation	UNP P00907
D	269	SER	CYS	engineered mutation	UNP P00907
F	269	SER	CYS	engineered mutation	UNP P00907
H	269	SER	CYS	engineered mutation	UNP P00907

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0
3	G	3	Total Mn 3 3	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total K 7 7	0	0
4	B	1	Total K 1 1	0	0
4	C	7	Total K 7 7	0	0
4	D	1	Total K 1 1	0	0
4	E	7	Total K 7 7	0	0
4	F	1	Total K 1 1	0	0
4	G	7	Total K 7 7	0	0
4	H	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

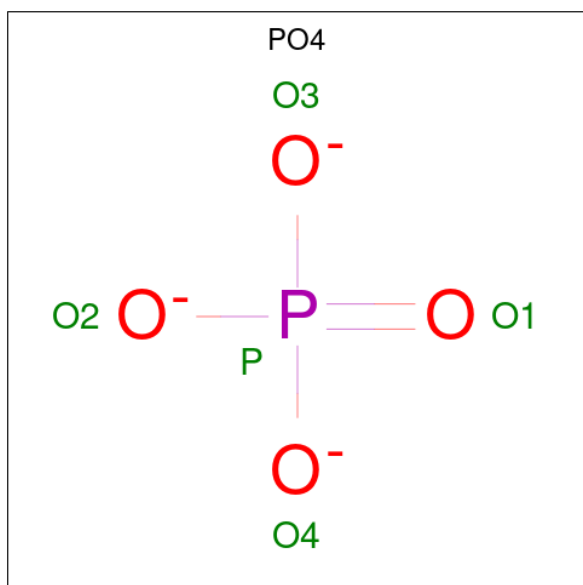
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0
5	D	1	Total Cl 1 1	0	0
5	E	3	Total Cl 3 3	0	0
5	F	1	Total Cl 1 1	0	0

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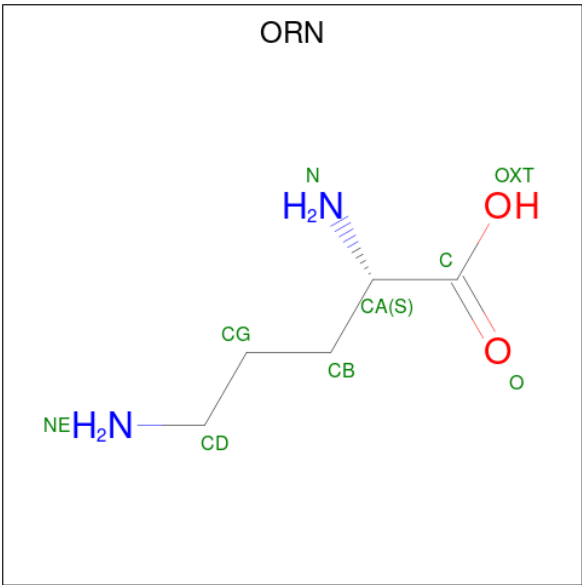
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	3	Total	Cl	0	0
			3	3		
5	H	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



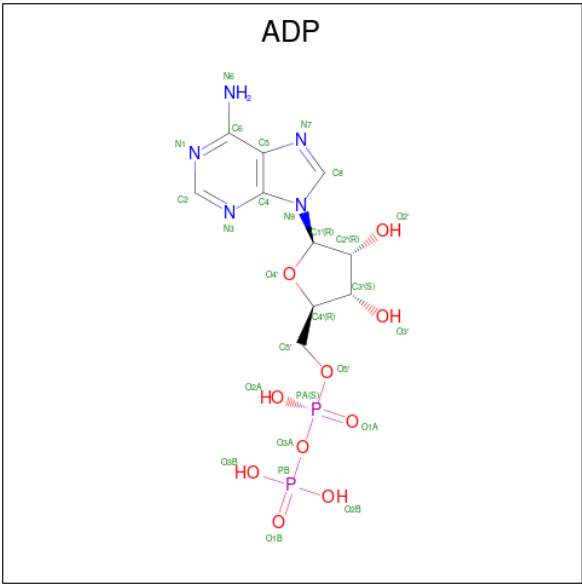
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is L-ornithine (CCD ID: ORN) (formula: $C_5H_{12}N_2O_2$).



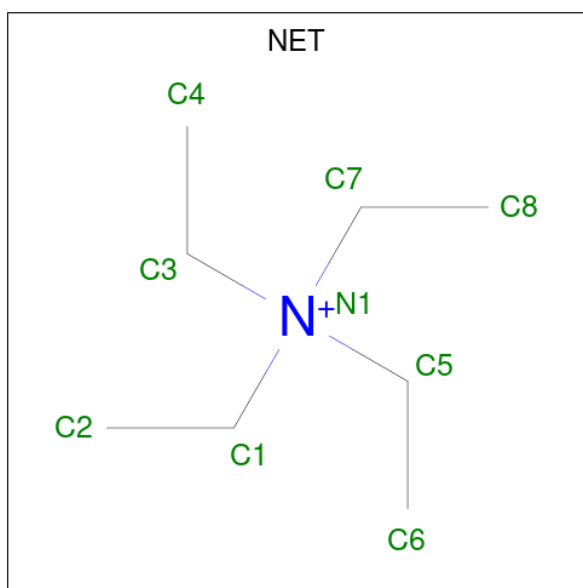
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			9	5	2	2		
7	A	1	Total	C	N	O	0	0
			8	5	2	1		
7	A	1	Total	C	N	O	0	0
			8	5	2	1		
7	A	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			9	8	1		
9	C	1	Total	C	N	0	0
			9	8	1		
9	E	1	Total	C	N	0	0
			9	8	1		
9	G	1	Total	C	N	0	0
			9	8	1		

- Molecule 10 is water.

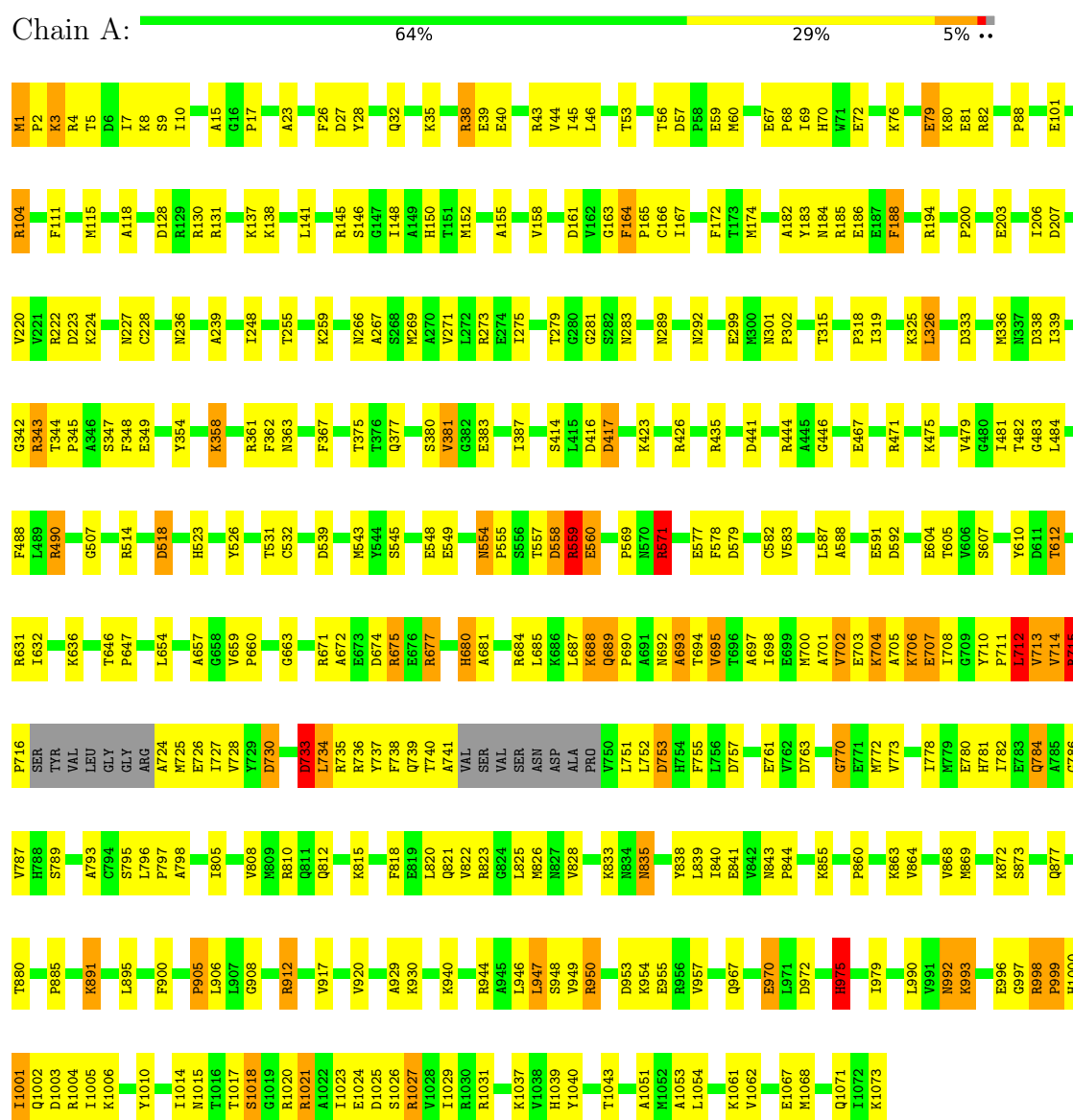
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	830	Total 830	O 830	0	0
10	B	230	Total 230	O 230	0	0
10	C	683	Total 683	O 683	0	0
10	D	238	Total 238	O 238	0	0
10	E	884	Total 884	O 884	0	0
10	F	272	Total 272	O 272	0	0
10	G	666	Total 666	O 666	0	0
10	H	184	Total 184	O 184	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

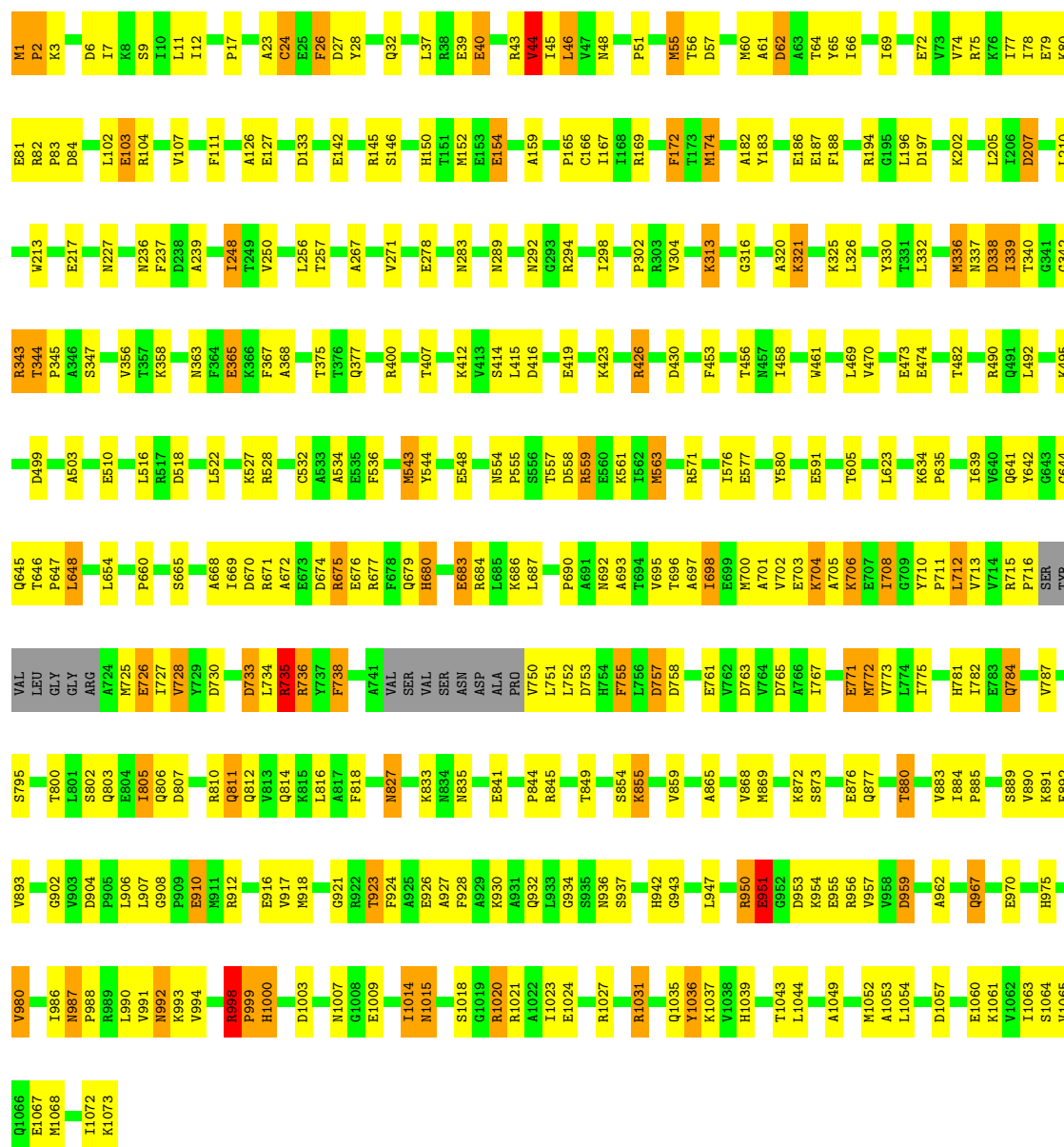
Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



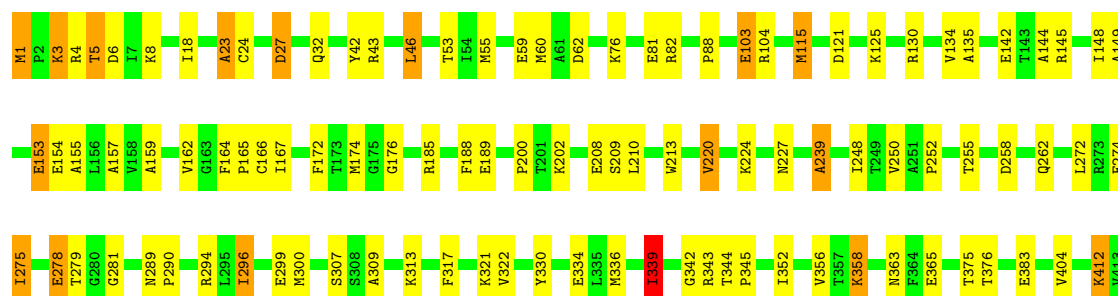
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain C:  64% 28% 6% .



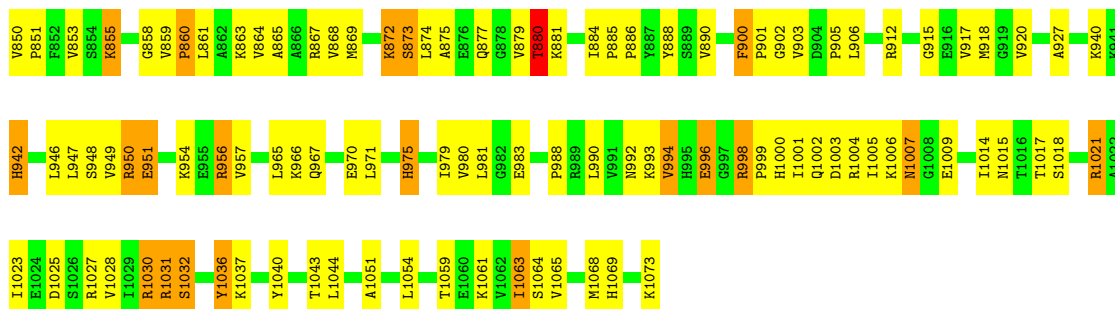
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain E:  69% 25% 5% .

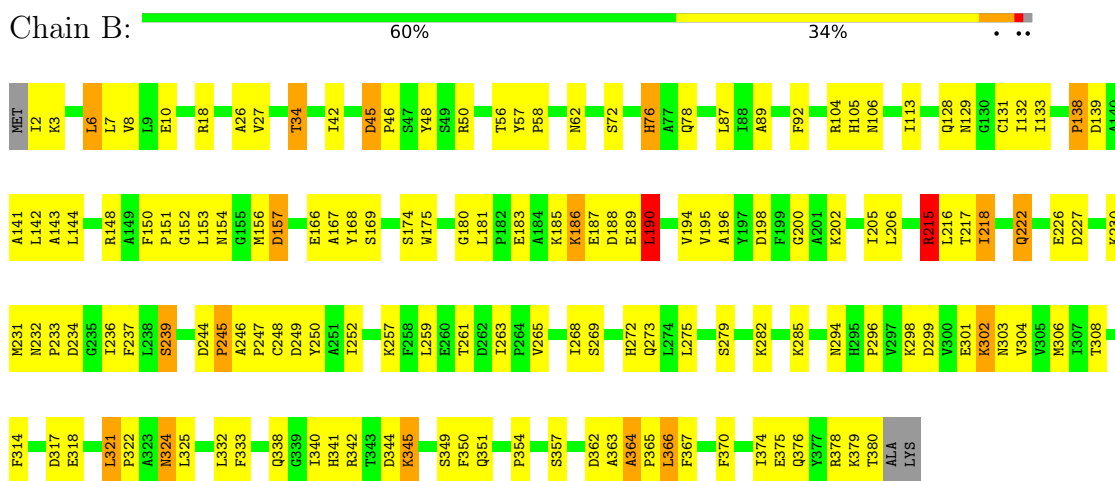




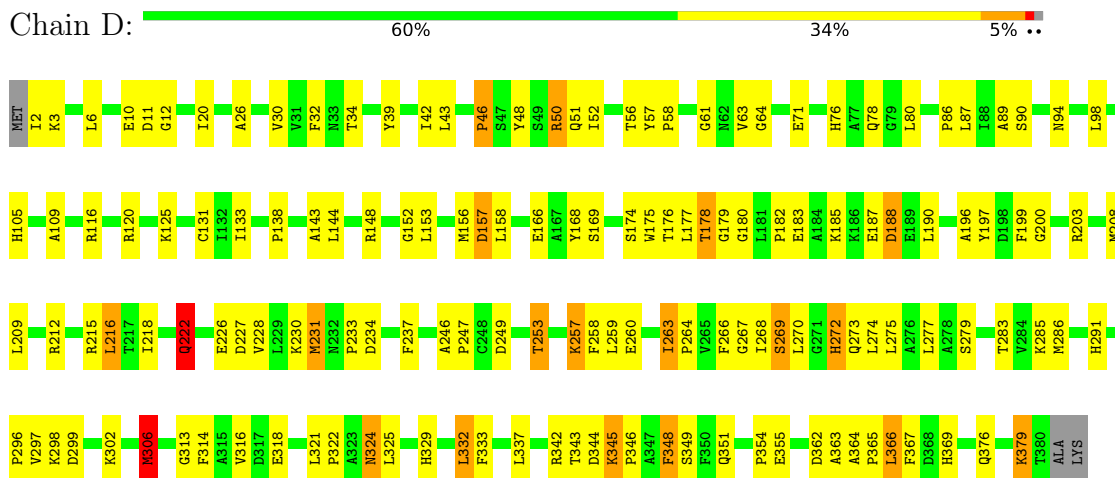
D769	E703	G641	Y547	L332	K202	L87	M1
G770	K704	G644	E548	F453	E203	P88	P2
E771	A705	G645	E549	T456	L204	E102	K3
M772	K706	G646	E550	T456	L205	L103	K8
E773	E707	G647	N554	N457	E208	R104	S9
L774	I708	P647	I458	I458	K214	Q105	I10
L775	G709	L648	P555	G341	K214	G106	L11
	Y710		S556	G342	K224	V107	
H781	A651		T557	R343	K224	L108	P17
L712	R652		D558	E473	F237	F111	I20
V713	A653		D558	E474	D246	A118	G21
G784	V714		R559	K475	S247	A126	Q22
A785	R715		P560	K475	I248	A126	A23
G786	P716		K561	E349	F237	F111	C24
	A656		M562		D246	A118	G21
S789	SER		M563	V479	D246	A118	Q22
	TYR		G658	T481	S247	A118	A23
A793	VAL		V659	T482	I248	A126	C24
	LEU		P660	G483	Q254	R130	E25
L796	GLY		V661		T255	F26	F26
P797	GLY		I662	F488	T255	V134	D27
	ARG		G663	L489	T257	A135	Y28
	A724		T684	Y580	M136	M136	S29
T800	M725		S665	L492	E260	K137	Q32
L801	E726		P666	K493	Y261	K138	
S802	I727		P667	R494	A267	T143	K35
Q803	V728		R590	L502	S268	A144	A36
E804	Y729		E591	L505	M269	R145	E39
Q806	D730		D592		V271	I148	E40
D807	E731		R671	V404	R272	A149	
V808	A732		A672	G405	L273	H150	R83
M809	D733		E673	A406	R273	T151	V44
	L734		D674	R509	E274	M152	I45
	R735		R675	E512	I275	M152	L46
			T605			E153	
A817	F733		R677	D410	F286	E154	M55
E818	Q739		F678	L412			T56
E819	T740		Q679	V413			D57
L820	A741		R615	D416	I296	P165	P58
Q821	VAL		A681	D417	P302	C166	
R822	SER		F618	E520	R303	I167	E59
R823	VAL		E619	D521	Q304	I168	M60
G824	SER		R694	L522	V304		
	ASP		L685	H523			A63
N827	ASP		K686	P524	K313	F172	T64
R828	ALA		L687	D625	A314	T173	Y65
Q829	PRO		K688	V525	T422	M174	
F830	V750		Q689	V626	K423	G175	I69
A831	L751		P690	L627	K527	G316	
R832	L752		A691	E628	F317	G176	H70
			R692	E629	P318	G180	H71
			R693	D530	I319	I181	W70
			A694	T531	A320	A182	V73
			V695	G432	K321	Y183	R74
L839	E761		E633	A534		N184	R75
I840	V762		K634	E535	K325	R185	K76
	D763		P635	F536	L326	E186	
P844	V764		K636		A327	E187	E79
R845	D765		G637	M543	V328	F188	
	A766		M700	Y544	G329	K540	K80
	V767		V638	A440	R329	E81	E81
R848	V768		I639	S545	Y330	L196	
	V769		T640	T546	Y330	T324	V86



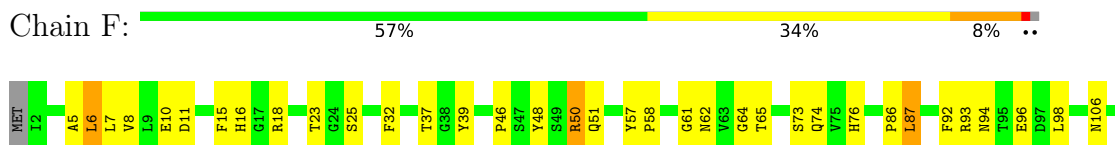
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

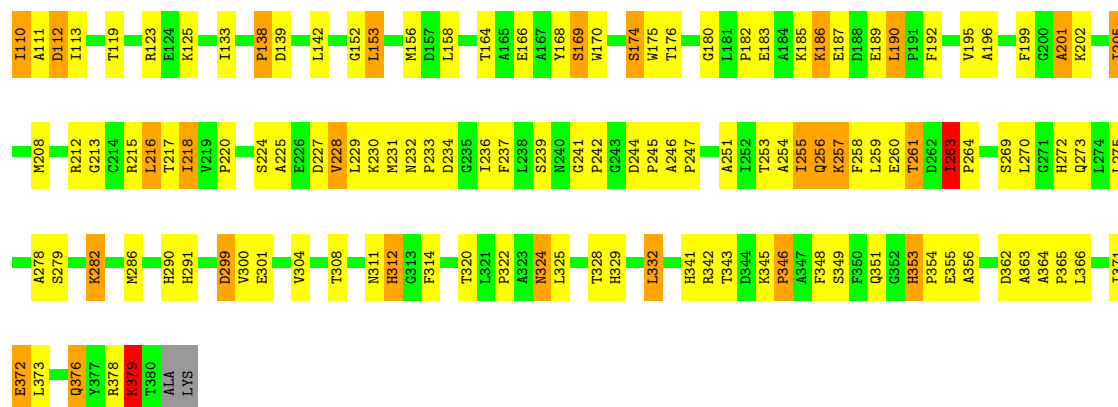


• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT



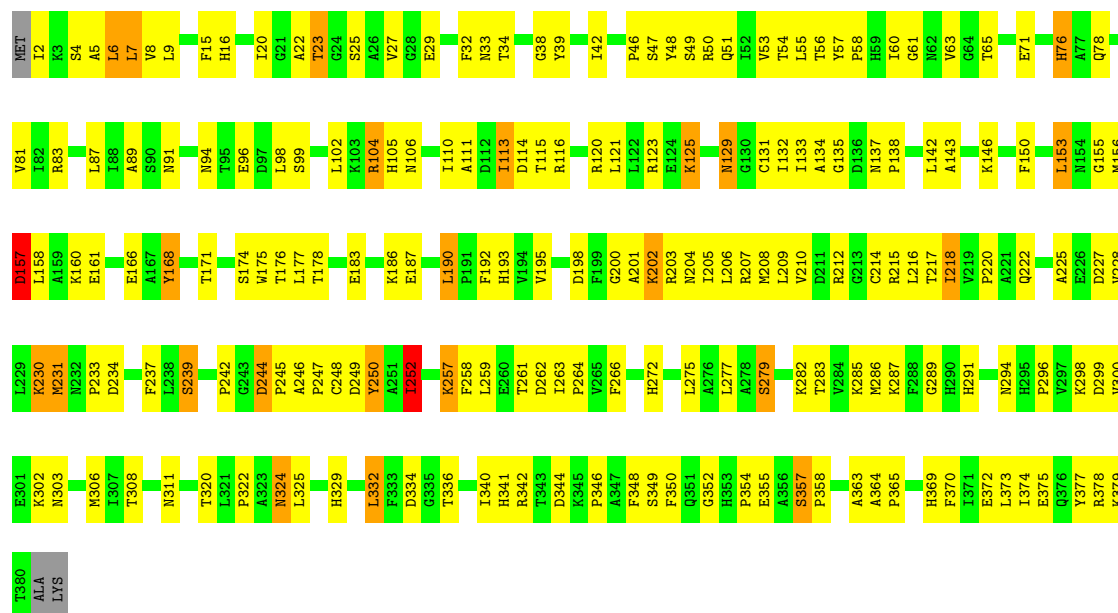
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT





● Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 48% 45% 6% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.60Å 164.60Å 332.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (30.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.189 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48668	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ORN, MN, PO4, ADP, NET, K

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	1.11	0/8339	1.59	80/11273 (0.7%)
1	C	1.15	10/8295 (0.1%)	1.62	77/11214 (0.7%)
1	E	1.15	3/8338 (0.0%)	1.58	71/11270 (0.6%)
1	G	1.10	1/8320 (0.0%)	1.63	95/11246 (0.8%)
2	B	1.05	0/2957	1.53	23/4016 (0.6%)
2	D	1.15	1/2957 (0.0%)	1.62	24/4016 (0.6%)
2	F	1.08	0/2957	1.61	27/4016 (0.7%)
2	H	1.06	0/2966	1.63	26/4028 (0.6%)
All	All	1.12	15/45129 (0.0%)	1.60	423/61079 (0.7%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	993	LYS	CE-NZ	6.12	1.67	1.49
1	C	40	GLU	CD-OE2	6.11	1.36	1.25
1	C	430	ASP	CG-OD2	6.09	1.36	1.25
1	C	955	GLU	CD-OE2	5.50	1.35	1.25
1	E	279	THR	CA-C	-5.45	1.46	1.53
1	C	959	ASP	CG-OD2	5.40	1.35	1.25
1	G	554	ASN	CA-C	-5.40	1.49	1.53
1	C	518	ASP	CG-OD2	5.34	1.35	1.25
1	C	951	GLU	CD-OE2	5.33	1.35	1.25
1	C	771	GLU	CD-OE2	5.30	1.35	1.25
1	C	72	GLU	CD-OE2	5.20	1.35	1.25
1	E	365	GLU	CD-OE2	5.20	1.35	1.25
2	D	234	ASP	CG-OD2	5.04	1.34	1.25
1	C	1024	GLU	CD-OE2	5.02	1.34	1.25
1	C	499	ASP	CG-OD2	5.00	1.34	1.25

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	16	HIS	CA-CB-CG	-9.26	104.54	113.80
1	G	557	THR	CA-C-N	9.12	132.68	120.65
1	G	557	THR	C-N-CA	9.12	132.68	120.65
1	C	885	PRO	O-C-N	9.09	125.42	121.15
1	G	660	PRO	N-CA-CB	8.91	108.49	102.25
1	G	605	THR	N-CA-C	8.89	123.61	110.46
1	G	319	ILE	N-CA-C	8.78	119.58	110.36
1	G	578	PHE	CA-CB-CG	-8.67	105.13	113.80
1	A	23	ALA	N-CA-C	8.54	121.33	109.29
2	B	105	HIS	CA-CB-CG	-8.47	105.33	113.80
1	C	207	ASP	CA-CB-CG	8.41	121.01	112.60
1	A	558	ASP	CA-CB-CG	8.37	120.97	112.60
2	D	157	ASP	CA-CB-CG	8.37	120.97	112.60
2	H	76	HIS	CA-CB-CG	-8.21	105.59	113.80
1	C	536	PHE	CA-CB-CG	-8.17	105.63	113.80
1	G	994	VAL	N-CA-C	8.02	118.82	110.72
1	E	404	VAL	N-CA-C	-7.95	105.12	112.43
1	C	605	THR	N-CA-C	7.90	122.21	110.52
1	G	998	ARG	N-CA-C	7.89	122.05	110.14
1	E	793	ALA	N-CA-C	-7.87	99.93	110.55
1	C	690	PRO	N-CA-CB	7.82	110.13	103.25
1	C	26	PHE	CA-CB-CG	-7.80	106.00	113.80
1	A	680	HIS	CA-CB-CG	-7.74	106.06	113.80
1	E	558	ASP	N-CA-C	7.71	119.37	110.97
1	C	716	PRO	N-CA-CB	7.70	111.47	103.00
1	G	453	PHE	CA-CB-CG	-7.67	106.13	113.80
1	E	559[A]	ARG	N-CA-C	7.66	121.85	110.52
1	E	559[B]	ARG	N-CA-C	7.66	121.85	110.52
1	C	998	ARG	N-CA-C	7.62	122.00	109.58
1	C	23	ALA	N-CA-C	7.58	119.98	109.29
1	E	560	GLU	N-CA-C	-7.54	96.97	108.96
1	E	339	ILE	N-CA-C	7.49	122.74	113.00
1	C	558	ASP	N-CA-CB	-7.42	97.94	110.49
2	F	11	ASP	CA-CB-CG	7.42	120.02	112.60
1	G	716	PRO	N-CA-CB	7.42	111.16	103.00
2	H	303	ASN	CA-CB-CG	-7.40	105.20	112.60
1	G	558	ASP	N-CA-C	7.38	119.02	110.97
1	A	188	PHE	CA-CB-CG	-7.35	106.45	113.80
1	G	88	PRO	CB-CA-C	-7.34	101.78	110.00
1	C	304	VAL	N-CA-C	-7.33	101.93	110.21
1	G	793	ALA	N-CA-C	-7.32	100.67	110.55
1	A	716	PRO	N-CA-CB	7.28	111.01	103.00
2	H	168	TYR	N-CA-C	7.21	119.10	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1039	HIS	CA-CB-CG	-7.18	106.62	113.80
1	C	154	GLU	CB-CG-CD	7.10	124.67	112.60
1	C	993	LYS	N-CA-C	-7.10	101.68	110.41
1	A	908	GLY	CA-C-N	7.08	127.24	119.87
1	A	908	GLY	C-N-CA	7.08	127.24	119.87
1	C	885	PRO	N-CA-CB	7.06	106.89	103.22
1	E	557	THR	CA-C-N	7.04	129.95	120.65
1	E	557	THR	C-N-CA	7.04	129.95	120.65
1	A	998	ARG	N-CA-C	7.02	119.61	108.23
1	A	15	ALA	N-CA-C	7.01	121.58	112.89
1	E	716	PRO	N-CA-CB	7.00	110.70	103.00
1	G	248	ILE	N-CA-C	-7.00	99.69	109.21
1	G	880	THR	N-CA-CB	-6.98	100.95	111.15
1	C	316	GLY	N-CA-C	-6.95	105.63	115.43
1	G	44	VAL	N-CA-C	6.92	117.82	107.51
1	E	1000	HIS	CA-CB-CG	-6.90	106.90	113.80
2	H	53	VAL	N-CA-C	6.87	118.02	107.99
1	C	660	PRO	N-CA-CB	6.86	107.31	102.65
1	G	738	PHE	CA-CB-CG	-6.83	106.97	113.80
1	G	317	PHE	CA-C-N	6.76	128.29	119.84
1	G	317	PHE	C-N-CA	6.76	128.29	119.84
1	G	558	ASP	N-CA-CB	-6.76	100.04	109.91
1	G	172	PHE	CA-CB-CG	-6.75	107.05	113.80
1	E	782	ILE	N-CA-C	-6.74	104.61	110.74
1	G	339	ILE	N-CA-C	6.73	121.58	111.89
2	F	362	ASP	CA-CB-CG	6.72	119.32	112.60
1	C	1000	HIS	CA-CB-CG	-6.71	107.09	113.80
1	E	558	ASP	CB-CA-C	-6.67	100.68	110.96
1	G	329	GLY	N-CA-C	6.66	123.00	115.08
1	C	210	LEU	N-CA-C	-6.64	103.77	112.41
2	D	222	GLN	N-CA-C	6.64	121.22	113.18
1	G	407	THR	N-CA-C	-6.64	105.08	113.72
2	F	346	PRO	N-CA-CB	6.64	106.90	102.25
1	C	1015	ASN	CA-CB-CG	6.63	119.23	112.60
1	G	107	VAL	N-CA-C	6.63	117.42	110.72
1	C	782	ILE	N-CA-C	-6.60	104.21	110.42
1	G	172	PHE	N-CA-C	6.59	120.63	111.74
1	E	1072	ILE	N-CA-C	6.59	117.58	108.89
1	G	27	ASP	N-CA-C	-6.57	103.61	111.69
1	A	612	THR	N-CA-C	6.56	120.39	112.38
1	A	554[A]	ASN	O-C-N	6.56	124.55	121.53
1	A	554[B]	ASN	O-C-N	6.56	124.55	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3	LYS	N-CA-C	6.53	119.44	110.24
1	C	645	GLN	N-CA-C	6.52	118.05	111.07
1	G	786	GLY	N-CA-C	-6.51	106.73	114.48
1	C	738	PHE	CA-CB-CG	-6.51	107.29	113.80
1	A	44	VAL	N-CA-C	6.49	117.25	108.17
1	E	454	ASN	N-CA-C	6.48	118.34	111.28
1	A	88	PRO	CB-CA-C	-6.47	102.81	109.92
1	E	209	SER	N-CA-C	6.46	120.04	109.76
1	C	27	ASP	N-CA-C	-6.45	103.76	111.69
1	C	755	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	694	THR	N-CA-CB	6.43	120.35	109.87
2	F	16	HIS	CA-C-N	-6.42	117.22	122.16
2	F	16	HIS	C-N-CA	-6.42	117.22	122.16
1	G	993	LYS	N-CA-C	-6.41	102.25	110.19
1	A	605	THR	N-CA-C	6.39	120.33	110.42
1	A	660	PRO	N-CA-CB	6.37	106.98	102.65
2	F	190	LEU	CA-C-N	6.36	125.86	119.24
2	F	190	LEU	C-N-CA	6.36	125.86	119.24
1	C	634	LYS	CB-CA-C	-6.34	105.48	111.00
1	C	955	GLU	CA-C-N	6.34	128.78	120.28
1	C	955	GLU	C-N-CA	6.34	128.78	120.28
1	C	999	PRO	N-CA-CB	6.34	109.57	102.60
1	G	316	GLY	N-CA-C	-6.33	106.40	115.64
1	E	523	HIS	O-C-N	-6.31	116.62	121.55
2	H	279	SER	CA-C-N	-6.31	116.01	123.08
2	H	279	SER	C-N-CA	-6.31	116.01	123.08
2	H	157	ASP	CA-CB-CG	6.30	118.91	112.60
1	E	557	THR	CA-C-O	6.30	125.98	119.05
2	D	348	PHE	CA-CB-CG	-6.29	107.50	113.80
2	D	297	VAL	CA-C-N	-6.28	114.06	122.72
2	D	297	VAL	C-N-CA	-6.28	114.06	122.72
2	B	45	ASP	CA-C-O	6.27	123.96	119.32
2	B	174	SER	N-CA-C	6.27	119.76	110.48
2	D	138	PRO	CB-CA-C	6.26	117.10	111.40
1	C	803	GLN	N-CA-C	-6.26	104.46	111.28
1	A	1039	HIS	CA-CB-CG	-6.24	107.56	113.80
1	C	904	ASP	CA-CB-CG	6.21	118.81	112.60
2	H	193	HIS	CA-C-N	-6.21	113.37	122.68
2	H	193	HIS	C-N-CA	-6.21	113.37	122.68
1	A	905	PRO	N-CA-CB	6.21	106.89	102.79
2	H	346	PRO	N-CA-CB	6.20	106.93	102.28
1	E	155	ALA	N-CA-C	6.18	117.68	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	157	ASP	CA-CB-CG	6.17	118.77	112.60
2	B	190	LEU	CA-C-N	6.17	125.39	118.97
2	B	190	LEU	C-N-CA	6.17	125.39	118.97
2	D	369	HIS	CA-CB-CG	-6.16	107.64	113.80
1	A	319	ILE	N-CA-C	6.15	116.82	110.36
2	F	372	GLU	N-CA-CB	-6.15	100.78	109.94
1	E	239	ALA	N-CA-C	6.13	117.80	110.19
2	H	129	ASN	N-CA-C	-6.13	100.30	110.17
1	A	715	ARG	N-CA-CB	6.13	119.46	109.90
1	G	1007	ASN	CA-CB-CG	-6.12	106.48	112.60
1	G	880	THR	CA-C-N	-6.12	114.36	122.99
1	G	880	THR	C-N-CA	-6.12	114.36	122.99
1	A	999	PRO	N-CA-CB	6.12	109.33	102.60
2	D	379	LYS	CA-C-N	6.09	132.66	121.70
2	D	379	LYS	C-N-CA	6.09	132.66	121.70
1	A	900	PHE	CA-C-N	6.08	125.77	119.56
1	A	900	PHE	C-N-CA	6.08	125.77	119.56
1	G	554	ASN	CA-CB-CG	-6.07	106.53	112.60
1	G	996	GLU	CA-C-N	-6.03	112.99	121.56
1	G	996	GLU	C-N-CA	-6.03	112.99	121.56
1	E	27	ASP	N-CA-C	-6.03	104.79	111.36
1	A	864	VAL	N-CA-C	6.03	116.20	110.42
1	A	543	MET	N-CA-C	6.02	119.37	109.85
2	F	138	PRO	N-CA-CB	6.02	108.66	103.36
1	G	682	VAL	N-CA-C	-6.02	104.64	110.72
1	C	1039	HIS	CA-CB-CG	-5.99	107.81	113.80
1	E	830	PHE	CB-CA-C	-5.97	98.08	109.66
1	G	942	HIS	CA-CB-CG	-5.96	107.84	113.80
1	C	283	ASN	CA-CB-CG	5.94	118.54	112.60
1	G	404	VAL	CB-CA-C	-5.94	104.30	111.85
2	H	252	ILE	CB-CA-C	-5.94	104.26	112.04
1	A	578	PHE	CA-CB-CG	-5.93	107.87	113.80
1	A	3	LYS	N-CA-C	5.92	118.41	110.35
1	G	316	GLY	CA-C-O	5.92	125.35	118.96
1	A	532	CYS	N-CA-C	5.90	119.71	111.56
1	C	559	ARG	N-CA-C	5.89	119.18	110.46
1	A	970	GLU	N-CA-C	-5.87	101.77	110.46
1	C	532	CYS	N-CA-C	5.87	120.28	112.30
1	C	674	ASP	CA-C-N	5.86	128.46	120.54
1	C	674	ASP	C-N-CA	5.86	128.46	120.54
1	A	560	GLU	N-CA-CB	5.86	119.03	109.95
1	G	550	GLU	N-CA-C	5.86	118.28	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PHE	CA-CB-CG	-5.85	107.95	113.80
1	A	592	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	582	CYS	N-CA-CB	5.85	118.72	110.12
2	B	196	ALA	N-CA-C	5.85	117.94	108.41
1	C	992	ASN	N-CA-C	5.85	119.44	110.20
2	B	138	PRO	N-CA-CB	5.84	108.36	103.17
2	D	10	GLU	CB-CA-C	-5.83	100.76	110.68
1	E	625	ASP	CA-CB-CG	-5.83	106.77	112.60
1	G	1036	TYR	CA-CB-CG	-5.83	103.40	113.90
2	B	362	ASP	N-CA-C	5.83	118.39	111.33
1	A	786	GLY	N-CA-C	-5.82	107.55	114.48
2	F	201	ALA	N-CA-C	5.82	118.89	110.28
2	D	209	LEU	N-CA-C	-5.80	105.04	111.36
1	C	557	THR	CA-C-N	5.79	132.59	121.54
1	C	557	THR	C-N-CA	5.79	132.59	121.54
1	C	194	ARG	CA-C-N	5.78	126.36	119.94
1	C	194	ARG	C-N-CA	5.78	126.36	119.94
1	A	338	ASP	N-CA-C	5.78	118.07	111.02
1	C	924	PHE	N-CA-C	-5.78	104.98	111.28
1	C	367	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	860	PRO	N-CA-CB	5.77	106.45	102.35
1	C	248	ILE	N-CA-C	-5.76	101.28	108.89
1	G	860	PRO	N-CA-CB	5.76	106.57	102.65
1	C	338	ASP	CA-CB-CG	5.76	118.36	112.60
2	F	217	THR	N-CA-CB	5.76	119.75	110.65
2	F	263	ILE	CB-CA-C	-5.75	105.36	111.00
1	A	164	PHE	CA-CB-CG	-5.75	108.05	113.80
1	G	23	ALA	N-CA-C	5.75	117.39	109.29
2	H	150	PHE	CA-C-O	5.74	124.53	119.71
1	E	23	ALA	N-CA-C	5.73	123.00	110.80
2	D	263	ILE	CB-CA-C	-5.72	105.39	111.00
1	C	24	CYS	N-CA-C	5.72	118.29	111.71
1	C	278	GLU	N-CA-CB	-5.72	103.43	110.98
1	A	733	ASP	CA-CB-CG	5.71	118.31	112.60
1	G	885	PRO	CA-C-N	5.71	127.95	121.04
1	G	885	PRO	C-N-CA	5.71	127.95	121.04
1	C	516	LEU	N-CA-CB	-5.71	101.72	110.12
1	E	757	ASP	CA-CB-CG	5.71	118.31	112.60
2	H	344	ASP	CA-CB-CG	5.71	118.31	112.60
1	E	818	PHE	CA-CB-CG	-5.71	108.09	113.80
2	H	244	ASP	CA-CB-CG	5.70	118.30	112.60
1	G	261	TYR	CB-CG-CD2	-5.70	112.25	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ILE	N-CA-C	-5.70	101.37	108.89
2	B	34	THR	N-CA-C	5.70	120.09	113.20
1	E	758	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	339	ILE	N-CA-C	5.69	120.00	112.04
1	G	135	ALA	CA-C-N	5.69	127.83	120.44
1	G	135	ALA	C-N-CA	5.69	127.83	120.44
1	C	557	THR	N-CA-C	-5.68	107.00	114.04
1	C	558	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	770	GLY	N-CA-C	-5.67	108.33	115.08
1	C	453	PHE	CA-CB-CG	-5.67	108.13	113.80
2	F	98	LEU	N-CA-C	5.66	117.91	111.11
1	E	651	ALA	N-CA-C	5.66	117.90	111.11
1	G	872	LYS	N-CA-C	5.66	118.54	107.57
1	G	536	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	69	ILE	N-CA-C	5.65	112.25	106.21
1	C	227	ASN	N-CA-C	-5.65	102.53	110.50
1	A	787	VAL	N-CA-C	-5.65	99.61	107.80
1	C	154	GLU	N-CA-C	-5.65	104.33	111.11
1	E	456	THR	N-CA-C	5.64	120.29	112.90
1	A	417	ASP	CA-C-O	5.64	123.80	119.46
1	C	543	MET	N-CA-C	5.64	118.43	109.81
1	E	255	THR	N-CA-C	5.63	119.46	112.59
1	C	44	VAL	CB-CA-C	5.63	118.49	110.84
1	G	342	GLY	N-CA-C	-5.61	107.22	115.30
2	D	272	HIS	CA-CB-CG	5.61	119.41	113.80
1	G	732	ALA	CA-C-N	5.61	128.06	120.38
1	G	732	ALA	C-N-CA	5.61	128.06	120.38
1	E	248	ILE	N-CA-C	-5.60	101.59	109.21
1	E	557	THR	N-CA-C	-5.60	106.44	113.72
2	B	245	PRO	CB-CA-C	-5.60	103.94	112.11
2	D	105	HIS	CA-CB-CG	-5.59	108.21	113.80
1	E	754	HIS	CA-CB-CG	-5.59	108.21	113.80
1	G	1005	ILE	N-CA-C	-5.58	105.06	110.42
2	H	23	THR	N-CA-CB	5.58	118.17	109.97
1	E	227	ASN	N-CA-C	-5.57	102.65	110.50
1	G	188	PHE	N-CA-CB	-5.56	101.95	110.01
2	H	204	ASN	N-CA-CB	5.56	118.40	110.06
1	G	432	GLY	O-C-N	-5.54	118.77	123.59
2	D	379	LYS	O-C-N	5.53	128.00	122.08
1	E	998	ARG	O-C-N	5.53	125.80	121.88
2	D	306	MET	N-CA-CB	5.52	120.44	110.83
1	E	900	PHE	O-C-N	5.52	125.70	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	THR	CA-C-N	5.52	125.98	120.52
1	C	344	THR	C-N-CA	5.52	125.98	120.52
1	G	108	LEU	CA-C-O	5.52	126.40	120.55
1	A	825	LEU	N-CA-C	5.51	118.00	110.55
1	G	651	ALA	N-CA-C	5.50	120.39	111.37
1	E	476	VAL	CB-CA-C	-5.50	104.72	112.14
1	E	860	PRO	N-CA-CB	5.49	106.74	102.73
2	F	312	HIS	CA-CB-CG	5.49	119.29	113.80
1	G	900	PHE	CA-C-N	5.49	125.32	119.28
1	G	900	PHE	C-N-CA	5.49	125.32	119.28
1	A	1025	ASP	CA-CB-CG	5.48	118.08	112.60
2	B	200	GLY	CA-C-N	5.48	128.54	120.82
2	B	200	GLY	C-N-CA	5.48	128.54	120.82
1	E	726	GLU	N-CA-CB	5.46	120.11	111.43
1	A	557	THR	N-CA-C	-5.46	106.53	114.12
1	C	1035	GLN	N-CA-C	5.46	117.99	111.71
1	E	558	ASP	N-CA-CB	-5.46	101.94	109.91
2	F	308	THR	N-CA-C	5.46	117.70	109.41
1	A	560	GLU	N-CA-C	-5.45	101.09	109.76
1	C	133	ASP	CA-CB-CG	5.45	118.05	112.60
2	D	46	PRO	N-CA-CB	5.45	108.93	103.48
2	B	76	HIS	CA-CB-CG	-5.44	108.36	113.80
1	C	708	ILE	N-CA-C	5.43	116.16	110.62
2	D	86	PRO	N-CA-CB	5.43	108.08	103.35
1	E	142	GLU	N-CA-C	5.42	119.07	109.96
2	F	346	PRO	CB-CA-C	-5.42	105.79	112.89
1	E	605	THR	N-CA-C	5.42	118.48	110.46
2	B	215	ARG	N-CA-C	-5.42	100.88	109.76
2	F	74	GLN	N-CA-C	5.42	116.50	108.86
2	F	195	VAL	N-CA-CB	5.42	117.55	111.21
2	H	257	LYS	N-CA-C	-5.40	105.31	111.14
1	A	523	HIS	CA-CB-CG	-5.40	108.40	113.80
1	E	162	VAL	N-CA-CB	5.40	119.57	110.56
2	H	308	THR	N-CA-C	5.39	118.37	109.85
1	E	486	ALA	N-CA-C	5.38	117.57	111.11
1	E	571	ARG	CD-NE-CZ	-5.38	116.87	124.40
2	F	10	GLU	CB-CA-C	-5.38	99.72	110.42
1	E	970	GLU	N-CA-C	-5.38	101.52	110.17
1	A	549	GLU	N-CA-C	5.37	119.36	111.04
1	A	949	VAL	N-CA-C	5.37	117.36	108.99
2	B	89	ALA	N-CA-C	-5.36	100.96	109.76
1	G	557	THR	CA-C-O	5.36	124.95	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	ARG	CD-NE-CZ	-5.36	116.90	124.40
2	F	216	LEU	N-CA-C	5.35	118.20	109.59
2	D	234	ASP	N-CA-C	-5.34	106.27	112.89
1	G	885	PRO	N-CA-CB	5.33	108.25	103.08
1	G	65	TYR	N-CA-C	5.33	117.42	107.99
1	A	435	ARG	N-CA-CB	5.33	117.88	109.94
1	A	782	ILE	N-CA-C	-5.32	105.66	110.82
1	G	286	PHE	CB-CA-C	-5.32	98.36	110.07
1	G	286	PHE	N-CA-C	5.32	117.28	109.24
1	G	902	GLY	N-CA-C	-5.32	108.71	115.31
1	A	557	THR	CA-C-N	5.32	131.70	121.54
1	A	557	THR	C-N-CA	5.32	131.70	121.54
1	E	210	LEU	N-CA-C	-5.31	105.50	112.41
1	E	679	GLN	CA-C-O	5.31	126.36	120.63
1	A	348	PHE	CA-CB-CG	-5.31	108.49	113.80
1	E	869	MET	N-CA-CB	5.31	117.92	110.12
1	A	885	PRO	N-CA-CB	5.29	108.22	103.08
1	G	152	MET	N-CA-C	-5.29	105.51	111.28
1	A	713	VAL	CB-CA-C	-5.29	105.89	112.45
1	G	612	THR	N-CA-C	5.29	117.96	111.82
1	G	558	ASP	CB-CA-C	-5.28	102.83	110.96
2	H	239	SER	N-CA-C	5.28	116.90	110.41
1	E	801	LEU	N-CA-C	5.27	117.87	110.23
1	C	987	ASN	CB-CA-C	-5.27	105.70	110.44
1	G	604	GLU	N-CA-C	5.27	119.42	112.89
1	A	953	ASP	CA-CB-CG	5.26	117.86	112.60
2	H	190	LEU	CA-C-O	5.26	123.51	119.46
2	B	92	PHE	CA-CB-CG	-5.26	108.54	113.80
1	G	186	GLU	CA-C-N	5.25	127.32	120.28
1	G	186	GLU	C-N-CA	5.25	127.32	120.28
1	A	975	HIS	CA-CB-CG	-5.25	108.55	113.80
1	C	642	TYR	N-CA-C	5.25	119.84	113.38
2	H	377	TYR	N-CA-C	-5.24	105.25	111.69
1	E	450	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	641	GLN	N-CA-C	5.22	119.50	113.18
1	A	900	PHE	CB-CA-C	-5.22	103.60	111.27
1	E	62	ASP	CA-CB-CG	-5.22	107.38	112.60
1	G	39	GLU	CB-CA-C	-5.22	101.81	110.68
1	C	62	ASP	CA-CB-CG	-5.21	107.39	112.60
1	E	334	GLU	CB-CG-CD	-5.21	103.75	112.60
1	A	283	ASN	CA-CB-CG	5.19	117.79	112.60
1	C	456	THR	N-CA-C	5.19	119.89	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	11	ASP	CA-CB-CG	5.18	117.78	112.60
2	B	141	ALA	N-CA-C	-5.18	105.81	111.82
1	E	536	PHE	CA-CB-CG	-5.18	108.62	113.80
1	C	239	ALA	N-CA-C	5.18	116.61	110.19
2	H	89	ALA	N-CA-C	-5.18	101.27	109.76
1	E	885	PRO	N-CA-CB	5.17	108.10	103.08
1	A	993	LYS	N-CA-C	-5.17	102.83	110.48
1	E	1028	VAL	N-CA-C	5.17	115.89	110.62
1	A	712	LEU	N-CA-C	5.17	117.83	109.40
2	F	299	ASP	N-CA-C	-5.16	98.91	107.99
2	F	353	HIS	CA-CB-CG	-5.15	108.65	113.80
1	C	172	PHE	N-CA-C	5.14	118.86	112.58
1	E	708	ILE	N-CA-C	5.14	115.92	110.72
1	C	980	VAL	N-CA-C	5.14	115.86	110.62
1	E	278	GLU	CA-C-N	-5.14	114.87	123.04
1	E	278	GLU	C-N-CA	-5.14	114.87	123.04
1	C	407	THR	N-CA-C	-5.13	105.91	113.61
1	A	1068	MET	CB-CA-C	-5.13	102.82	110.88
2	F	379	LYS	N-CA-C	-5.13	105.87	111.82
1	G	543	MET	N-CA-C	5.13	117.66	109.81
2	B	133	ILE	N-CA-CB	5.12	118.30	111.64
1	E	1012	TYR	N-CA-C	5.12	117.51	108.75
1	A	239	ALA	N-CA-C	5.12	116.54	110.19
1	A	255	THR	N-CA-C	5.11	118.82	112.59
1	C	735	ARG	O-C-N	5.11	127.55	122.08
1	G	625	ASP	CA-CB-CG	-5.11	107.49	112.60
1	G	666	PRO	N-CA-C	-5.11	106.88	113.57
1	C	987	ASN	N-CA-CB	5.10	117.77	110.11
1	E	712	LEU	N-CA-C	5.10	117.42	109.52
2	F	362	ASP	N-CA-C	5.10	118.28	111.75
1	A	381	VAL	CB-CA-C	-5.10	104.88	111.20
1	G	345	PRO	CB-CA-C	-5.10	103.21	110.75
2	B	364	ALA	CA-C-O	5.09	123.02	118.33
1	A	558	ASP	CA-C-N	5.09	128.94	120.94
1	A	558	ASP	C-N-CA	5.09	128.94	120.94
1	G	136	MET	CA-C-O	5.09	126.17	120.82
1	A	56	THR	CA-C-N	-5.09	113.85	120.67
1	A	56	THR	C-N-CA	-5.09	113.85	120.67
1	G	26	PHE	CA-CB-CG	-5.09	108.71	113.80
2	D	200	GLY	CA-C-N	5.08	127.98	120.82
2	D	200	GLY	C-N-CA	5.08	127.98	120.82
1	A	367	PHE	CA-CB-CG	-5.07	108.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	89	ALA	N-CA-C	-5.07	101.44	109.96
1	C	680	HIS	CA-CB-CG	-5.07	108.73	113.80
1	E	88	PRO	CB-CA-C	-5.07	103.19	111.56
2	F	112	ASP	N-CA-C	5.07	118.77	112.58
1	A	484	LEU	N-CA-C	5.07	118.55	110.70
2	B	62	ASN	CA-C-N	-5.07	114.81	122.76
2	B	62	ASN	C-N-CA	-5.07	114.81	122.76
2	B	308	THR	N-CA-C	5.07	117.11	109.41
2	D	216	LEU	N-CA-C	5.06	117.82	109.72
2	F	168	TYR	N-CA-C	5.06	116.22	108.42
1	C	880	THR	N-CA-CB	-5.06	104.27	111.00
2	H	220	PRO	N-CA-CB	5.06	107.57	103.32
1	C	557	THR	CA-C-O	5.06	125.38	119.06
1	E	908	GLY	CA-C-N	5.06	124.72	119.56
1	E	908	GLY	C-N-CA	5.06	124.72	119.56
1	G	660	PRO	CB-CA-C	-5.06	106.27	112.89
2	H	200	GLY	N-CA-C	-5.06	101.20	113.18
1	E	904	ASP	CA-CB-CG	5.05	117.65	112.60
1	G	775	ILE	CB-CA-C	5.05	116.68	111.23
1	E	971	LEU	N-CA-C	5.04	117.71	109.59
1	G	859	VAL	O-C-N	5.04	125.81	121.12
1	A	1005	ILE	CB-CA-C	-5.04	105.52	111.97
1	E	521	ASP	CA-CB-CG	5.04	117.64	112.60
1	G	886	PRO	CA-C-O	5.04	124.07	118.38
1	G	682	VAL	O-C-N	5.03	127.02	121.83
1	E	579	ASP	CA-CB-CG	-5.03	107.57	112.60
1	G	727	ILE	N-CA-CB	-5.03	104.41	111.25
1	G	683	GLU	N-CA-C	-5.03	104.88	111.02
1	A	57	ASP	CA-C-N	5.03	126.12	119.84
1	A	57	ASP	C-N-CA	5.03	126.12	119.84
2	F	346	PRO	N-CA-C	-5.03	105.69	112.48
1	C	316	GLY	CA-C-O	5.02	124.84	119.06
1	A	518	ASP	CA-CB-CG	-5.02	107.58	112.60
1	C	1036	TYR	CA-CB-CG	-5.02	104.87	113.90
1	E	999	PRO	N-CA-CB	5.02	108.12	102.60
1	G	949	VAL	CA-CB-CG1	-5.02	101.87	110.40
1	G	1028[A]	VAL	CA-C-N	-5.02	114.60	120.72
1	G	1028[A]	VAL	C-N-CA	-5.02	114.60	120.72
1	G	1028[B]	VAL	CA-C-N	-5.02	114.60	120.72
1	G	1028[B]	VAL	C-N-CA	-5.02	114.60	120.72
1	G	43	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	G	809	MET	CA-CB-CG	-5.01	104.08	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	547	TYR	CA-CB-CG	-5.01	104.88	113.90
1	A	559	ARG	N-CA-C	5.01	117.56	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8189	0	8227	258	0
1	C	8165	0	8199	250	0
1	E	8188	0	8225	216	0
1	G	8178	0	8221	351	0
2	B	2895	0	2861	109	0
2	D	2895	0	2861	101	0
2	F	2895	0	2861	117	0
2	H	2900	0	2863	146	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	1	0
5	F	1	0	0	0	0
5	G	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	10	0	0	1	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	34	0	44	2	0
8	A	54	0	24	2	0
8	C	54	0	24	0	0
8	E	54	0	24	3	0
8	G	54	0	24	1	0
9	A	9	0	20	0	0
9	C	9	0	20	0	0
9	E	9	0	20	0	0
9	G	9	0	20	0	0
10	A	830	0	0	24	0
10	B	230	0	0	5	0
10	C	683	0	0	23	0
10	D	238	0	0	4	0
10	E	884	0	0	21	0
10	F	272	0	0	2	0
10	G	666	0	0	20	0
10	H	184	0	0	4	0
All	All	48668	0	44538	1528	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 17.

All (1528) 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:E:993:LYS:CE	1:E:993:LYS:NZ	1.67	1.55
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.21	1.19
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.28	1.12
1:C:998:ARG:HG3	1:C:999:PRO:HA	1.30	1.11
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.34	1.09
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.31	1.07
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.22	1.06
1:G:559:ARG:HG3	1:G:559:ARG:HH11	1.23	1.04
1:E:1002:GLN:HE22	1:E:1006:LYS:HE3	1.19	1.03
1:G:784:GLN:H	1:G:784:GLN:NE2	1.56	1.01
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.46	0.98
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.42	0.98
2:H:286:MET:HE2	2:H:289:GLY:HA2	1.46	0.95
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.45	0.94
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.48	0.94
2:D:324:ASN:H	2:D:324:ASN:HD22	1.12	0.93
1:A:784:GLN:HE21	1:A:784:GLN:H	1.15	0.92
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.85	0.92
1:E:59:GLU:HG2	1:E:60:MET:HE2	1.50	0.92
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.51	0.92
1:G:784:GLN:HE21	1:G:784:GLN:N	1.67	0.92
1:C:698:ILE:HD12	1:C:698:ILE:H	1.33	0.91
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.49	0.91
1:G:1051:ALA:HA	1:G:1054:LEU:HD12	1.53	0.91
1:A:559:ARG:HG3	1:A:559:ARG:HH11	1.36	0.90
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.85	0.90
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.51	0.90
1:E:784:GLN:H	1:E:784:GLN:NE2	1.70	0.90
1:C:1:MET:HG3	1:C:2:PRO:HD2	1.53	0.90
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.54	0.90
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.53	0.89
2:F:228:VAL:HA	2:F:231:MET:CE	2.02	0.89
1:E:696:THR:N	1:E:700:MET:HE3	1.88	0.89
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.03	0.89
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.36	0.88
1:G:1001:ILE:HD12	1:G:1002:GLN:N	1.89	0.88
1:E:696:THR:H	1:E:700:MET:HE3	1.37	0.87
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.04	0.87
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.04	0.87
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.91	0.86
1:A:1027[B]:ARG:HH22	1:A:1031:ARG:HH11	1.24	0.85
1:C:559:ARG:NH1	10:C:4442:HOH:O	2.09	0.85
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.57	0.85
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.12	0.85
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.59	0.85
2:B:324:ASN:HD22	2:B:324:ASN:N	1.73	0.85
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.11	0.85
1:E:726:GLU:HG2	1:E:727:ILE:H	1.40	0.84
2:H:324:ASN:HD22	2:H:324:ASN:H	1.25	0.84
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.58	0.84
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:PHE:CZ	2:D:268:ILE:HD12	2.13	0.84
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.38	0.83
1:E:646:THR:HB	1:E:647:PRO:HD3	1.60	0.83
1:E:59:GLU:CG	1:E:60:MET:HE2	2.08	0.83
1:A:1027[B]:ARG:NH2	1:A:1031:ARG:HH11	1.76	0.83
2:D:259:LEU:HD13	2:D:342:ARG:NH1	1.93	0.83
1:C:998:ARG:CG	1:C:999:PRO:HA	2.08	0.82
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.14	0.82
2:F:324:ASN:H	2:F:324:ASN:HD22	1.25	0.82
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.62	0.82
1:E:1001:ILE:HD12	1:E:1002:GLN:N	1.95	0.82
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.62	0.81
1:G:726:GLU:HG3	1:G:727:ILE:N	1.95	0.81
1:E:702:VAL:HG11	1:E:735:ARG:NH2	1.94	0.81
1:A:726:GLU:HG3	1:A:727:ILE:N	1.95	0.81
1:A:1027[B]:ARG:HH22	1:A:1031:ARG:NH1	1.78	0.81
1:C:726:GLU:HG3	1:C:727:ILE:N	1.96	0.81
1:G:865:ALA:O	1:G:869:MET:HG3	1.81	0.81
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.63	0.81
1:A:873:SER:O	1:A:877:GLN:HG3	1.81	0.80
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.64	0.79
1:G:1:MET:H3	1:G:1:MET:HE2	1.47	0.79
2:B:185:LYS:HD3	2:B:190:LEU:HD21	1.64	0.79
1:C:715:ARG:HG2	1:C:725:MET:HE2	1.63	0.79
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.98	0.79
1:G:682:VAL:HG11	1:G:689:GLN:NE2	1.98	0.78
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.12	0.78
1:G:860:PRO:HB2	1:G:863:LYS:HG3	1.63	0.78
1:C:883:VAL:O	1:C:884:ILE:HD13	1.83	0.78
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.31	0.78
1:G:682:VAL:HG11	1:G:689:GLN:HE21	1.49	0.78
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.64	0.78
1:E:772[B]:MET:HE3	10:E:4886:HOH:O	1.83	0.78
1:A:999:PRO:HD2	1:G:983:GLU:OE2	1.84	0.77
2:B:324:ASN:HD22	2:B:324:ASN:H	1.30	0.77
2:F:254:ALA:O	2:F:257:LYS:HB2	1.83	0.77
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.67	0.77
1:E:784:GLN:H	1:E:784:GLN:HE21	1.32	0.77
1:G:994:VAL:HG22	1:G:1000:HIS:CG	2.20	0.77
1:E:558:ASP:HB3	1:E:559[B]:ARG:HG3	1.67	0.77
1:A:784:GLN:H	1:A:784:GLN:NE2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:LEU:HD12	1:A:751:LEU:H	1.50	0.76
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.21	0.76
2:F:324:ASN:O	2:F:342:ARG:HD2	1.84	0.76
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.65	0.76
1:G:1021:ARG:HG2	1:G:1021:ARG:HH11	1.48	0.76
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.51	0.76
2:B:298:LYS:HE2	2:B:303:ASN:OD1	1.86	0.76
2:H:324:ASN:HD22	2:H:324:ASN:N	1.82	0.76
1:G:784:GLN:H	1:G:784:GLN:HE21	0.82	0.75
1:G:1063:ILE:HD13	1:G:1068:MET:HG2	1.68	0.75
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.69	0.75
1:E:698:ILE:O	1:E:702:VAL:HG23	1.85	0.75
10:E:4794:HOH:O	2:F:304:VAL:HB	1.85	0.75
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.16	0.75
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.21	0.74
1:C:675:ARG:H	1:C:675:ARG:CD	1.99	0.74
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.16	0.74
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.68	0.74
1:C:1020:ARG:NH2	1:C:1023:ILE:HG21	2.02	0.74
1:E:1027:ARG:HE	1:E:1031:ARG:HE	1.32	0.74
1:G:509:ARG:HH11	1:G:509:ARG:HB2	1.52	0.74
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.03	0.74
1:A:28:TYR:O	1:A:32:GLN:HG3	1.86	0.74
2:H:46:PRO:O	2:H:242:PRO:HG3	1.88	0.74
2:H:299:ASP:OD1	2:H:302:LYS:HD3	1.88	0.74
1:C:400:ARG:HD3	10:C:4363:HOH:O	1.86	0.73
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.18	0.73
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.87	0.73
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.71	0.73
2:H:71:GLU:C	2:H:203:ARG:HG3	2.13	0.73
2:B:324:ASN:ND2	2:B:324:ASN:H	1.86	0.73
1:A:1027[B]:ARG:NH1	10:A:4891:HOH:O	2.21	0.72
1:G:704:LYS:O	1:G:708:ILE:HD12	1.87	0.72
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.71	0.72
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.69	0.72
2:F:228:VAL:HA	2:F:231:MET:HE3	1.70	0.72
1:C:1064:SER:OG	1:C:1067:GLU:HG3	1.88	0.72
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.89	0.72
2:B:156:MET:HA	10:B:4197:HOH:O	1.90	0.72
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.54	0.72
1:G:1:MET:H3	1:G:224:LYS:HE3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:ILE:O	1:A:701:ALA:HB3	1.89	0.72
1:G:1:MET:HB3	10:G:4163:HOH:O	1.89	0.72
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.17	0.72
1:A:1020:ARG:NH2	1:A:1023:ILE:HG21	2.05	0.72
1:C:865:ALA:O	1:C:869:MET:HG3	1.90	0.72
1:G:702:VAL:HG21	1:G:735:ARG:NH2	2.04	0.72
1:G:873:SER:O	1:G:877:GLN:HG3	1.90	0.71
1:G:872:LYS:HG2	1:G:877:GLN:HG2	1.71	0.71
1:A:79:GLU:HB2	1:A:111:PHE:CZ	2.25	0.71
2:D:226:GLU:O	2:D:230:LYS:HG3	1.90	0.71
1:E:135:ALA:HB1	1:E:274:GLU:HG3	1.72	0.71
2:H:275:LEU:HD23	2:H:349:SER:OG	1.91	0.71
2:F:228:VAL:HA	2:F:231:MET:HE2	1.72	0.71
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.91	0.71
1:E:726:GLU:HG2	1:E:727:ILE:N	2.06	0.71
2:B:375:GLU:HA	10:B:4246:HOH:O	1.90	0.70
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.72	0.70
2:H:153:LEU:HA	2:H:156:MET:HE3	1.72	0.70
2:H:34:THR:HA	2:H:56:THR:OG1	1.90	0.70
2:B:259:LEU:O	2:B:345:LYS:HD2	1.91	0.70
1:G:563:MET:HE3	1:G:635:PRO:CG	2.12	0.70
1:C:954:LYS:O	1:C:957:VAL:HG12	1.91	0.70
1:C:698:ILE:H	1:C:698:ILE:CD1	2.05	0.70
2:D:324:ASN:HD22	2:D:324:ASN:N	1.83	0.70
1:E:698:ILE:HD12	1:E:698:ILE:H	1.56	0.70
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.22	0.70
1:G:340:THR:O	1:G:343:ARG:HB2	1.91	0.70
1:C:146:SER:CB	1:C:205:LEU:HD11	2.22	0.70
1:E:1021:ARG:HG2	1:E:1021:ARG:HH11	1.56	0.70
1:A:1037:LYS:HA	10:A:4585:HOH:O	1.92	0.70
1:G:130:ARG:O	1:G:134:VAL:HG23	1.92	0.70
1:G:946:LEU:C	1:G:947:LEU:HD12	2.17	0.70
2:H:286:MET:CE	2:H:289:GLY:HA2	2.19	0.70
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.54	0.70
1:C:890:VAL:HG23	1:C:927:ALA:HB1	1.74	0.70
1:A:751:LEU:HD12	1:A:751:LEU:N	2.07	0.69
1:C:51:PRO:O	1:C:855:LYS:HD3	1.91	0.69
2:D:78:GLN:NE2	10:D:1966:HOH:O	2.25	0.69
1:E:998:ARG:HA	1:E:999:PRO:C	2.17	0.69
1:A:954:LYS:O	1:A:957:VAL:HG12	1.93	0.69
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:LEU:O	1:C:734:LEU:HD12	1.93	0.69
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.75	0.69
1:C:802:SER:O	1:C:806:GLN:HG3	1.93	0.69
2:F:269:SER:O	2:F:272:HIS:HB3	1.92	0.69
1:G:534:ALA:O	2:H:123:ARG:HD3	1.92	0.69
1:G:559:ARG:HG3	1:G:559:ARG:NH1	1.97	0.69
1:A:1027[B]:ARG:NH2	1:A:1031:ARG:NH1	2.39	0.69
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.23	0.69
2:F:232:ASN:N	2:F:233:PRO:HD3	2.07	0.69
1:G:327:ALA:HB2	10:G:4226:HOH:O	1.92	0.69
1:E:872:LYS:HD3	1:E:877:GLN:HG2	1.75	0.68
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.75	0.68
1:A:1001:ILE:HD13	1:A:1029:ILE:HG13	1.73	0.68
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.23	0.68
1:G:35:LYS:NZ	10:G:4207:HOH:O	2.26	0.68
1:C:363:ASN:HA	1:C:365:GLU:OE2	1.93	0.68
2:D:212:ARG:HG3	2:D:212:ARG:HH11	1.59	0.68
2:F:224:SER:OG	2:F:227:ASP:HB2	1.93	0.68
1:E:679:GLN:O	1:E:683:GLU:HB2	1.92	0.68
1:A:490:ARG:HD3	10:A:4644:HOH:O	1.93	0.68
1:E:1002:GLN:NE2	1:E:1006:LYS:HE3	2.03	0.68
1:G:166:CYS:C	1:G:167:ILE:HD12	2.18	0.68
1:A:726:GLU:HG3	1:A:727:ILE:H	1.59	0.68
1:A:228:CYS:SG	1:A:269:MET:HG2	2.34	0.68
2:B:222:GLN:H	2:B:222:GLN:HE21	1.42	0.68
1:E:1027:ARG:HE	1:E:1031:ARG:NE	1.91	0.68
2:F:186:LYS:NZ	10:F:3117:HOH:O	2.27	0.68
1:G:676:GLU:O	1:G:680:HIS:ND1	2.27	0.67
1:A:822:VAL:O	1:A:823:ARG:HD3	1.94	0.67
1:E:670:ASP:HB2	10:E:4867:HOH:O	1.94	0.67
2:H:286:MET:HE2	2:H:289:GLY:CA	2.21	0.67
1:G:690:PRO:HG3	1:G:756:LEU:HD11	1.76	0.67
1:E:145:ARG:O	1:E:208:GLU:HG2	1.95	0.67
1:A:279:THR:HG22	10:A:4322:HOH:O	1.93	0.67
1:C:677:ARG:O	1:C:680:HIS:HB2	1.95	0.67
2:H:121:LEU:CD1	2:H:125:LYS:HD3	2.25	0.67
1:A:38:ARG:HG2	1:A:38:ARG:NH1	1.94	0.67
1:C:890:VAL:HG23	1:C:927:ALA:CB	2.24	0.67
1:G:588:ALA:O	1:G:591:GLU:HB3	1.95	0.67
1:G:802:SER:O	1:G:806:GLN:HG3	1.95	0.67
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:ARG:HG2	2:B:378:ARG:HH11	1.60	0.67
1:G:58:PRO:HD2	1:G:59[A]:GLU:OE2	1.95	0.67
1:G:516:LEU:HD11	1:G:520:TYR:CZ	2.29	0.67
1:G:698:ILE:HD12	1:G:698:ILE:N	2.10	0.67
1:A:1020:ARG:O	1:A:1024:GLU:HG3	1.94	0.67
2:B:268:ILE:HD13	2:B:354:PRO:HD2	1.77	0.67
1:G:805:ILE:HD12	1:G:832:VAL:HG11	1.77	0.67
1:A:695:VAL:CG1	1:A:701:ALA:HB2	2.13	0.67
1:G:354:TYR:HB2	1:G:388:GLY:O	1.94	0.67
1:G:803:GLN:N	10:G:4710:HOH:O	2.27	0.67
2:D:222:GLN:H	2:D:222:GLN:HE21	1.43	0.66
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.25	0.66
1:G:875:ALA:HB2	10:G:4718:HOH:O	1.93	0.66
1:A:944:ARG:HD3	1:A:972:ASP:OD1	1.96	0.66
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.77	0.66
1:A:863:LYS:HE2	10:A:4593:HOH:O	1.94	0.66
1:E:998:ARG:CB	1:E:999:PRO:HA	2.26	0.66
1:G:475[B]:LYS:HG2	1:G:488:PHE:CZ	2.30	0.66
2:H:202:LYS:NZ	2:H:355:GLU:OE1	2.27	0.66
2:B:226:GLU:O	2:B:230:LYS:HG3	1.96	0.65
1:E:559[B]:ARG:HD2	1:E:595:GLU:HB2	1.77	0.65
1:E:806:GLN:HA	1:E:809:MET:CE	2.26	0.65
1:G:331:THR:N	1:G:334:GLU:OE1	2.28	0.65
1:C:784:GLN:H	1:C:784:GLN:HE21	1.44	0.65
1:E:698:ILE:HD12	1:E:698:ILE:N	2.10	0.65
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.79	0.65
2:D:64:GLY:HA3	2:D:94:ASN:OD1	1.96	0.65
1:E:5:THR:O	1:E:8:LYS:NZ	2.29	0.65
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.42	0.65
2:B:6:LEU:HD11	2:B:8:VAL:HG22	1.76	0.65
1:C:954:LYS:HG2	1:C:980:VAL:HG21	1.77	0.65
1:E:417:ASP:OD2	1:E:418:PRO:HD2	1.96	0.65
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.31	0.65
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.78	0.65
1:A:693:ALA:O	1:A:752:LEU:HB2	1.97	0.65
1:C:802:SER:OG	1:C:805:ILE:HB	1.97	0.65
1:C:807:ASP:O	1:C:811:GLN:HB2	1.96	0.65
1:E:6:ASP:OD2	1:E:6:ASP:N	2.30	0.65
1:C:56:THR:OG1	1:C:855:LYS:NZ	2.26	0.65
1:C:693:ALA:CB	1:C:704:LYS:HG3	2.27	0.65
2:F:324:ASN:ND2	2:F:324:ASN:H	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:LEU:HD23	2:H:15:PHE:CD2	2.32	0.65
1:E:922:ARG:NH2	1:E:926:GLU:OE1	2.27	0.65
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.97	0.65
2:B:194:VAL:HB	2:B:216:LEU:HD23	1.79	0.64
1:E:563:MET:CE	1:E:635:PRO:HG3	2.27	0.64
2:F:300:VAL:HG22	2:F:328:THR:O	1.96	0.64
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.30	0.64
1:G:343:ARG:NH1	10:G:4538:HOH:O	2.29	0.64
1:G:663:GLY:HA3	1:G:869:MET:HE2	1.78	0.64
1:C:1009[A]:GLU:OE2	10:C:4707:HOH:O	2.14	0.64
1:E:998:ARG:HG2	1:E:999:PRO:HA	1.80	0.64
1:A:947:LEU:HA	1:A:1014:ILE:HG23	1.79	0.64
2:D:259:LEU:HD13	2:D:342:ARG:HH12	1.62	0.64
1:G:954:LYS:O	1:G:957:VAL:HG12	1.96	0.64
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.78	0.64
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.79	0.64
2:D:363:ALA:O	2:D:366:LEU:HD12	1.98	0.64
1:A:1037:LYS:HD2	10:A:4879:HOH:O	1.97	0.64
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.33	0.64
2:H:324:ASN:ND2	2:H:324:ASN:H	1.95	0.64
1:C:103:GLU:HG3	1:C:104:ARG:N	2.08	0.64
2:D:26:ALA:O	2:D:131:CYS:HA	1.98	0.64
1:E:278:GLU:HG2	10:E:4232:HOH:O	1.97	0.64
2:B:144:LEU:O	2:B:148:ARG:HG3	1.97	0.64
1:A:145:ARG:NH2	1:A:161:ASP:OD2	2.29	0.64
1:C:697:ALA:O	1:C:700:MET:HB3	1.98	0.64
1:E:954:LYS:O	1:E:980:VAL:HG11	1.98	0.64
1:C:676:GLU:O	1:C:680:HIS:ND1	2.31	0.64
1:G:426:ARG:HD3	1:G:426:ARG:C	2.23	0.64
1:E:153:GLU:HB3	10:E:4782:HOH:O	1.98	0.64
1:A:636:LYS:NZ	10:A:4502:HOH:O	2.30	0.63
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.80	0.63
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.80	0.63
1:C:735:ARG:O	1:C:738:PHE:N	2.32	0.63
1:E:998:ARG:CG	1:E:999:PRO:HA	2.27	0.63
2:H:71:GLU:O	2:H:203:ARG:HG3	1.98	0.63
1:A:1001:ILE:CD1	1:A:1029:ILE:HG13	2.27	0.63
1:C:197:ASP:OD2	1:C:1037:LYS:NZ	2.30	0.63
2:D:324:ASN:H	2:D:324:ASN:ND2	1.93	0.63
2:D:324:ASN:C	2:D:343:THR:HG23	2.24	0.63
2:F:190:LEU:HD23	2:F:213:GLY:HA2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:N	10:G:4316:HOH:O	2.31	0.63
2:H:244:ASP:OD2	2:H:245:PRO:HD2	1.98	0.63
1:G:482:THR:HG22	1:G:483:GLY:N	2.14	0.63
1:A:318:PRO:HG3	1:A:610:TYR:OH	1.98	0.63
1:C:772:MET:HE1	1:C:880:THR:O	1.98	0.63
1:E:713:VAL:HB	1:E:753:ASP:HB2	1.79	0.63
2:B:8:VAL:HG21	2:B:143:ALA:HB3	1.81	0.62
2:H:218:ILE:N	2:H:218:ILE:HD13	2.14	0.62
1:C:7:ILE:HG23	1:C:84:ASP:HB2	1.81	0.62
1:C:730:ASP:OD2	1:C:733:ASP:HB2	1.99	0.62
1:C:1027:ARG:O	1:C:1031:ARG:HG3	1.99	0.62
2:D:71:GLU:O	2:D:203:ARG:HG3	1.99	0.62
1:G:269:MET:O	1:G:273:ARG:HG3	1.99	0.62
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.29	0.62
1:E:1027:ARG:NE	1:E:1031:ARG:HE	1.98	0.62
2:F:5:ALA:HB3	2:F:110:ILE:HG13	1.81	0.62
1:A:663:GLY:CA	1:A:869:MET:HG2	2.29	0.62
1:E:515:LYS:O	1:E:515:LYS:HD3	2.00	0.62
1:G:561:LYS:HE2	10:G:4461:HOH:O	1.99	0.62
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.81	0.62
1:C:1063:ILE:HD13	1:C:1068:MET:HG2	1.82	0.62
2:D:266:PHE:HA	2:D:348:PHE:O	1.98	0.62
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.81	0.62
1:E:481:ILE:HD12	1:E:508:VAL:HG21	1.81	0.62
1:E:734:LEU:HD12	1:E:734:LEU:O	2.00	0.62
1:E:904:ASP:O	1:E:906:LEU:N	2.31	0.62
1:E:994:VAL:HG23	1:E:1001:ILE:HD11	1.82	0.62
1:G:641:GLN:OE1	1:G:869:MET:HE1	1.99	0.62
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.82	0.61
2:F:376:GLN:HA	2:F:379:LYS:HZ2	1.64	0.61
2:H:264:PRO:HB3	2:H:373:LEU:HB3	1.81	0.61
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.18	0.61
2:F:236:ILE:HD11	2:F:263:ILE:HG21	1.82	0.61
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.99	0.61
2:B:6:LEU:HD12	2:B:7:LEU:N	2.16	0.61
1:G:698:ILE:HD12	1:G:698:ILE:H	1.66	0.61
1:G:772:MET:HE1	1:G:880:THR:HA	1.83	0.61
2:H:228:VAL:O	2:H:231:MET:HG3	1.99	0.61
1:A:1021:ARG:HH11	1:A:1021:ARG:CG	2.14	0.61
2:D:344:ASP:O	2:D:345:LYS:HG2	2.01	0.61
1:G:1:MET:HB2	1:G:224:LYS:NZ	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ALA:O	1:A:271:VAL:HG23	2.00	0.61
1:C:639:ILE:HD13	1:C:869:MET:HE3	1.81	0.61
1:C:74:VAL:HG11	1:C:102:LEU:HD11	1.83	0.61
2:F:186:LYS:O	2:F:189:GLU:HB2	2.01	0.61
2:F:286:MET:HE1	2:F:312:HIS:ND1	2.16	0.61
2:H:187:GLU:HG2	2:H:215:ARG:CD	2.20	0.61
1:C:146:SER:HB2	1:C:205:LEU:CD1	2.31	0.61
2:H:248:CYS:O	2:H:252:ILE:HG13	2.01	0.61
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.36	0.60
2:H:334:ASP:OD2	2:H:336:THR:HG23	2.00	0.60
1:A:27:ASP:OD2	1:A:53:THR:HB	2.01	0.60
1:A:675:ARG:CD	1:A:675:ARG:H	2.14	0.60
1:G:675:ARG:CD	1:G:675:ARG:H	2.13	0.60
2:H:50:ARG:HG2	2:H:158:LEU:CD1	2.31	0.60
1:A:514:ARG:NE	10:A:4660:HOH:O	2.26	0.60
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.47	0.60
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.84	0.60
1:A:559:ARG:HG3	1:A:559:ARG:NH1	2.05	0.60
2:B:378:ARG:HG2	2:B:378:ARG:NH1	2.16	0.60
1:C:32:GLN:OE1	1:C:320:ALA:HB3	2.01	0.60
1:G:641:GLN:CD	1:G:869:MET:HE1	2.27	0.60
1:E:185:ARG:O	1:E:189:GLU:HG3	2.01	0.60
2:F:201:ALA:HB2	2:F:239:SER:CB	2.32	0.60
1:G:563:MET:HE1	1:G:630:VAL:HA	1.83	0.60
1:G:679:GLN:O	1:G:683:GLU:HB2	2.02	0.60
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.37	0.60
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.83	0.60
2:H:279:SER:O	2:H:322:PRO:HG3	2.02	0.60
1:A:712:LEU:HD23	1:A:752:LEU:HG	1.84	0.60
1:C:936:ASN:HB2	10:C:4085:HOH:O	2.02	0.60
1:E:954:LYS:HE2	1:E:976:GLY:C	2.26	0.60
1:G:22:GLN:HG3	1:G:174:MET:HE1	1.84	0.60
1:G:1021:ARG:HG2	1:G:1021:ARG:NH1	2.17	0.60
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.37	0.60
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.83	0.59
2:B:232:ASN:N	2:B:233:PRO:HD3	2.17	0.59
1:C:711:PRO:HG2	1:C:755:PHE:HD2	1.67	0.59
2:H:195:VAL:HG11	2:H:228:VAL:HG13	1.84	0.59
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.02	0.59
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.65	0.59
2:F:354:PRO:HB3	2:F:363:ALA:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:947:LEU:HD12	1:G:947:LEU:N	2.17	0.59
1:G:950:ARG:NH1	10:G:4728:HOH:O	2.33	0.59
1:A:35:LYS:O	1:A:39:GLU:HG3	2.02	0.59
1:A:222:ARG:CZ	1:A:273:ARG:HG2	2.32	0.59
1:A:358:LYS:HE3	10:A:4174:HOH:O	2.01	0.59
2:B:249:ASP:OD2	2:B:250:TYR:N	2.36	0.59
1:C:930:LYS:HE3	10:C:4170:HOH:O	2.01	0.59
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.29	0.59
2:H:155:GLY:O	2:H:247:PRO:HG3	2.02	0.59
1:A:1001:ILE:HG13	1:A:1002:GLN:H	1.67	0.59
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.20	0.59
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.84	0.59
1:E:734:LEU:HD12	1:E:734:LEU:C	2.27	0.59
1:G:954:LYS:O	1:G:980:VAL:HG11	2.01	0.59
2:B:279:SER:O	2:B:322:PRO:HG3	2.03	0.59
1:C:646:THR:HB	1:C:647:PRO:HD3	1.85	0.59
1:A:737:TYR:CE1	1:A:741:ALA:HB2	2.37	0.59
1:C:24:CYS:HB3	1:C:576:ILE:HD12	1.85	0.59
1:C:337:ASN:HB3	1:C:340:THR:OG1	2.03	0.59
1:C:415:LEU:HB2	10:C:4581:HOH:O	2.02	0.59
1:E:167:ILE:N	1:E:167:ILE:HD12	2.18	0.59
2:F:261:THR:OG1	2:F:263:ILE:HG13	2.02	0.59
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.37	0.59
1:C:1063:ILE:HD13	1:C:1068:MET:CG	2.33	0.59
1:G:436:ILE:HG22	10:G:4327:HOH:O	2.02	0.59
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.84	0.58
2:F:251:ALA:O	2:F:255:ILE:HD12	2.02	0.58
2:H:142:LEU:O	2:H:146:LYS:HG3	2.02	0.58
1:A:770:GLY:HA2	1:A:823:ARG:NH1	2.18	0.58
1:A:998:ARG:CB	1:A:999:PRO:HA	2.33	0.58
2:B:344:ASP:OD2	2:B:344:ASP:N	2.28	0.58
1:G:863:LYS:O	1:G:867:ARG:HG3	2.02	0.58
1:C:426:ARG:HD3	1:C:426:ARG:C	2.28	0.58
1:E:854:SER:HA	1:E:859:VAL:O	2.02	0.58
1:G:686:LYS:O	1:G:687:LEU:HD23	2.03	0.58
1:G:701:ALA:O	1:G:705:ALA:N	2.29	0.58
1:G:659:VAL:HG13	1:G:660:PRO:HD2	1.85	0.58
2:D:43:LEU:HD21	2:D:80:LEU:HD13	1.85	0.58
1:A:220:VAL:O	1:A:281:GLY:HA2	2.04	0.58
1:C:75:ARG:HD3	10:C:4173:HOH:O	2.04	0.58
1:E:1:MET:N	10:E:4636:HOH:O	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.30	0.58
2:B:364:ALA:N	2:B:365:PRO:HD2	2.19	0.58
1:C:1063:ILE:HG12	1:C:1064:SER:N	2.18	0.58
1:E:1001:ILE:HD12	1:E:1002:GLN:H	1.69	0.58
1:G:64:THR:O	1:G:1065:VAL:HG23	2.03	0.58
1:G:57:ASP:HB3	1:G:59[A]:GLU:OE2	2.03	0.58
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.19	0.58
1:G:775:ILE:HD11	1:G:813:VAL:HG11	1.86	0.58
1:C:1014:ILE:HD12	1:C:1015:ASN:N	2.18	0.58
2:H:168:TYR:CE2	2:H:218:ILE:HG12	2.39	0.58
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.50	0.57
1:C:267:ALA:O	1:C:271:VAL:HG23	2.04	0.57
1:C:998:ARG:HA	1:C:999:PRO:C	2.27	0.57
2:D:50:ARG:NH2	10:D:1965:HOH:O	2.37	0.57
1:E:274:GLU:OE2	1:E:274:GLU:HA	2.03	0.57
2:H:171:THR:HG22	2:H:190:LEU:HD12	1.86	0.57
2:H:208:MET:HB3	2:H:212:ARG:NH1	2.19	0.57
1:A:1027[B]:ARG:CZ	1:A:1031:ARG:HD3	2.34	0.57
2:F:286:MET:HE2	2:F:314:PHE:O	2.03	0.57
1:G:28:TYR:CE1	1:G:313:LYS:HE3	2.39	0.57
1:G:646:THR:HB	1:G:647:PRO:HD3	1.87	0.57
2:F:152:GLY:O	2:F:156:MET:HE3	2.04	0.57
1:C:482:THR:HG23	10:C:4408:HOH:O	2.04	0.57
2:D:257:LYS:O	2:D:260:GLU:HB2	2.05	0.57
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.19	0.57
1:E:922:ARG:HH21	1:E:926:GLU:CD	2.10	0.57
2:D:318:GLU:O	2:D:321:LEU:HB2	2.04	0.57
2:H:23:THR:HG23	2:H:134:ALA:O	2.05	0.57
1:A:972:ASP:OD2	1:A:1004[B]:ARG:NH1	2.38	0.57
1:C:1061:LYS:HG2	10:C:4542:HOH:O	2.05	0.57
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.39	0.57
2:B:273:GLN:HE21	2:B:351:GLN:HE22	1.52	0.57
2:D:228:VAL:HA	2:D:231:MET:HE3	1.85	0.57
1:G:509:ARG:HB2	1:G:509:ARG:NH1	2.17	0.57
1:G:768:CYS:HB2	1:G:773:VAL:HG22	1.85	0.57
1:A:826:MET:HE2	1:A:828:VAL:CG2	2.35	0.57
1:A:1001:ILE:HG13	1:A:1002:GLN:N	2.19	0.57
1:C:186:GLU:HB2	10:C:4561:HOH:O	2.02	0.57
1:C:693:ALA:HB2	1:C:708:ILE:HD11	1.87	0.57
1:E:417:ASP:OD2	1:E:419:GLU:HB2	2.05	0.57
1:E:966:LYS:O	1:E:966:LYS:HG3	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:361:ARG:CZ	1:G:571:ARG:HG2	2.35	0.57
1:A:82:ARG:HG3	1:A:82:ARG:NH1	2.15	0.56
1:C:6:ASP:OD2	1:C:6:ASP:N	2.31	0.56
2:F:299:ASP:HA	2:F:329:HIS:CD2	2.40	0.56
1:C:686:LYS:O	1:C:687:LEU:HD23	2.04	0.56
1:C:698:ILE:HD12	1:C:698:ILE:N	2.12	0.56
1:A:692:ASN:HB3	1:A:753:ASP:CG	2.31	0.56
1:C:336:MET:HE3	1:C:342:GLY:O	2.04	0.56
1:C:923:THR:OG1	1:C:926:GLU:HB2	2.05	0.56
1:E:32:GLN:HB3	1:E:321:LYS:HG3	1.87	0.56
1:E:691:ALA:CB	1:E:708:ILE:HG23	2.36	0.56
1:E:809:MET:HG2	1:E:830:PHE:CE2	2.41	0.56
2:H:363:ALA:C	2:H:365:PRO:HD2	2.31	0.56
1:E:1021:ARG:HG2	1:E:1021:ARG:NH1	2.21	0.56
2:F:279:SER:HB2	2:F:325:LEU:HD11	1.87	0.56
1:G:797:PRO:HD2	1:G:888:TYR:CD1	2.40	0.56
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.40	0.56
1:C:702:VAL:O	1:C:706:LYS:HD3	2.06	0.56
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.41	0.56
1:C:986:ILE:O	1:C:988:PRO:HD3	2.05	0.56
1:C:1036:TYR:C	1:C:1037:LYS:HG2	2.30	0.56
2:D:174:SER:O	2:D:182:PRO:HD3	2.05	0.56
1:E:18:ILE:HD12	1:E:23:ALA:C	2.31	0.56
1:E:901:PRO:HD2	5:E:4055:CL:CL	2.43	0.56
1:E:993:LYS:NZ	1:E:993:LYS:CD	2.60	0.56
2:F:261:THR:O	2:F:345:LYS:NZ	2.38	0.56
1:G:79:GLU:HG2	1:G:111:PHE:HE2	1.70	0.56
1:G:679:GLN:NE2	1:G:692:ASN:OD1	2.38	0.56
1:G:784:GLN:NE2	1:G:784:GLN:N	2.39	0.56
1:A:979:ILE:HG12	1:G:990:LEU:HD23	1.88	0.56
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.52	0.56
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.36	0.56
1:G:1:MET:N	1:G:224:LYS:HE3	2.18	0.56
1:G:17:PRO:HG3	1:G:917:VAL:HG13	1.87	0.56
1:G:151:THR:HG21	10:G:4266:HOH:O	2.05	0.56
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.35	0.56
1:E:712:LEU:O	1:E:727:ILE:HA	2.05	0.56
1:E:991:VAL:CG2	1:E:1004:ARG:HE	2.19	0.56
2:B:341:HIS:ND1	2:B:342:ARG:N	2.53	0.56
1:G:412:LYS:HD3	1:G:437:TRP:HB2	1.87	0.56
1:G:710:TYR:HB3	1:G:729:TYR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:918:MET:HE2	1:G:920:VAL:CG2	2.36	0.55
1:A:164:PHE:HA	1:A:165:PRO:C	2.30	0.55
1:A:715:ARG:NH2	8:A:4006:ADP:O1A	2.27	0.55
1:C:695:VAL:CG2	1:C:752:LEU:HD22	2.36	0.55
1:G:339:ILE:HD11	1:G:531:THR:HG23	1.88	0.55
1:G:766:ALA:HB2	1:G:775:ILE:HD13	1.87	0.55
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.21	0.55
1:A:998:ARG:HA	1:A:999:PRO:C	2.28	0.55
1:G:695:VAL:CG1	1:G:701:ALA:HB2	2.18	0.55
1:G:734:LEU:HD12	1:G:734:LEU:O	2.06	0.55
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.88	0.55
1:A:992:ASN:ND2	1:G:975:HIS:NE2	2.55	0.55
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.67	0.55
1:A:692:ASN:O	1:A:693:ALA:HB2	2.06	0.55
1:A:698:ILE:O	1:A:702:VAL:HG23	2.06	0.55
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.19	0.55
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.36	0.55
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.31	0.55
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.21	0.55
2:H:46:PRO:HA	2:H:76:HIS:CG	2.41	0.55
2:H:78:GLN:HA	2:H:78:GLN:NE2	2.22	0.55
1:G:663:GLY:HA3	1:G:869:MET:CE	2.37	0.55
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.28	0.55
1:G:767:ILE:HA	1:G:824:GLY:O	2.07	0.55
2:H:168:TYR:O	2:H:218:ILE:N	2.31	0.55
2:D:237:PHE:HZ	2:D:268:ILE:HD12	1.68	0.55
1:E:941:LYS:HE2	10:E:4911:HOH:O	2.06	0.55
2:B:272:HIS:ND1	2:B:349:SER:OG	2.36	0.55
1:G:563:MET:CE	1:G:635:PRO:HG3	2.15	0.55
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.42	0.54
1:E:556[A]:SER:HB2	1:E:558:ASP:HB2	1.89	0.54
1:C:1007:ASN:HB3	1:C:1009[B]:GLU:OE2	2.06	0.54
1:E:336:MET:HB3	1:E:342:GLY:HA2	1.88	0.54
2:F:212:ARG:HG3	2:F:212:ARG:HH11	1.72	0.54
1:G:738:PHE:HA	1:G:741:ALA:HB3	1.89	0.54
1:C:419:GLU:HG3	10:C:4722:HOH:O	2.07	0.54
1:E:735:ARG:O	1:E:738:PHE:HB2	2.07	0.54
1:G:473:GLU:HG2	1:G:505:LEU:HD11	1.89	0.54
1:G:901:PRO:HD2	5:G:4076:CL:CL	2.44	0.54
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.87	0.54
1:C:712:LEU:HD23	1:C:753:ASP:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:ALA:O	1:G:271:VAL:HG23	2.07	0.54
2:H:249:ASP:OD2	2:H:250:TYR:HD2	1.91	0.54
1:C:39:GLU:HG3	10:C:4675:HOH:O	2.07	0.54
1:G:588:ALA:HB2	1:G:863:LYS:HB3	1.89	0.54
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.88	0.54
1:A:734:LEU:HD12	1:A:734:LEU:O	2.06	0.54
2:B:325:LEU:HD22	2:B:340:ILE:HB	1.89	0.54
1:C:1014:ILE:HD12	1:C:1014:ILE:C	2.33	0.54
1:E:46:LEU:HG	1:E:46:LEU:O	2.02	0.54
1:E:46:LEU:HD13	1:E:55:MET:HE2	1.88	0.54
1:A:1001:ILE:HD13	1:A:1029:ILE:CG1	2.38	0.54
1:C:639:ILE:HD13	1:C:869:MET:CE	2.38	0.54
1:E:344:THR:HB	1:E:345:PRO:HD2	1.90	0.54
2:F:324:ASN:HA	2:F:343:THR:OG1	2.07	0.54
1:G:427:GLU:HG3	1:G:438:TYR:CE1	2.43	0.54
1:A:417:ASP:OD1	1:A:423:LYS:NZ	2.29	0.54
1:G:165:PRO:HA	1:G:182:ALA:O	2.07	0.54
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.38	0.54
2:F:169:SER:HA	2:F:216:LEU:O	2.08	0.54
1:E:891:LYS:HG2	1:E:892:GLU:N	2.23	0.54
1:G:637:GLY:HA3	1:G:662:ILE:HG23	1.89	0.54
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.89	0.54
1:A:689:GLN:HG3	1:A:690:PRO:HD2	1.89	0.53
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.22	0.53
1:G:1:MET:HE2	1:G:1:MET:N	2.21	0.53
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.37	0.53
2:H:324:ASN:ND2	2:H:324:ASN:N	2.56	0.53
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.23	0.53
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.43	0.53
1:G:900:PHE:O	1:G:903:VAL:HB	2.08	0.53
2:B:296:PRO:HB2	2:B:332:LEU:HB2	1.90	0.53
1:E:802:SER:OG	1:E:805:ILE:HB	2.08	0.53
1:A:165:PRO:HB3	1:A:183:TYR:CD1	2.43	0.53
1:C:1:MET:HG3	1:C:2:PRO:CD	2.30	0.53
1:C:39:GLU:OE1	1:C:325:LYS:NZ	2.36	0.53
1:C:78:ILE:O	1:C:82:ARG:N	2.27	0.53
1:C:1052:MET:HG3	10:C:4623:HOH:O	2.08	0.53
2:H:259:LEU:HD13	2:H:342:ARG:NH1	2.24	0.53
1:A:315:THR:O	1:A:531:THR:HG22	2.08	0.53
1:A:711:PRO:HG2	1:A:755:PHE:HD2	1.74	0.53
1:C:470:VAL:O	1:C:474:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.38	0.53
2:H:6:LEU:HD12	2:H:7:LEU:N	2.24	0.53
1:A:948:SER:O	1:A:1015:ASN:HA	2.09	0.53
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.09	0.53
1:C:561:LYS:HE2	10:C:4441:HOH:O	2.07	0.53
2:D:175:TRP:CZ2	2:D:177:LEU:HA	2.44	0.53
2:D:188:ASP:OD2	2:D:188:ASP:N	2.41	0.53
2:H:198:ASP:HB2	2:H:218:ILE:CG2	2.39	0.53
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.31	0.53
2:B:245:PRO:HG3	2:B:273:GLN:OE1	2.09	0.53
1:E:18:ILE:HD12	1:E:23:ALA:HA	1.91	0.53
1:G:640:VAL:HG21	1:G:651:ALA:HB2	1.89	0.53
1:C:784:GLN:H	1:C:784:GLN:NE2	2.07	0.53
2:D:178:THR:HB	10:D:1683:HOH:O	2.08	0.53
1:A:363:ASN:OD1	1:A:381:VAL:HG21	2.09	0.53
2:B:364:ALA:HB3	2:B:365:PRO:HD3	1.91	0.53
1:E:166:CYS:C	1:E:167:ILE:HD12	2.34	0.53
1:E:809:MET:HG2	1:E:830:PHE:CD2	2.44	0.53
2:F:153:LEU:HD23	10:F:2053:HOH:O	2.07	0.53
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.73	0.53
1:A:146:SER:HB3	1:A:207:ASP:OD1	2.09	0.53
1:A:1021:ARG:HH11	1:A:1021:ARG:HG3	1.74	0.53
2:D:324:ASN:O	2:D:343:THR:HG23	2.09	0.53
1:A:663:GLY:HA2	1:A:869:MET:HG2	1.90	0.52
2:B:299:ASP:OD1	2:B:302:LYS:HG3	2.10	0.52
1:C:344:THR:HB	1:C:345:PRO:CD	2.39	0.52
2:D:46:PRO:HA	2:D:76:HIS:CG	2.44	0.52
2:H:227:ASP:O	2:H:230:LYS:HB2	2.09	0.52
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.43	0.52
1:C:69:ILE:O	1:C:69:ILE:HG22	2.09	0.52
2:F:225:ALA:HB3	2:F:257:LYS:HG2	1.91	0.52
1:G:136:MET:N	1:G:136:MET:HE2	2.24	0.52
1:G:592:ASP:OD1	1:G:867:ARG:NE	2.34	0.52
1:G:665:SER:OG	1:G:667:ASP:N	2.43	0.52
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.92	0.52
1:E:144:ALA:HB1	1:E:208:GLU:CG	2.39	0.52
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.91	0.52
2:H:50:ARG:HG2	2:H:158:LEU:HD11	1.91	0.52
1:C:77:ILE:O	1:C:81:GLU:N	2.30	0.52
2:F:236:ILE:CD1	2:F:263:ILE:HG21	2.39	0.52
1:A:693:ALA:HB3	1:A:708:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:698:ILE:HG23	1:E:738:PHE:CD2	2.45	0.52
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.39	0.52
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.91	0.52
2:H:160:LYS:HE3	2:H:161:GLU:OE2	2.08	0.52
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.90	0.52
1:G:683:GLU:HA	1:G:683:GLU:OE2	2.09	0.52
1:G:693:ALA:HB2	1:G:708:ILE:CD1	2.29	0.52
2:H:272:HIS:CB	2:H:349:SER:HB2	2.40	0.52
1:G:145:ARG:HB2	1:G:208:GLU:OE1	2.09	0.52
1:G:695:VAL:HG13	1:G:700:MET:HG2	1.92	0.52
1:A:724:ALA:O	1:A:725:MET:HG3	2.09	0.52
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.09	0.52
1:C:298:ILE:HG13	10:C:4272:HOH:O	2.09	0.52
2:D:178:THR:HG22	2:D:179:GLY:N	2.25	0.52
1:A:579:ASP:O	1:A:583:VAL:HG23	2.10	0.52
1:A:730:ASP:OD2	1:A:733:ASP:OD2	2.28	0.52
1:C:503:ALA:HB2	1:C:510:GLU:HA	1.91	0.52
1:C:561:LYS:NZ	10:C:4456:HOH:O	2.42	0.52
1:G:145:ARG:HB2	1:G:208:GLU:CD	2.35	0.52
1:G:361:ARG:NH2	1:G:571:ARG:HG2	2.25	0.52
1:A:166:CYS:C	1:A:167:ILE:HD12	2.35	0.52
1:A:194:ARG:NH2	10:A:4618:HOH:O	2.38	0.52
1:C:142:GLU:OE2	1:C:294:ARG:NH2	2.42	0.52
1:C:889:SER:OG	1:C:918:MET:HE3	2.08	0.52
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.92	0.52
2:F:234:ASP:OD1	2:F:378:ARG:HD2	2.09	0.52
2:B:46:PRO:HA	2:B:76:HIS:CG	2.45	0.51
2:F:62:ASN:OD1	2:F:86:PRO:HG3	2.10	0.51
1:G:185:ARG:O	1:G:185:ARG:HG2	2.10	0.51
1:A:82:ARG:HE	1:A:111:PHE:HB3	1.76	0.51
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.41	0.51
1:C:257:THR:HG22	2:D:63:VAL:HG21	1.92	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.51
1:E:755:PHE:CE1	8:E:4047:ADP:C2	2.99	0.51
2:F:272:HIS:HA	2:F:349:SER:OG	2.10	0.51
1:A:796:LEU:HD23	1:A:796:LEU:C	2.35	0.51
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.29	0.51
1:E:979:ILE:O	1:E:983:GLU:HG3	2.11	0.51
1:G:761:GLU:HG2	1:G:781:HIS:CE1	2.45	0.51
2:H:135:GLY:O	2:H:138:PRO:HD3	2.11	0.51
7:A:4030:ORN:NE	1:C:892:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:GLN:NE2	10:B:4164:HOH:O	2.31	0.51
2:D:168:TYR:O	2:D:218:ILE:N	2.35	0.51
1:G:726:GLU:HG3	1:G:727:ILE:H	1.71	0.51
1:A:795:SER:OG	1:A:797:PRO:O	2.29	0.51
1:A:929:ALA:HB2	1:A:1053:ALA:HB1	1.92	0.51
1:A:1037:LYS:HB2	10:A:4564:HOH:O	2.10	0.51
1:C:693:ALA:HB3	1:C:708:ILE:HD11	1.92	0.51
1:G:32:GLN:OE1	1:G:320:ALA:HB3	2.11	0.51
1:A:698:ILE:HD12	1:A:698:ILE:H	1.76	0.51
1:E:121:ASP:O	1:E:125:LYS:HB2	2.11	0.51
1:G:654:LEU:HB3	1:G:659:VAL:HB	1.91	0.51
1:A:559:ARG:HH11	1:A:559:ARG:CG	2.16	0.51
7:A:4051:ORN:NE	1:E:783:GLU:OE1	2.44	0.51
2:D:71:GLU:C	2:D:203:ARG:HG3	2.35	0.51
1:C:703:GLU:HA	1:C:703:GLU:OE2	2.11	0.51
1:C:735:ARG:O	1:C:738:PHE:HB2	2.11	0.51
1:E:646:THR:HB	1:E:647:PRO:CD	2.38	0.51
1:G:1:MET:HE2	10:G:4316:HOH:O	2.10	0.51
2:B:378:ARG:C	2:B:380:THR:H	2.17	0.51
1:C:40:GLU:OE1	1:C:325:LYS:HE2	2.11	0.51
1:C:1049:ALA:HA	1:C:1052:MET:HE3	1.93	0.51
1:E:309:ALA:O	1:E:313:LYS:HG2	2.11	0.51
1:E:698:ILE:H	1:E:698:ILE:CD1	2.22	0.51
1:G:735:ARG:O	1:G:738:PHE:HB2	2.11	0.51
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.91	0.51
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.76	0.51
1:A:569:PRO:O	1:A:571:ARG:HD2	2.10	0.50
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.76	0.50
1:E:678:PHE:O	1:E:681:ALA:N	2.43	0.50
1:G:167:ILE:HD12	1:G:167:ILE:N	2.26	0.50
1:G:1003:ASP:O	1:G:1007:ASN:OD1	2.28	0.50
2:H:277:LEU:HD21	2:H:283:THR:HG23	1.92	0.50
1:A:79:GLU:HA	1:A:111:PHE:CE2	2.46	0.50
1:A:375:THR:HG23	1:A:377:GLN:H	1.75	0.50
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.92	0.50
2:H:47:SER:HB2	2:H:311:ASN:ND2	2.27	0.50
2:B:322:PRO:HG2	2:B:324:ASN:HD21	1.76	0.50
1:C:695:VAL:HG23	1:C:752:LEU:HD22	1.92	0.50
1:C:921:GLY:HA3	1:C:926:GLU:HB3	1.91	0.50
1:C:942:HIS:C	1:C:942:HIS:CD2	2.89	0.50
1:E:440:ALA:O	1:E:444:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:625:ASP:O	1:G:629:ILE:HG13	2.11	0.50
1:G:901:PRO:C	1:G:903:VAL:H	2.19	0.50
1:A:757:ASP:OD2	1:A:833:LYS:NZ	2.45	0.50
2:B:370:PHE:O	2:B:374:ILE:HG13	2.11	0.50
1:C:126:ALA:HB3	1:C:302:PRO:HG3	1.92	0.50
1:C:910:GLU:HB2	10:C:4668:HOH:O	2.11	0.50
1:G:59[A]:GLU:OE1	1:G:60:MET:HE2	2.11	0.50
1:G:829:GLN:O	1:G:840:ILE:HB	2.10	0.50
2:H:25:SER:HA	2:H:132:ILE:O	2.12	0.50
1:E:426:ARG:C	1:E:426:ARG:HD3	2.36	0.50
2:B:364:ALA:N	2:B:365:PRO:CD	2.74	0.50
1:C:644:GLY:O	1:C:647:PRO:HD2	2.12	0.50
1:C:680:HIS:HA	1:C:683:GLU:OE2	2.11	0.50
1:C:998:ARG:HE	1:C:1000:HIS:CE1	2.29	0.50
2:H:322:PRO:CB	2:H:324:ASN:HD21	2.24	0.50
1:A:688:LYS:HD3	1:A:838:TYR:CE1	2.47	0.50
1:C:908:GLY:HA3	10:C:4505:HOH:O	2.11	0.50
2:H:275:LEU:HD23	2:H:349:SER:CB	2.42	0.50
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.35	0.50
1:C:767:ILE:HD13	1:C:865:ALA:HB2	1.94	0.50
1:C:872:LYS:HG3	1:C:876:GLU:HB3	1.93	0.50
2:F:174:SER:O	2:F:182:PRO:HD3	2.12	0.50
1:G:29:SER:HB3	1:G:304:VAL:HG21	1.92	0.50
1:G:353:ASP:OD1	2:H:116:ARG:HD2	2.12	0.50
1:G:998:ARG:HA	1:G:999:PRO:C	2.31	0.50
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.46	0.50
1:C:734:LEU:HD12	1:C:734:LEU:C	2.35	0.50
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.46	0.50
1:G:656:ALA:C	1:G:658:GLY:H	2.20	0.50
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.38	0.49
2:B:222:GLN:HE21	2:B:222:GLN:N	2.10	0.49
1:C:79:GLU:HB2	1:C:111:PHE:CZ	2.47	0.49
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.47	0.49
1:E:703:GLU:O	1:E:706:LYS:HB2	2.12	0.49
1:G:668:ALA:O	1:G:671:ARG:HB2	2.11	0.49
2:H:298:LYS:O	2:H:329:HIS:HA	2.11	0.49
1:A:115:MET:HG2	1:A:118:ALA:O	2.12	0.49
1:A:692:ASN:HB3	1:A:753:ASP:OD1	2.12	0.49
2:F:257:LYS:O	2:F:260:GLU:HB2	2.12	0.49
2:F:328:THR:HG21	2:F:341:HIS:HB2	1.94	0.49
1:G:11:LEU:O	1:G:86:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:509:ARG:NH1	1:G:512:GLU:HG3	2.27	0.49
2:B:206:LEU:N	2:B:206:LEU:HD23	2.27	0.49
2:B:246:ALA:N	2:B:247:PRO:HD2	2.26	0.49
2:F:229:LEU:C	2:F:231:MET:H	2.18	0.49
1:G:315:THR:O	1:G:531:THR:HG22	2.13	0.49
2:H:202:LYS:HZ3	2:H:355:GLU:CG	2.26	0.49
1:A:446:GLY:O	1:E:447:LEU:HD23	2.12	0.49
2:H:208:MET:SD	2:H:355:GLU:HA	2.53	0.49
1:A:1067:GLU:O	1:A:1071:GLN:HG3	2.12	0.49
2:D:98:LEU:HD12	2:D:98:LEU:O	2.13	0.49
2:D:212:ARG:HH11	2:D:212:ARG:CG	2.24	0.49
2:D:316:VAL:HB	2:D:337:LEU:HD23	1.94	0.49
1:E:710:TYR:HB3	1:E:729:TYR:O	2.13	0.49
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.73	0.49
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.47	0.49
1:G:951:GLU:OE1	1:G:954:LYS:HD2	2.13	0.49
1:A:698:ILE:HD12	1:A:698:ILE:N	2.27	0.49
1:A:930:LYS:HE3	10:A:4205:HOH:O	2.12	0.49
2:B:26:ALA:O	2:B:131:CYS:HA	2.12	0.49
1:G:1064:SER:O	1:G:1068:MET:HG3	2.12	0.49
2:H:50:ARG:HG2	2:H:158:LEU:HD13	1.94	0.49
1:A:1:MET:HB3	1:A:224:LYS:NZ	2.27	0.49
1:A:101:GLU:OE2	1:A:101:GLU:HA	2.12	0.49
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.95	0.49
2:B:185:LYS:CD	2:B:190:LEU:HD21	2.39	0.49
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.47	0.49
1:E:252:PRO:HD3	1:E:352:ILE:HD11	1.94	0.49
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.13	0.49
2:F:300:VAL:HG22	2:F:328:THR:C	2.38	0.49
2:F:364:ALA:N	2:F:365:PRO:HD2	2.27	0.49
1:G:148:ILE:O	10:G:4640:HOH:O	2.19	0.49
1:G:494:ARG:HG3	1:G:547:TYR:CB	2.43	0.49
1:A:163:GLY:O	1:A:166:CYS:HB3	2.11	0.49
1:A:946:LEU:C	1:A:947:LEU:HD12	2.38	0.49
2:B:27:VAL:O	2:B:78:GLN:HG2	2.12	0.49
1:C:956:ARG:HD3	1:C:1044:LEU:HD23	1.95	0.49
1:E:144:ALA:HB1	1:E:208:GLU:HG3	1.94	0.49
1:G:590:ARG:HB2	1:G:596:THR:CG2	2.42	0.49
1:G:864:VAL:O	1:G:868:VAL:HG23	2.13	0.49
1:G:1032:SER:O	1:G:1036:TYR:HD1	1.95	0.49
1:C:713:VAL:HG23	1:C:755:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.29	0.49
2:D:168:TYR:CZ	2:D:218:ILE:HG21	2.48	0.49
1:E:702:VAL:HG11	1:E:735:ARG:HH22	1.75	0.49
1:E:772[A]:MET:HG3	1:E:874:LEU:HD12	1.95	0.49
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.47	0.49
2:H:192:PHE:O	2:H:215:ARG:HB3	2.12	0.49
2:H:202:LYS:NZ	2:H:355:GLU:CG	2.76	0.49
1:A:734:LEU:HD11	1:A:738:PHE:HE2	1.76	0.49
1:A:997:GLY:O	1:A:998:ARG:HG3	2.13	0.49
1:C:321:LYS:NZ	1:C:338:ASP:OD1	2.43	0.49
1:E:164:PHE:HD2	1:E:166:CYS:HG	1.57	0.49
1:E:514:ARG:HD3	10:E:4452:HOH:O	2.13	0.49
1:E:942:HIS:CD2	1:E:942:HIS:C	2.90	0.49
1:A:167:ILE:HD12	1:A:167:ILE:N	2.28	0.48
1:C:237:PHE:HB3	1:C:248:ILE:O	2.12	0.48
1:C:693:ALA:HB1	1:C:704:LYS:HG3	1.95	0.48
2:D:185:LYS:HB2	2:D:190:LEU:HD11	1.95	0.48
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.78	0.48
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.78	0.48
1:G:35:LYS:HD2	10:G:4199:HOH:O	2.11	0.48
1:G:70:HIS:ND1	1:G:72:GLU:HB2	2.27	0.48
1:G:890:VAL:HG23	1:G:927:ALA:CB	2.43	0.48
2:H:22:ALA:HB2	2:H:106:ASN:HA	1.95	0.48
2:H:324:ASN:O	2:H:342:ARG:HD2	2.13	0.48
1:C:675:ARG:H	1:C:675:ARG:HD3	1.74	0.48
2:F:272:HIS:HA	2:F:349:SER:CB	2.43	0.48
1:G:1:MET:HB2	1:G:224:LYS:CE	2.44	0.48
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.42	0.48
1:A:663:GLY:HA3	1:A:869:MET:HG2	1.95	0.48
1:C:883:VAL:C	1:C:884:ILE:HD13	2.37	0.48
2:F:133:ILE:CG2	2:F:138:PRO:HB3	2.43	0.48
2:F:341:HIS:CD2	2:F:348:PHE:HB3	2.49	0.48
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.20	0.48
1:A:704:LYS:O	1:A:707:GLU:HB2	2.13	0.48
1:A:947:LEU:CD1	1:A:947:LEU:N	2.77	0.48
2:F:205:ILE:HG21	2:F:237:PHE:CZ	2.49	0.48
1:G:804:GLU:HB2	10:G:4603:HOH:O	2.14	0.48
1:A:467:GLU:O	1:A:471:ARG:HG2	2.14	0.48
1:A:646:THR:HB	1:A:647:PRO:HD3	1.95	0.48
1:C:668:ALA:O	1:C:671:ARG:HB2	2.14	0.48
1:G:224:LYS:HE2	1:G:329:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:796:LEU:C	1:G:796:LEU:HD23	2.39	0.48
2:H:113:ILE:O	2:H:115:THR:N	2.47	0.48
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.46	0.48
1:A:912:ARG:NH1	10:A:4528:HOH:O	2.47	0.48
1:A:947:LEU:HD12	1:A:947:LEU:N	2.29	0.48
2:B:237:PHE:HE1	2:B:268:ILE:HG13	1.78	0.48
1:C:107:VAL:HG12	1:C:107:VAL:O	2.14	0.48
2:D:20:ILE:HG13	2:D:109:ALA:HB3	1.96	0.48
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.39	0.48
1:G:1:MET:HB2	1:G:224:LYS:HE3	1.95	0.48
1:G:36:ALA:HB1	1:G:325:LYS:HE3	1.96	0.48
1:G:57:ASP:HB2	1:G:60:MET:HG2	1.96	0.48
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.11	0.48
2:B:248:CYS:C	2:B:252:ILE:HD12	2.38	0.48
1:C:872:LYS:HG2	1:C:877:GLN:HG2	1.94	0.48
2:D:363:ALA:C	2:D:365:PRO:HD2	2.39	0.48
1:E:4:ARG:NH2	1:E:6:ASP:OD1	2.37	0.48
1:G:412:LYS:HG2	1:G:438:TYR:CE1	2.48	0.48
1:G:417:ASP:OD2	1:G:418:PRO:HD2	2.14	0.48
1:G:695:VAL:HG13	1:G:700:MET:CG	2.42	0.48
1:E:159:ALA:HB2	1:E:188:PHE:CZ	2.49	0.48
1:E:809:MET:HE3	1:E:809:MET:HB2	1.69	0.48
1:G:622:THR:OG1	1:G:625:ASP:OD1	2.29	0.48
1:G:637:GLY:HA3	1:G:662:ILE:CG2	2.43	0.48
1:G:695:VAL:HG12	1:G:697:ALA:O	2.13	0.48
2:H:20:ILE:O	2:H:99:SER:OG	2.28	0.48
2:H:296:PRO:HB2	2:H:332:LEU:HB2	1.95	0.48
1:A:361:ARG:HG2	1:A:571:ARG:HG3	1.94	0.48
1:C:28:TYR:CZ	1:C:313:LYS:HE3	2.48	0.48
1:G:246:ASP:C	1:G:360:PRO:HG3	2.39	0.48
1:G:994:VAL:HG22	1:G:1000:HIS:CD2	2.49	0.48
2:H:201:ALA:HB2	2:H:239:SER:CB	2.43	0.48
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.41	0.48
2:B:232:ASN:N	2:B:233:PRO:CD	2.77	0.48
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.78	0.48
1:E:467:GLU:O	1:E:471:ARG:HG2	2.14	0.48
1:G:69:ILE:HG22	1:G:69:ILE:O	2.13	0.48
1:G:470:VAL:O	1:G:474:GLU:HG3	2.13	0.48
1:G:681:ALA:O	1:G:685:LEU:HG	2.14	0.48
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.39	0.48
1:A:715:ARG:HG2	1:A:725:MET:SD	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:GLN:HE21	1:A:784:GLN:N	1.97	0.47
2:B:218:ILE:HD13	2:B:218:ILE:N	2.29	0.47
1:C:773:VAL:HG23	1:C:818:PHE:CZ	2.49	0.47
1:C:892:GLU:HG3	1:C:893:VAL:N	2.27	0.47
2:D:246:ALA:N	2:D:247:PRO:HD2	2.28	0.47
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.49	0.47
1:E:845:ARG:NH1	1:E:846:ALA:O	2.47	0.47
1:A:700:MET:O	1:A:704:LYS:HB2	2.14	0.47
1:E:490:ARG:HD3	10:E:4665:HOH:O	2.13	0.47
1:E:682:VAL:CG1	1:E:687:LEU:HB2	2.44	0.47
2:F:7:LEU:HB3	2:F:15:PHE:HB2	1.96	0.47
2:F:208:MET:O	2:F:212:ARG:HG3	2.13	0.47
2:F:228:VAL:O	2:F:231:MET:HB2	2.14	0.47
1:G:772:MET:HG3	1:G:773:VAL:N	2.30	0.47
1:A:778:ILE:HD11	1:A:810:ARG:HG3	1.96	0.47
2:D:299:ASP:OD1	2:D:302:LYS:HD2	2.13	0.47
1:G:257:THR:OG1	1:G:260:GLU:HG3	2.15	0.47
1:G:772:MET:HE1	1:G:880:THR:CA	2.43	0.47
1:G:853:VAL:HG12	1:G:861:LEU:HD11	1.96	0.47
2:H:175:TRP:CZ2	2:H:177:LEU:HA	2.49	0.47
1:A:577:GLU:OE2	1:A:577:GLU:N	2.37	0.47
1:A:681:ALA:O	1:A:685:LEU:HG	2.13	0.47
1:A:975:HIS:C	1:A:975:HIS:CD2	2.93	0.47
1:C:12:ILE:HD11	1:C:37:LEU:HD12	1.95	0.47
1:C:64:THR:O	1:C:1065:VAL:HG23	2.14	0.47
1:C:957:VAL:O	1:C:957:VAL:HG22	2.13	0.47
2:F:286:MET:CE	2:F:312:HIS:ND1	2.77	0.47
1:A:344:THR:HB	1:A:345:PRO:HD2	1.96	0.47
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.49	0.47
1:A:1027[A]:ARG:HD3	10:A:4891:HOH:O	2.14	0.47
2:B:168:TYR:CE2	2:B:218:ILE:HG12	2.49	0.47
2:B:322:PRO:CG	2:B:324:ASN:HD21	2.27	0.47
1:C:670:ASP:HB3	1:C:677:ARG:HH21	1.79	0.47
2:D:2:ILE:HG13	2:D:3:LYS:N	2.30	0.47
2:D:39:TYR:CZ	2:D:61:GLY:HA2	2.49	0.47
1:E:571:ARG:HD3	1:E:571:ARG:N	2.28	0.47
2:F:244:ASP:OD2	2:F:245:PRO:HD2	2.15	0.47
1:G:559:ARG:HH11	1:G:559:ARG:CG	2.12	0.47
1:G:1031:ARG:HE	1:G:1031:ARG:HB3	1.42	0.47
2:H:63:VAL:HG12	2:H:91:ASN:HB2	1.96	0.47
1:C:152:MET:HE2	1:C:152:MET:HB2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ARG:HH21	1:C:207:ASP:CG	2.22	0.47
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.49	0.47
2:H:364:ALA:N	2:H:365:PRO:CD	2.78	0.47
1:A:223:ASP:CG	1:A:227:ASN:HB2	2.40	0.47
1:A:675:ARG:HG3	1:A:751:LEU:HD21	1.96	0.47
1:C:358:LYS:HE3	10:C:4142:HOH:O	2.13	0.47
1:C:679:GLN:HG2	1:C:683:GLU:OE1	2.15	0.47
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.97	0.47
1:C:953:ASP:HB3	1:C:1044:LEU:HD22	1.97	0.47
2:F:111:ALA:O	2:F:112:ASP:HB2	2.14	0.47
1:G:148:ILE:HD13	1:G:204:LEU:O	2.15	0.47
1:G:330:TYR:HA	1:G:334:GLU:OE1	2.15	0.47
1:G:453:PHE:CD1	1:G:453:PHE:C	2.92	0.47
1:G:494:ARG:HG3	1:G:547:TYR:HB2	1.96	0.47
1:G:516:LEU:HD11	1:G:520:TYR:CE2	2.49	0.47
1:G:702:VAL:HG21	1:G:735:ARG:CZ	2.44	0.47
1:G:1004:ARG:O	1:G:1009:GLU:HG3	2.15	0.47
2:H:156:MET:HE2	2:H:156:MET:HB2	1.66	0.47
2:H:282:LYS:HB2	2:H:320:THR:HG21	1.97	0.47
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.97	0.47
1:E:735:ARG:O	1:E:738:PHE:N	2.47	0.47
1:E:1019:GLY:O	1:E:1023:ILE:HG13	2.15	0.47
2:F:272:HIS:HB2	2:F:349:SER:HB2	1.97	0.47
1:G:151:THR:OG1	1:G:154:GLU:HG3	2.15	0.47
1:G:524:PRO:HD2	1:G:628:GLU:OE2	2.15	0.47
1:G:548:GLU:OE1	2:H:114:ASP:HA	2.15	0.47
1:G:699:GLU:OE2	1:G:699:GLU:HA	2.15	0.47
1:G:716:PRO:HA	1:G:750:VAL:HG22	1.95	0.47
2:H:98:LEU:O	2:H:102:LEU:HG	2.15	0.47
1:A:1061:LYS:HG2	1:A:1062:VAL:N	2.28	0.47
2:B:269:SER:O	2:B:272:HIS:HB3	2.15	0.47
1:E:1028:VAL:O	1:E:1032:SER:HB2	2.14	0.47
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.96	0.47
1:A:76:LYS:O	1:A:80:LYS:HB3	2.14	0.47
2:B:317:ASP:O	2:B:321:LEU:HD13	2.14	0.47
1:C:891:LYS:HG2	1:C:892:GLU:N	2.29	0.47
1:E:503:ALA:HB1	1:E:508:VAL:O	2.14	0.47
1:G:400:ARG:HD3	10:G:4399:HOH:O	2.14	0.47
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.50	0.47
1:G:695:VAL:HG11	1:G:701:ALA:N	2.30	0.47
2:H:158:LEU:CB	2:H:242:PRO:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:ARG:NH2	10:H:3959:HOH:O	2.48	0.47
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.96	0.46
1:A:698:ILE:H	1:A:698:ILE:CD1	2.29	0.46
1:A:992:ASN:HB2	1:A:999:PRO:O	2.16	0.46
2:B:217:THR:HG21	2:B:231:MET:HE1	1.97	0.46
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.47	0.46
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.49	0.46
2:D:208:MET:SD	2:D:355:GLU:HA	2.55	0.46
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.32	0.46
2:F:353:HIS:N	2:F:353:HIS:CD2	2.83	0.46
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.48	0.46
1:G:681:ALA:HA	1:G:684:ARG:HB3	1.96	0.46
1:G:704:LYS:O	1:G:707:GLU:HB2	2.14	0.46
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.96	0.46
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.15	0.46
1:A:333:ASP:OD1	1:A:333:ASP:N	2.48	0.46
2:D:285:LYS:HB2	2:D:314:PHE:CE1	2.50	0.46
1:E:27:ASP:OD2	1:E:53:THR:HB	2.14	0.46
1:E:154:GLU:O	1:E:157:ALA:HB3	2.16	0.46
1:G:135:ALA:O	1:G:138:LYS:HB3	2.16	0.46
1:G:344:THR:HB	1:G:345:PRO:HD2	1.97	0.46
1:G:730:ASP:H	1:G:733:ASP:HB2	1.80	0.46
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.29	0.46
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.75	0.46
1:A:713:VAL:HG12	1:A:713:VAL:O	2.15	0.46
1:A:714:VAL:HG23	1:A:728:VAL:HG23	1.97	0.46
2:B:186:LYS:O	2:B:189:GLU:HB2	2.15	0.46
1:C:701:ALA:O	1:C:705:ALA:N	2.39	0.46
1:E:698:ILE:N	1:E:698:ILE:CD1	2.79	0.46
2:F:164:THR:O	2:F:220:PRO:HB3	2.16	0.46
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.53	0.46
1:G:9:SER:HA	1:G:43:ARG:O	2.15	0.46
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.79	0.46
2:H:325:LEU:HA	2:H:325:LEU:HD23	1.56	0.46
2:B:237:PHE:CE2	2:B:239:SER:HA	2.49	0.46
1:C:563:MET:CE	1:C:635:PRO:HG3	2.46	0.46
1:E:889:SER:HB3	1:E:918:MET:HE3	1.97	0.46
2:H:266:PHE:CD2	2:H:370:PHE:CD2	3.04	0.46
1:A:165:PRO:HA	1:A:182:ALA:O	2.16	0.46
1:C:715:ARG:CG	1:C:725:MET:HE2	2.41	0.46
1:C:873:SER:O	1:C:877:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:THR:HA	2:D:56:THR:OG1	2.15	0.46
1:E:164:PHE:HA	1:E:165:PRO:C	2.41	0.46
2:F:87:LEU:HA	2:F:87:LEU:HD12	1.58	0.46
2:H:206:LEU:O	2:H:210:VAL:HG23	2.15	0.46
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.46	0.46
1:C:325:LYS:O	1:C:330:TYR:HB2	2.15	0.46
2:F:290:HIS:HB2	2:F:312:HIS:CD2	2.50	0.46
1:G:1:MET:CB	1:G:224:LYS:NZ	2.79	0.46
1:G:948:SER:O	1:G:1015:ASN:HA	2.16	0.46
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.43	0.46
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.96	0.46
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.16	0.46
1:E:708:ILE:HG22	1:E:754:HIS:HB2	1.97	0.46
1:E:728:VAL:HG13	1:E:733:ASP:CB	2.33	0.46
1:G:29:SER:CB	1:G:304:VAL:HG21	2.46	0.46
1:G:577:GLU:O	1:G:580:TYR:HB3	2.16	0.46
1:A:266:ASN:ND2	10:A:4760:HOH:O	2.46	0.46
1:A:780:GLU:OE2	1:A:798:ALA:HB1	2.15	0.46
2:B:128:GLN:HG3	10:B:4129:HOH:O	2.14	0.46
1:C:46:LEU:HD13	1:C:55:MET:HE2	1.98	0.46
1:C:775:ILE:HG13	1:C:810:ARG:HG2	1.97	0.46
2:D:272:HIS:HA	2:D:349:SER:CB	2.45	0.46
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.98	0.46
2:F:379:LYS:HB2	2:F:379:LYS:NZ	2.30	0.46
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.51	0.46
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.51	0.46
2:D:12:GLY:HA2	2:D:144:LEU:HD13	1.98	0.46
2:D:156:MET:SD	2:D:158:LEU:HD21	2.55	0.46
1:E:415:LEU:HA	10:E:4432:HOH:O	2.15	0.46
1:E:805:ILE:HD13	1:E:805:ILE:HA	1.78	0.46
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.51	0.46
1:G:153:GLU:O	1:G:153:GLU:HG2	2.14	0.46
1:G:561:LYS:HG2	1:G:595:GLU:OE2	2.16	0.46
1:G:563:MET:HB2	1:G:638:VAL:HG22	1.98	0.46
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.51	0.46
1:A:772:MET:SD	1:A:880:THR:HG22	2.56	0.46
2:D:306:MET:HB3	2:D:362:ASP:HB3	1.97	0.46
1:G:24:CYS:HB2	1:G:604:GLU:HB2	1.98	0.46
1:G:947:LEU:N	1:G:947:LEU:CD1	2.78	0.46
2:H:225:ALA:HA	2:H:258:PHE:CE1	2.51	0.46
1:A:702:VAL:O	1:A:706:LYS:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:LEU:HD21	1:C:669:ILE:CG2	2.46	0.45
1:G:809:MET:HG2	1:G:837:VAL:HG11	1.98	0.45
2:H:352:GLY:O	2:H:354:PRO:HD3	2.16	0.45
1:A:223:ASP:OD1	1:A:227:ASN:HB2	2.16	0.45
1:A:343:ARG:HD3	1:A:343:ARG:N	2.32	0.45
1:A:612:THR:HG22	1:A:612:THR:O	2.16	0.45
1:C:994:VAL:HG22	1:C:1000:HIS:CG	2.50	0.45
2:D:269:SER:O	2:D:272:HIS:HB3	2.16	0.45
1:E:994:VAL:CG2	1:E:1001:ILE:HD11	2.46	0.45
1:G:75:ARG:HD3	10:G:4220:HOH:O	2.16	0.45
1:G:358:LYS:HG2	1:G:359:ILE:N	2.27	0.45
2:H:91:ASN:O	2:H:94:ASN:HB3	2.16	0.45
2:H:168:TYR:O	2:H:217:THR:HA	2.16	0.45
1:A:695:VAL:HG13	1:A:697:ALA:O	2.17	0.45
1:A:703:GLU:O	1:A:706:LYS:HB2	2.17	0.45
1:C:890:VAL:HG23	1:C:927:ALA:HB3	1.97	0.45
2:D:324:ASN:O	2:D:342:ARG:HD2	2.17	0.45
1:E:796:LEU:C	1:E:796:LEU:HD23	2.42	0.45
1:G:423[B]:LYS:NZ	10:G:4420:HOH:O	2.48	0.45
1:G:577:GLU:HG2	1:G:848:ARG:O	2.17	0.45
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.44	0.45
1:C:332:LEU:HB3	1:C:347:SER:HB3	1.99	0.45
1:C:375:THR:HG23	1:C:377:GLN:H	1.81	0.45
1:C:469:LEU:O	1:C:473:GLU:HG3	2.17	0.45
1:E:258:ASP:O	1:E:262:GLN:HG2	2.16	0.45
1:E:773:VAL:HG21	1:E:814:GLN:HA	1.99	0.45
2:H:27:VAL:HG22	2:H:131:CYS:CB	2.33	0.45
1:A:426:ARG:HD3	1:A:426:ARG:C	2.41	0.45
1:A:1020:ARG:HH21	1:A:1023:ILE:HG21	1.80	0.45
2:D:185:LYS:HD3	2:D:190:LEU:HD21	1.98	0.45
2:D:212:ARG:HG3	2:D:212:ARG:NH1	2.29	0.45
1:E:995:HIS:CD2	1:E:995:HIS:H	2.35	0.45
2:F:6:LEU:HD12	2:F:7:LEU:N	2.32	0.45
1:G:45:ILE:HG23	1:G:63:ALA:HB3	1.99	0.45
1:G:632:ILE:HG13	1:G:633:GLU:N	2.31	0.45
1:G:775:ILE:HD13	1:G:775:ILE:HA	1.79	0.45
2:H:264:PRO:HG2	2:H:374:ILE:HA	1.97	0.45
2:B:153:LEU:N	2:B:153:LEU:HD12	2.31	0.45
1:C:9:SER:OG	1:C:83:PRO:HA	2.16	0.45
1:C:686:LYS:C	1:C:687:LEU:HD23	2.42	0.45
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:LEU:HD13	2:H:214:CYS:O	2.16	0.45
1:C:490:ARG:HG3	1:C:522:LEU:HD11	1.99	0.45
1:C:648:LEU:HD13	1:C:845:ARG:HD3	1.99	0.45
1:C:1027:ARG:NH2	10:C:4504:HOH:O	2.48	0.45
2:D:197:TYR:HB3	2:D:199:PHE:CZ	2.51	0.45
2:D:324:ASN:ND2	2:D:324:ASN:N	2.56	0.45
2:D:332:LEU:HD12	2:D:332:LEU:HA	1.66	0.45
1:E:130:ARG:O	1:E:134:VAL:HG23	2.17	0.45
1:G:176:GLY:N	8:G:4062:ADP:O2B	2.46	0.45
2:H:153:LEU:HD12	2:H:156:MET:HE3	1.99	0.45
1:A:481:ILE:HG22	10:A:4638:HOH:O	2.16	0.45
1:A:993:LYS:HB2	1:A:996:GLU:HG3	1.99	0.45
2:B:153:LEU:N	2:B:153:LEU:CD1	2.79	0.45
2:B:236:ILE:HG13	2:B:263:ILE:HG21	1.98	0.45
1:E:239:ALA:HB2	10:E:4316:HOH:O	2.15	0.45
1:E:1003:ASP:O	1:E:1007:ASN:OD1	2.34	0.45
2:F:364:ALA:N	2:F:365:PRO:CD	2.79	0.45
2:B:34:THR:HA	2:B:56:THR:OG1	2.17	0.45
1:C:250:VAL:HA	1:C:356:VAL:O	2.17	0.45
1:E:317:PHE:CE1	1:E:322:VAL:HG21	2.52	0.45
2:F:376:GLN:HA	2:F:379:LYS:NZ	2.31	0.45
1:G:214:LYS:NZ	1:G:255:THR:OG1	2.37	0.45
1:C:854:SER:HA	1:C:859:VAL:O	2.17	0.45
1:E:436:ILE:HG22	1:E:437:TRP:CE3	2.52	0.45
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.78	0.45
1:G:11:LEU:HA	1:G:45:ILE:O	2.16	0.45
1:G:752:LEU:HD12	1:G:752:LEU:HA	1.47	0.45
2:H:266:PHE:HD2	2:H:370:PHE:CD2	2.33	0.45
1:A:583:VAL:O	1:A:587:LEU:HG	2.16	0.44
1:C:959:ASP:O	1:C:962:ALA:HB3	2.17	0.44
1:E:145:ARG:H	1:E:208:GLU:CD	2.23	0.44
1:G:773:VAL:HG21	1:G:817:ALA:HB3	1.99	0.44
1:G:901:PRO:C	1:G:903:VAL:N	2.75	0.44
2:D:152:GLY:O	2:D:156:MET:HE3	2.18	0.44
2:D:286:MET:HG3	2:D:313:GLY:O	2.18	0.44
1:E:1:MET:HE2	1:E:1:MET:H3	1.80	0.44
1:G:770:GLY:HA3	1:G:823:ARG:CZ	2.47	0.44
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.99	0.44
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.48	0.44
1:A:730:ASP:H	1:A:733:ASP:HB2	1.82	0.44
1:C:765:ASP:OD2	1:C:827:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:SER:HA	2:D:216:LEU:O	2.16	0.44
2:F:236:ILE:HD12	2:F:263:ILE:CG2	2.48	0.44
2:F:279:SER:O	2:F:322:PRO:HG3	2.17	0.44
1:G:803:GLN:HG3	1:G:807:ASP:OD1	2.17	0.44
1:G:830:PHE:CD1	1:G:837:VAL:CG1	3.01	0.44
1:A:4:ARG:NE	1:A:7:ILE:HD12	2.32	0.44
1:A:1017:THR:HG22	1:A:1018:SER:N	2.32	0.44
2:B:6:LEU:HD23	2:B:138:PRO:HB2	1.98	0.44
2:B:363:ALA:C	2:B:365:PRO:HD2	2.42	0.44
1:C:44:VAL:HG22	1:C:61:ALA:HB1	2.00	0.44
2:D:249:ASP:O	2:D:253:THR:HB	2.17	0.44
1:G:407:THR:OG1	1:G:410:ASP:OD1	2.35	0.44
1:G:965:LEU:HA	1:G:965:LEU:HD23	1.80	0.44
2:H:6:LEU:HD11	2:H:8:VAL:HG22	1.95	0.44
2:H:48:TYR:O	2:H:51:GLN:HB2	2.16	0.44
2:H:218:ILE:N	2:H:218:ILE:CD1	2.80	0.44
1:A:482:THR:HB	10:A:4453:HOH:O	2.17	0.44
1:A:734:LEU:CD1	1:A:738:PHE:CE2	2.99	0.44
2:B:181:LEU:HD23	2:B:181:LEU:HA	1.74	0.44
2:D:279:SER:O	2:D:322:PRO:HG3	2.17	0.44
2:F:291:HIS:HD2	2:F:311:ASN:OD1	2.01	0.44
1:G:672:ALA:HB3	1:G:844:PRO:HG3	1.99	0.44
1:G:713:VAL:O	1:G:713:VAL:HG12	2.17	0.44
1:G:981:LEU:CD1	1:G:988:PRO:HG3	2.39	0.44
1:A:9:SER:C	1:A:10:ILE:HG13	2.41	0.44
1:A:185:ARG:O	1:A:188:PHE:HB3	2.17	0.44
1:A:654:LEU:O	1:A:659:VAL:HG23	2.17	0.44
2:B:317:ASP:OD2	2:B:318:GLU:N	2.51	0.44
1:C:994:VAL:HA	1:C:1000:HIS:CB	2.48	0.44
1:C:1063:ILE:CD1	1:C:1068:MET:HG3	2.46	0.44
1:E:375:THR:OG1	1:E:376:THR:N	2.48	0.44
2:F:92:PHE:CE1	2:F:93:ARG:HG2	2.53	0.44
1:G:1063:ILE:HD13	1:G:1068:MET:CG	2.43	0.44
1:A:130:ARG:HB2	1:A:148:ILE:HG13	1.99	0.44
1:A:1054:LEU:HD23	1:A:1054:LEU:HA	1.83	0.44
2:B:10:GLU:HG3	2:B:129:ASN:HB2	2.00	0.44
2:B:378:ARG:C	2:B:380:THR:N	2.76	0.44
1:C:805:ILE:HG22	1:C:806:GLN:N	2.32	0.44
1:E:422:THR:HA	10:E:4063:HOH:O	2.18	0.44
1:E:436:ILE:CG2	1:E:437:TRP:CE3	3.00	0.44
2:F:32:PHE:CG	2:F:119:THR:HG23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:187:GLU:HG2	2:F:215:ARG:HD3	2.00	0.44
1:G:70:HIS:CE1	1:G:72:GLU:HB2	2.53	0.44
1:G:648:LEU:HD13	1:G:845:ARG:HD3	2.00	0.44
1:A:362:PHE:CE1	1:A:380:SER:HB3	2.53	0.44
1:A:947:LEU:HG	1:A:1014:ILE:HG21	1.99	0.44
1:C:74:VAL:CG1	1:C:102:LEU:HD11	2.48	0.44
1:G:534:ALA:HB1	2:H:120:ARG:HG2	1.98	0.44
1:G:830:PHE:CE1	1:G:839:LEU:HD13	2.53	0.44
1:G:906:LEU:HD13	1:G:1030:ARG:CD	2.48	0.44
2:H:348:PHE:CD1	2:H:369:HIS:HD2	2.36	0.44
1:A:734:LEU:HD12	1:A:734:LEU:C	2.38	0.44
2:B:8:VAL:CG2	2:B:143:ALA:CB	2.96	0.44
2:B:350:PHE:HB2	2:B:366:LEU:HD23	1.98	0.44
1:C:934:GLY:C	1:C:936:ASN:H	2.25	0.44
1:E:375:THR:HA	10:E:4307:HOH:O	2.18	0.44
1:E:819:GLU:HB2	10:E:4897:HOH:O	2.16	0.44
2:F:275:LEU:HD23	2:F:349:SER:OG	2.18	0.44
1:G:956:ARG:HB3	1:G:1044:LEU:HD23	2.00	0.44
2:H:33:ASN:HA	2:H:291:HIS:O	2.18	0.44
2:H:234:ASP:OD1	2:H:378:ARG:NH1	2.49	0.44
1:A:128:ASP:CG	1:A:131:ARG:HG3	2.43	0.43
1:A:695:VAL:CG2	1:A:701:ALA:HA	2.39	0.43
2:B:350:PHE:CB	2:B:366:LEU:CD2	2.96	0.43
1:E:563:MET:HE2	1:E:563:MET:HB2	1.84	0.43
1:E:921:GLY:HA3	1:E:926:GLU:HB3	1.99	0.43
1:G:340:THR:C	1:G:343:ARG:HH11	2.25	0.43
2:H:209:LEU:HA	2:H:209:LEU:HD23	1.84	0.43
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.48	0.43
1:C:237:PHE:CE2	1:C:458:ILE:HD13	2.53	0.43
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.18	0.43
2:D:175:TRP:CH2	2:D:177:LEU:HA	2.53	0.43
1:E:339:ILE:HD13	1:E:339:ILE:HG21	1.68	0.43
1:G:71:TRP:CZ3	1:G:105:GLN:HG3	2.52	0.43
1:G:493:LYS:HA	1:G:493:LYS:HD2	1.76	0.43
1:G:627:LEU:HD23	1:G:627:LEU:HA	1.81	0.43
2:H:341:HIS:CD2	2:H:348:PHE:HB3	2.53	0.43
2:H:373:LEU:HD23	2:H:373:LEU:HA	1.86	0.43
1:A:354:TYR:CD2	1:A:387:ILE:HG23	2.53	0.43
1:C:26:PHE:HB2	10:C:4133:HOH:O	2.18	0.43
1:C:332:LEU:CB	1:C:347:SER:HB3	2.48	0.43
1:C:577:GLU:O	1:C:580:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:ILE:HA	2:D:264:PRO:HD3	1.81	0.43
1:E:946:LEU:HB3	1:E:1013:ILE:HG12	2.01	0.43
2:F:227:ASP:O	2:F:231:MET:HE2	2.18	0.43
2:F:236:ILE:HD12	2:F:263:ILE:HG22	2.00	0.43
1:G:519:GLN:C	1:G:521:ASP:N	2.76	0.43
1:G:867:ARG:HB2	1:G:877:GLN:NE2	2.32	0.43
2:H:205:ILE:HG21	2:H:237:PHE:CZ	2.54	0.43
1:A:1021:ARG:CG	1:A:1021:ARG:NH1	2.80	0.43
1:C:365:GLU:H	1:C:365:GLU:HG3	1.31	0.43
1:E:493:LYS:HE2	1:E:517:ARG:HD3	2.00	0.43
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.99	0.43
2:F:324:ASN:ND2	2:F:324:ASN:N	2.64	0.43
1:G:698:ILE:N	1:G:698:ILE:CD1	2.79	0.43
1:G:770:GLY:CA	1:G:823:ARG:CZ	2.97	0.43
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.77	0.43
1:A:588:ALA:HB2	1:A:863:LYS:HG2	2.01	0.43
1:C:213:TRP:HH2	1:C:294:ARG:HD3	1.83	0.43
1:E:681:ALA:O	1:E:684:ARG:HB3	2.19	0.43
1:E:695:VAL:CG1	1:E:696:THR:N	2.81	0.43
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.41	0.43
1:G:820:LEU:O	1:G:821:GLN:HB2	2.19	0.43
1:G:858:GLY:HA2	1:G:1069:HIS:ND1	2.30	0.43
2:H:157:ASP:HB2	2:H:247:PRO:HB2	1.99	0.43
2:H:322:PRO:HD2	2:H:325:LEU:HD12	2.00	0.43
1:A:820:LEU:O	1:A:821:GLN:HB2	2.17	0.43
2:B:275:LEU:HD12	2:B:275:LEU:O	2.17	0.43
1:C:623:LEU:HD12	1:C:654:LEU:HD23	2.00	0.43
1:C:712:LEU:O	1:C:727:ILE:HA	2.19	0.43
2:D:157:ASP:HA	10:D:1865:HOH:O	2.18	0.43
2:D:269:SER:HB3	2:D:270:LEU:H	1.64	0.43
2:F:269:SER:OG	2:F:270:LEU:N	2.51	0.43
1:G:40:GLU:HG2	1:G:325:LYS:HE2	2.01	0.43
1:G:550:GLU:OE2	2:H:120:ARG:NH2	2.46	0.43
1:G:556:SER:O	1:G:561:LYS:NZ	2.50	0.43
1:A:475:LYS:HE2	1:A:488:PHE:CZ	2.53	0.43
1:A:872:LYS:HB2	10:A:4818:HOH:O	2.19	0.43
1:A:1014:ILE:HG23	1:A:1014:ILE:O	2.18	0.43
2:D:325:LEU:HA	2:D:325:LEU:HD23	1.76	0.43
1:G:9:SER:C	1:G:10:ILE:HG13	2.43	0.43
2:H:210:VAL:HA	2:H:214:CYS:O	2.19	0.43
2:H:234:ASP:HB3	2:H:374:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.79	0.43
1:A:631:ARG:HG2	1:A:632:ILE:HG23	2.00	0.43
1:A:751:LEU:O	1:A:752:LEU:HD12	2.18	0.43
1:A:840:ILE:O	1:A:841:GLU:HB3	2.18	0.43
2:B:367:PHE:O	2:B:370:PHE:HB3	2.19	0.43
1:C:787:VAL:HG13	1:C:907:LEU:HB3	2.00	0.43
2:D:227:ASP:O	2:D:230:LYS:HB2	2.19	0.43
2:D:342:ARG:HD2	2:D:342:ARG:HA	1.75	0.43
1:E:710:TYR:HB3	1:E:711:PRO:HA	2.01	0.43
1:E:1000:HIS:CD2	1:E:1000:HIS:C	2.97	0.43
1:G:822:VAL:C	1:G:823:ARG:HG2	2.44	0.43
1:A:347:SER:O	2:B:296:PRO:HB3	2.19	0.43
1:A:736:ARG:O	1:A:740:THR:HG23	2.18	0.43
2:B:175:TRP:HA	2:B:180:GLY:O	2.18	0.43
1:C:1064:SER:O	1:C:1068:MET:HG3	2.19	0.43
1:E:697:ALA:O	1:E:700:MET:HB2	2.19	0.43
2:F:202:LYS:NZ	2:F:356:ALA:O	2.45	0.43
2:F:228:VAL:HG22	2:F:231:MET:CE	2.49	0.43
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.49	0.43
1:G:703:GLU:OE2	1:G:703:GLU:HA	2.19	0.43
2:H:249:ASP:OD2	2:H:249:ASP:N	2.51	0.43
1:A:579:ASP:OD2	1:A:607:SER:OG	2.35	0.43
1:C:127:GLU:HB2	1:C:172:PHE:CZ	2.54	0.43
1:C:150:HIS:ND1	1:C:154:GLU:OE2	2.44	0.43
1:C:340:THR:O	1:C:343:ARG:HB2	2.18	0.43
1:C:492:LEU:O	1:C:495:LYS:HB2	2.19	0.43
1:C:1057:ASP:HB3	1:C:1060:GLU:HB2	1.99	0.43
2:F:246:ALA:N	2:F:247:PRO:HD2	2.33	0.43
1:A:712:LEU:O	1:A:727:ILE:HA	2.19	0.42
2:D:196:ALA:HA	2:D:237:PHE:O	2.19	0.42
2:D:258:PHE:C	2:D:260:GLU:H	2.26	0.42
1:E:755:PHE:CD1	8:E:4047:ADP:C2	3.07	0.42
2:H:266:PHE:HA	2:H:348:PHE:O	2.19	0.42
1:A:4:ARG:CD	1:A:7:ILE:HD12	2.48	0.42
1:A:657:ALA:HB1	10:A:4512:HOH:O	2.18	0.42
1:C:44:VAL:N	1:C:62:ASP:OD2	2.44	0.42
1:C:65:TYR:OH	1:C:80:LYS:NZ	2.30	0.42
1:C:183:TYR:HB2	1:C:187:GLU:OE1	2.19	0.42
2:D:212:ARG:CG	2:D:212:ARG:NH1	2.77	0.42
1:E:176:GLY:N	8:E:4041:ADP:O2B	2.38	0.42
1:E:294:ARG:NH1	10:E:4632:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:769:ASP:OD2	1:G:769:ASP:N	2.50	0.42
1:G:801:LEU:HD22	1:G:805:ILE:HG21	2.00	0.42
2:H:287:LYS:NZ	10:H:3683:HOH:O	2.52	0.42
1:C:165:PRO:HA	1:C:182:ALA:O	2.20	0.42
1:C:196:LEU:HA	1:C:196:LEU:HD23	1.80	0.42
1:C:812:GLN:O	1:C:816:LEU:HD12	2.18	0.42
1:E:202:LYS:O	1:E:202:LYS:HG2	2.19	0.42
1:E:250:VAL:HA	1:E:356:VAL:O	2.19	0.42
1:E:659:VAL:HG13	1:E:660:PRO:HD2	2.01	0.42
2:F:176:THR:O	2:F:180:GLY:N	2.47	0.42
2:F:263:ILE:HA	2:F:264:PRO:HD3	1.75	0.42
1:G:735:ARG:O	1:G:738:PHE:N	2.52	0.42
1:A:150:HIS:NE2	1:A:203:GLU:HG3	2.34	0.42
1:A:383:GLU:OE2	1:A:604:GLU:OE1	2.38	0.42
1:A:1004[A]:ARG:HD2	1:A:1010:TYR:OH	2.19	0.42
1:C:669:ILE:HA	1:C:844:PRO:HG2	2.02	0.42
1:E:784:GLN:HE21	1:E:784:GLN:N	2.09	0.42
2:F:373:LEU:HA	2:F:373:LEU:HD23	1.79	0.42
1:G:118:ALA:HA	10:G:4550:HOH:O	2.19	0.42
2:H:8:VAL:HG12	2:H:9:LEU:N	2.33	0.42
2:H:175:TRP:CH2	2:H:177:LEU:HA	2.55	0.42
1:A:441:ASP:OD2	1:A:444:ARG:NH1	2.50	0.42
1:A:701:ALA:O	1:A:705:ALA:HB2	2.18	0.42
1:A:773:VAL:HG23	1:A:818:PHE:CE2	2.55	0.42
1:C:693:ALA:N	1:C:708:ILE:HD11	2.35	0.42
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.85	0.42
1:E:436:ILE:HD12	1:E:436:ILE:HA	1.88	0.42
1:G:74:VAL:HG11	1:G:102:LEU:HD11	2.00	0.42
1:G:103:GLU:HG3	1:G:104:ARG:N	2.28	0.42
1:G:205:LEU:HD12	1:G:205:LEU:HA	1.89	0.42
1:G:426:ARG:HD3	1:G:427:GLU:N	2.35	0.42
1:A:128:ASP:OD2	1:A:131:ARG:HG3	2.20	0.42
1:C:461:TRP:HB2	2:D:90:SER:HB3	2.01	0.42
2:D:187:GLU:HG2	2:D:215:ARG:CD	2.47	0.42
2:D:222:GLN:H	2:D:222:GLN:NE2	2.15	0.42
2:D:298:LYS:O	2:D:329:HIS:HA	2.19	0.42
1:E:1052:MET:HG2	10:E:4939:HOH:O	2.18	0.42
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.54	0.42
1:G:456:THR:O	1:G:457:ASN:HB2	2.19	0.42
1:A:35:LYS:HD2	10:A:4186:HOH:O	2.18	0.42
1:C:734:LEU:HD11	1:C:738:PHE:HE2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:932:GLN:HG2	1:C:937:SER:HB3	2.01	0.42
1:C:950:ARG:H	1:C:950:ARG:HG3	1.59	0.42
2:D:264:PRO:HA	2:D:346:PRO:O	2.20	0.42
1:E:82:ARG:HD3	10:E:4592:HOH:O	2.18	0.42
1:E:475:LYS:HE2	1:E:488:PHE:CZ	2.55	0.42
2:F:205:ILE:HG12	2:F:355:GLU:CD	2.45	0.42
2:H:348:PHE:CE1	2:H:369:HIS:HD2	2.37	0.42
1:A:843:ASN:HA	1:A:844:PRO:HD3	1.83	0.42
1:A:1027[B]:ARG:CZ	1:A:1031:ARG:CD	2.98	0.42
1:C:166:CYS:C	1:C:167:ILE:HD12	2.44	0.42
1:C:339:ILE:HD13	1:C:339:ILE:HG21	1.87	0.42
1:C:528:ARG:HG2	1:C:543:MET:HG2	2.02	0.42
1:C:954:LYS:CG	1:C:980:VAL:HG21	2.48	0.42
1:C:990:LEU:HD23	1:E:979:ILE:HG12	2.02	0.42
1:E:4:ARG:HA	10:E:4159:HOH:O	2.19	0.42
2:F:218:ILE:HD13	2:F:218:ILE:N	2.34	0.42
2:F:253:THR:O	2:F:256:GLN:HB2	2.19	0.42
1:G:56:THR:OG1	1:G:855:LYS:NZ	2.45	0.42
1:G:406:ALA:HA	1:G:410:ASP:OD2	2.20	0.42
1:G:890:VAL:HG23	1:G:927:ALA:HB3	2.02	0.42
2:H:29:GLU:HA	2:H:129:ASN:HA	2.01	0.42
2:H:176:THR:HB	10:H:3971:HOH:O	2.19	0.42
1:A:38:ARG:NH1	1:A:38:ARG:CG	2.76	0.42
1:A:70:HIS:ND1	1:A:72:GLU:HB2	2.35	0.42
1:A:167:ILE:HG12	8:A:4000:ADP:C2	2.55	0.42
1:E:1:MET:N	1:E:1:MET:HE2	2.34	0.42
1:E:630:VAL:O	1:E:634[B]:LYS:HD2	2.19	0.42
1:E:991:VAL:HG23	1:E:1004:ARG:HE	1.84	0.42
2:F:187:GLU:HG2	2:F:215:ARG:HD2	2.00	0.42
1:G:196:LEU:HD23	1:G:196:LEU:HA	1.89	0.42
1:G:333:ASP:OD1	1:G:333:ASP:N	2.48	0.42
1:A:339:ILE:HD13	1:A:339:ILE:HG21	1.88	0.42
1:A:507:GLY:HA2	10:A:4692:HOH:O	2.19	0.42
1:A:583:VAL:HG12	1:A:587:LEU:HD11	2.02	0.42
1:C:692:ASN:HA	1:C:752:LEU:O	2.20	0.42
1:C:693:ALA:HB1	1:C:704:LYS:CG	2.50	0.42
2:D:116:ARG:O	2:D:120:ARG:HG3	2.20	0.42
2:D:233:PRO:HG2	2:D:263:ILE:HD13	2.02	0.42
1:E:220:VAL:O	1:E:281:GLY:HA2	2.20	0.42
2:F:282:LYS:HB2	2:F:320:THR:HG21	2.02	0.42
1:G:618:PHE:C	1:G:619:GLU:HG2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:644:GLY:O	1:G:647:PRO:HD2	2.20	0.42
1:G:860:PRO:HB2	1:G:863:LYS:CG	2.42	0.42
2:H:65:THR:OG1	2:H:96:GLU:O	2.32	0.42
2:H:357:SER:HA	2:H:358:PRO:HA	1.85	0.42
1:A:343:ARG:HD3	1:A:343:ARG:H	1.84	0.41
2:B:222:GLN:HG3	2:B:250:TYR:CE1	2.54	0.41
1:C:534:ALA:HB2	2:D:116:ARG:NH1	2.35	0.41
2:D:228:VAL:HA	2:D:231:MET:CE	2.50	0.41
1:E:258:ASP:OD1	2:F:37:THR:OG1	2.37	0.41
1:E:631:ARG:HD3	10:E:4457:HOH:O	2.20	0.41
2:F:65:THR:OG1	2:F:96:GLU:O	2.27	0.41
1:G:561:LYS:O	1:G:636:LYS:N	2.46	0.41
1:A:349:GLU:O	2:B:294:ASN:HB2	2.20	0.41
1:A:680:HIS:N	1:A:680:HIS:ND1	2.66	0.41
1:E:103:GLU:HG2	10:E:4707:HOH:O	2.20	0.41
1:E:709:GLY:O	1:E:754:HIS:ND1	2.53	0.41
2:F:253:THR:O	2:F:257:LYS:HD3	2.20	0.41
1:G:1:MET:N	1:G:224:LYS:CE	2.83	0.41
1:G:148:ILE:CG2	1:G:149:ALA:N	2.80	0.41
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.19	0.41
1:G:738:PHE:O	1:G:741:ALA:HB3	2.20	0.41
1:G:1004:ARG:HA	1:G:1009:GLU:HG3	2.02	0.41
2:H:32:PHE:O	2:H:291:HIS:HB2	2.20	0.41
1:A:479:VAL:CG2	1:A:483:GLY:HA3	2.50	0.41
1:A:784:GLN:HE22	1:A:1043:THR:HB	1.84	0.41
1:A:793:ALA:HA	1:A:891:LYS:O	2.21	0.41
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.55	0.41
2:B:248:CYS:O	2:B:252:ILE:HD12	2.20	0.41
1:E:738:PHE:O	1:E:741:ALA:HB3	2.19	0.41
2:F:236:ILE:CD1	2:F:263:ILE:CG2	2.98	0.41
1:G:698:ILE:H	1:G:698:ILE:CD1	2.31	0.41
1:G:762:VAL:HG12	1:G:763:ASP:N	2.34	0.41
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.76	0.41
1:A:950:ARG:HD3	10:A:4709:HOH:O	2.21	0.41
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.56	0.41
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.86	0.41
1:E:1020:ARG:HD3	1:E:1020:ARG:HA	1.95	0.41
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.54	0.41
2:B:152:GLY:O	2:B:156:MET:HE3	2.20	0.41
2:B:296:PRO:HD3	2:B:333:PHE:CZ	2.55	0.41
1:C:11:LEU:HA	1:C:45:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:TYR:HA	1:C:711:PRO:C	2.44	0.41
2:D:296:PRO:HB2	2:D:332:LEU:HB2	2.01	0.41
2:F:196:ALA:HA	2:F:237:PHE:O	2.20	0.41
2:F:232:ASN:N	2:F:233:PRO:CD	2.80	0.41
2:F:255:ILE:CG2	2:F:278:ALA:CB	2.98	0.41
1:G:492:LEU:HD13	1:G:502:LEU:HD22	2.01	0.41
1:G:784:GLN:HE22	1:G:1043:THR:HB	1.86	0.41
1:G:1023:ILE:HG23	1:G:1030:ARG:NH2	2.35	0.41
1:A:770:GLY:HA2	1:A:823:ARG:CZ	2.50	0.41
2:B:72:SER:HB2	10:B:4107:HOH:O	2.19	0.41
1:C:1063:ILE:CD1	1:C:1068:MET:CG	2.99	0.41
1:E:148:ILE:CG2	1:E:149:ALA:N	2.84	0.41
1:E:358:LYS:HE3	10:E:4183:HOH:O	2.21	0.41
2:F:255:ILE:HA	2:F:258:PHE:CD2	2.56	0.41
1:G:489:LEU:HA	1:G:489:LEU:HD23	1.83	0.41
2:H:38:GLY:HA3	2:H:358:PRO:HB3	2.01	0.41
2:B:167:ALA:O	2:B:168:TYR:HB3	2.20	0.41
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	2.02	0.41
2:D:32:PHE:O	2:D:291:HIS:HB2	2.19	0.41
1:E:115:MET:HE3	1:E:115:MET:HB2	1.83	0.41
1:E:571:ARG:HH11	1:E:571:ARG:HD2	1.65	0.41
1:G:850:VAL:HB	1:G:851:PRO:HD3	2.03	0.41
1:G:942:HIS:CD2	1:G:942:HIS:C	2.98	0.41
1:G:1021:ARG:NH1	1:G:1021:ARG:CG	2.84	0.41
2:H:369:HIS:O	2:H:372:GLU:HB2	2.20	0.41
1:A:326:LEU:HA	1:A:326:LEU:HD12	1.85	0.41
1:C:167:ILE:HD12	1:C:167:ILE:N	2.35	0.41
1:C:942:HIS:CD2	1:C:943:GLY:N	2.89	0.41
1:C:991:VAL:HG22	1:C:992:ASN:N	2.36	0.41
1:C:1000:HIS:CD2	1:C:1000:HIS:C	2.97	0.41
2:D:267:GLY:O	2:D:349:SER:HB2	2.21	0.41
1:E:412:LYS:HG2	1:E:438:TYR:CZ	2.56	0.41
1:E:469:LEU:O	1:E:473:GLU:HG3	2.20	0.41
1:G:764:VAL:O	1:G:827:ASN:HA	2.21	0.41
1:G:874:LEU:HB3	1:G:879:VAL:O	2.20	0.41
1:G:915:GLY:HA2	10:G:4181:HOH:O	2.21	0.41
1:G:992:ASN:ND2	1:G:996:GLU:HB3	2.36	0.41
1:A:184:ASN:OD1	1:A:186:GLU:HB2	2.20	0.41
2:B:132:ILE:HG21	2:B:132:ILE:HD13	1.84	0.41
2:B:246:ALA:N	2:B:247:PRO:CD	2.84	0.41
1:C:1:MET:CG	1:C:2:PRO:HD2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASN:O	1:C:66:ILE:HA	2.21	0.41
1:C:174:MET:HB2	6:C:4025:PO4:O1	2.20	0.41
1:C:841:GLU:HB2	10:C:4535:HOH:O	2.21	0.41
1:C:868:VAL:HG23	1:C:877:GLN:NE2	2.35	0.41
1:C:902:GLY:O	1:C:1027:ARG:NH2	2.49	0.41
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.51	0.41
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.35	0.41
1:E:59:GLU:HG3	1:E:60:MET:HE2	1.96	0.41
1:E:714:VAL:HG13	1:E:752:LEU:HD12	2.03	0.41
2:F:46:PRO:HA	2:F:76:HIS:CG	2.55	0.41
2:F:50:ARG:HG3	2:F:158:LEU:HD13	2.02	0.41
2:F:273:GLN:HE21	2:F:351:GLN:HE22	1.67	0.41
1:G:440:ALA:O	1:G:444:ARG:HG3	2.21	0.41
1:G:517:ARG:HG2	1:G:522:LEU:HD23	2.03	0.41
1:G:518:ASP:OD1	1:G:523:HIS:HE1	2.04	0.41
1:G:872:LYS:HG2	1:G:872:LYS:O	2.19	0.41
1:G:1021:ARG:HD3	1:G:1025:ASP:OD2	2.21	0.41
2:H:5:ALA:HB3	2:H:110:ILE:HG13	2.03	0.41
2:H:54:THR:HA	2:H:81:VAL:HB	2.03	0.41
2:B:8:VAL:HG21	2:B:143:ALA:CB	2.49	0.41
2:B:45:ASP:O	2:B:76:HIS:HB2	2.20	0.41
1:C:426:ARG:HD3	1:C:426:ARG:O	2.21	0.41
2:F:229:LEU:C	2:F:231:MET:N	2.79	0.41
1:G:349:GLU:O	2:H:294:ASN:HB2	2.22	0.41
1:G:412:LYS:HD3	1:G:437:TRP:CB	2.50	0.41
2:H:110:ILE:HG12	2:H:111:ALA:N	2.36	0.41
1:A:1051:ALA:O	1:A:1054:LEU:HB2	2.20	0.40
2:B:202:LYS:HB3	2:B:202:LYS:HE2	1.80	0.40
2:B:222:GLN:HG3	2:B:250:TYR:CD1	2.55	0.40
1:C:51:PRO:HG2	1:C:916:GLU:OE2	2.22	0.40
1:C:336:MET:HB3	1:C:342:GLY:HA2	2.03	0.40
1:E:213:TRP:CZ2	1:E:289:ASN:HB2	2.56	0.40
2:F:199:PHE:O	2:F:241:GLY:HA3	2.22	0.40
1:G:359:ILE:HD13	1:G:359:ILE:HG21	1.79	0.40
1:A:152:MET:O	1:A:155:ALA:HB3	2.21	0.40
1:A:539:ASP:HB2	10:A:4472:HOH:O	2.22	0.40
1:A:687:LEU:HD22	1:A:812:GLN:CD	2.47	0.40
1:A:781:HIS:HE1	1:A:789:SER:HB3	1.85	0.40
2:B:236:ILE:HB	2:B:265:VAL:HG22	2.03	0.40
2:D:30:VAL:HG22	2:D:52:ILE:HB	2.03	0.40
2:D:277:LEU:HD21	2:D:283:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ILE:HD12	1:E:275:ILE:HA	1.80	0.40
1:E:534:ALA:O	2:F:123:ARG:HD3	2.20	0.40
1:E:651:ALA:HB1	1:E:666:PRO:HG3	2.02	0.40
2:F:6:LEU:HD11	2:F:8:VAL:CG2	2.51	0.40
1:G:143:THR:HA	1:G:296:ILE:HG23	2.03	0.40
1:A:475:LYS:HA	10:A:4792:HOH:O	2.21	0.40
1:A:835:ASN:HD22	1:A:835:ASN:HA	1.76	0.40
1:C:503:ALA:CB	1:C:510:GLU:HA	2.51	0.40
1:C:757:ASP:C	1:C:833:LYS:HZ2	2.28	0.40
1:E:734:LEU:O	1:E:737:TYR:HB3	2.21	0.40
1:E:1006:LYS:O	1:E:1006:LYS:HG3	2.19	0.40
2:F:170:TRP:CD1	2:F:170:TRP:C	2.98	0.40
1:G:317:PHE:C	1:G:317:PHE:CD1	3.00	0.40
1:G:671:ARG:NH2	1:G:819:GLU:O	2.54	0.40
1:A:59:GLU:CG	1:A:60:MET:HE2	2.52	0.40
1:A:868:VAL:HA	1:A:872:LYS:O	2.21	0.40
1:A:1017:THR:CG2	1:A:1018:SER:N	2.84	0.40
2:B:227:ASP:HA	2:B:230:LYS:HD2	2.03	0.40
2:B:296:PRO:CD	2:B:333:PHE:CE1	3.05	0.40
1:C:928:PHE:HD1	1:C:1053:ALA:HB2	1.87	0.40
2:D:364:ALA:N	2:D:365:PRO:CD	2.85	0.40
2:F:46:PRO:O	2:F:242:PRO:HG3	2.22	0.40
1:C:554:ASN:N	1:C:555:PRO:HD3	2.37	0.40
1:C:987:ASN:ND2	10:C:4516:HOH:O	2.46	0.40
2:D:176:THR:O	2:D:180:GLY:N	2.40	0.40
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.76	0.40
1:G:165:PRO:HB3	1:G:183:TYR:CD1	2.57	0.40
1:G:423[B]:LYS:HE3	1:G:427:GLU:HG2	2.04	0.40
1:G:637:GLY:HA2	1:G:660:PRO:O	2.21	0.40
1:G:905:PRO:HB2	1:G:1040:TYR:HH	1.86	0.40
2:H:25:SER:HB2	2:H:133:ILE:HG12	2.03	0.40
2:H:38:GLY:HA3	2:H:358:PRO:CB	2.52	0.40
2:H:153:LEU:HA	2:H:153:LEU:HD12	1.79	0.40
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.51	0.40
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1058/1073 (99%)	1012 (96%)	42 (4%)	4 (0%)	30	27
1	C	1053/1073 (98%)	996 (95%)	51 (5%)	6 (1%)	21	17
1	E	1058/1073 (99%)	1014 (96%)	44 (4%)	0	100	100
1	G	1056/1073 (98%)	1000 (95%)	50 (5%)	6 (1%)	21	17
2	B	377/382 (99%)	361 (96%)	16 (4%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	377/382 (99%)	358 (95%)	18 (5%)	1 (0%)	36	35
2	H	378/382 (99%)	355 (94%)	23 (6%)	0	100	100
All	All	5734/5820 (98%)	5460 (95%)	257 (4%)	17 (0%)	36	35

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	ASP
1	A	975	HIS
1	C	698	ILE
1	A	693	ALA
1	C	758	ASP
1	G	738	PHE
1	G	739	GLN
1	G	873	SER
1	C	975	HIS
1	C	368	ALA
1	C	736	ARG
1	G	519	GLN
1	G	975	HIS
2	F	185	LYS
1	C	2	PRO
1	G	2	PRO
1	A	2	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	871/878 (99%)	795 (91%)	76 (9%)	9	6
1	C	866/878 (99%)	794 (92%)	72 (8%)	10	7
1	E	871/878 (99%)	795 (91%)	76 (9%)	9	6
1	G	869/878 (99%)	780 (90%)	89 (10%)	7	4
2	B	308/310 (99%)	273 (89%)	35 (11%)	5	3
2	D	308/310 (99%)	283 (92%)	25 (8%)	11	7
2	F	308/310 (99%)	271 (88%)	37 (12%)	5	3
2	H	309/310 (100%)	271 (88%)	38 (12%)	4	3
All	All	4710/4752 (99%)	4262 (90%)	448 (10%)	8	5

All (448) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	5	THR
1	A	8	LYS
1	A	38	ARG
1	A	46	LEU
1	A	79	GLU
1	A	104	ARG
1	A	137	LYS
1	A	138	LYS
1	A	174	MET
1	A	236	ASN
1	A	275	ILE
1	A	299	GLU
1	A	326	LEU
1	A	343	ARG
1	A	358	LYS
1	A	414	SER
1	A	416	ASP

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Mol	Chain	Res	Type
1	A	490	ARG
1	A	518	ASP
1	A	548	GLU
1	A	554[A]	ASN
1	A	554[B]	ASN
1	A	559	ARG
1	A	560	GLU
1	A	571	ARG
1	A	591	GLU
1	A	671	ARG
1	A	675	ARG
1	A	677	ARG
1	A	684	ARG
1	A	688	LYS
1	A	689	GLN
1	A	695	VAL
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	707	GLU
1	A	712	LEU
1	A	714	VAL
1	A	715	ARG
1	A	730	ASP
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	739	GLN
1	A	753	ASP
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE
1	A	808	VAL
1	A	815	LYS
1	A	835	ASN
1	A	839	LEU
1	A	855	LYS
1	A	891	LYS
1	A	895	LEU
1	A	906	LEU
1	A	912	ARG
1	A	920	VAL

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Mol	Chain	Res	Type
1	A	940	LYS
1	A	947	LEU
1	A	950	ARG
1	A	955	GLU
1	A	967	GLN
1	A	970	GLU
1	A	992	ASN
1	A	1001	ILE
1	A	1006	LYS
1	A	1018	SER
1	A	1021	ARG
1	A	1026	SER
1	A	1027[A]	ARG
1	A	1027[B]	ARG
1	A	1073	LYS
2	B	2	ILE
2	B	3	LYS
2	B	6	LEU
2	B	18	ARG
2	B	50	ARG
2	B	87	LEU
2	B	104	ARG
2	B	106	ASN
2	B	113	ILE
2	B	154	ASN
2	B	157	ASP
2	B	166	GLU
2	B	169	SER
2	B	183	GLU
2	B	186	LYS
2	B	188	ASP
2	B	190	LEU
2	B	215	ARG
2	B	218	ILE
2	B	222	GLN
2	B	239	SER
2	B	257	LYS
2	B	261	THR
2	B	282	LYS
2	B	301	GLU
2	B	302	LYS
2	B	304	VAL

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Mol	Chain	Res	Type
2	B	306	MET
2	B	321	LEU
2	B	324	ASN
2	B	345	LYS
2	B	357	SER
2	B	366	LEU
2	B	376	GLN
2	B	379	LYS
1	C	1	MET
1	C	43	ARG
1	C	44	VAL
1	C	46	LEU
1	C	55	MET
1	C	103	GLU
1	C	145	ARG
1	C	174	MET
1	C	202	LYS
1	C	217	GLU
1	C	236	ASN
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	336	MET
1	C	343	ARG
1	C	365	GLU
1	C	412	LYS
1	C	414	SER
1	C	416	ASP
1	C	423	LYS
1	C	426	ARG
1	C	548	GLU
1	C	563	MET
1	C	571	ARG
1	C	591	GLU
1	C	648	LEU
1	C	665	SER
1	C	675	ARG
1	C	683	GLU
1	C	684	ARG
1	C	696	THR
1	C	704	LYS
1	C	706	LYS

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Mol	Chain	Res	Type
1	C	712	LEU
1	C	726	GLU
1	C	728	VAL
1	C	733	ASP
1	C	735	ARG
1	C	736	ARG
1	C	750	VAL
1	C	751	LEU
1	C	757	ASP
1	C	763	ASP
1	C	771	GLU
1	C	772	MET
1	C	784	GLN
1	C	795	SER
1	C	800	THR
1	C	805	ILE
1	C	811	GLN
1	C	814	GLN
1	C	827	ASN
1	C	835	ASN
1	C	849	THR
1	C	855	LYS
1	C	906	LEU
1	C	910	GLU
1	C	912	ARG
1	C	923	THR
1	C	950	ARG
1	C	951	GLU
1	C	967	GLN
1	C	970	GLU
1	C	998	ARG
1	C	1014	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1031	ARG
1	C	1072	ILE
1	C	1073	LYS
2	D	6	LEU
2	D	42	ILE
2	D	50	ARG
2	D	87	LEU

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Mol	Chain	Res	Type
2	D	125	LYS
2	D	148	ARG
2	D	153	LEU
2	D	166	GLU
2	D	178	THR
2	D	183	GLU
2	D	188	ASP
2	D	222	GLN
2	D	231	MET
2	D	253	THR
2	D	257	LYS
2	D	269	SER
2	D	275	LEU
2	D	306	MET
2	D	324	ASN
2	D	332	LEU
2	D	333	PHE
2	D	345	LYS
2	D	366	LEU
2	D	376	GLN
2	D	379	LYS
1	E	1	MET
1	E	3	LYS
1	E	5	THR
1	E	24	CYS
1	E	46	LEU
1	E	76	LYS
1	E	103	GLU
1	E	104	ARG
1	E	115	MET
1	E	153	GLU
1	E	174	MET
1	E	220	VAL
1	E	272	LEU
1	E	275	ILE
1	E	296	ILE
1	E	299	GLU
1	E	300	MET
1	E	307	SER
1	E	339	ILE
1	E	343	ARG
1	E	358	LYS

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Mol	Chain	Res	Type
1	E	363	ASN
1	E	412	LYS
1	E	414	SER
1	E	428	LEU
1	E	548	GLU
1	E	558	ASP
1	E	559[A]	ARG
1	E	559[B]	ARG
1	E	562	ILE
1	E	571	ARG
1	E	591	GLU
1	E	671	ARG
1	E	675	ARG
1	E	676	GLU
1	E	677	ARG
1	E	680	HIS
1	E	695	VAL
1	E	696	THR
1	E	698	ILE
1	E	700	MET
1	E	704	LYS
1	E	706	LYS
1	E	707	GLU
1	E	712	LEU
1	E	734	LEU
1	E	735	ARG
1	E	750	VAL
1	E	751	LEU
1	E	784	GLN
1	E	805	ILE
1	E	809	MET
1	E	835	ASN
1	E	836	GLU
1	E	839	LEU
1	E	855	LYS
1	E	881	LYS
1	E	906	LEU
1	E	936	ASN
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU
1	E	956	ARG

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Mol	Chain	Res	Type
1	E	957	VAL
1	E	966	LYS
1	E	967	GLN
1	E	991	VAL
1	E	1014	ILE
1	E	1018	SER
1	E	1020	ARG
1	E	1021	ARG
1	E	1027	ARG
1	E	1031	ARG
1	E	1052	MET
1	E	1072	ILE
1	E	1073	LYS
2	F	6	LEU
2	F	18	ARG
2	F	23	THR
2	F	25	SER
2	F	50	ARG
2	F	73	SER
2	F	87	LEU
2	F	106	ASN
2	F	110	ILE
2	F	113	ILE
2	F	125	LYS
2	F	153	LEU
2	F	166	GLU
2	F	169	SER
2	F	174	SER
2	F	175	TRP
2	F	183	GLU
2	F	186	LYS
2	F	192	PHE
2	F	205	ILE
2	F	218	ILE
2	F	228	VAL
2	F	230	LYS
2	F	255	ILE
2	F	256	GLN
2	F	257	LYS
2	F	261	THR
2	F	263	ILE
2	F	282	LYS

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Mol	Chain	Res	Type
2	F	301	GLU
2	F	324	ASN
2	F	332	LEU
2	F	366	LEU
2	F	371	ILE
2	F	372	GLU
2	F	376	GLN
2	F	379	LYS
1	G	1	MET
1	G	8	LYS
1	G	20	ILE
1	G	43	ARG
1	G	46	LEU
1	G	55	MET
1	G	59[A]	GLU
1	G	59[B]	GLU
1	G	76	LYS
1	G	145	ARG
1	G	174	MET
1	G	185	ARG
1	G	202	LYS
1	G	275	ILE
1	G	321	LYS
1	G	326	LEU
1	G	339	ILE
1	G	343	ARG
1	G	358	LYS
1	G	413	VAL
1	G	416	ASP
1	G	422	THR
1	G	426	ARG
1	G	428	LEU
1	G	479	VAL
1	G	481	ILE
1	G	482	THR
1	G	489	LEU
1	G	509	ARG
1	G	519	GLN
1	G	548	GLU
1	G	554	ASN
1	G	559	ARG
1	G	571	ARG

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Mol	Chain	Res	Type
1	G	591	GLU
1	G	648	LEU
1	G	652	ARG
1	G	665	SER
1	G	673	GLU
1	G	675	ARG
1	G	682	VAL
1	G	683	GLU
1	G	688	LYS
1	G	698	ILE
1	G	704	LYS
1	G	706	LYS
1	G	712	LEU
1	G	714	VAL
1	G	730	ASP
1	G	733	ASP
1	G	734	LEU
1	G	735	ARG
1	G	751	LEU
1	G	752	LEU
1	G	767	ILE
1	G	772	MET
1	G	775	ILE
1	G	784	GLN
1	G	789	SER
1	G	800	THR
1	G	805	ILE
1	G	808	VAL
1	G	840	ILE
1	G	845	ARG
1	G	849	THR
1	G	855	LYS
1	G	880	THR
1	G	881	LYS
1	G	884	ILE
1	G	912	ARG
1	G	940	LYS
1	G	950	ARG
1	G	951	GLU
1	G	956	ARG
1	G	966	LYS
1	G	967	GLN

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Mol	Chain	Res	Type
1	G	970	GLU
1	G	1006	LYS
1	G	1014	ILE
1	G	1018	SER
1	G	1021	ARG
1	G	1027	ARG
1	G	1030	ARG
1	G	1031	ARG
1	G	1032	SER
1	G	1059	THR
1	G	1061	LYS
1	G	1063	ILE
1	G	1073	LYS
2	H	2	ILE
2	H	4	SER
2	H	6	LEU
2	H	7	LEU
2	H	42	ILE
2	H	49	SER
2	H	87	LEU
2	H	104	ARG
2	H	113	ILE
2	H	125	LYS
2	H	137	ASN
2	H	153	LEU
2	H	157	ASP
2	H	166	GLU
2	H	174	SER
2	H	178	THR
2	H	183	GLU
2	H	186	LYS
2	H	202	LYS
2	H	216	LEU
2	H	218	ILE
2	H	222	GLN
2	H	230	LYS
2	H	231	MET
2	H	250	TYR
2	H	252	ILE
2	H	257	LYS
2	H	261	THR
2	H	262	ASP

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Mol	Chain	Res	Type
2	H	263	ILE
2	H	300	VAL
2	H	306	MET
2	H	324	ASN
2	H	332	LEU
2	H	340	ILE
2	H	357	SER
2	H	375	GLU
2	H	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	266	ASN
1	A	391	GLN
1	A	645	GLN
1	A	692	ASN
1	A	784	GLN
1	A	811	GLN
1	A	812	GLN
1	A	834	ASN
1	A	835	ASN
1	A	932	GLN
1	A	936	ASN
1	A	987	ASN
1	A	992	ASN
1	A	995	HIS
1	A	1000	HIS
1	A	1035	GLN
1	A	1071	GLN
2	B	16	HIS
2	B	51	GLN
2	B	78	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	457	ASN
1	C	645	GLN
1	C	679	GLN

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Mol	Chain	Res	Type
1	C	689	GLN
1	C	692	ASN
1	C	784	GLN
1	C	814	GLN
1	C	835	ASN
1	C	843	ASN
1	C	942	HIS
1	C	992	ASN
1	C	1000	HIS
1	C	1007	ASN
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	154	ASN
2	D	222	GLN
2	D	273	GLN
2	D	324	ASN
2	D	351	GLN
1	E	150	HIS
1	E	266	ASN
1	E	337	ASN
1	E	679	GLN
1	E	689	GLN
1	E	692	ASN
1	E	784	GLN
1	E	803	GLN
1	E	812	GLN
1	E	827	ASN
1	E	843	ASN
1	E	898	ASN
1	E	936	ASN
1	E	942	HIS
1	E	992	ASN
1	E	995	HIS
1	E	1002	GLN
1	E	1007	ASN
1	E	1015	ASN
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	51	GLN

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Mol	Chain	Res	Type
2	F	154	ASN
2	F	324	ASN
2	F	329	HIS
2	F	351	GLN
2	F	353	HIS
1	G	105	GLN
1	G	266	ASN
1	G	523	HIS
1	G	645	GLN
1	G	679	GLN
1	G	689	GLN
1	G	784	GLN
1	G	803	GLN
1	G	812	GLN
1	G	835	ASN
1	G	936	ASN
1	G	992	ASN
1	G	1055	ASN
2	H	16	HIS
2	H	51	GLN
2	H	78	GLN
2	H	105	HIS
2	H	154	ASN
2	H	222	GLN
2	H	232	ASN
2	H	324	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 82 ligands modelled in this entry, 60 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	C	4040	-	4,4,4	1.28	0	6,6,6	0.84	0
8	ADP	G	4068	4,3	28,29,29	1.25	4 (14%)	43,45,45	0.95	4 (9%)
9	NET	E	4052	-	8,8,8	0.71	0	10,10,10	0.65	0
8	ADP	A	4000	3	28,29,29	1.33	3 (10%)	43,45,45	0.92	0
6	PO4	E	4061	-	4,4,4	2.31	3 (75%)	6,6,6	0.96	0
7	ORN	A	4030	-	6,7,8	1.07	1 (16%)	2,7,9	0.95	0
8	ADP	E	4041	3	28,29,29	1.37	6 (21%)	43,45,45	1.01	3 (6%)
6	PO4	C	4025	4,3	4,4,4	2.41	4 (100%)	6,6,6	1.15	0
9	NET	A	4011	-	8,8,8	0.70	0	10,10,10	0.58	0
9	NET	C	4031	-	8,8,8	0.58	0	10,10,10	0.53	0
8	ADP	A	4006	4,3	28,29,29	1.39	4 (14%)	43,45,45	0.98	2 (4%)
6	PO4	E	4046	4,3	4,4,4	2.09	2 (50%)	6,6,6	1.10	0
7	ORN	A	4010	-	7,8,8	1.04	1 (14%)	6,9,9	1.34	1 (16%)
8	ADP	E	4047	4,3	28,29,29	1.21	3 (10%)	43,45,45	1.00	2 (4%)
9	NET	G	4073	-	8,8,8	0.82	0	10,10,10	0.44	0
6	PO4	A	4005	4,3	4,4,4	2.37	2 (50%)	6,6,6	1.30	1 (16%)
7	ORN	A	4051	-	6,7,8	1.16	1 (16%)	2,7,9	0.44	0
8	ADP	G	4062	3	28,29,29	1.12	3 (10%)	43,45,45	1.00	3 (6%)
8	ADP	C	4020	3	28,29,29	1.38	4 (14%)	43,45,45	1.03	1 (2%)
8	ADP	C	4026	4,3	28,29,29	1.10	3 (10%)	43,45,45	0.95	3 (6%)
6	PO4	G	4067	4,3	4,4,4	2.40	2 (50%)	6,6,6	1.16	0
7	ORN	A	4072	-	7,8,8	0.82	0	6,9,9	1.14	0

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
9	NET	G	4073	-	-	0/12/12/12	-
8	ADP	G	4068	4,3	-	4/16/32/32	0/3/3/3
8	ADP	G	4062	3	-	0/16/32/32	0/3/3/3
9	NET	A	4011	-	-	0/12/12/12	-
9	NET	E	4052	-	-	3/12/12/12	-
8	ADP	C	4020	3	-	2/16/32/32	0/3/3/3
8	ADP	C	4026	4,3	-	0/16/32/32	0/3/3/3
7	ORN	A	4051	-	-	3/5/6/8	-
9	NET	C	4031	-	-	0/12/12/12	-
8	ADP	A	4006	4,3	-	3/16/32/32	0/3/3/3
8	ADP	A	4000	3	-	1/16/32/32	0/3/3/3
8	ADP	E	4041	3	-	2/16/32/32	0/3/3/3
7	ORN	A	4030	-	-	4/5/6/8	-
7	ORN	A	4010	-	-	6/8/8/8	-
8	ADP	E	4047	4,3	-	3/16/32/32	0/3/3/3
7	ORN	A	4072	-	-	6/8/8/8	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4000	ADP	PA-O3A	-4.40	1.54	1.59
8	C	4020	ADP	PA-O3A	-4.24	1.54	1.59
8	A	4006	ADP	PA-O3A	-4.00	1.55	1.59
6	G	4067	PO4	P-O2	-3.78	1.43	1.54
8	G	4068	ADP	PA-O3A	-3.20	1.56	1.59
6	E	4046	PO4	P-O2	-3.02	1.45	1.54
6	A	4005	PO4	P-O4	-2.92	1.46	1.54
8	G	4068	ADP	O3'-C3'	2.90	1.50	1.43
8	E	4047	ADP	O2'-C2'	2.88	1.50	1.43
8	E	4041	ADP	O2'-C2'	2.87	1.50	1.43
6	A	4005	PO4	P-O2	-2.77	1.46	1.54
8	E	4041	ADP	PA-O3A	-2.76	1.56	1.59
8	E	4047	ADP	O3'-C3'	2.74	1.49	1.43
8	C	4020	ADP	O2'-C2'	2.74	1.49	1.43
6	E	4061	PO4	P-O4	-2.60	1.47	1.54
8	A	4006	ADP	C2-N3	-2.59	1.29	1.33
8	E	4047	ADP	C2-N1	2.58	1.38	1.33
6	E	4061	PO4	P-O2	-2.56	1.47	1.54
6	C	4025	PO4	P-O3	-2.55	1.47	1.54
8	C	4026	ADP	O3'-C3'	2.54	1.49	1.43
7	A	4030	ORN	O-C	2.50	1.29	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	4025	PO4	P-O1	-2.47	1.45	1.50
6	C	4025	PO4	P-O2	-2.45	1.47	1.54
8	A	4000	ADP	C2-N1	2.42	1.38	1.33
8	A	4006	ADP	C8-N7	2.40	1.36	1.31
8	E	4041	ADP	O3'-C3'	2.38	1.48	1.43
8	A	4006	ADP	O3'-C3'	2.36	1.48	1.43
8	G	4062	ADP	C2-N3	-2.29	1.29	1.33
8	C	4026	ADP	O2'-C2'	2.27	1.48	1.43
8	E	4041	ADP	C8-N7	2.26	1.36	1.31
7	A	4051	ORN	O-C	2.25	1.28	1.20
8	G	4062	ADP	O2'-C2'	2.18	1.48	1.43
6	G	4067	PO4	P-O3	-2.17	1.48	1.54
7	A	4010	ORN	O-C	2.16	1.28	1.22
8	C	4026	ADP	PA-O3A	-2.15	1.57	1.59
6	E	4061	PO4	P-O3	-2.15	1.48	1.54
6	C	4025	PO4	P-O4	-2.14	1.48	1.54
8	G	4068	ADP	C2-N1	2.14	1.37	1.33
8	C	4020	ADP	O4'-C1'	-2.13	1.37	1.42
6	E	4046	PO4	P-O3	-2.13	1.48	1.54
8	G	4068	ADP	O2'-C2'	2.13	1.48	1.43
8	G	4062	ADP	PA-O3A	-2.11	1.57	1.59
8	A	4000	ADP	C8-N7	2.09	1.35	1.31
8	E	4041	ADP	O4'-C1'	-2.08	1.37	1.42
8	E	4041	ADP	C2-N1	2.08	1.37	1.33
8	C	4020	ADP	C2-N1	2.05	1.37	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	4047	ADP	O2A-PA-O3A	3.13	115.74	107.27
8	A	4006	ADP	O3'-C3'-C2'	2.86	120.99	111.82
8	G	4062	ADP	O2A-PA-O3A	2.71	114.59	107.27
8	G	4068	ADP	O3'-C3'-C2'	2.65	120.33	111.82
8	G	4068	ADP	O3B-PB-O3A	2.58	113.29	104.64
8	G	4062	ADP	O4'-C1'-N9	-2.57	103.15	108.09
8	E	4041	ADP	O3'-C3'-C2'	2.53	119.91	111.82
8	C	4026	ADP	O2A-PA-O3A	2.51	114.07	107.27
8	C	4026	ADP	O2'-C2'-C3'	2.51	119.85	111.82
8	A	4006	ADP	O2'-C2'-C3'	2.48	119.78	111.82
8	G	4062	ADP	O3'-C3'-C2'	2.41	119.53	111.82
8	C	4020	ADP	N6-C6-N1	-2.40	113.02	118.38
8	E	4047	ADP	C2'-C3'-C4'	-2.28	98.21	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	4068	ADP	O2'-C2'-C3'	2.27	119.08	111.82
8	E	4041	ADP	O2'-C2'-C3'	2.19	118.83	111.82
8	G	4068	ADP	O2A-PA-O3A	2.15	113.09	107.27
7	A	4010	ORN	CB-CA-C	-2.13	104.79	110.45
8	E	4041	ADP	O2A-PA-O3A	2.10	112.94	107.27
8	C	4026	ADP	C2'-C3'-C4'	-2.08	98.59	102.61
6	A	4005	PO4	O4-P-O2	2.06	114.33	107.91

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4010	ORN	N-CA-CB-CG
7	A	4010	ORN	C-CA-CB-CG
7	A	4030	ORN	N-CA-CB-CG
7	A	4030	ORN	C-CA-CB-CG
7	A	4051	ORN	N-CA-CB-CG
7	A	4051	ORN	C-CA-CB-CG
7	A	4072	ORN	N-CA-CB-CG
7	A	4072	ORN	C-CA-CB-CG
8	E	4047	ADP	PA-O3A-PB-O3B
8	G	4068	ADP	C5'-O5'-PA-O3A
7	A	4010	ORN	OXT-C-CA-N
7	A	4072	ORN	OXT-C-CA-N
8	A	4006	ADP	PA-O3A-PB-O1B
7	A	4010	ORN	CA-CB-CG-CD
7	A	4072	ORN	CA-CB-CG-CD
7	A	4051	ORN	CA-CB-CG-CD
7	A	4010	ORN	O-C-CA-N
7	A	4072	ORN	O-C-CA-N
7	A	4030	ORN	CA-CB-CG-CD
8	E	4041	ADP	PB-O3A-PA-O1A
7	A	4010	ORN	NE-CD-CG-CB
7	A	4030	ORN	NE-CD-CG-CB
9	E	4052	NET	C4-C3-N1-C7
8	G	4068	ADP	C5'-O5'-PA-O2A
9	E	4052	NET	C4-C3-N1-C5
8	A	4006	ADP	PB-O3A-PA-O2A
8	C	4020	ADP	PB-O3A-PA-O1A
8	E	4047	ADP	PB-O3A-PA-O2A
8	G	4068	ADP	PA-O3A-PB-O1B
7	A	4072	ORN	NE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
9	E	4052	NET	C4-C3-N1-C1
8	C	4020	ADP	PA-O3A-PB-O2B
8	A	4006	ADP	PB-O3A-PA-O1A
8	E	4047	ADP	PA-O3A-PB-O1B
8	A	4000	ADP	PB-O3A-PA-O2A
8	E	4041	ADP	PB-O3A-PA-O2A
8	G	4068	ADP	PB-O3A-PA-O2A

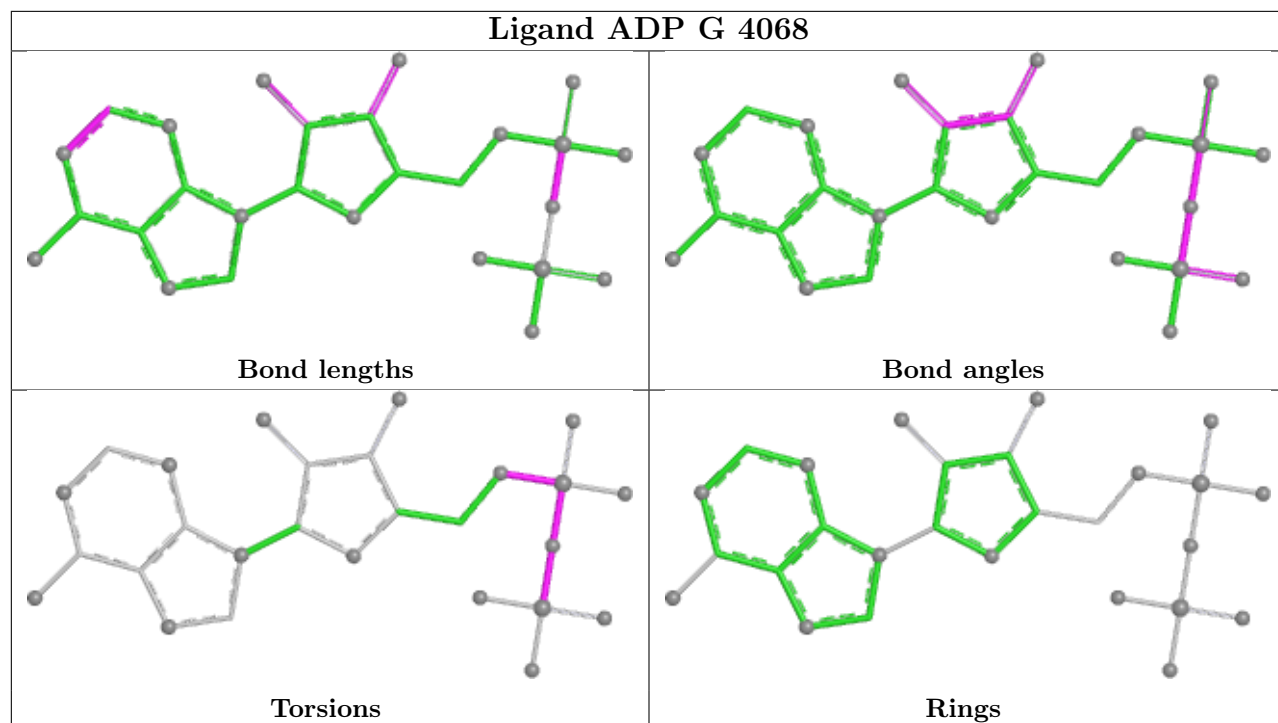
There are no ring outliers.

8 monomers are involved in 9 short contacts:

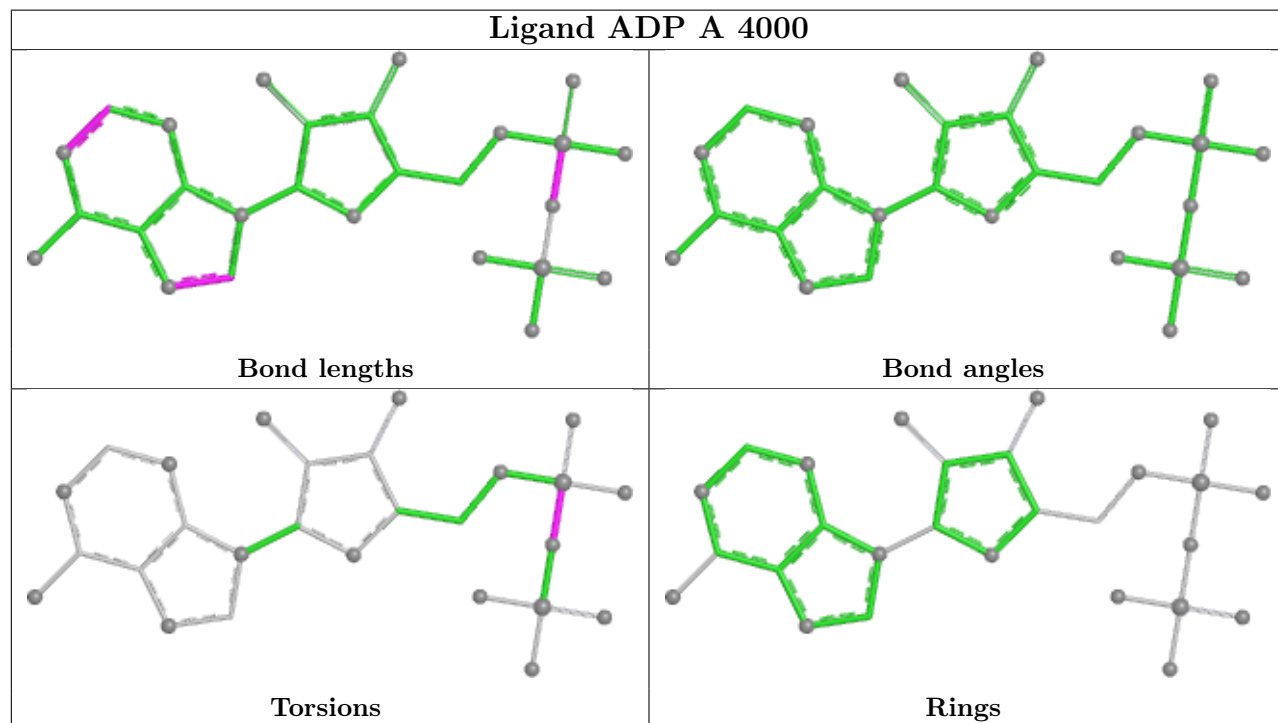
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4000	ADP	1	0
7	A	4030	ORN	1	0
8	E	4041	ADP	1	0
6	C	4025	PO4	1	0
8	A	4006	ADP	1	0
8	E	4047	ADP	2	0
7	A	4051	ORN	1	0
8	G	4062	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

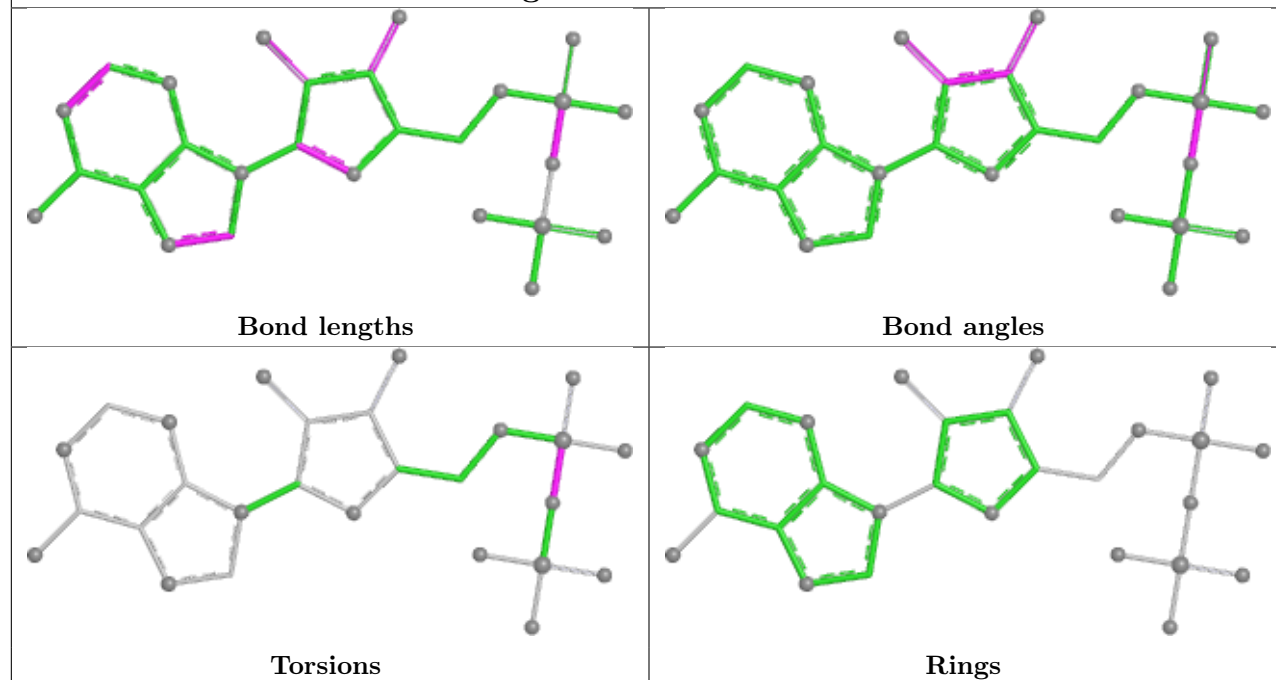
Ligand ADP G 4068



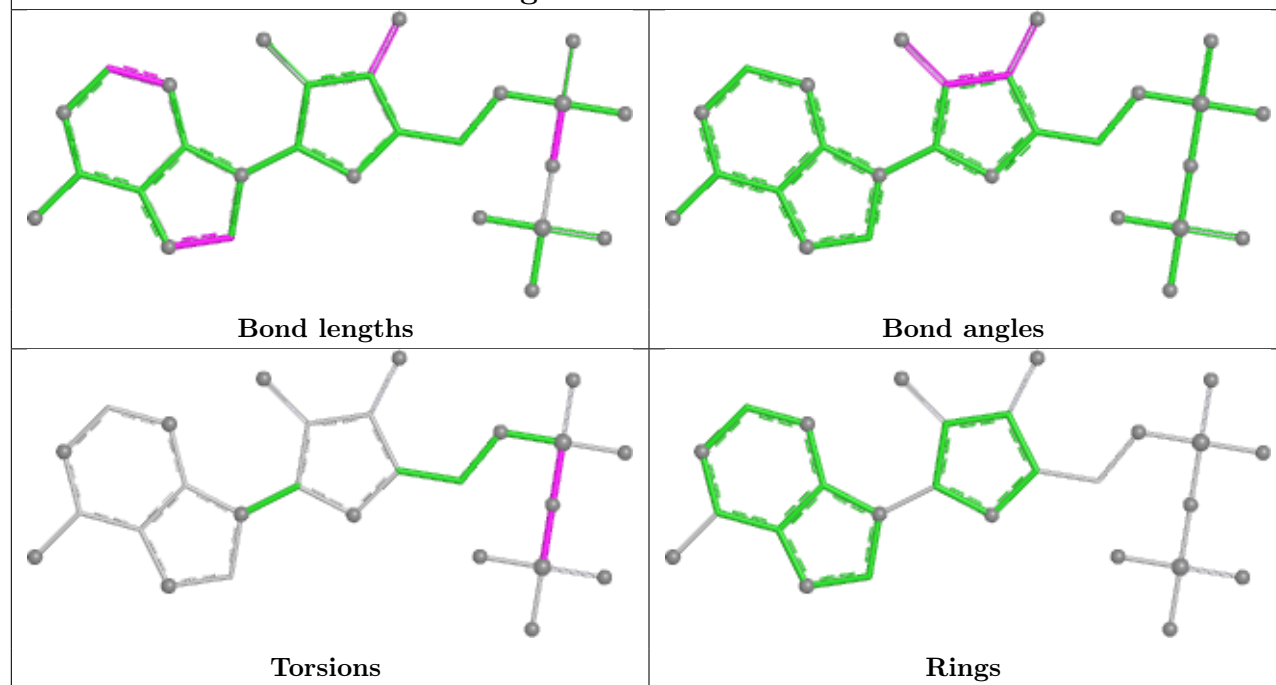
Ligand ADP A 4000



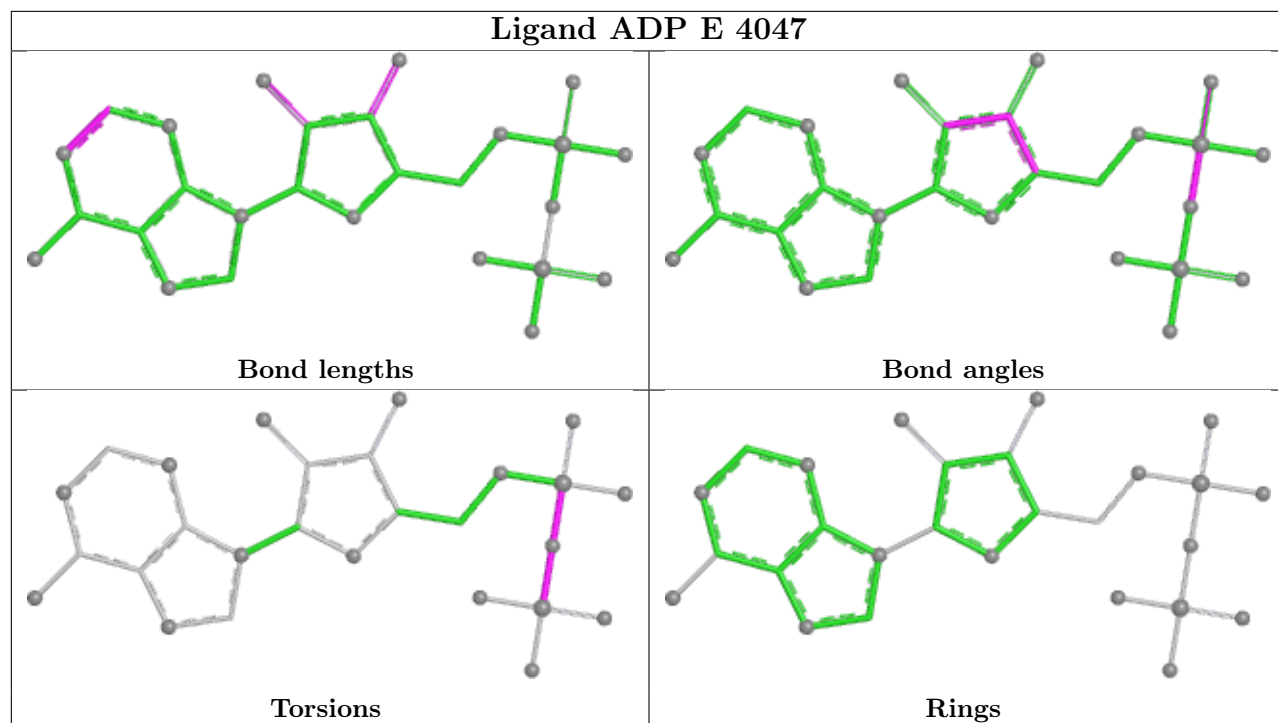
Ligand ADP E 4041



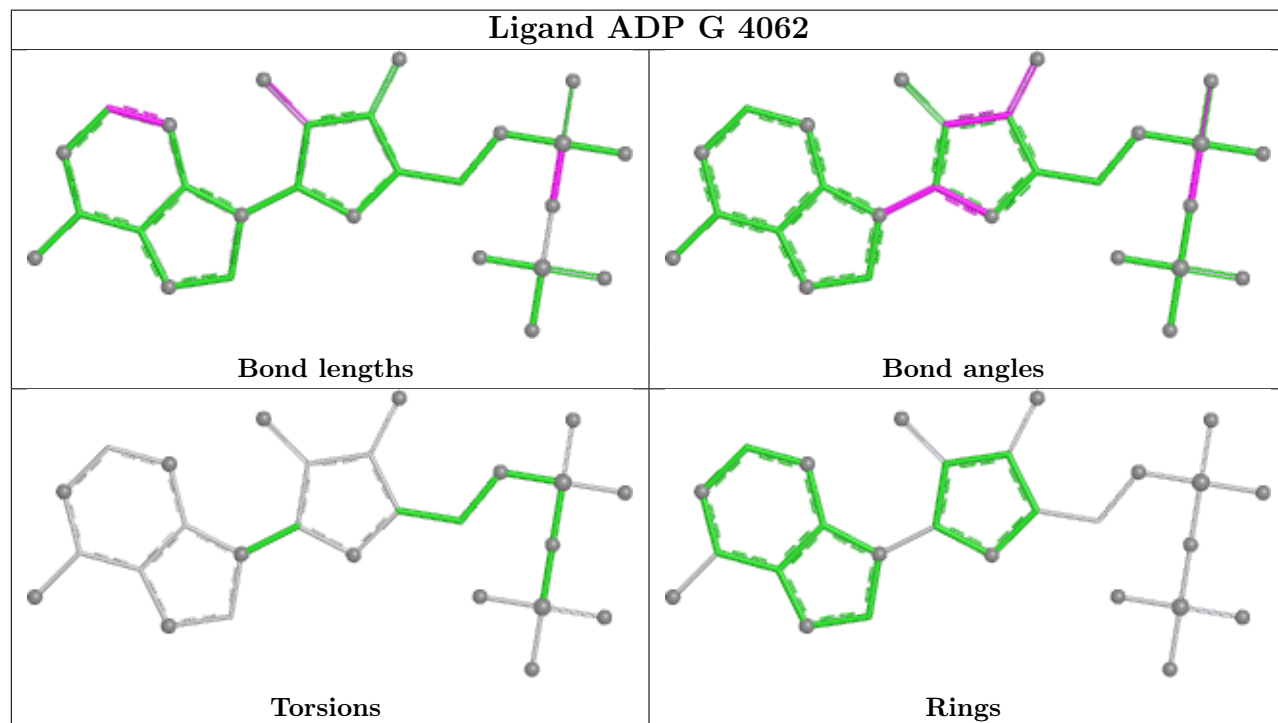
Ligand ADP A 4006

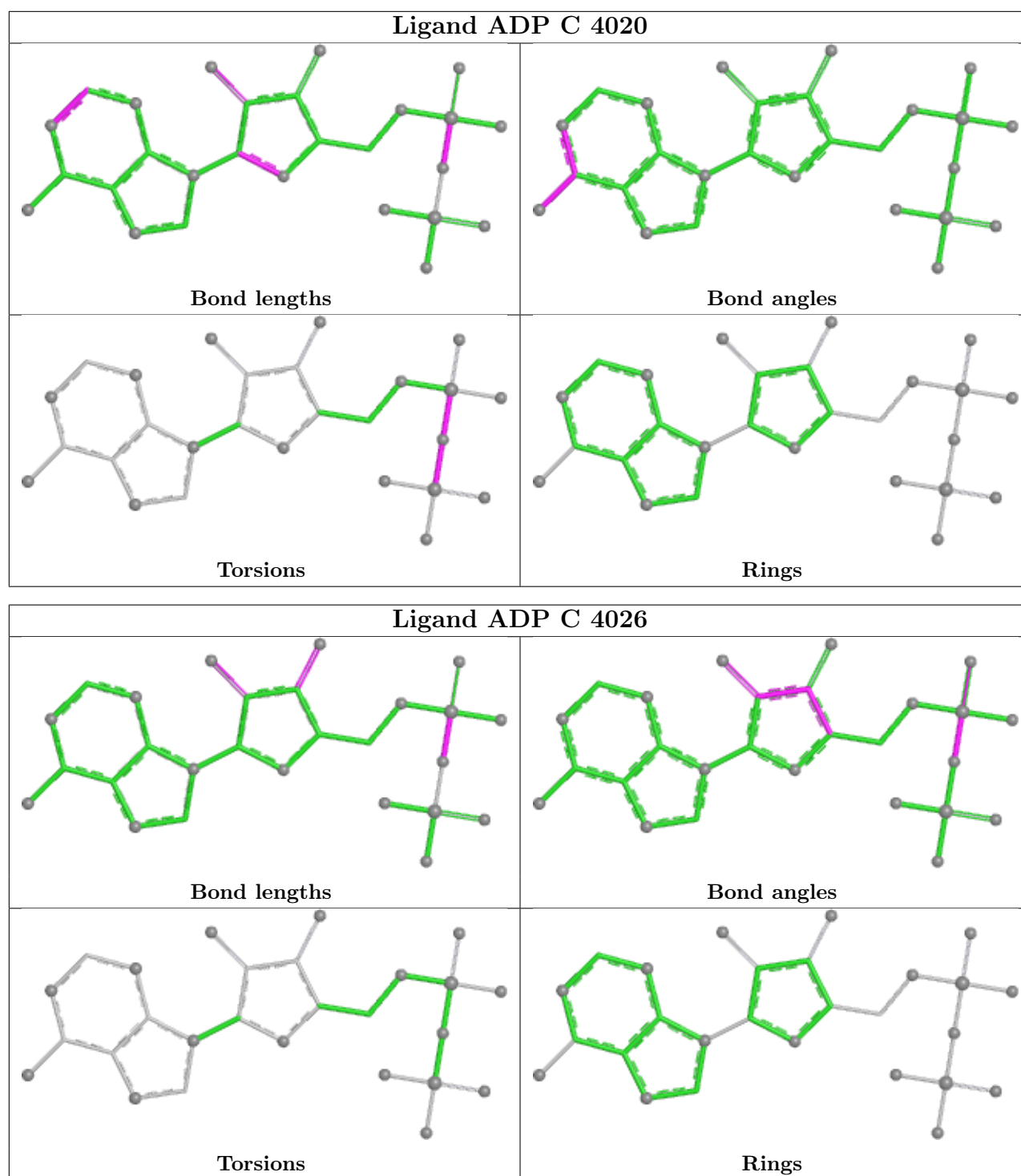


Ligand ADP E 4047



Ligand ADP G 4062





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.