



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1I41
Title : CYSTATHIONINE GAMMA-SYNTHASE IN COMPLEX WITH THE INHIBITOR APPA
Authors : Steegborn, C.; Laber, B.; Messerschmidt, A.; Huber, R.; Clausen, T.
Deposited on : 2001-02-19
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

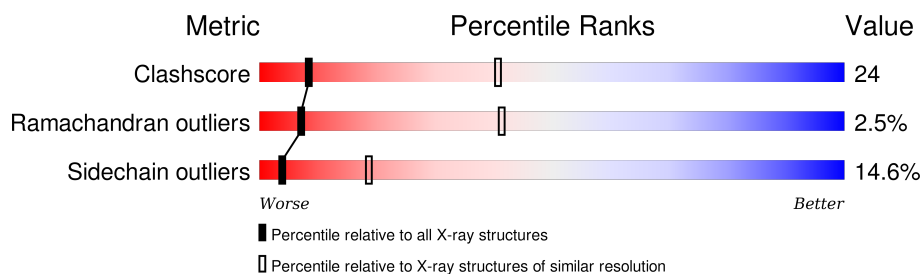
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)




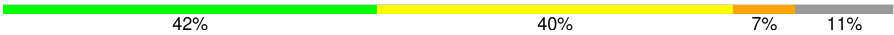
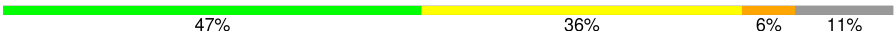
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	
1	B	445	
1	C	445	
1	D	445	
1	E	445	
1	F	445	
1	G	445	

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Mol	Chain	Length	Quality of chain
1	H	445	 42% 41% 7% 11%
1	I	445	 48% 36% 5% 11%
1	J	445	 43% 40% 6% 11%
1	K	445	 42% 40% 7% 11%
1	L	445	 47% 36% 6% 11%

2 Entry composition

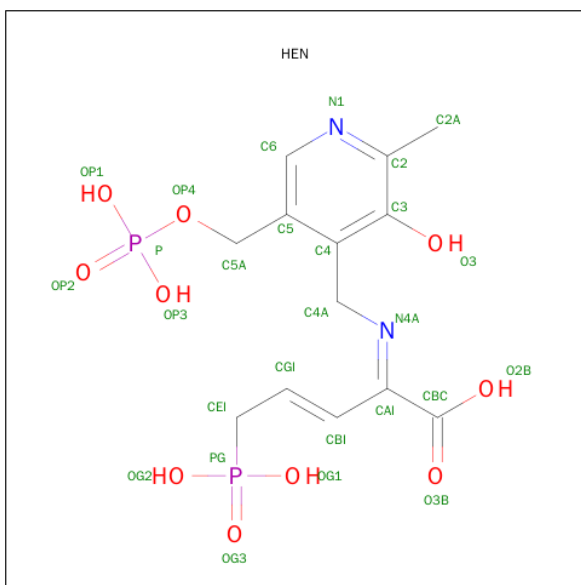
There are 2 unique types of molecules in this entry. The entry contains 36600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYSTATHIONINE GAMMA-SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	B	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	C	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	D	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	E	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	F	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	G	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	H	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	I	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	J	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	K	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	L	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYL)-IMINO]-5-PHOSPHONO-PENT-3-ENOIC ACID (three-letter code: HEN) (formula: C₁₃H₁₈N₂O₁₀P₂).

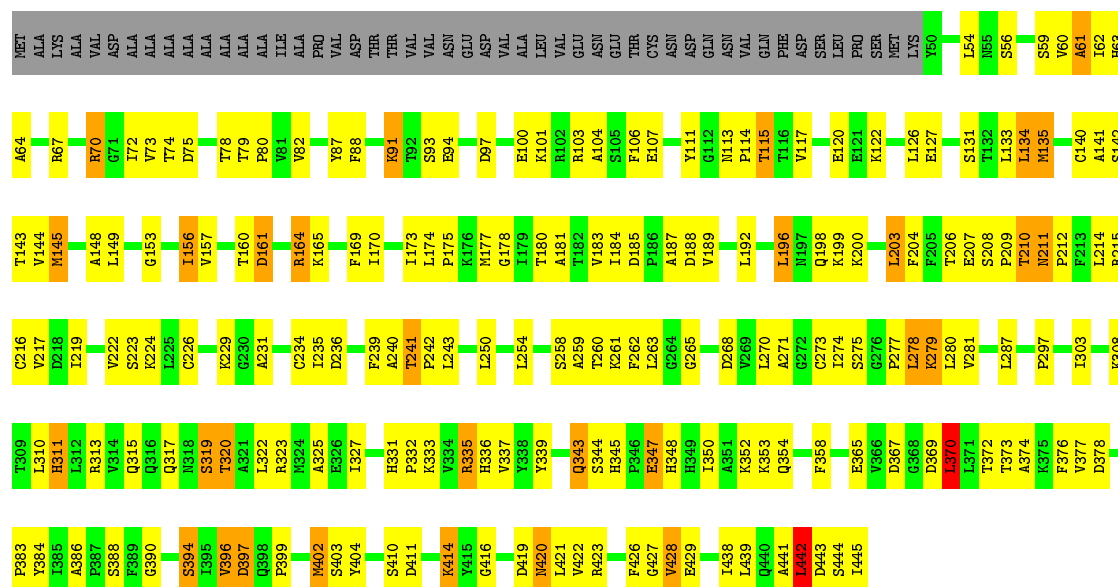


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	B	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	C	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	D	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	E	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	F	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	G	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	H	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	I	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	J	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	K	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	L	1	Total 27	C 13	N 2	O 10	P 2	0	0



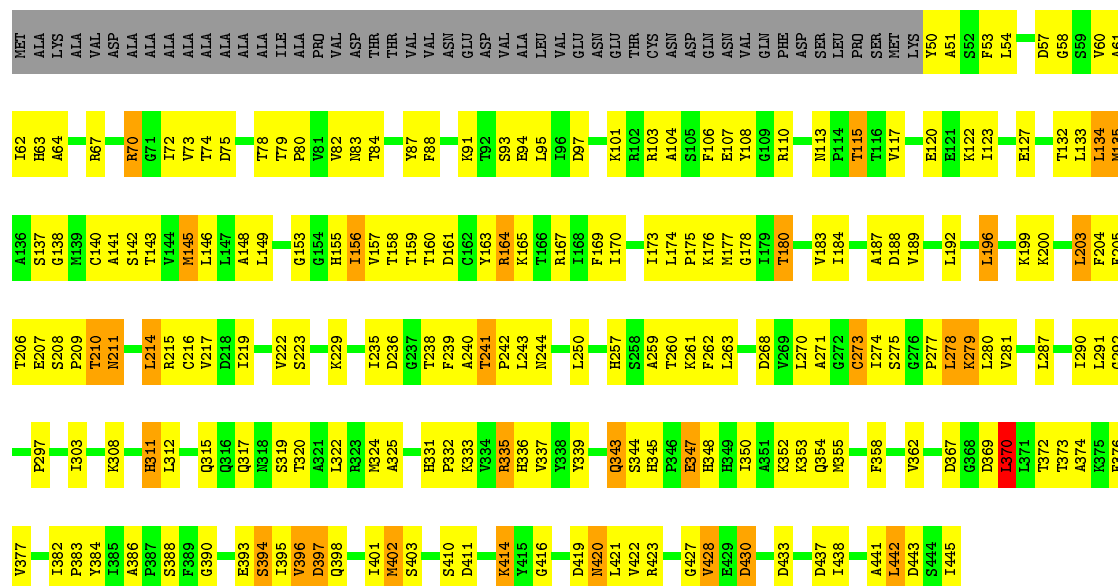
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain C: 44% 38% 7% 11%



• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain D: 42% 40% 7% 11%

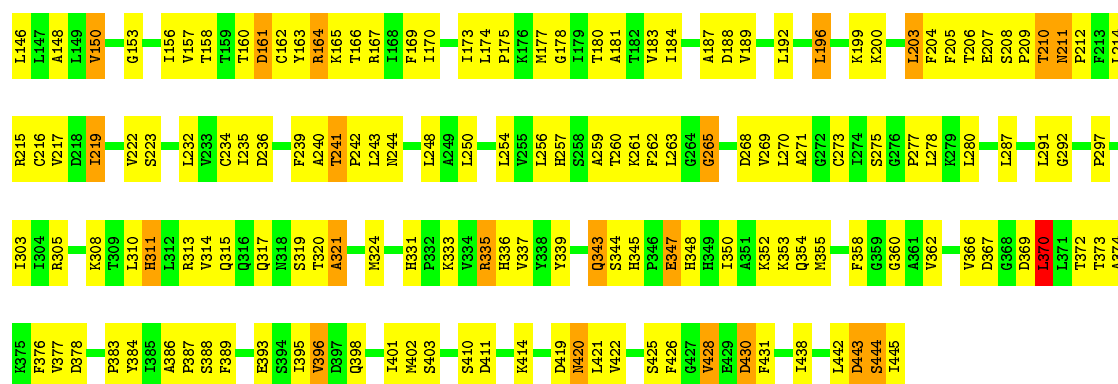


• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

D387	Q318	T238	V157	A64	MET
Q398	S319	F239	T158		ALA
P399	T320	A240	T159	R67	LVS
	A321	T241	T160		ALA
A401	L322	P242	D161	R70	VAL
M402		L243	C162	G71	ASP
S403	A325	D244	V163	I72	ALA
		Q245	R164		ALA
S408	H331	L250	K165	T78	ALA
A409	P332			T79	ALA
S410	K333		I170	P80	ALA
D411	V334	L254		R61	ALA
	R335		I173	R82	ALA
K414	H336	H257	L174		ALA
Y415	V337	S258	P175	F88	IIE
G416	V338	A259	K176		ALA
I417	Y339	T260	M177	K91	P90
M418		K261	G178	I92	VAL
D419	Q343	F262	I179	S93	ASP
M420	S344	L263	T180	R94	THR
L421	H345	L264	A181	L95	THR
V422	P346				VAL
R423	E347	D268	I184	K101	VAL
	H348	V269			ASN
G427	H349	L270	A187	R110	GLU
V428	T350	A271	D188		ASP
E429	A351	C272	V189	M113	VAL
D430	K352	I274		P114	ALA
	K353	S275	L192	T115	LEU
I438	Q354	G276		T116	VAL
L439		T277	L196	V117	GLU
Q440	F358	L278		V118	ASN
A441		K279	K199	L119	GLU
L442	F364	L280	K200	E120	THR
D443		V281		F121	CYS
S444	D367		L203	K122	ASN
I445	G368	P285	P204		ASP
	P369	T286	F205	L126	GLU
	L370	L287	T206	E127	ASN
	L371		E207		VAL
	T372	I290	S208	L133	GLN
	K373	L291	P209	L134	PHE
	A374		T210	M135	ASP
	K375	A294	M211		SER
	F376		P212	C140	LEU
	V377	P297	F213	A141	P90
			L214	S142	SER
	P383	L302	R215	T143	THR
	K384	I303	C216	V144	MET
	L385	L304	V217	M145	LVS
	A386	R305	D218	L146	Y50
	P387		I219	L147	F54
	S388	L310		A148	L54
	G390	H311	V222	L149	N55
		R312	S223	V150	
		R313			S59
	E393	V314	C234	G153	V60
	S394	Q315	I235	G154	A61
	L395	G316	D236	H155	I62
	T396	R317	C237	T156	H63

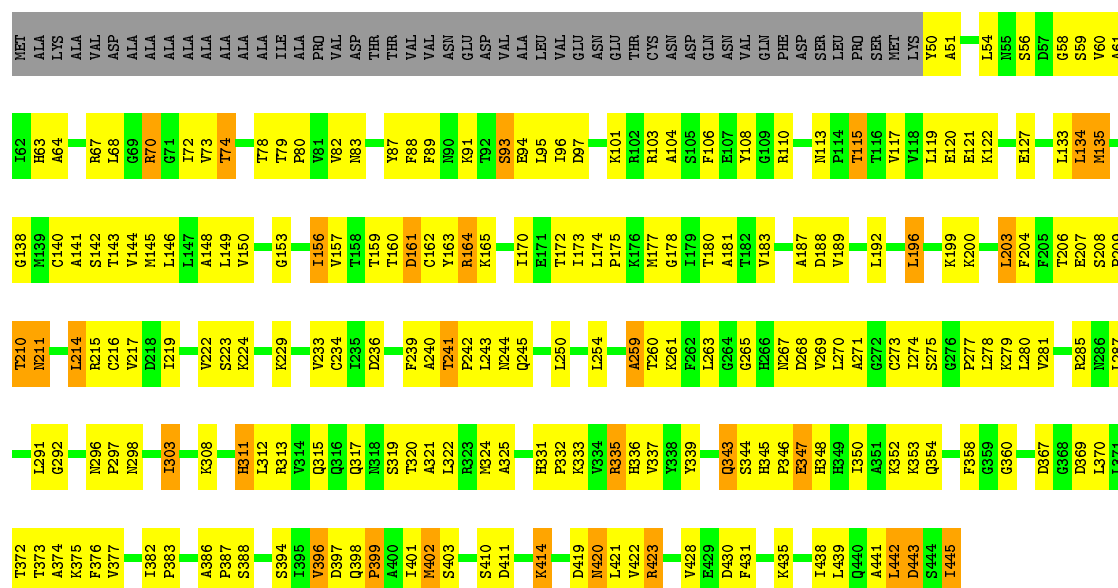
A386	P297	S208	G138	A61	MET
P387	I303	P209	M139	I62	LYS
S388		T210	C140	H63	ALA
		N211	A141	A64	ALA
E393	K308	P212	S142	R67	VAL
	T309	F213	T143		ASP
V396	L310	L214	V144		ALA
D397	R311	R215	M145	R70	ALA
K398	H312	C216	L146	G71	ALA
P399	R313	V217	L147	I72	ALA
A400		D218	A148	V73	ALA
I401	Q317	I219	L149	T74	ALA
M402	N318	V222	V150		ALA
S403	T320	S223	G153	T78	ALA
		K224		P80	ILE
S410				V81	ALA
D411	K324	K229	I156	V82	PRO
			V157	N83	VAL
K414	K333	V233	T158		ASP
Y415	V334	C234	T159	T84	THR
G416	K335	D235	D161	S85	THR
I417	H336	D236	I162	A86	VAL
H418	V337		V163	Y87	VAL
D419	T338	A240	R164	F88	ASN
M420	Y339	T241	T165	S93	GLU
L421		P242	K166	E94	ASP
V422	Q343	L243	R167		VAL
	S344			D97	ALA
G427	H345	L250	I170		LEU
V428	P346			K101	VAL
E429	E347	H257	I173	R102	GLU
D430	H348	S258	L174	R103	ASN
F431	K349	A259	P175	A104	GLU
	T350	T260	K176	S105	THR
D437	K351	K261	K177	F106	CYS
	K352	F262	G178	E107	ASN
L442	K353	L263	I179		ASP
D443	K354	D268	T180	G112	GLN
I444		V269	A181	N113	ASN
I445	F358	L270	L182	P114	VAL
			V183	T115	GLN
	E365	C273	I184	T116	PHE
	V366	I274	A187	V117	ASP
	D367	S275	D188	V118	SER
	G368	G276	V189	L119	LEU
	D369	T277		E120	PRO
L370	L371	L278	L192	E121	SER
T372	T373	K279		E121	MET
A374	A374	V281	L196	K122	LYS
K375	K375	S282	K199	L126	Y50
F376	F376	R285	K200	E127	A51
V377	V377	N286			S52
		L287			F53
					S54
					L54
					N55
					S56
					D57
					G58
					S59
					V60
					S197

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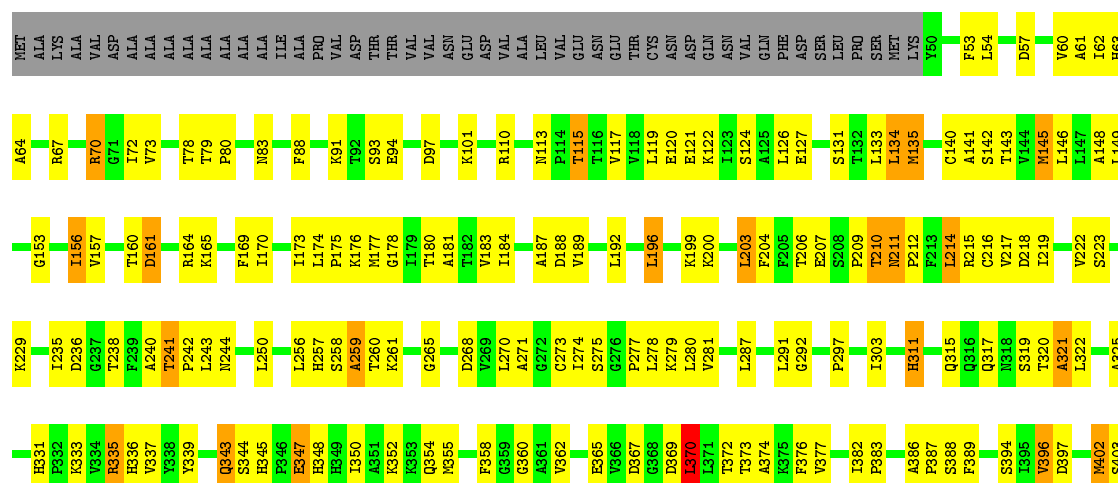
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain H: 42% 41% 7% 11%



• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

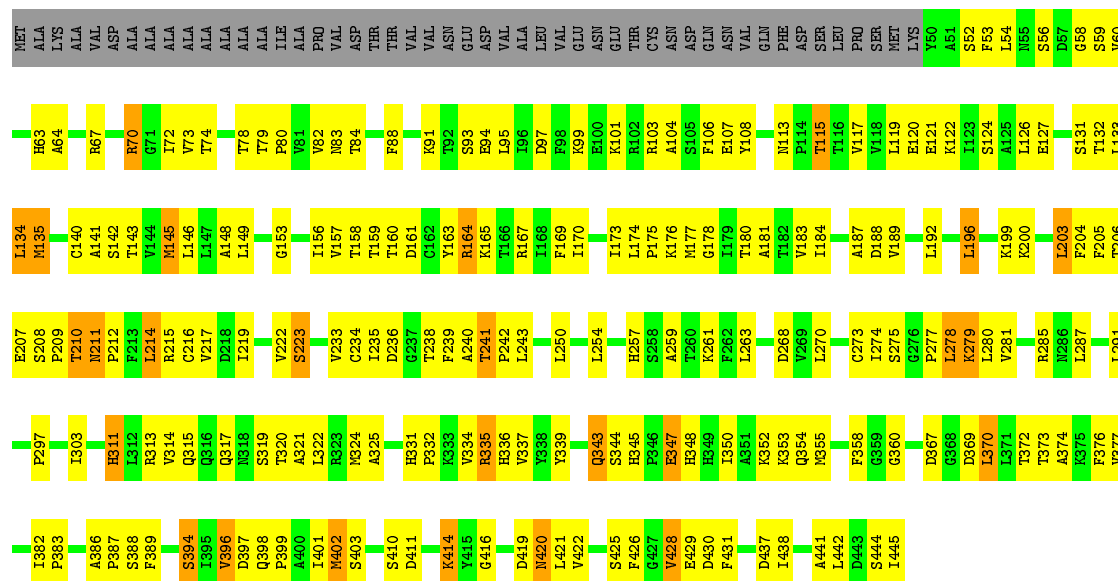
Chain I: 48% 36% 5% 11%





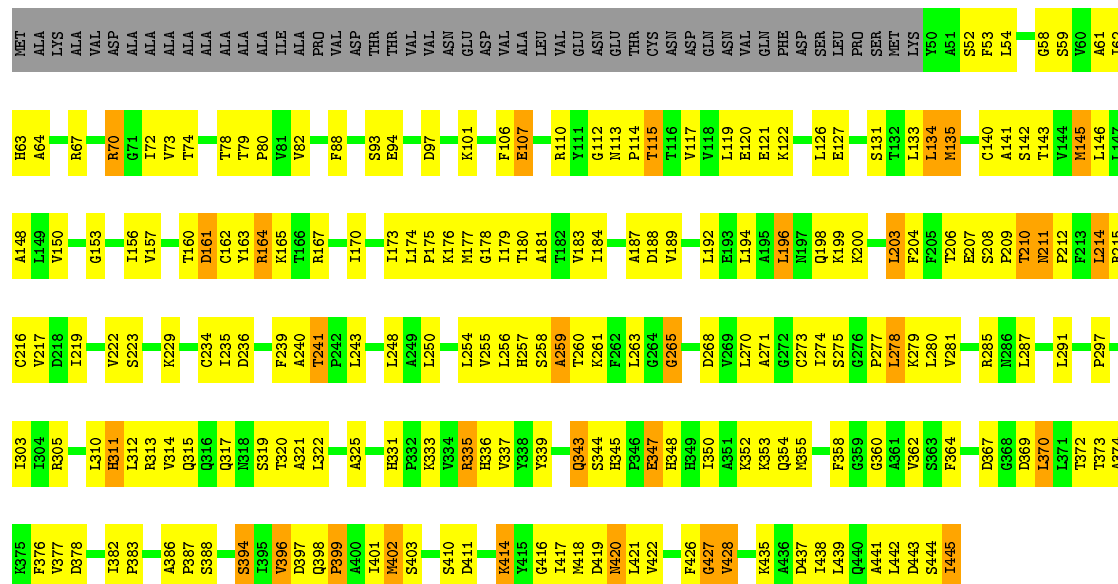
- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain J: 43% 40% 6% 11%



- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain K: 42% 40% 7% 11%



- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain L:  47% 36% 6% 11%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	312.20Å 166.00Å 161.80Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.239 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36600	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: HEN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3082	0.53	0/4179
1	B	0.31	0/3082	0.52	0/4179
1	C	0.32	0/3082	0.52	0/4179
1	D	0.32	0/3082	0.52	0/4179
1	E	0.33	0/3082	0.53	0/4179
1	F	0.32	0/3082	0.53	0/4179
1	G	0.33	0/3082	0.52	0/4179
1	H	0.33	0/3082	0.53	0/4179
1	I	0.32	0/3082	0.52	0/4179
1	J	0.31	0/3082	0.52	0/4179
1	K	0.31	0/3082	0.52	0/4179
1	L	0.31	0/3082	0.52	0/4179
All	All	0.32	0/36984	0.52	0/50148

There are no bond length outliers.

There are no bond angle outliers.

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	3023	0	3054	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3023	0	3054	167	0
1	C	3023	0	3054	159	0
1	D	3023	0	3054	159	0
1	E	3023	0	3054	155	0
1	F	3023	0	3054	160	0
1	G	3023	0	3054	156	0
1	H	3023	0	3054	164	0
1	I	3023	0	3054	141	0
1	J	3023	0	3054	155	0
1	K	3023	0	3054	153	0
1	L	3023	0	3054	131	0
2	A	27	0	12	3	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	27	0	12	2	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	1	0
2	H	27	0	12	2	0
2	I	27	0	12	2	0
2	J	27	0	12	1	0
2	K	27	0	12	1	0
2	L	27	0	12	1	0
All	All	36600	0	36792	1765	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 24.

All (1765) 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:F:64:ALA:HB3	1:F:122:LYS:HG3	1.44	0.98
1:L:54:LEU:HD22	1:L:59:SER:HB3	1.45	0.97
1:A:145:MET:HE1	1:A:146:LEU:HD23	1.47	0.96
1:A:383:PRO:HB2	1:A:396:VAL:HG22	1.49	0.93
1:H:241:THR:HG22	1:H:243:LEU:H	1.31	0.92
1:C:54:LEU:HD22	1:C:59:SER:HB3	1.49	0.92
1:B:78:THR:HG21	1:C:268:ASP:HB3	1.47	0.92
1:L:383:PRO:HB2	1:L:396:VAL:HG22	1.51	0.90
1:H:383:PRO:HB2	1:H:396:VAL:HG22	1.53	0.90
1:D:383:PRO:HB2	1:D:396:VAL:HG22	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:PHE:HB2	1:D:445:ILE:HD11	1.54	0.90
1:I:241:THR:HG22	1:I:243:LEU:H	1.36	0.89
1:D:64:ALA:HB3	1:D:122:LYS:HG3	1.53	0.89
1:D:241:THR:HG22	1:D:243:LEU:H	1.38	0.89
1:J:241:THR:HG22	1:J:243:LEU:H	1.35	0.88
1:J:383:PRO:HB2	1:J:396:VAL:HG22	1.54	0.88
1:K:438:ILE:O	1:K:441:ALA:HB3	1.73	0.87
1:G:383:PRO:HB2	1:G:396:VAL:HG22	1.56	0.87
1:F:383:PRO:HB2	1:F:396:VAL:HG22	1.56	0.86
1:K:241:THR:HG22	1:K:243:LEU:H	1.40	0.86
1:E:383:PRO:HB2	1:E:396:VAL:HG22	1.55	0.86
1:C:241:THR:HG22	1:C:243:LEU:H	1.39	0.86
1:J:207:GLU:HB3	1:J:236:ASP:HB3	1.58	0.86
1:I:383:PRO:HB2	1:I:396:VAL:HG22	1.57	0.85
1:G:210:THR:HG22	1:G:215:ARG:H	1.40	0.85
1:C:383:PRO:HB2	1:C:396:VAL:HG22	1.58	0.84
1:D:207:GLU:HB3	1:D:236:ASP:HB3	1.57	0.84
1:L:207:GLU:HB3	1:L:236:ASP:HB3	1.59	0.84
1:B:383:PRO:HB2	1:B:396:VAL:HG22	1.59	0.84
1:E:64:ALA:HB3	1:E:122:LYS:HG3	1.59	0.83
1:J:210:THR:HG22	1:J:215:ARG:H	1.41	0.83
1:I:207:GLU:HB3	1:I:236:ASP:HB3	1.59	0.82
1:A:64:ALA:HB3	1:A:122:LYS:HG3	1.59	0.82
1:L:115:THR:HG21	1:L:297:PRO:HB3	1.61	0.82
1:B:207:GLU:HB3	1:B:236:ASP:HB3	1.61	0.82
1:G:64:ALA:HB3	1:G:122:LYS:HG3	1.58	0.82
1:J:240:ALA:O	1:J:241:THR:HB	1.78	0.82
1:B:268:ASP:HB3	1:C:78:THR:HG21	1.61	0.82
1:J:170:ILE:HA	1:J:174:LEU:HD12	1.59	0.82
1:C:210:THR:HG22	1:C:215:ARG:H	1.44	0.82
1:F:442:LEU:HA	1:F:445:ILE:HD12	1.59	0.82
1:K:145:MET:HE1	1:K:146:LEU:HD23	1.60	0.82
1:I:64:ALA:HB3	1:I:122:LYS:HG3	1.61	0.81
1:K:210:THR:HG22	1:K:215:ARG:H	1.44	0.81
1:A:207:GLU:HB3	1:A:236:ASP:HB3	1.63	0.81
1:I:240:ALA:O	1:I:241:THR:HB	1.79	0.81
1:K:240:ALA:O	1:K:241:THR:HB	1.80	0.81
1:H:210:THR:HG22	1:H:215:ARG:H	1.43	0.81
1:F:120:GLU:HG3	1:F:134:LEU:HD12	1.63	0.81
1:K:207:GLU:HB3	1:K:236:ASP:HB3	1.63	0.81
1:H:207:GLU:HB3	1:H:236:ASP:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ALA:O	1:B:241:THR:HB	1.80	0.80
1:E:145:MET:HE1	1:E:146:LEU:HD23	1.64	0.80
1:L:240:ALA:O	1:L:241:THR:HB	1.81	0.80
1:B:115:THR:HG21	1:B:297:PRO:HB3	1.63	0.80
1:C:64:ALA:HB3	1:C:122:LYS:HG3	1.62	0.79
1:F:241:THR:HG22	1:F:243:LEU:H	1.47	0.79
1:I:210:THR:HG22	1:I:215:ARG:H	1.47	0.79
1:B:210:THR:HG22	1:B:215:ARG:H	1.45	0.79
1:D:240:ALA:O	1:D:241:THR:HB	1.82	0.79
1:F:216:CYS:H	1:F:347:GLU:HG3	1.48	0.79
1:E:54:LEU:HD22	1:E:59:SER:HB3	1.65	0.79
1:E:210:THR:HG22	1:E:215:ARG:H	1.48	0.79
1:L:241:THR:HG22	1:L:243:LEU:H	1.49	0.78
1:H:240:ALA:O	1:H:241:THR:HB	1.83	0.78
1:C:207:GLU:HB3	1:C:236:ASP:HB3	1.66	0.78
1:C:170:ILE:HA	1:C:174:LEU:HD12	1.64	0.78
1:C:115:THR:HG21	1:C:297:PRO:HB3	1.66	0.77
1:D:135:MET:HE2	1:D:141:ALA:HA	1.65	0.77
1:I:261:LYS:NZ	1:I:388:SER:HA	1.99	0.77
1:C:240:ALA:O	1:C:241:THR:HB	1.82	0.77
1:L:210:THR:HG22	1:L:215:ARG:H	1.48	0.77
1:C:120:GLU:HG3	1:C:134:LEU:HD12	1.66	0.77
1:B:241:THR:HG22	1:B:243:LEU:H	1.48	0.77
1:E:216:CYS:H	1:E:347:GLU:HG3	1.47	0.77
1:E:207:GLU:HB3	1:E:236:ASP:HB3	1.67	0.77
1:F:261:LYS:HZ3	1:F:388:SER:HA	1.49	0.76
1:G:241:THR:HG22	1:G:243:LEU:H	1.49	0.76
1:A:240:ALA:O	1:A:241:THR:HB	1.84	0.76
1:B:53:PHE:HZ	1:B:68:LEU:HD21	1.50	0.76
1:G:207:GLU:HB3	1:G:236:ASP:HB3	1.67	0.75
1:G:135:MET:HE2	1:G:141:ALA:HA	1.68	0.75
1:K:383:PRO:HB2	1:K:396:VAL:HG22	1.69	0.75
1:B:216:CYS:H	1:B:347:GLU:HG3	1.51	0.75
1:G:120:GLU:HG3	1:G:134:LEU:HD12	1.69	0.75
1:D:210:THR:HG22	1:D:215:ARG:H	1.51	0.75
1:E:240:ALA:O	1:E:241:THR:HB	1.85	0.75
1:C:370:LEU:HD23	1:C:419:ASP:HB3	1.69	0.75
1:G:240:ALA:O	1:G:241:THR:HB	1.87	0.75
1:L:120:GLU:HG3	1:L:134:LEU:HD12	1.67	0.75
1:I:120:GLU:HG3	1:I:134:LEU:HD12	1.69	0.74
1:J:156:ILE:HG13	1:J:203:LEU:HD23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:113:ASN:ND2	1:K:297:PRO:HG3	2.02	0.73
1:A:238:THR:HB	2:A:500:HEN:H2A2	1.70	0.73
1:A:210:THR:HG22	1:A:215:ARG:H	1.52	0.73
1:F:261:LYS:NZ	1:F:388:SER:HA	2.03	0.73
1:I:211:ASN:HD22	1:I:211:ASN:C	1.92	0.73
1:J:120:GLU:HG3	1:J:134:LEU:HD12	1.71	0.73
1:F:250:LEU:HD11	1:F:354:GLN:HB2	1.71	0.73
1:E:241:THR:HG22	1:E:243:LEU:H	1.52	0.72
1:A:170:ILE:HA	1:A:174:LEU:HD12	1.70	0.72
1:A:241:THR:HG22	1:A:243:LEU:H	1.54	0.72
1:L:64:ALA:HB3	1:L:122:LYS:HG3	1.71	0.72
1:K:115:THR:HG21	1:K:297:PRO:HB3	1.70	0.72
1:G:170:ILE:HA	1:G:174:LEU:HD12	1.71	0.72
1:D:120:GLU:HG3	1:D:134:LEU:HD12	1.70	0.72
1:A:211:ASN:HD22	1:A:211:ASN:C	1.93	0.72
1:E:261:LYS:NZ	1:E:388:SER:HA	2.05	0.72
1:G:145:MET:HE1	1:G:146:LEU:HD23	1.71	0.72
1:A:261:LYS:NZ	1:A:388:SER:HA	2.05	0.72
1:A:370:LEU:HD23	1:A:419:ASP:HB3	1.72	0.71
1:D:250:LEU:HD11	1:D:354:GLN:HB2	1.72	0.71
1:F:210:THR:HG22	1:F:215:ARG:H	1.55	0.71
1:G:370:LEU:HD23	1:G:419:ASP:HB3	1.70	0.71
1:K:170:ILE:HA	1:K:174:LEU:HD12	1.73	0.71
1:J:54:LEU:HD22	1:J:59:SER:HB3	1.71	0.71
1:K:313:ARG:O	1:K:317:GLN:HG3	1.90	0.71
1:B:335:ARG:HH21	1:B:367:ASP:HA	1.55	0.71
1:J:216:CYS:H	1:J:347:GLU:HG3	1.56	0.70
1:D:335:ARG:HH21	1:D:367:ASP:HA	1.55	0.70
1:G:216:CYS:H	1:G:347:GLU:HG3	1.54	0.70
1:J:64:ALA:HB3	1:J:122:LYS:HG3	1.73	0.70
1:F:240:ALA:O	1:F:241:THR:HB	1.91	0.70
1:L:216:CYS:H	1:L:347:GLU:HG3	1.57	0.70
1:L:347:GLU:HB3	1:L:350:ILE:HD12	1.72	0.70
1:H:64:ALA:HB3	1:H:122:LYS:HG3	1.73	0.70
1:E:250:LEU:HD11	1:E:354:GLN:HB2	1.72	0.70
1:E:261:LYS:HZ3	1:E:388:SER:HA	1.57	0.69
1:K:411:ASP:O	1:K:414:LYS:HB2	1.92	0.69
1:H:156:ILE:HG12	1:H:157:VAL:N	2.07	0.69
1:A:216:CYS:H	1:A:347:GLU:HG3	1.57	0.69
1:C:127:GLU:OE2	1:C:242:PRO:HB3	1.93	0.69
1:A:438:ILE:O	1:A:442:LEU:HD12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HD3	1:B:79:THR:OG1	1.90	0.69
1:A:259:ALA:HB3	1:A:271:ALA:HB3	1.73	0.69
1:E:78:THR:HG21	1:H:268:ASP:HB3	1.74	0.69
1:F:268:ASP:HB3	1:G:78:THR:HG21	1.73	0.69
1:K:64:ALA:HB3	1:K:122:LYS:HG3	1.75	0.69
1:K:343:GLN:HA	1:K:348:HIS:CD2	2.28	0.68
1:L:335:ARG:HH21	1:L:367:ASP:HA	1.59	0.68
1:D:343:GLN:HA	1:D:348:HIS:CD2	2.28	0.68
1:B:64:ALA:HB3	1:B:122:LYS:HG3	1.74	0.68
1:H:120:GLU:HG3	1:H:134:LEU:HD12	1.75	0.68
1:J:343:GLN:HA	1:J:348:HIS:CD2	2.28	0.68
1:K:277:PRO:HG2	1:K:280:LEU:HB2	1.74	0.68
1:H:170:ILE:HA	1:H:174:LEU:HD12	1.76	0.67
1:E:140:CYS:O	1:E:144:VAL:HG23	1.93	0.67
1:K:211:ASN:HD22	1:K:211:ASN:C	1.97	0.67
1:H:145:MET:HE3	1:H:149:LEU:HD12	1.74	0.67
1:G:211:ASN:HD22	1:G:211:ASN:C	1.97	0.67
1:L:145:MET:HE1	1:L:146:LEU:HD23	1.75	0.67
1:G:115:THR:HG21	1:G:297:PRO:HB3	1.75	0.67
1:K:370:LEU:HD23	1:K:419:ASP:HB3	1.76	0.67
1:C:211:ASN:HD22	1:C:211:ASN:C	1.98	0.67
1:E:268:ASP:HB3	1:H:78:THR:HG21	1.76	0.67
1:L:250:LEU:HD11	1:L:354:GLN:HB2	1.76	0.67
1:J:78:THR:HG21	1:K:268:ASP:HB3	1.76	0.67
1:E:170:ILE:HA	1:E:174:LEU:HD12	1.77	0.67
1:E:291:LEU:HD22	1:G:143:THR:HG21	1.76	0.67
1:I:145:MET:HE1	1:I:146:LEU:HD23	1.77	0.67
1:G:54:LEU:CD2	1:G:59:SER:HB3	2.25	0.66
1:B:133:LEU:HD23	1:B:135:MET:HE3	1.76	0.66
1:E:345:HIS:CE1	1:E:347:GLU:HG2	2.30	0.66
1:B:331:HIS:CD2	1:B:442:LEU:HD13	2.30	0.66
1:C:156:ILE:HG13	1:C:203:LEU:HD23	1.77	0.66
1:A:156:ILE:HG12	1:A:157:VAL:N	2.08	0.66
1:J:347:GLU:HB3	1:J:350:ILE:HD12	1.78	0.66
1:J:115:THR:HG21	1:J:297:PRO:HB3	1.78	0.66
1:G:54:LEU:HD22	1:G:59:SER:HB3	1.78	0.66
1:H:148:ALA:HB2	1:H:287:LEU:HD23	1.77	0.66
1:H:115:THR:HG21	1:H:297:PRO:HB3	1.77	0.66
1:I:115:THR:HG21	1:I:297:PRO:HB3	1.78	0.66
1:J:268:ASP:HB3	1:K:78:THR:HG21	1.78	0.66
1:K:216:CYS:H	1:K:347:GLU:HG3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:156:ILE:HG12	1:L:157:VAL:N	2.11	0.65
1:E:115:THR:HG21	1:E:297:PRO:HB3	1.76	0.65
1:B:62:ILE:HD11	1:C:428:VAL:HG12	1.78	0.65
1:L:113:ASN:ND2	1:L:297:PRO:HG3	2.12	0.65
1:F:78:THR:HG21	1:G:268:ASP:HB3	1.78	0.65
1:I:261:LYS:HZ3	1:I:388:SER:HA	1.60	0.65
1:K:135:MET:HE2	1:K:141:ALA:HA	1.79	0.65
1:E:156:ILE:HG12	1:E:157:VAL:N	2.12	0.65
1:D:370:LEU:HD23	1:D:419:ASP:HB3	1.78	0.65
1:A:250:LEU:HD11	1:A:354:GLN:HB2	1.78	0.65
1:D:115:THR:HG21	1:D:297:PRO:HB3	1.78	0.65
1:H:335:ARG:HH21	1:H:367:ASP:HA	1.61	0.65
1:B:369:ASP:H	1:B:372:THR:HB	1.61	0.65
1:J:145:MET:HE1	1:J:146:LEU:HD23	1.79	0.64
1:D:261:LYS:NZ	1:D:388:SER:HA	2.12	0.64
1:C:148:ALA:HB2	1:C:287:LEU:HD23	1.79	0.64
1:F:343:GLN:HA	1:F:348:HIS:CD2	2.33	0.64
1:A:78:THR:HG21	1:D:268:ASP:HB3	1.78	0.64
1:I:421:LEU:HD12	1:I:422:VAL:N	2.13	0.64
1:I:156:ILE:HG12	1:I:157:VAL:N	2.11	0.64
1:H:216:CYS:H	1:H:347:GLU:HG3	1.63	0.64
1:H:343:GLN:HA	1:H:348:HIS:CD2	2.33	0.64
1:G:148:ALA:HB2	1:G:287:LEU:HD23	1.79	0.64
1:F:277:PRO:HG2	1:F:280:LEU:HB2	1.78	0.64
1:H:261:LYS:NZ	1:H:388:SER:HA	2.11	0.64
1:E:331:HIS:CE1	1:E:333:LYS:HB2	2.33	0.64
1:K:250:LEU:HD11	1:K:354:GLN:HB2	1.79	0.64
1:D:63:HIS:HB3	1:D:67:ARG:HB2	1.79	0.64
1:G:51:ALA:HB3	1:G:54:LEU:HB2	1.79	0.64
1:F:207:GLU:HB3	1:F:236:ASP:HB3	1.78	0.64
1:D:170:ILE:HA	1:D:174:LEU:HD12	1.78	0.63
1:A:113:ASN:ND2	1:A:297:PRO:HG3	2.14	0.63
1:H:54:LEU:HD23	1:H:59:SER:HB3	1.81	0.63
1:G:345:HIS:CE1	1:G:347:GLU:HG2	2.34	0.63
1:F:335:ARG:HH21	1:F:367:ASP:HA	1.64	0.63
1:I:216:CYS:H	1:I:347:GLU:HG3	1.62	0.63
1:F:170:ILE:HA	1:F:174:LEU:HD12	1.80	0.63
1:E:370:LEU:HD23	1:E:419:ASP:HB3	1.78	0.63
1:G:343:GLN:HA	1:G:348:HIS:CD2	2.34	0.63
1:D:148:ALA:HB2	1:D:287:LEU:HD23	1.81	0.63
1:C:153:GLY:HA2	1:C:178:GLY:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HD23	1:B:419:ASP:HB3	1.80	0.63
1:G:156:ILE:HG12	1:G:157:VAL:N	2.14	0.63
1:L:343:GLN:HA	1:L:348:HIS:CD2	2.34	0.63
1:C:210:THR:HG23	1:C:211:ASN:N	2.13	0.62
1:B:438:ILE:O	1:B:441:ALA:HB3	1.99	0.62
1:B:156:ILE:HG12	1:B:157:VAL:N	2.12	0.62
1:G:113:ASN:ND2	1:G:297:PRO:HG3	2.14	0.62
1:A:115:THR:HG21	1:A:297:PRO:HB3	1.82	0.62
1:L:411:ASP:O	1:L:414:LYS:HB2	1.99	0.62
1:D:156:ILE:HG12	1:D:157:VAL:N	2.13	0.62
1:K:120:GLU:HG3	1:K:134:LEU:HD12	1.80	0.62
1:K:153:GLY:HA2	1:K:178:GLY:O	1.99	0.62
1:E:421:LEU:HD12	1:E:422:VAL:N	2.14	0.62
1:C:277:PRO:HG2	1:C:280:LEU:HB2	1.82	0.62
1:E:174:LEU:N	1:E:175:PRO:HD2	2.15	0.62
1:H:51:ALA:HB3	1:H:54:LEU:HD12	1.81	0.62
1:I:153:GLY:HA2	1:I:178:GLY:O	1.98	0.62
1:K:421:LEU:HD12	1:K:422:VAL:N	2.15	0.62
1:A:210:THR:HG23	1:A:211:ASN:N	2.15	0.62
1:H:397:ASP:HB2	1:H:402:MET:HG2	1.82	0.62
1:J:63:HIS:HB3	1:J:67:ARG:HB2	1.80	0.62
1:K:210:THR:HG23	1:K:211:ASN:N	2.15	0.61
1:E:120:GLU:HG3	1:E:134:LEU:HD12	1.82	0.61
1:E:345:HIS:HE1	1:E:347:GLU:HG2	1.63	0.61
1:A:261:LYS:HZ2	1:A:388:SER:HA	1.64	0.61
1:E:397:ASP:HB2	1:E:402:MET:HG2	1.83	0.61
1:K:369:ASP:H	1:K:372:THR:HB	1.64	0.61
1:C:373:THR:O	1:C:376:PHE:HB3	2.01	0.61
1:A:335:ARG:HH21	1:A:367:ASP:HA	1.65	0.61
1:A:277:PRO:HG2	1:A:280:LEU:HB2	1.80	0.61
1:D:53:PHE:CD1	1:D:54:LEU:HG	2.35	0.61
1:A:339:TYR:CZ	1:A:358:PHE:HB2	2.36	0.61
1:B:261:LYS:NZ	1:B:388:SER:HA	2.16	0.61
1:D:238:THR:HB	2:D:503:HEN:H2A2	1.83	0.61
1:D:421:LEU:HD12	1:D:422:VAL:N	2.16	0.61
1:H:210:THR:HG23	1:H:211:ASN:N	2.15	0.61
1:E:335:ARG:HH21	1:E:367:ASP:HA	1.66	0.61
1:F:113:ASN:ND2	1:F:297:PRO:HG3	2.16	0.61
1:B:120:GLU:HG3	1:B:134:LEU:HD12	1.82	0.61
1:H:347:GLU:HB3	1:H:350:ILE:HD12	1.83	0.61
1:I:211:ASN:HD22	1:I:212:PRO:N	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:370:LEU:HD23	1:L:419:ASP:HB3	1.82	0.61
1:B:127:GLU:OE2	1:B:242:PRO:HB3	2.01	0.61
1:I:343:GLN:HA	1:I:348:HIS:CD2	2.34	0.61
1:J:339:TYR:CZ	1:J:358:PHE:HB2	2.35	0.61
1:J:261:LYS:NZ	1:J:388:SER:HA	2.16	0.60
1:F:211:ASN:C	1:F:211:ASN:HD22	2.04	0.60
1:E:333:LYS:HE2	1:E:445:ILE:HG22	1.82	0.60
1:I:268:ASP:HB3	1:L:78:THR:HG21	1.84	0.60
1:C:335:ARG:HH21	1:C:367:ASP:HA	1.66	0.60
1:J:174:LEU:N	1:J:175:PRO:HD2	2.16	0.60
1:G:210:THR:HG23	1:G:211:ASN:N	2.16	0.60
1:J:250:LEU:HD11	1:J:354:GLN:HB2	1.83	0.60
1:H:250:LEU:HD11	1:H:354:GLN:HB2	1.83	0.60
1:C:216:CYS:H	1:C:347:GLU:HG3	1.66	0.60
1:G:173:ILE:C	1:G:175:PRO:HD2	2.22	0.60
1:K:347:GLU:HB3	1:K:350:ILE:HD12	1.82	0.60
1:E:53:PHE:CD1	1:E:54:LEU:HG	2.36	0.60
1:I:148:ALA:HB2	1:I:287:LEU:HD23	1.84	0.60
1:B:143:THR:HG21	1:D:291:LEU:HD22	1.83	0.60
1:F:386:ALA:HB2	1:H:88:PHE:HA	1.83	0.60
1:E:343:GLN:HA	1:E:348:HIS:CD2	2.36	0.60
1:F:204:PHE:CE2	1:F:222:VAL:HG11	2.36	0.60
1:B:113:ASN:ND2	1:B:297:PRO:HG3	2.15	0.60
1:I:210:THR:HG23	1:I:211:ASN:N	2.16	0.60
1:B:331:HIS:CE1	1:B:333:LYS:HB2	2.37	0.60
1:F:347:GLU:HB3	1:F:350:ILE:HD12	1.83	0.60
1:K:174:LEU:N	1:K:175:PRO:HD2	2.16	0.60
1:A:120:GLU:HG3	1:A:134:LEU:HD12	1.84	0.60
1:C:261:LYS:NZ	1:C:388:SER:HA	2.16	0.60
1:J:113:ASN:ND2	1:J:297:PRO:HG3	2.17	0.59
1:J:339:TYR:OH	1:J:358:PHE:HB2	2.02	0.59
1:G:331:HIS:CE1	1:G:333:LYS:HB2	2.37	0.59
1:C:80:PRO:HB3	1:D:82:VAL:HG22	1.84	0.59
1:H:369:ASP:H	1:H:372:THR:HB	1.67	0.59
1:E:211:ASN:HD22	1:E:211:ASN:C	2.04	0.59
1:H:204:PHE:CE2	1:H:222:VAL:HG11	2.36	0.59
1:C:442:LEU:HA	1:C:445:ILE:HD13	1.83	0.59
1:G:133:LEU:HD23	1:G:135:MET:HE1	1.85	0.59
1:D:211:ASN:C	1:D:211:ASN:HD22	2.05	0.59
1:D:216:CYS:H	1:D:347:GLU:HG3	1.67	0.59
1:K:70:ARG:HD3	1:K:79:THR:OG1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LEU:N	1:D:175:PRO:HD2	2.18	0.59
1:G:156:ILE:HG13	1:G:203:LEU:HD23	1.83	0.59
1:L:421:LEU:HD12	1:L:422:VAL:N	2.17	0.59
1:H:127:GLU:OE2	1:H:242:PRO:HB3	2.03	0.59
1:J:421:LEU:HD12	1:J:422:VAL:N	2.18	0.59
1:C:156:ILE:HG12	1:C:157:VAL:N	2.16	0.59
1:D:156:ILE:HG13	1:D:203:LEU:HD23	1.84	0.59
1:H:370:LEU:HD23	1:H:419:ASP:HB3	1.83	0.59
1:H:211:ASN:C	1:H:211:ASN:HD22	2.06	0.59
1:H:70:ARG:HD3	1:H:79:THR:OG1	2.03	0.59
1:A:343:GLN:HA	1:A:348:HIS:CD2	2.38	0.59
1:C:331:HIS:CE1	1:C:333:LYS:HB2	2.37	0.59
1:H:210:THR:HG22	1:H:215:ARG:N	2.16	0.59
1:E:113:ASN:ND2	1:E:297:PRO:HG3	2.17	0.59
1:L:153:GLY:HA2	1:L:178:GLY:O	2.02	0.59
1:A:347:GLU:HB3	1:A:350:ILE:HD12	1.85	0.58
1:D:441:ALA:C	1:D:443:ASP:H	2.05	0.58
1:G:335:ARG:HH21	1:G:367:ASP:HA	1.68	0.58
1:G:204:PHE:N	1:G:232:LEU:O	2.32	0.58
1:I:277:PRO:HG2	1:I:280:LEU:HB2	1.84	0.58
1:D:261:LYS:HZ3	1:D:388:SER:HA	1.67	0.58
1:I:373:THR:O	1:I:376:PHE:HB3	2.02	0.58
1:D:204:PHE:CE2	1:D:222:VAL:HG11	2.39	0.58
1:A:373:THR:O	1:A:376:PHE:HB3	2.03	0.58
1:C:343:GLN:HA	1:C:348:HIS:CD2	2.37	0.58
1:J:153:GLY:HA2	1:J:178:GLY:O	2.03	0.58
1:J:211:ASN:C	1:J:211:ASN:HD22	2.06	0.58
1:C:277:PRO:O	1:C:281:VAL:HG12	2.03	0.58
1:L:261:LYS:NZ	1:L:388:SER:HA	2.18	0.58
1:K:335:ARG:HH21	1:K:367:ASP:HA	1.69	0.58
1:B:240:ALA:O	1:B:241:THR:CB	2.50	0.58
1:F:210:THR:HG23	1:F:211:ASN:N	2.17	0.58
1:C:250:LEU:HD11	1:C:354:GLN:HB2	1.85	0.58
1:L:373:THR:O	1:L:376:PHE:HB3	2.04	0.58
1:C:113:ASN:ND2	1:C:297:PRO:HG3	2.19	0.58
1:E:240:ALA:O	1:E:241:THR:CB	2.52	0.58
1:I:376:PHE:HB2	1:I:445:ILE:HD11	1.86	0.58
1:I:376:PHE:HB2	1:I:445:ILE:CD1	2.33	0.58
1:L:174:LEU:N	1:L:175:PRO:HD2	2.18	0.58
1:A:204:PHE:CE2	1:A:222:VAL:HG11	2.39	0.58
1:D:241:THR:HG23	1:D:242:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:ILE:HG13	1:I:203:LEU:HD23	1.85	0.58
1:E:369:ASP:H	1:E:372:THR:HB	1.67	0.58
1:K:54:LEU:CD2	1:K:59:SER:HB3	2.34	0.58
1:J:173:ILE:C	1:J:175:PRO:HD2	2.24	0.58
1:F:215:ARG:HD2	1:F:347:GLU:OE2	2.03	0.58
1:A:331:HIS:CG	1:A:332:PRO:HD2	2.38	0.58
1:D:369:ASP:H	1:D:372:THR:HB	1.69	0.58
1:G:261:LYS:NZ	1:G:388:SER:HA	2.19	0.58
1:B:343:GLN:HA	1:B:348:HIS:CD2	2.38	0.58
1:B:291:LEU:HD22	1:D:143:THR:HG21	1.84	0.58
1:I:113:ASN:ND2	1:I:297:PRO:HG3	2.17	0.58
1:F:156:ILE:HG13	1:F:203:LEU:HD23	1.84	0.58
1:G:170:ILE:HG23	1:G:174:LEU:HD12	1.85	0.58
1:I:174:LEU:N	1:I:175:PRO:HD2	2.18	0.58
1:G:63:HIS:HB3	1:G:67:ARG:HB2	1.85	0.57
1:A:397:ASP:HB2	1:A:402:MET:HG2	1.86	0.57
1:K:119:LEU:HG	1:K:134:LEU:HD11	1.85	0.57
1:G:70:ARG:HD3	1:G:79:THR:OG1	2.04	0.57
1:L:140:CYS:O	1:L:144:VAL:HG23	2.03	0.57
1:F:345:HIS:CE1	1:F:347:GLU:HG2	2.38	0.57
1:E:393:GLU:OE2	1:H:308:LYS:HD2	2.05	0.57
1:E:277:PRO:HG2	1:E:280:LEU:HB2	1.86	0.57
1:G:313:ARG:O	1:G:317:GLN:HG3	2.04	0.57
1:L:211:ASN:C	1:L:211:ASN:HD22	2.07	0.57
1:F:115:THR:HG21	1:F:297:PRO:HB3	1.85	0.57
1:D:336:HIS:ND1	1:D:337:VAL:N	2.53	0.57
1:B:210:THR:HG23	1:B:211:ASN:N	2.18	0.57
1:L:331:HIS:CE1	1:L:333:LYS:HB2	2.40	0.57
1:J:261:LYS:HZ3	1:J:388:SER:HA	1.69	0.57
1:A:153:GLY:HA2	1:A:178:GLY:O	2.04	0.57
1:B:347:GLU:HB3	1:B:350:ILE:HD12	1.86	0.57
1:H:438:ILE:O	1:H:442:LEU:HD12	2.04	0.57
1:B:148:ALA:HB2	1:B:287:LEU:HD23	1.87	0.57
1:I:335:ARG:HH21	1:I:367:ASP:HA	1.68	0.57
1:F:127:GLU:OE2	1:F:257:HIS:NE2	2.37	0.57
1:H:174:LEU:N	1:H:175:PRO:HD2	2.20	0.57
1:H:421:LEU:HD12	1:H:422:VAL:N	2.20	0.57
1:K:127:GLU:OE2	1:K:257:HIS:NE2	2.38	0.57
1:C:60:VAL:HG12	1:C:64:ALA:HB2	1.87	0.56
1:B:211:ASN:C	1:B:211:ASN:HD22	2.09	0.56
1:B:250:LEU:HD11	1:B:354:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:210:THR:O	1:I:214:LEU:HA	2.05	0.56
1:G:127:GLU:OE2	1:G:242:PRO:HB3	2.05	0.56
1:J:373:THR:O	1:J:376:PHE:HB3	2.05	0.56
1:E:145:MET:HE2	1:E:149:LEU:HD12	1.86	0.56
1:B:386:ALA:HB2	1:D:88:PHE:HA	1.87	0.56
1:H:50:TYR:CE1	1:H:68:LEU:HD12	2.40	0.56
1:L:313:ARG:O	1:L:317:GLN:HG3	2.05	0.56
1:J:156:ILE:HG12	1:J:157:VAL:N	2.21	0.56
1:G:174:LEU:N	1:G:175:PRO:HD2	2.21	0.56
1:C:438:ILE:O	1:C:441:ALA:HB3	2.06	0.56
1:J:345:HIS:CE1	1:J:347:GLU:HG2	2.41	0.56
1:G:240:ALA:O	1:G:244:ASN:HB2	2.04	0.56
1:A:339:TYR:OH	1:A:358:PHE:HB2	2.06	0.56
1:A:135:MET:HE1	1:A:274:ILE:HD12	1.88	0.56
1:E:386:ALA:HB2	1:G:88:PHE:HA	1.87	0.56
1:J:141:ALA:HB1	1:J:274:ILE:HD11	1.88	0.56
1:F:88:PHE:HA	1:H:386:ALA:HB2	1.88	0.56
1:I:369:ASP:H	1:I:372:THR:HB	1.70	0.56
1:G:161:ASP:HB3	1:G:210:THR:OG1	2.06	0.56
1:B:140:CYS:O	1:B:144:VAL:HG23	2.05	0.56
1:G:250:LEU:HD11	1:G:354:GLN:HB2	1.86	0.56
1:G:241:THR:HG23	1:G:242:PRO:HD2	1.87	0.56
1:F:187:ALA:O	1:F:189:VAL:N	2.38	0.56
1:E:394:SER:OG	1:E:427:GLY:N	2.36	0.56
1:D:347:GLU:HB3	1:D:350:ILE:HD12	1.87	0.56
1:A:211:ASN:ND2	1:A:211:ASN:C	2.59	0.56
1:G:143:THR:HG23	1:G:169:PHE:CE1	2.41	0.56
1:C:63:HIS:HB3	1:C:67:ARG:HB2	1.88	0.56
1:A:369:ASP:H	1:A:372:THR:HB	1.70	0.56
1:F:174:LEU:N	1:F:175:PRO:HD2	2.21	0.56
1:B:110:ARG:HH21	2:D:503:HEN:P	2.29	0.56
1:I:78:THR:HG21	1:L:268:ASP:HB3	1.87	0.56
1:I:217:VAL:HG13	1:I:222:VAL:HG21	1.88	0.56
1:G:310:LEU:HA	1:G:313:ARG:NH2	2.20	0.55
1:F:336:HIS:ND1	1:F:337:VAL:N	2.54	0.55
1:F:140:CYS:O	1:F:143:THR:HB	2.05	0.55
1:B:113:ASN:OD1	1:B:115:THR:HG22	2.06	0.55
1:K:135:MET:CE	1:K:141:ALA:HA	2.36	0.55
1:L:170:ILE:HA	1:L:174:LEU:HD12	1.89	0.55
1:J:321:ALA:HB2	1:J:360:GLY:HA2	1.89	0.55
1:J:335:ARG:HH21	1:J:367:ASP:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:PRO:HB3	2:A:500:HEN:OG3	2.06	0.55
1:K:64:ALA:O	1:K:122:LYS:HE2	2.07	0.55
1:D:339:TYR:CZ	1:D:358:PHE:HB2	2.42	0.55
1:A:63:HIS:HB3	1:A:67:ARG:HB2	1.88	0.55
1:I:170:ILE:HA	1:I:174:LEU:HD12	1.87	0.55
1:K:435:LYS:HG2	1:K:439:LEU:HD12	1.89	0.55
1:G:209:PRO:HG3	1:G:355:MET:HE1	1.89	0.55
1:A:174:LEU:N	1:A:175:PRO:HD2	2.21	0.55
1:H:156:ILE:HG23	1:H:181:ALA:HB2	1.87	0.55
1:G:336:HIS:ND1	1:G:337:VAL:N	2.54	0.55
1:L:135:MET:HE1	1:L:141:ALA:HA	1.87	0.55
1:D:133:LEU:HD23	1:D:135:MET:HE1	1.89	0.55
1:A:310:LEU:O	1:A:314:VAL:HG23	2.07	0.55
1:F:173:ILE:C	1:F:175:PRO:HD2	2.26	0.55
1:L:319:SER:O	1:L:320:THR:C	2.45	0.55
1:D:317:GLN:HG2	1:D:427:GLY:O	2.07	0.55
1:A:56:SER:HB3	1:D:433:ASP:OD2	2.07	0.55
1:L:115:THR:CG2	1:L:297:PRO:HB3	2.34	0.55
1:I:250:LEU:HD11	1:I:354:GLN:HB2	1.89	0.55
1:F:259:ALA:HA	1:F:263:LEU:HB2	1.89	0.55
1:G:82:VAL:HG22	1:H:80:PRO:HB3	1.89	0.55
1:I:240:ALA:O	1:I:241:THR:CB	2.54	0.55
1:C:161:ASP:HB3	1:C:210:THR:OG1	2.07	0.55
1:F:292:GLY:O	1:H:140:CYS:HB2	2.07	0.55
1:E:259:ALA:HA	1:E:263:LEU:HB2	1.88	0.55
1:E:173:ILE:C	1:E:175:PRO:HD2	2.27	0.55
1:E:156:ILE:HG13	1:E:203:LEU:HD23	1.89	0.55
1:B:394:SER:OG	1:B:427:GLY:N	2.33	0.55
1:L:240:ALA:O	1:L:241:THR:CB	2.54	0.55
1:A:345:HIS:CE1	1:A:347:GLU:HG2	2.42	0.55
1:D:339:TYR:OH	1:D:358:PHE:HB2	2.07	0.55
1:E:155:HIS:HA	1:E:180:THR:O	2.07	0.55
1:B:345:HIS:CE1	1:B:347:GLU:HG2	2.43	0.54
1:K:206:THR:O	1:K:235:ILE:HA	2.07	0.54
1:L:70:ARG:HD3	1:L:79:THR:OG1	2.07	0.54
1:J:210:THR:O	1:J:214:LEU:HA	2.07	0.54
1:L:345:HIS:CE1	1:L:347:GLU:HG2	2.42	0.54
1:H:223:SER:HA	1:H:233:VAL:HG21	1.90	0.54
1:L:63:HIS:HB3	1:L:67:ARG:HB2	1.89	0.54
1:K:322:LEU:O	1:K:325:ALA:HB3	2.07	0.54
1:A:145:MET:HE1	1:A:146:LEU:CD2	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:243:LEU:HD12	1:J:314:VAL:HG21	1.89	0.54
1:L:127:GLU:OE2	1:L:257:HIS:NE2	2.40	0.54
1:F:127:GLU:OE2	1:F:242:PRO:HB3	2.07	0.54
1:J:374:ALA:O	1:J:377:VAL:HG22	2.07	0.54
1:I:321:ALA:HB2	1:I:360:GLY:HA2	1.88	0.54
1:G:259:ALA:HB3	1:G:271:ALA:HB3	1.88	0.54
1:I:217:VAL:O	1:I:219:ILE:N	2.41	0.54
1:E:339:TYR:CZ	1:E:358:PHE:HB2	2.43	0.54
1:L:72:ILE:HG23	1:L:72:ILE:O	2.08	0.54
1:G:210:THR:HG22	1:G:215:ARG:N	2.18	0.54
1:H:173:ILE:C	1:H:175:PRO:HD2	2.28	0.54
1:H:345:HIS:CE1	1:H:347:GLU:HG2	2.42	0.54
1:H:156:ILE:HG13	1:H:203:LEU:HD23	1.89	0.54
1:C:174:LEU:N	1:C:175:PRO:HD2	2.23	0.54
1:B:83:ASN:O	1:D:268:ASP:HB2	2.07	0.54
1:A:88:PHE:HA	1:C:386:ALA:HB2	1.90	0.54
1:B:94:GLU:O	1:B:97:ASP:HB2	2.08	0.54
1:F:411:ASP:O	1:F:414:LYS:HB2	2.08	0.54
1:A:321:ALA:HB2	1:A:360:GLY:HA2	1.90	0.54
1:E:238:THR:HB	2:E:504:HEN:H2A2	1.90	0.54
1:H:72:ILE:O	1:H:72:ILE:HG23	2.08	0.54
1:K:211:ASN:HB2	1:K:239:PHE:HE2	1.73	0.54
1:K:210:THR:CG2	1:K:215:ARG:H	2.17	0.54
1:H:373:THR:O	1:H:376:PHE:HB3	2.07	0.54
1:I:70:ARG:HD3	1:I:79:THR:OG1	2.07	0.54
1:A:242:PRO:HD3	1:A:257:HIS:CE1	2.42	0.54
1:J:88:PHE:HA	1:L:386:ALA:HB2	1.89	0.54
1:I:331:HIS:CE1	1:I:333:LYS:HB2	2.42	0.54
1:L:277:PRO:O	1:L:281:VAL:HG12	2.07	0.54
1:H:153:GLY:HA2	1:H:178:GLY:O	2.07	0.54
1:I:319:SER:O	1:I:320:THR:C	2.46	0.54
1:I:370:LEU:HD23	1:I:419:ASP:HB3	1.89	0.54
1:G:369:ASP:H	1:G:372:THR:HB	1.72	0.54
1:E:160:THR:HG23	1:E:184:ILE:O	2.07	0.54
1:F:55:ASN:HD22	1:F:55:ASN:N	2.06	0.54
1:L:60:VAL:HG12	1:L:64:ALA:HB2	1.88	0.54
1:A:140:CYS:O	1:A:144:VAL:HG23	2.08	0.54
1:K:398:GLN:HB3	1:K:401:ILE:HD12	1.90	0.54
1:E:63:HIS:HB3	1:E:67:ARG:HB2	1.90	0.54
1:B:174:LEU:N	1:B:175:PRO:HD2	2.23	0.54
1:K:156:ILE:HG13	1:K:203:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:HIS:ND1	1:G:311:HIS:N	2.56	0.54
1:D:277:PRO:O	1:D:281:VAL:HG12	2.08	0.54
1:J:210:THR:HG23	1:J:211:ASN:N	2.23	0.53
1:C:421:LEU:HD12	1:C:422:VAL:N	2.23	0.53
1:C:445:ILE:HD12	1:C:445:ILE:N	2.23	0.53
1:C:313:ARG:O	1:C:317:GLN:HG3	2.07	0.53
1:J:148:ALA:HB2	1:J:287:LEU:HD23	1.90	0.53
1:H:277:PRO:O	1:H:281:VAL:HG12	2.08	0.53
1:F:160:THR:HG23	1:F:184:ILE:O	2.08	0.53
1:D:155:HIS:HD1	1:D:180:THR:HG23	1.73	0.53
1:I:62:ILE:HD11	1:L:428:VAL:HG12	1.90	0.53
1:K:215:ARG:HD2	1:K:347:GLU:OE2	2.08	0.53
1:D:210:THR:HG23	1:D:211:ASN:N	2.24	0.53
1:E:277:PRO:O	1:E:281:VAL:HG12	2.08	0.53
1:H:140:CYS:O	1:H:144:VAL:HG23	2.08	0.53
1:K:374:ALA:O	1:K:377:VAL:HG22	2.08	0.53
1:J:70:ARG:HD3	1:J:79:THR:OG1	2.08	0.53
1:L:148:ALA:HB2	1:L:287:LEU:HD23	1.90	0.53
1:C:411:ASP:O	1:C:414:LYS:HB2	2.08	0.53
1:B:72:ILE:HG23	1:B:72:ILE:O	2.08	0.53
1:G:215:ARG:HD2	1:G:347:GLU:OE2	2.09	0.53
1:I:211:ASN:ND2	1:I:211:ASN:C	2.61	0.53
1:K:133:LEU:HD23	1:K:135:MET:HE1	1.91	0.53
1:B:63:HIS:HB3	1:B:67:ARG:HB2	1.91	0.53
1:A:87:TYR:HA	1:B:75:ASP:O	2.09	0.53
1:D:145:MET:CE	1:D:146:LEU:HD23	2.39	0.53
1:D:215:ARG:HD2	1:D:347:GLU:OE2	2.09	0.53
1:I:145:MET:HE2	1:I:149:LEU:HD12	1.91	0.53
1:E:398:GLN:HB3	1:E:401:ILE:HD12	1.90	0.53
1:F:135:MET:HE1	1:F:274:ILE:HD12	1.90	0.53
1:J:277:PRO:O	1:J:281:VAL:HG12	2.08	0.53
1:G:277:PRO:HG2	1:G:280:LEU:HB2	1.90	0.53
1:D:153:GLY:HA2	1:D:178:GLY:O	2.07	0.53
1:G:345:HIS:HE1	1:G:347:GLU:HG2	1.73	0.53
1:E:210:THR:HG23	1:E:211:ASN:N	2.23	0.53
1:K:173:ILE:O	1:K:176:LYS:HB2	2.08	0.53
1:K:133:LEU:CD1	1:K:285:ARG:HD3	2.39	0.53
1:G:160:THR:HG23	1:G:184:ILE:O	2.07	0.53
1:K:117:VAL:O	1:K:121:GLU:HG3	2.09	0.53
1:H:145:MET:HE2	1:H:146:LEU:HD23	1.90	0.53
1:J:287:LEU:O	1:J:287:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:THR:HG21	1:K:291:LEU:HD22	1.90	0.53
1:B:248:LEU:HG	1:B:255:VAL:HG12	1.91	0.53
1:E:153:GLY:HA2	1:E:178:GLY:O	2.08	0.53
1:G:210:THR:CG2	1:G:215:ARG:H	2.19	0.53
1:K:211:ASN:ND2	1:K:211:ASN:C	2.62	0.53
1:F:120:GLU:HG2	1:F:132:THR:O	2.09	0.53
1:E:438:ILE:O	1:E:441:ALA:HB3	2.08	0.53
1:F:370:LEU:HD23	1:F:419:ASP:HB3	1.91	0.53
1:A:70:ARG:HD3	1:A:79:THR:OG1	2.09	0.53
1:K:161:ASP:HB3	1:K:210:THR:OG1	2.09	0.53
1:E:211:ASN:ND2	1:E:211:ASN:C	2.62	0.53
1:A:240:ALA:O	1:A:241:THR:CB	2.56	0.53
1:F:374:ALA:O	1:F:377:VAL:HG22	2.09	0.53
1:A:268:ASP:HB3	1:D:78:THR:HG21	1.91	0.53
1:B:397:ASP:HB2	1:B:402:MET:HG2	1.91	0.53
1:H:117:VAL:O	1:H:121:GLU:HG3	2.09	0.52
1:C:261:LYS:HZ3	1:C:388:SER:HA	1.74	0.52
1:G:373:THR:O	1:G:376:PHE:HB3	2.09	0.52
1:C:336:HIS:ND1	1:C:337:VAL:N	2.57	0.52
1:F:63:HIS:HB3	1:F:67:ARG:HB2	1.90	0.52
1:H:374:ALA:O	1:H:377:VAL:HG22	2.08	0.52
1:J:210:THR:CG2	1:J:215:ARG:H	2.18	0.52
1:A:240:ALA:O	1:A:244:ASN:HB2	2.10	0.52
1:H:399:PRO:HG2	1:H:421:LEU:HG	1.90	0.52
1:J:135:MET:HE1	1:J:274:ILE:HD12	1.92	0.52
1:C:319:SER:O	1:C:320:THR:C	2.48	0.52
1:A:270:LEU:N	1:A:270:LEU:HD23	2.25	0.52
1:L:210:THR:HG22	1:L:215:ARG:N	2.22	0.52
1:D:345:HIS:CE1	1:D:347:GLU:HG2	2.44	0.52
1:B:135:MET:HE1	1:B:141:ALA:HA	1.92	0.52
1:D:192:LEU:HD21	1:D:222:VAL:HG13	1.91	0.52
1:J:397:ASP:HB2	1:J:402:MET:HG2	1.90	0.52
1:F:369:ASP:H	1:F:372:THR:HB	1.74	0.52
1:G:72:ILE:HD13	1:G:80:PRO:HG2	1.91	0.52
1:J:426:PHE:HE1	1:J:438:ILE:HD11	1.75	0.52
1:H:211:ASN:HB2	1:H:239:PHE:HE2	1.74	0.52
1:F:310:LEU:HA	1:F:313:ARG:NH2	2.25	0.52
1:G:321:ALA:HB2	1:G:360:GLY:HA2	1.91	0.52
1:A:187:ALA:O	1:A:189:VAL:N	2.43	0.52
1:A:207:GLU:CB	1:A:236:ASP:HB3	2.38	0.52
1:E:135:MET:CE	1:E:141:ALA:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:441:ALA:C	1:H:443:ASP:H	2.12	0.52
1:F:373:THR:O	1:F:376:PHE:HB3	2.09	0.52
1:C:210:THR:CG2	1:C:215:ARG:H	2.17	0.52
1:C:60:VAL:CG1	1:C:64:ALA:HB2	2.39	0.52
1:D:173:ILE:C	1:D:175:PRO:HD2	2.30	0.52
1:L:170:ILE:HG23	1:L:174:LEU:HD12	1.90	0.52
1:G:310:LEU:O	1:G:314:VAL:HG23	2.09	0.52
1:L:133:LEU:HD23	1:L:135:MET:HE3	1.92	0.52
1:F:291:LEU:HD22	1:H:143:THR:HG21	1.91	0.52
1:G:442:LEU:HA	1:G:445:ILE:HD12	1.92	0.52
1:A:135:MET:HE2	1:A:141:ALA:HA	1.90	0.52
1:I:217:VAL:CG1	1:I:222:VAL:HG21	2.39	0.52
1:H:277:PRO:HG2	1:H:280:LEU:HB2	1.91	0.52
1:D:210:THR:O	1:D:214:LEU:HA	2.10	0.52
1:E:143:THR:HG21	1:G:291:LEU:HD22	1.92	0.52
1:K:160:THR:HG23	1:K:184:ILE:O	2.10	0.52
1:K:336:HIS:ND1	1:K:337:VAL:N	2.58	0.52
1:K:240:ALA:O	1:K:241:THR:CB	2.52	0.52
1:A:331:HIS:ND1	1:A:332:PRO:HD2	2.25	0.52
1:C:374:ALA:O	1:C:377:VAL:HG22	2.10	0.52
1:A:374:ALA:O	1:A:377:VAL:HG22	2.10	0.52
1:L:210:THR:HG23	1:L:211:ASN:N	2.24	0.52
1:C:204:PHE:CE2	1:C:222:VAL:HG11	2.45	0.52
1:G:374:ALA:O	1:G:377:VAL:HG22	2.09	0.52
1:I:261:LYS:HZ2	1:I:388:SER:HA	1.73	0.51
1:C:70:ARG:HD3	1:C:79:THR:OG1	2.10	0.51
1:A:421:LEU:HD12	1:A:422:VAL:N	2.25	0.51
1:F:377:VAL:HA	1:F:380:LEU:HD12	1.91	0.51
1:I:63:HIS:HB3	1:I:67:ARG:HB2	1.92	0.51
1:K:311:HIS:N	1:K:311:HIS:ND1	2.57	0.51
1:F:156:ILE:HG12	1:F:157:VAL:N	2.24	0.51
1:L:277:PRO:HG2	1:L:280:LEU:HB2	1.91	0.51
1:H:313:ARG:O	1:H:317:GLN:HG3	2.10	0.51
1:B:210:THR:CG2	1:B:215:ARG:H	2.21	0.51
1:J:217:VAL:CG1	1:J:222:VAL:HG21	2.41	0.51
1:B:384:TYR:CZ	1:C:67:ARG:HD2	2.45	0.51
1:D:145:MET:HE3	1:D:149:LEU:HD12	1.91	0.51
1:A:80:PRO:HB3	1:B:82:VAL:HG22	1.92	0.51
1:J:369:ASP:H	1:J:372:THR:HB	1.75	0.51
1:K:187:ALA:O	1:K:189:VAL:N	2.43	0.51
1:A:77:ILE:HD12	1:B:86:ALA:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:133:LEU:HD23	1:I:135:MET:HE3	1.91	0.51
1:A:305:ARG:O	1:A:308:LYS:HB2	2.10	0.51
1:F:54:LEU:HD13	1:F:59:SER:HB3	1.93	0.51
1:G:211:ASN:ND2	1:G:211:ASN:C	2.62	0.51
1:E:60:VAL:O	1:E:64:ALA:N	2.43	0.51
1:C:192:LEU:HD21	1:C:222:VAL:HG13	1.92	0.51
1:B:421:LEU:HD12	1:B:422:VAL:N	2.25	0.51
1:A:148:ALA:HB2	1:A:287:LEU:HD23	1.93	0.51
1:G:319:SER:O	1:G:320:THR:C	2.48	0.51
1:F:240:ALA:O	1:F:241:THR:CB	2.57	0.51
1:H:146:LEU:O	1:H:150:VAL:HG23	2.09	0.51
1:I:156:ILE:HG23	1:I:181:ALA:HB2	1.91	0.51
1:D:311:HIS:N	1:D:311:HIS:ND1	2.58	0.51
1:K:382:ILE:HD12	1:K:437:ASP:HB2	1.93	0.51
1:I:411:ASP:O	1:I:414:LYS:HB2	2.10	0.51
1:F:60:VAL:HG12	1:F:64:ALA:HB2	1.92	0.51
1:A:438:ILE:HG22	1:A:442:LEU:HD11	1.93	0.51
1:L:261:LYS:HZ3	1:L:388:SER:HA	1.76	0.51
1:K:156:ILE:HG12	1:K:157:VAL:N	2.25	0.51
1:G:411:ASP:O	1:G:414:LYS:HB2	2.10	0.51
1:I:428:VAL:HG12	1:L:62:ILE:HD11	1.92	0.51
1:E:88:PHE:HA	1:G:386:ALA:HB2	1.93	0.51
1:K:319:SER:O	1:K:320:THR:C	2.48	0.51
1:D:240:ALA:O	1:D:241:THR:CB	2.57	0.51
1:B:268:ASP:HB2	1:D:83:ASN:O	2.11	0.51
1:E:240:ALA:HB1	1:E:245:GLN:HG2	1.93	0.51
1:E:135:MET:HE1	1:E:274:ILE:HD12	1.92	0.51
1:E:339:TYR:OH	1:E:358:PHE:HB2	2.10	0.51
1:J:322:LEU:O	1:J:325:ALA:HB3	2.10	0.51
1:F:62:ILE:HD11	1:G:428:VAL:HG12	1.92	0.51
1:C:173:ILE:C	1:C:175:PRO:HD2	2.32	0.51
1:E:311:HIS:N	1:E:311:HIS:ND1	2.59	0.51
1:A:211:ASN:HD22	1:A:212:PRO:N	2.08	0.51
1:B:217:VAL:O	1:B:219:ILE:N	2.44	0.51
1:E:140:CYS:HB2	1:G:292:GLY:O	2.11	0.51
1:B:88:PHE:HA	1:D:386:ALA:HB2	1.91	0.51
1:B:411:ASP:O	1:B:414:LYS:HB2	2.11	0.51
1:A:311:HIS:ND1	1:A:311:HIS:N	2.57	0.51
1:E:163:TYR:CE2	1:E:165:LYS:HB2	2.46	0.51
1:L:311:HIS:N	1:L:311:HIS:ND1	2.59	0.51
1:C:211:ASN:ND2	1:C:211:ASN:C	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:O	1:B:354:GLN:HG2	2.11	0.50
1:F:153:GLY:HA2	1:F:178:GLY:O	2.11	0.50
1:I:88:PHE:HA	1:K:386:ALA:HB2	1.92	0.50
1:F:56:SER:OG	1:G:430:ASP:HB2	2.10	0.50
1:K:82:VAL:HG22	1:L:80:PRO:HB3	1.93	0.50
1:C:187:ALA:O	1:C:189:VAL:N	2.45	0.50
1:K:170:ILE:HG23	1:K:174:LEU:HD12	1.92	0.50
1:G:53:PHE:CD1	1:G:54:LEU:HG	2.46	0.50
1:F:170:ILE:HG23	1:F:174:LEU:HD12	1.92	0.50
1:I:277:PRO:O	1:I:281:VAL:HG12	2.11	0.50
1:I:428:VAL:O	1:I:428:VAL:CG1	2.59	0.50
1:J:209:PRO:HG3	1:J:355:MET:HE1	1.93	0.50
1:C:135:MET:CE	1:C:141:ALA:HA	2.41	0.50
1:C:135:MET:HE2	1:C:141:ALA:HA	1.93	0.50
1:E:70:ARG:HD3	1:E:79:THR:OG1	2.11	0.50
1:I:259:ALA:HB3	1:I:271:ALA:HB3	1.93	0.50
1:J:160:THR:HG22	1:J:183:VAL:HG12	1.92	0.50
1:B:428:VAL:O	1:B:428:VAL:CG1	2.59	0.50
1:B:53:PHE:O	1:B:54:LEU:HD23	2.10	0.50
1:F:55:ASN:N	1:F:55:ASN:ND2	2.59	0.50
1:C:133:LEU:HD23	1:C:135:MET:HE1	1.92	0.50
1:H:324:MET:HG2	1:H:431:PHE:CE1	2.47	0.50
1:F:319:SER:O	1:F:320:THR:C	2.50	0.50
1:J:140:CYS:O	1:J:143:THR:HB	2.10	0.50
1:K:148:ALA:HB2	1:K:287:LEU:HD23	1.93	0.50
1:J:240:ALA:O	1:J:241:THR:CB	2.53	0.50
1:F:215:ARG:NH1	1:F:347:GLU:OE2	2.42	0.50
1:D:210:THR:HG22	1:D:215:ARG:N	2.24	0.50
1:I:173:ILE:C	1:I:175:PRO:HD2	2.32	0.50
1:D:277:PRO:HG2	1:D:280:LEU:HB2	1.92	0.50
1:I:63:HIS:HD2	1:I:67:ARG:HD3	1.75	0.50
1:H:324:MET:HG2	1:H:431:PHE:HE1	1.76	0.50
1:F:421:LEU:HD12	1:F:422:VAL:N	2.26	0.50
1:H:336:HIS:ND1	1:H:337:VAL:N	2.60	0.50
1:B:373:THR:O	1:B:376:PHE:HB3	2.11	0.50
1:D:397:ASP:HB2	1:D:402:MET:HG2	1.92	0.50
1:K:217:VAL:CG1	1:K:222:VAL:HG21	2.42	0.50
1:I:215:ARG:HD2	1:I:347:GLU:OE2	2.11	0.50
1:F:345:HIS:HE1	1:F:347:GLU:HG2	1.76	0.50
1:L:347:GLU:CB	1:L:350:ILE:HD12	2.40	0.50
1:I:397:ASP:HB2	1:I:402:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:398:GLN:HB3	1:H:401:ILE:HD12	1.94	0.50
1:H:58:GLY:HA3	1:H:311:HIS:CD2	2.46	0.50
1:H:211:ASN:ND2	1:H:211:ASN:C	2.65	0.50
1:B:156:ILE:HG23	1:B:181:ALA:HB2	1.93	0.50
1:K:160:THR:HG22	1:K:183:VAL:HG12	1.93	0.50
1:E:82:VAL:HG22	1:F:80:PRO:HB3	1.93	0.50
1:D:438:ILE:HG22	1:D:442:LEU:HD12	1.94	0.50
1:A:394:SER:OG	1:A:427:GLY:N	2.39	0.50
1:C:127:GLU:CD	1:C:242:PRO:HB3	2.31	0.50
1:L:210:THR:O	1:L:214:LEU:HA	2.11	0.50
1:E:140:CYS:O	1:E:143:THR:HB	2.12	0.50
1:E:259:ALA:HB3	1:E:271:ALA:HB3	1.93	0.50
1:K:397:ASP:HB2	1:K:402:MET:HG2	1.92	0.50
1:J:320:THR:O	1:J:324:MET:HB2	2.11	0.50
1:J:234:CYS:HA	1:J:254:LEU:O	2.12	0.50
1:A:72:ILE:HG23	1:A:72:ILE:O	2.12	0.50
1:D:373:THR:O	1:D:376:PHE:HB3	2.12	0.50
1:E:347:GLU:HB3	1:E:350:ILE:HD12	1.94	0.50
1:C:87:TYR:CE1	1:C:106:PHE:HB2	2.46	0.50
1:A:411:ASP:O	1:A:414:LYS:HB2	2.12	0.50
1:A:248:LEU:HG	1:A:255:VAL:HG12	1.92	0.50
1:E:110:ARG:HH21	2:G:506:HEN:P	2.35	0.50
1:J:270:LEU:HD23	1:J:270:LEU:N	2.27	0.50
1:I:72:ILE:HG12	1:I:72:ILE:O	2.12	0.50
1:L:336:HIS:ND1	1:L:337:VAL:N	2.60	0.50
1:C:428:VAL:O	1:C:428:VAL:CG1	2.60	0.49
1:F:317:GLN:HG2	1:F:427:GLY:O	2.11	0.49
1:L:159:THR:HG23	1:L:206:THR:HB	1.94	0.49
1:A:336:HIS:ND1	1:A:337:VAL:N	2.59	0.49
1:K:331:HIS:CE1	1:K:333:LYS:HB2	2.47	0.49
1:C:311:HIS:N	1:C:311:HIS:ND1	2.60	0.49
1:D:113:ASN:ND2	1:D:297:PRO:HG3	2.27	0.49
1:C:103:ARG:HG2	1:C:104:ALA:N	2.26	0.49
1:H:187:ALA:O	1:H:189:VAL:N	2.45	0.49
1:F:277:PRO:O	1:F:281:VAL:HG12	2.12	0.49
1:E:331:HIS:HE1	1:E:333:LYS:HB2	1.76	0.49
1:J:215:ARG:NH1	1:J:347:GLU:OE2	2.42	0.49
1:L:215:ARG:HD2	1:L:347:GLU:OE2	2.13	0.49
1:A:386:ALA:HB2	1:C:88:PHE:HA	1.94	0.49
1:C:310:LEU:HA	1:C:313:ARG:NH2	2.27	0.49
1:F:260:THR:HG23	1:F:270:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:SER:O	1:E:320:THR:C	2.50	0.49
1:F:192:LEU:HG	1:F:196:LEU:HD23	1.94	0.49
1:F:211:ASN:C	1:F:211:ASN:ND2	2.65	0.49
1:G:240:ALA:O	1:G:241:THR:CB	2.59	0.49
1:A:438:ILE:O	1:A:441:ALA:HB3	2.12	0.49
1:K:204:PHE:CE2	1:K:222:VAL:HG11	2.48	0.49
1:I:206:THR:O	1:I:235:ILE:HA	2.12	0.49
1:E:127:GLU:OE2	1:E:257:HIS:NE2	2.45	0.49
1:J:345:HIS:HE1	1:J:347:GLU:HG2	1.77	0.49
1:F:397:ASP:HB2	1:F:402:MET:HG2	1.94	0.49
1:D:145:MET:HE2	1:D:146:LEU:HA	1.94	0.49
1:G:421:LEU:HD12	1:G:422:VAL:N	2.28	0.49
1:E:217:VAL:O	1:E:219:ILE:N	2.46	0.49
1:D:319:SER:O	1:D:320:THR:C	2.51	0.49
1:G:428:VAL:CG1	1:G:428:VAL:O	2.61	0.49
1:E:54:LEU:CD2	1:E:59:SER:HB3	2.38	0.49
1:F:250:LEU:CD1	1:F:354:GLN:HB2	2.40	0.49
1:C:217:VAL:HG13	1:C:222:VAL:HG21	1.95	0.49
1:H:63:HIS:HB3	1:H:67:ARG:HB2	1.93	0.49
1:I:210:THR:CG2	1:I:215:ARG:H	2.21	0.49
1:B:215:ARG:HD2	1:B:347:GLU:OE2	2.12	0.49
1:I:117:VAL:HA	1:I:120:GLU:HB2	1.95	0.49
1:E:331:HIS:CG	1:E:332:PRO:HD2	2.47	0.49
1:H:339:TYR:CZ	1:H:358:PHE:HB2	2.48	0.49
1:K:209:PRO:HG3	1:K:355:MET:HE1	1.95	0.49
1:E:72:ILE:O	1:E:72:ILE:HG23	2.12	0.49
1:B:428:VAL:HG12	1:C:62:ILE:HD11	1.94	0.49
1:I:215:ARG:NH1	1:I:347:GLU:OE2	2.38	0.49
1:L:145:MET:HE2	1:L:149:LEU:HD12	1.95	0.49
1:G:114:PRO:O	1:G:117:VAL:HG22	2.13	0.49
1:D:72:ILE:O	1:D:72:ILE:HG23	2.13	0.49
1:K:145:MET:CE	1:K:146:LEU:HD23	2.37	0.49
1:L:211:ASN:C	1:L:211:ASN:ND2	2.66	0.49
1:D:159:THR:HG23	1:D:206:THR:HB	1.95	0.49
1:H:259:ALA:HB3	1:H:271:ALA:HB3	1.95	0.49
1:J:428:VAL:O	1:J:428:VAL:CG1	2.61	0.49
1:F:145:MET:HG2	1:F:149:LEU:HD12	1.95	0.49
1:C:369:ASP:H	1:C:372:THR:HB	1.77	0.49
1:J:211:ASN:C	1:J:211:ASN:ND2	2.66	0.48
1:J:52:SER:C	1:J:54:LEU:H	2.16	0.48
1:E:187:ALA:O	1:E:189:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:ASP:HB3	1:H:210:THR:OG1	2.12	0.48
1:A:310:LEU:HA	1:A:313:ARG:NH2	2.28	0.48
1:J:156:ILE:CG2	1:J:181:ALA:HB2	2.44	0.48
1:B:60:VAL:HG12	1:B:64:ALA:HB2	1.96	0.48
1:H:113:ASN:ND2	1:H:297:PRO:HG3	2.28	0.48
1:H:261:LYS:HZ3	1:H:388:SER:HA	1.75	0.48
1:I:322:LEU:O	1:I:325:ALA:HB3	2.14	0.48
1:B:146:LEU:O	1:B:150:VAL:HG23	2.13	0.48
1:D:127:GLU:OE2	1:D:242:PRO:HB3	2.13	0.48
1:G:166:THR:O	1:G:170:ILE:HG13	2.13	0.48
1:F:291:LEU:O	1:H:140:CYS:HA	2.12	0.48
1:J:438:ILE:HG22	1:J:442:LEU:HD11	1.94	0.48
1:F:51:ALA:HB1	1:F:53:PHE:CE2	2.48	0.48
1:J:370:LEU:HD23	1:J:419:ASP:HB3	1.95	0.48
1:D:374:ALA:O	1:D:377:VAL:HG22	2.13	0.48
1:D:70:ARG:HD3	1:D:79:THR:OG1	2.12	0.48
1:D:73:VAL:O	1:D:74:THR:HG23	2.13	0.48
1:E:336:HIS:ND1	1:E:337:VAL:N	2.61	0.48
1:L:54:LEU:CD2	1:L:59:SER:HB3	2.32	0.48
1:A:145:MET:HE2	1:A:149:LEU:HD12	1.95	0.48
1:H:54:LEU:CD2	1:H:59:SER:HB3	2.43	0.48
1:B:156:ILE:HG23	1:B:181:ALA:CB	2.44	0.48
1:E:127:GLU:OE2	1:E:242:PRO:HB3	2.14	0.48
1:D:206:THR:O	1:D:235:ILE:HA	2.13	0.48
1:E:80:PRO:HB3	1:F:82:VAL:HG22	1.94	0.48
1:L:217:VAL:CG1	1:L:222:VAL:HG21	2.43	0.48
1:K:173:ILE:C	1:K:175:PRO:HD2	2.34	0.48
1:H:435:LYS:HG2	1:H:439:LEU:HD12	1.96	0.48
1:L:135:MET:CE	1:L:141:ALA:HA	2.43	0.48
1:F:145:MET:CE	1:F:146:LEU:HD23	2.43	0.48
1:K:196:LEU:HD12	1:K:229:LYS:HB2	1.96	0.48
1:D:411:ASP:O	1:D:414:LYS:HB2	2.12	0.48
1:I:53:PHE:O	1:I:54:LEU:HD23	2.14	0.48
1:B:211:ASN:C	1:B:211:ASN:ND2	2.67	0.48
1:J:64:ALA:O	1:J:122:LYS:HE2	2.14	0.48
1:A:133:LEU:HD13	1:A:285:ARG:HD3	1.96	0.48
1:E:386:ALA:HB1	1:E:387:PRO:CD	2.44	0.48
1:F:223:SER:HA	1:F:233:VAL:HG21	1.95	0.48
1:J:210:THR:HG22	1:J:215:ARG:N	2.19	0.48
1:H:207:GLU:CB	1:H:236:ASP:HB3	2.40	0.48
1:L:60:VAL:CG1	1:L:64:ALA:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ILE:HD12	1:C:250:LEU:HD12	1.95	0.48
1:J:428:VAL:HG12	1:K:62:ILE:HD11	1.96	0.48
1:E:373:THR:O	1:E:376:PHE:HB3	2.14	0.48
1:B:321:ALA:HB2	1:B:360:GLY:HA2	1.96	0.48
1:C:339:TYR:CZ	1:C:358:PHE:HB2	2.48	0.48
1:K:164:ARG:O	1:K:167:ARG:HB3	2.14	0.48
1:L:426:PHE:HE1	1:L:438:ILE:HD11	1.79	0.48
1:K:345:HIS:CE1	1:K:347:GLU:HG2	2.49	0.48
1:E:53:PHE:CE1	1:E:54:LEU:HG	2.49	0.48
1:K:277:PRO:O	1:K:281:VAL:HG12	2.13	0.48
1:C:94:GLU:O	1:C:97:ASP:HB2	2.13	0.48
1:H:428:VAL:CG1	1:H:428:VAL:O	2.62	0.48
1:F:382:ILE:HD12	1:F:437:ASP:HB2	1.95	0.48
1:H:270:LEU:HD23	1:H:270:LEU:N	2.28	0.48
1:B:311:HIS:N	1:B:311:HIS:ND1	2.61	0.48
1:A:370:LEU:HD23	1:A:419:ASP:CB	2.43	0.48
1:B:60:VAL:O	1:B:64:ALA:N	2.44	0.48
1:K:278:LEU:O	1:K:280:LEU:N	2.47	0.48
1:F:234:CYS:O	1:F:235:ILE:HD13	2.13	0.48
1:H:240:ALA:O	1:H:241:THR:CB	2.56	0.48
1:E:216:CYS:N	1:E:347:GLU:HG3	2.25	0.48
1:I:119:LEU:HG	1:I:134:LEU:HD11	1.96	0.48
1:A:161:ASP:HB3	1:A:210:THR:OG1	2.13	0.48
1:H:442:LEU:HA	1:H:445:ILE:HD12	1.96	0.48
1:E:317:GLN:HG2	1:E:427:GLY:O	2.14	0.48
1:E:374:ALA:O	1:E:377:VAL:HG22	2.13	0.48
1:H:60:VAL:O	1:H:61:ALA:C	2.51	0.48
1:B:277:PRO:O	1:B:281:VAL:HG12	2.13	0.48
1:L:428:VAL:O	1:L:428:VAL:CG1	2.62	0.47
1:H:210:THR:O	1:H:214:LEU:HA	2.14	0.47
1:I:209:PRO:HG3	1:I:355:MET:HE1	1.96	0.47
1:I:135:MET:CE	1:I:141:ALA:HA	2.44	0.47
1:H:135:MET:HE1	1:H:274:ILE:HD12	1.96	0.47
1:L:208:SER:HA	1:L:209:PRO:C	2.34	0.47
1:F:148:ALA:HB2	1:F:287:LEU:HD23	1.96	0.47
1:I:365:GLU:HB3	1:I:420:ASN:HB2	1.95	0.47
1:D:428:VAL:CG1	1:D:428:VAL:O	2.61	0.47
1:I:292:GLY:O	1:K:140:CYS:HB2	2.14	0.47
1:K:210:THR:O	1:K:214:LEU:HA	2.14	0.47
1:C:64:ALA:O	1:C:122:LYS:HE2	2.14	0.47
1:A:435:LYS:HG2	1:A:439:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HG	1:B:134:LEU:HD11	1.95	0.47
1:L:173:ILE:C	1:L:175:PRO:HD2	2.34	0.47
1:C:206:THR:O	1:C:235:ILE:HA	2.14	0.47
1:I:317:GLN:HG2	1:I:427:GLY:O	2.14	0.47
1:D:123:ILE:HD13	1:D:273:CYS:SG	2.55	0.47
1:I:311:HIS:ND1	1:I:311:HIS:N	2.62	0.47
1:J:127:GLU:OE2	1:J:257:HIS:NE2	2.46	0.47
1:E:215:ARG:NH1	1:E:347:GLU:OE2	2.42	0.47
1:I:120:GLU:CG	1:I:134:LEU:HD12	2.43	0.47
1:C:217:VAL:O	1:C:219:ILE:N	2.48	0.47
1:I:173:ILE:O	1:I:176:LYS:HB2	2.13	0.47
1:C:73:VAL:O	1:C:74:THR:HG23	2.14	0.47
1:G:187:ALA:O	1:G:189:VAL:N	2.47	0.47
1:E:156:ILE:HG23	1:E:181:ALA:HB2	1.96	0.47
1:K:261:LYS:NZ	1:K:388:SER:HA	2.29	0.47
1:E:260:THR:HG23	1:E:270:LEU:HD22	1.97	0.47
1:I:127:GLU:OE2	1:I:257:HIS:NE2	2.48	0.47
1:B:336:HIS:ND1	1:B:337:VAL:N	2.61	0.47
1:E:428:VAL:CG1	1:E:428:VAL:O	2.62	0.47
1:G:127:GLU:OE2	1:G:257:HIS:NE2	2.47	0.47
1:L:60:VAL:O	1:L:61:ALA:C	2.53	0.47
1:A:261:LYS:HZ3	1:A:388:SER:HA	1.78	0.47
1:C:426:PHE:HE1	1:C:438:ILE:HD11	1.78	0.47
1:J:208:SER:HA	1:J:209:PRO:C	2.33	0.47
1:E:217:VAL:CG1	1:E:222:VAL:HG21	2.44	0.47
1:B:196:LEU:HD12	1:B:229:LYS:HB2	1.96	0.47
1:B:322:LEU:O	1:B:325:ALA:HB3	2.14	0.47
1:B:260:THR:HG23	1:B:270:LEU:HD22	1.95	0.47
1:J:336:HIS:ND1	1:J:337:VAL:N	2.62	0.47
1:I:57:ASP:HB3	1:I:243:LEU:CD2	2.45	0.47
1:J:207:GLU:CB	1:J:236:ASP:HB3	2.38	0.47
1:J:146:LEU:HD13	1:J:174:LEU:HD11	1.95	0.47
1:C:211:ASN:HD22	1:C:212:PRO:N	2.13	0.47
1:I:60:VAL:CG1	1:I:64:ALA:HB2	2.45	0.47
1:B:210:THR:O	1:B:214:LEU:HA	2.14	0.47
1:B:335:ARG:HB2	1:B:335:ARG:HE	1.57	0.47
1:H:438:ILE:HG22	1:H:442:LEU:CD1	2.45	0.47
1:A:322:LEU:O	1:A:325:ALA:HB3	2.13	0.47
1:D:382:ILE:HD12	1:D:437:ASP:HB2	1.96	0.47
1:G:339:TYR:CZ	1:G:358:PHE:HB2	2.49	0.47
1:L:339:TYR:CZ	1:L:358:PHE:HB2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:313:ARG:O	1:J:317:GLN:HG3	2.13	0.47
1:H:103:ARG:HG2	1:H:104:ALA:N	2.30	0.47
1:K:339:TYR:CZ	1:K:358:PHE:HB2	2.49	0.47
1:K:347:GLU:CB	1:K:350:ILE:HD12	2.44	0.47
1:L:127:GLU:OE2	1:L:242:PRO:HB3	2.15	0.47
1:I:216:CYS:SG	1:I:355:MET:HE1	2.54	0.47
1:I:345:HIS:CE1	1:I:347:GLU:HG2	2.50	0.47
1:F:217:VAL:CG1	1:F:222:VAL:HG21	2.45	0.47
1:A:173:ILE:C	1:A:175:PRO:HD2	2.34	0.47
1:D:335:ARG:HB2	1:D:335:ARG:HE	1.64	0.47
1:B:331:HIS:ND1	1:B:332:PRO:HD2	2.30	0.47
1:K:373:THR:OG1	1:K:420:ASN:HA	2.15	0.47
1:K:420:ASN:O	1:K:422:VAL:HG23	2.15	0.47
1:J:217:VAL:O	1:J:219:ILE:N	2.46	0.47
1:B:140:CYS:HA	1:D:291:LEU:O	2.15	0.47
1:A:217:VAL:O	1:A:219:ILE:N	2.47	0.47
1:A:217:VAL:HG13	1:A:222:VAL:HG21	1.97	0.47
1:H:373:THR:OG1	1:H:420:ASN:HA	2.15	0.47
1:L:310:LEU:HA	1:L:313:ARG:NH2	2.30	0.47
1:B:72:ILE:HD13	1:B:80:PRO:HG2	1.96	0.47
1:B:204:PHE:CE2	1:B:222:VAL:HG11	2.50	0.47
1:D:438:ILE:HG22	1:D:442:LEU:CD1	2.45	0.47
1:F:145:MET:HE2	1:F:146:LEU:HA	1.96	0.47
1:E:373:THR:OG1	1:E:420:ASN:HA	2.14	0.47
1:H:135:MET:HE2	1:H:141:ALA:HA	1.97	0.47
1:F:339:TYR:CZ	1:F:358:PHE:HB2	2.50	0.47
1:K:248:LEU:HG	1:K:255:VAL:HG12	1.97	0.47
1:G:153:GLY:HA2	1:G:178:GLY:O	2.12	0.47
1:H:331:HIS:CG	1:H:332:PRO:HD2	2.49	0.47
1:C:270:LEU:O	1:C:271:ALA:HB2	2.14	0.47
1:B:159:THR:HG23	1:B:206:THR:HB	1.96	0.47
1:B:58:GLY:HA3	1:B:311:HIS:CD2	2.50	0.47
1:D:211:ASN:C	1:D:211:ASN:ND2	2.67	0.47
1:G:217:VAL:CG1	1:G:222:VAL:HG21	2.44	0.47
1:B:140:CYS:HB2	1:D:292:GLY:O	2.15	0.47
1:C:217:VAL:CG1	1:C:222:VAL:HG21	2.44	0.47
1:A:217:VAL:CG1	1:A:222:VAL:HG21	2.44	0.47
1:F:135:MET:CE	1:F:141:ALA:HA	2.45	0.47
1:I:140:CYS:O	1:I:143:THR:HB	2.14	0.47
1:C:226:CYS:HB3	1:C:231:ALA:HB3	1.97	0.47
1:K:73:VAL:O	1:K:74:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:CG2	1:B:297:PRO:HB3	2.41	0.47
1:K:115:THR:CG2	1:K:297:PRO:HB3	2.43	0.47
1:E:140:CYS:HA	1:G:291:LEU:O	2.14	0.47
1:F:106:PHE:CD1	1:F:112:GLY:HA3	2.50	0.47
1:I:204:PHE:CE2	1:I:222:VAL:HG11	2.50	0.47
1:G:72:ILE:HG12	1:G:72:ILE:O	2.15	0.47
1:F:53:PHE:O	1:F:54:LEU:HD23	2.15	0.47
1:E:163:TYR:O	1:E:164:ARG:C	2.54	0.47
1:K:442:LEU:HA	1:K:445:ILE:CD1	2.45	0.47
1:H:87:TYR:CE1	1:H:106:PHE:HB2	2.50	0.47
1:G:234:CYS:SG	1:G:256:LEU:HD23	2.54	0.47
1:G:163:TYR:O	1:G:164:ARG:C	2.53	0.47
1:K:63:HIS:HB3	1:K:67:ARG:HB2	1.96	0.47
1:J:94:GLU:O	1:J:97:ASP:HB2	2.15	0.47
1:K:428:VAL:O	1:K:428:VAL:CG1	2.62	0.47
1:I:113:ASN:O	1:I:117:VAL:HG13	2.15	0.47
1:C:441:ALA:C	1:C:443:ASP:N	2.68	0.47
1:F:159:THR:HG23	1:F:206:THR:HB	1.96	0.47
1:J:442:LEU:C	1:J:444:SER:H	2.17	0.47
1:F:313:ARG:O	1:F:317:GLN:HG3	2.14	0.47
1:E:429:GLU:OE2	1:H:63:HIS:HE1	1.98	0.47
1:H:73:VAL:O	1:H:74:THR:HG23	2.15	0.47
1:B:443:ASP:O	1:B:445:ILE:N	2.47	0.47
1:B:63:HIS:HE1	1:C:429:GLU:OE2	1.99	0.46
1:H:319:SER:O	1:H:320:THR:C	2.52	0.46
1:A:428:VAL:O	1:A:428:VAL:CG1	2.62	0.46
1:B:320:THR:O	1:B:324:MET:HB2	2.14	0.46
1:K:94:GLU:O	1:K:97:ASP:HB2	2.15	0.46
1:A:145:MET:HG2	1:A:149:LEU:CD1	2.46	0.46
1:J:311:HIS:N	1:J:311:HIS:ND1	2.62	0.46
1:K:310:LEU:HA	1:K:313:ARG:NH2	2.29	0.46
1:E:250:LEU:CD1	1:E:354:GLN:HB2	2.41	0.46
1:D:173:ILE:O	1:D:176:LYS:HB2	2.14	0.46
1:L:443:ASP:C	1:L:445:ILE:H	2.17	0.46
1:G:219:ILE:HG21	1:G:250:LEU:HB2	1.97	0.46
1:G:259:ALA:HA	1:G:263:LEU:HB2	1.98	0.46
1:B:160:THR:HG22	1:B:183:VAL:HG12	1.96	0.46
1:D:312:LEU:HD23	1:D:312:LEU:N	2.30	0.46
1:D:260:THR:HG23	1:D:270:LEU:HD22	1.98	0.46
1:D:170:ILE:HG23	1:D:174:LEU:HD12	1.96	0.46
1:B:343:GLN:HB3	1:B:343:GLN:HE21	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:443:ASP:C	1:G:445:ILE:H	2.18	0.46
1:D:384:TYR:O	1:D:395:ILE:HG23	2.16	0.46
1:C:241:THR:HG23	1:C:242:PRO:HD2	1.98	0.46
1:G:64:ALA:O	1:G:122:LYS:HE2	2.15	0.46
1:I:60:VAL:O	1:I:62:ILE:N	2.49	0.46
1:F:311:HIS:N	1:F:311:HIS:ND1	2.63	0.46
1:H:156:ILE:HG23	1:H:181:ALA:CB	2.46	0.46
1:E:313:ARG:O	1:E:317:GLN:HG3	2.15	0.46
1:G:420:ASN:O	1:G:422:VAL:HG23	2.15	0.46
1:I:63:HIS:CD2	1:I:67:ARG:HD3	2.50	0.46
1:L:209:PRO:HG3	1:L:355:MET:HE1	1.97	0.46
1:C:322:LEU:O	1:C:325:ALA:HB3	2.16	0.46
1:L:397:ASP:HB2	1:L:402:MET:HG2	1.98	0.46
1:C:211:ASN:HB2	1:C:239:PHE:HE2	1.79	0.46
1:G:135:MET:CE	1:G:141:ALA:HA	2.42	0.46
1:F:140:CYS:HA	1:H:291:LEU:O	2.14	0.46
1:G:80:PRO:HB3	1:H:82:VAL:HG22	1.97	0.46
1:H:133:LEU:CD1	1:H:285:ARG:HD3	2.46	0.46
1:C:234:CYS:HA	1:C:254:LEU:O	2.15	0.46
1:K:426:PHE:HE1	1:K:438:ILE:HD11	1.81	0.46
1:J:133:LEU:HD23	1:J:135:MET:HE3	1.98	0.46
1:A:127:GLU:OE2	1:A:257:HIS:NE2	2.48	0.46
1:C:208:SER:HA	1:C:209:PRO:C	2.36	0.46
1:I:336:HIS:ND1	1:I:337:VAL:N	2.63	0.46
1:L:207:GLU:CB	1:L:236:ASP:HB3	2.39	0.46
1:A:185:ASP:OD1	1:A:215:ARG:NH2	2.48	0.46
1:A:259:ALA:HA	1:A:263:LEU:HD12	1.98	0.46
1:E:135:MET:HB3	1:E:140:CYS:HB3	1.98	0.46
1:H:443:ASP:C	1:H:445:ILE:H	2.18	0.46
1:F:87:TYR:CE1	1:F:106:PHE:HB2	2.51	0.46
1:C:192:LEU:CD2	1:C:222:VAL:HG13	2.45	0.46
1:H:375:LYS:HD3	1:H:445:ILE:HG23	1.97	0.46
1:D:145:MET:HE2	1:D:146:LEU:HD23	1.98	0.46
1:C:135:MET:HE2	1:C:274:ILE:HD12	1.97	0.46
1:K:339:TYR:OH	1:K:358:PHE:HB2	2.16	0.46
1:D:94:GLU:O	1:D:97:ASP:HB2	2.16	0.46
1:E:234:CYS:HA	1:E:254:LEU:O	2.15	0.46
1:F:72:ILE:HG23	1:F:72:ILE:O	2.16	0.46
1:H:382:ILE:HB	1:H:383:PRO:CD	2.46	0.46
1:L:113:ASN:O	1:L:117:VAL:HG13	2.16	0.46
1:J:145:MET:CE	1:J:149:LEU:HD12	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:ASN:ND2	1:I:212:PRO:N	2.64	0.46
1:E:173:ILE:O	1:E:176:LYS:HB2	2.16	0.46
1:G:343:GLN:HB3	1:G:343:GLN:HE21	1.55	0.46
1:A:343:GLN:HE21	1:A:343:GLN:HB3	1.56	0.46
1:G:261:LYS:HZ3	1:G:388:SER:HA	1.79	0.46
1:C:441:ALA:O	1:C:443:ASP:N	2.48	0.46
1:G:160:THR:HG22	1:G:183:VAL:HG12	1.97	0.46
1:B:160:THR:HG23	1:B:184:ILE:O	2.16	0.46
1:K:260:THR:HG23	1:K:270:LEU:HD22	1.98	0.46
1:D:103:ARG:HG2	1:D:104:ALA:N	2.31	0.46
1:F:398:GLN:O	1:F:401:ILE:N	2.48	0.46
1:D:331:HIS:CE1	1:D:333:LYS:HB2	2.51	0.46
1:I:260:THR:CG2	1:I:270:LEU:HD22	2.46	0.46
1:L:192:LEU:HG	1:L:196:LEU:HD23	1.98	0.46
1:H:312:LEU:HD23	1:H:312:LEU:N	2.30	0.46
1:H:311:HIS:ND1	1:H:311:HIS:N	2.64	0.46
1:F:157:VAL:O	1:F:204:PHE:CD1	2.69	0.46
1:B:83:ASN:O	1:D:268:ASP:CB	2.63	0.46
1:G:350:ILE:O	1:G:354:GLN:HG2	2.17	0.46
1:G:208:SER:HA	1:G:209:PRO:C	2.35	0.46
1:A:82:VAL:HG22	1:B:80:PRO:HB3	1.98	0.46
1:H:269:VAL:C	1:H:270:LEU:HD23	2.37	0.46
1:K:259:ALA:HA	1:K:263:LEU:HB2	1.98	0.46
1:I:196:LEU:HD12	1:I:229:LYS:HB2	1.98	0.46
1:I:121:GLU:O	1:I:124:SER:HB2	2.16	0.46
1:D:164:ARG:O	1:D:167:ARG:HB3	2.16	0.46
1:K:126:LEU:HA	1:K:126:LEU:HD23	1.82	0.46
1:G:53:PHE:HD1	1:G:54:LEU:HG	1.81	0.45
1:I:143:THR:HG23	1:I:169:PHE:CE1	2.50	0.45
1:E:439:LEU:HA	1:E:442:LEU:HD12	1.98	0.45
1:J:444:SER:C	1:J:445:ILE:HG13	2.36	0.45
1:A:308:LYS:HD2	1:D:393:GLU:OE2	2.17	0.45
1:L:159:THR:HA	1:L:184:ILE:O	2.16	0.45
1:B:319:SER:O	1:B:320:THR:C	2.55	0.45
1:I:260:THR:HG23	1:I:270:LEU:HD22	1.96	0.45
1:A:319:SER:O	1:A:320:THR:C	2.54	0.45
1:G:270:LEU:N	1:G:270:LEU:HD23	2.30	0.45
1:G:384:TYR:O	1:G:395:ILE:HG23	2.16	0.45
1:J:382:ILE:HD12	1:J:437:ASP:HB2	1.98	0.45
1:B:113:ASN:OD1	1:B:115:THR:N	2.40	0.45
1:E:210:THR:O	1:E:214:LEU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:TYR:CD2	1:B:54:LEU:HD12	2.52	0.45
1:B:156:ILE:CG2	1:B:181:ALA:HB2	2.47	0.45
1:B:127:GLU:CD	1:B:242:PRO:HB3	2.36	0.45
1:H:438:ILE:HG22	1:H:442:LEU:HD11	1.97	0.45
1:B:259:ALA:HA	1:B:263:LEU:HB2	1.97	0.45
1:A:60:VAL:CG1	1:A:64:ALA:HB2	2.46	0.45
1:K:211:ASN:HD22	1:K:212:PRO:N	2.15	0.45
1:H:345:HIS:HE1	1:H:347:GLU:HG2	1.81	0.45
1:H:217:VAL:O	1:H:219:ILE:N	2.48	0.45
1:K:156:ILE:HG23	1:K:181:ALA:HB2	1.98	0.45
1:D:58:GLY:HA3	1:D:311:HIS:CD2	2.51	0.45
1:B:145:MET:HE3	1:B:149:LEU:HD12	1.98	0.45
1:I:192:LEU:HG	1:I:196:LEU:HD23	1.97	0.45
1:E:126:LEU:HA	1:E:126:LEU:HD23	1.77	0.45
1:A:83:ASN:O	1:C:268:ASP:HB2	2.16	0.45
1:E:397:ASP:O	1:E:399:PRO:HD3	2.16	0.45
1:D:441:ALA:C	1:D:443:ASP:N	2.68	0.45
1:B:287:LEU:HD12	1:B:287:LEU:O	2.17	0.45
1:K:192:LEU:HG	1:K:196:LEU:HD23	1.99	0.45
1:J:103:ARG:HG2	1:J:104:ALA:N	2.31	0.45
1:D:398:GLN:HB3	1:D:401:ILE:HD12	1.98	0.45
1:F:324:MET:HG2	1:F:431:PHE:HE1	1.81	0.45
1:D:57:ASP:HB3	1:D:243:LEU:CD2	2.47	0.45
1:F:243:LEU:CD1	1:F:311:HIS:HA	2.47	0.45
1:A:211:ASN:HB2	1:A:239:PHE:HE2	1.81	0.45
1:D:441:ALA:O	1:D:443:ASP:N	2.50	0.45
1:A:398:GLN:O	1:A:401:ILE:N	2.49	0.45
1:F:324:MET:HG2	1:F:431:PHE:CE1	2.52	0.45
1:C:75:ASP:O	1:D:87:TYR:HA	2.17	0.45
1:A:60:VAL:O	1:A:64:ALA:N	2.44	0.45
1:D:208:SER:HA	1:D:209:PRO:C	2.37	0.45
1:C:373:THR:OG1	1:C:420:ASN:HA	2.16	0.45
1:F:386:ALA:HA	1:F:402:MET:CE	2.47	0.45
1:K:54:LEU:HD22	1:K:59:SER:HB3	1.97	0.45
1:K:54:LEU:HD23	1:K:59:SER:HB3	1.97	0.45
1:B:339:TYR:CZ	1:B:358:PHE:HB2	2.51	0.45
1:J:121:GLU:O	1:J:124:SER:HB2	2.17	0.45
1:F:442:LEU:CA	1:F:445:ILE:HD12	2.40	0.45
1:I:64:ALA:O	1:I:122:LYS:HE2	2.16	0.45
1:H:215:ARG:NH1	1:H:347:GLU:OE2	2.43	0.45
1:B:52:SER:C	1:B:54:LEU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:HZ3	1:B:388:SER:HA	1.80	0.45
1:J:389:PHE:HB2	1:J:425:SER:OG	2.17	0.45
1:H:420:ASN:O	1:H:422:VAL:HG23	2.17	0.45
1:J:133:LEU:CD1	1:J:285:ARG:HD3	2.46	0.45
1:F:140:CYS:O	1:F:144:VAL:HG23	2.17	0.45
1:K:312:LEU:N	1:K:312:LEU:HD23	2.31	0.45
1:I:386:ALA:HB1	1:I:387:PRO:CD	2.47	0.45
1:L:114:PRO:O	1:L:117:VAL:HG22	2.16	0.45
1:I:347:GLU:HB3	1:I:350:ILE:HD12	1.98	0.45
1:A:210:THR:CG2	1:A:215:ARG:H	2.25	0.45
1:C:196:LEU:HD12	1:C:229:LYS:HB2	1.99	0.45
1:D:143:THR:HG23	1:D:169:PHE:CE1	2.52	0.45
1:H:265:GLY:HA3	1:H:313:ARG:NH1	2.32	0.45
1:B:196:LEU:HD13	1:B:196:LEU:HA	1.82	0.45
1:G:339:TYR:CD1	1:G:362:VAL:HG22	2.52	0.45
1:F:398:GLN:O	1:F:399:PRO:C	2.55	0.45
1:I:80:PRO:HB3	1:J:82:VAL:HG22	1.99	0.45
1:C:115:THR:CG2	1:C:297:PRO:HB3	2.42	0.45
1:G:206:THR:OG1	1:G:207:GLU:N	2.48	0.45
1:E:312:LEU:N	1:E:312:LEU:HD23	2.32	0.45
1:A:215:ARG:HD2	1:A:347:GLU:OE2	2.17	0.45
1:G:217:VAL:HG13	1:G:222:VAL:HG21	1.98	0.45
1:C:335:ARG:HB2	1:C:335:ARG:HE	1.67	0.45
1:F:206:THR:O	1:F:235:ILE:HA	2.16	0.45
1:J:441:ALA:O	1:J:444:SER:HB2	2.17	0.45
1:I:386:ALA:HB2	1:K:88:PHE:HA	1.98	0.45
1:G:324:MET:HG2	1:G:431:PHE:HE1	1.82	0.45
1:B:163:TYR:CE2	1:B:165:LYS:HB2	2.52	0.45
1:I:339:TYR:CZ	1:I:358:PHE:HB2	2.52	0.45
1:B:153:GLY:HA2	1:B:178:GLY:O	2.16	0.45
1:D:160:THR:HG23	1:D:184:ILE:O	2.17	0.45
1:H:382:ILE:HB	1:H:383:PRO:HD3	1.98	0.45
1:L:156:ILE:HG23	1:L:181:ALA:HB2	1.98	0.45
1:B:84:THR:HA	1:D:268:ASP:HA	1.99	0.45
1:H:261:LYS:HZ2	1:H:388:SER:HA	1.78	0.45
1:B:277:PRO:HG2	1:B:280:LEU:HB2	1.99	0.45
1:J:398:GLN:O	1:J:401:ILE:N	2.49	0.45
1:L:398:GLN:O	1:L:401:ILE:N	2.50	0.45
1:G:215:ARG:NH1	1:G:347:GLU:OE2	2.49	0.44
1:B:53:PHE:CZ	1:B:68:LEU:HD21	2.41	0.44
1:F:217:VAL:HG13	1:F:222:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:O	1:C:280:LEU:N	2.50	0.44
1:K:373:THR:O	1:K:376:PHE:HB3	2.17	0.44
1:J:63:HIS:HB3	1:J:67:ARG:CB	2.47	0.44
1:J:204:PHE:CE2	1:J:222:VAL:HG11	2.52	0.44
1:E:242:PRO:HD3	1:E:257:HIS:CE1	2.53	0.44
1:E:148:ALA:HB2	1:E:287:LEU:HD23	2.00	0.44
1:C:397:ASP:HB2	1:C:402:MET:HG2	1.99	0.44
1:A:196:LEU:HD13	1:A:196:LEU:HA	1.79	0.44
1:J:383:PRO:HA	1:J:394:SER:O	2.17	0.44
1:F:442:LEU:HA	1:F:445:ILE:CD1	2.39	0.44
1:E:243:LEU:CD1	1:E:311:HIS:HA	2.47	0.44
1:C:72:ILE:HG12	1:C:72:ILE:O	2.18	0.44
1:L:331:HIS:CG	1:L:332:PRO:HD2	2.52	0.44
1:B:384:TYR:OH	1:C:67:ARG:HA	2.17	0.44
2:F:505:HEN:P	1:H:110:ARG:HH21	2.40	0.44
1:G:377:VAL:CG2	1:G:378:ASP:N	2.80	0.44
1:J:319:SER:O	1:J:320:THR:C	2.55	0.44
1:C:339:TYR:OH	1:C:358:PHE:HB2	2.17	0.44
1:I:127:GLU:OE2	1:I:242:PRO:HB3	2.17	0.44
1:B:258:SER:C	1:B:260:THR:N	2.71	0.44
1:G:324:MET:HG2	1:G:431:PHE:CE1	2.52	0.44
1:J:72:ILE:HG23	1:J:72:ILE:O	2.17	0.44
1:K:106:PHE:CD1	1:K:112:GLY:HA3	2.53	0.44
1:F:70:ARG:HD3	1:F:79:THR:OG1	2.17	0.44
1:J:119:LEU:HG	1:J:134:LEU:HD11	1.98	0.44
1:G:63:HIS:HD2	1:G:67:ARG:HD3	1.81	0.44
1:A:133:LEU:HD23	1:A:135:MET:CE	2.48	0.44
1:A:256:LEU:HB2	1:A:274:ILE:HG12	1.98	0.44
1:J:132:THR:HG22	1:J:133:LEU:N	2.33	0.44
1:F:260:THR:CG2	1:F:270:LEU:HD22	2.47	0.44
1:B:260:THR:CG2	1:B:270:LEU:HD22	2.48	0.44
1:H:321:ALA:HB2	1:H:360:GLY:HA2	1.98	0.44
1:K:394:SER:OG	1:K:427:GLY:N	2.36	0.44
1:B:292:GLY:O	1:D:140:CYS:HB2	2.17	0.44
1:D:373:THR:OG1	1:D:420:ASN:HA	2.17	0.44
1:C:60:VAL:O	1:C:62:ILE:N	2.50	0.44
1:A:386:ALA:HB1	1:A:387:PRO:CD	2.48	0.44
1:F:280:LEU:HD23	1:F:280:LEU:HA	1.80	0.44
1:B:261:LYS:HZ2	1:B:388:SER:HA	1.83	0.44
1:I:291:LEU:HD22	1:K:143:THR:HG21	1.99	0.44
1:A:94:GLU:O	1:A:97:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ARG:HG2	1:F:167:ARG:HH11	1.82	0.44
1:D:106:PHE:O	1:D:108:TYR:N	2.50	0.44
1:H:322:LEU:O	1:H:325:ALA:HB3	2.18	0.44
1:C:60:VAL:O	1:C:61:ALA:C	2.55	0.44
1:F:127:GLU:CD	1:F:242:PRO:HB3	2.37	0.44
1:G:335:ARG:HB2	1:G:335:ARG:HE	1.66	0.44
1:J:83:ASN:O	1:L:268:ASP:HB2	2.18	0.44
1:C:103:ARG:HG2	1:C:104:ALA:H	1.80	0.44
1:B:258:SER:O	1:B:260:THR:N	2.51	0.44
1:D:163:TYR:O	1:D:164:ARG:C	2.55	0.44
1:F:164:ARG:O	1:F:167:ARG:HB3	2.17	0.44
1:F:167:ARG:HG2	1:F:167:ARG:NH1	2.32	0.44
1:L:259:ALA:HA	1:L:263:LEU:HB2	2.00	0.44
1:J:223:SER:HA	1:J:233:VAL:HG21	1.98	0.44
1:G:398:GLN:HB3	1:G:401:ILE:HD12	1.98	0.44
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.84	0.44
1:A:145:MET:HG2	1:A:149:LEU:HD12	1.98	0.44
1:A:393:GLU:OE2	1:D:308:LYS:HD2	2.17	0.44
1:D:217:VAL:CG1	1:D:222:VAL:HG21	2.47	0.44
1:F:159:THR:HA	1:F:184:ILE:O	2.17	0.44
1:J:159:THR:HA	1:J:184:ILE:O	2.17	0.44
1:B:106:PHE:O	1:B:108:TYR:N	2.51	0.44
1:B:208:SER:HA	1:B:209:PRO:C	2.38	0.44
1:F:308:LYS:HD2	1:G:393:GLU:OE2	2.17	0.44
1:K:72:ILE:HG23	1:K:72:ILE:O	2.17	0.44
1:L:113:ASN:OD1	1:L:115:THR:N	2.49	0.44
1:F:241:THR:HG23	1:F:242:PRO:HD2	1.98	0.44
1:B:215:ARG:NH1	1:B:347:GLU:OE2	2.46	0.44
1:C:113:ASN:O	1:C:117:VAL:HG13	2.18	0.44
1:D:250:LEU:CD1	1:D:354:GLN:HB2	2.46	0.44
1:A:133:LEU:HD23	1:A:135:MET:HE3	1.99	0.44
1:J:135:MET:CE	1:J:141:ALA:HA	2.48	0.44
1:A:127:GLU:OE2	1:A:242:PRO:HB3	2.18	0.44
1:B:145:MET:HE1	1:B:146:LEU:HD23	2.00	0.44
1:B:258:SER:C	1:B:260:THR:H	2.21	0.44
1:H:234:CYS:HA	1:H:254:LEU:O	2.18	0.44
1:A:106:PHE:O	1:A:107:GLU:HB3	2.18	0.44
1:F:428:VAL:O	1:F:428:VAL:CG1	2.65	0.44
1:D:60:VAL:O	1:D:64:ALA:N	2.50	0.44
1:A:345:HIS:HE1	1:A:347:GLU:HG2	1.83	0.44
1:K:343:GLN:HE21	1:K:343:GLN:HB3	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:VAL:O	1:D:219:ILE:N	2.50	0.44
1:F:160:THR:HG22	1:F:183:VAL:HG12	1.99	0.44
1:K:217:VAL:HG13	1:K:222:VAL:HG21	1.99	0.44
1:B:393:GLU:OE2	1:C:308:LYS:HD2	2.17	0.44
1:J:259:ALA:HA	1:J:263:LEU:HB2	1.98	0.44
1:G:167:ARG:HG2	1:G:167:ARG:HH11	1.83	0.44
1:F:333:LYS:HE2	1:F:445:ILE:C	2.38	0.44
1:G:206:THR:O	1:G:235:ILE:HA	2.18	0.44
1:E:208:SER:HA	1:E:209:PRO:C	2.38	0.44
1:F:83:ASN:O	1:H:268:ASP:HB2	2.18	0.44
1:C:347:GLU:HB3	1:C:350:ILE:HD12	2.00	0.44
1:H:217:VAL:CG1	1:H:222:VAL:HG21	2.48	0.44
1:L:333:LYS:HE2	1:L:445:ILE:HG22	2.00	0.44
1:D:320:THR:O	1:D:324:MET:HB2	2.18	0.44
1:B:209:PRO:HG3	1:B:355:MET:HE1	1.99	0.44
1:L:374:ALA:O	1:L:377:VAL:HG22	2.17	0.44
1:E:94:GLU:O	1:E:95:LEU:C	2.55	0.44
1:H:244:ASN:O	1:H:245:GLN:HB3	2.18	0.43
1:C:114:PRO:O	1:C:117:VAL:HG22	2.18	0.43
1:D:117:VAL:HA	1:D:120:GLU:HB2	2.00	0.43
1:E:291:LEU:O	1:G:140:CYS:HA	2.17	0.43
1:F:278:LEU:O	1:F:280:LEU:N	2.51	0.43
1:I:343:GLN:HE21	1:I:343:GLN:HB3	1.62	0.43
1:A:331:HIS:CE1	1:A:333:LYS:HB2	2.52	0.43
1:G:386:ALA:HB1	1:G:387:PRO:CD	2.48	0.43
1:H:93:SER:O	1:H:96:ILE:HB	2.18	0.43
1:J:215:ARG:HD2	1:J:347:GLU:OE2	2.18	0.43
1:F:217:VAL:O	1:F:219:ILE:N	2.51	0.43
1:B:64:ALA:O	1:B:122:LYS:HE2	2.18	0.43
1:H:115:THR:CG2	1:H:297:PRO:HB3	2.48	0.43
1:E:116:THR:O	1:E:119:LEU:N	2.51	0.43
1:C:317:GLN:HG2	1:C:427:GLY:O	2.18	0.43
1:I:258:SER:O	1:I:260:THR:N	2.51	0.43
1:J:386:ALA:HB1	1:J:387:PRO:CD	2.48	0.43
1:H:411:ASP:O	1:H:414:LYS:HB2	2.18	0.43
1:J:73:VAL:O	1:J:74:THR:HG23	2.18	0.43
1:D:122:LYS:NZ	1:D:308:LYS:HE2	2.33	0.43
1:L:113:ASN:OD1	1:L:115:THR:HG22	2.17	0.43
1:H:423:ARG:NH2	2:H:507:HEN:O2B	2.51	0.43
1:E:161:ASP:HB3	1:E:210:THR:OG1	2.17	0.43
1:D:141:ALA:HB1	1:D:274:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:370:LEU:HD23	1:G:419:ASP:CB	2.45	0.43
1:G:287:LEU:HD12	1:G:287:LEU:O	2.19	0.43
1:E:421:LEU:HD12	1:E:422:VAL:H	1.83	0.43
1:B:192:LEU:HD21	1:B:222:VAL:HG13	2.01	0.43
1:H:260:THR:HG23	1:H:270:LEU:HD22	2.00	0.43
1:D:94:GLU:O	1:D:95:LEU:C	2.56	0.43
1:F:73:VAL:O	1:F:74:THR:HG23	2.19	0.43
1:I:243:LEU:CD1	1:I:311:HIS:HA	2.48	0.43
1:L:241:THR:HG23	1:L:242:PRO:HD2	1.98	0.43
1:I:161:ASP:HB3	1:I:210:THR:OG1	2.17	0.43
1:C:428:VAL:O	1:C:428:VAL:HG13	2.18	0.43
1:H:320:THR:O	1:H:324:MET:HB2	2.17	0.43
1:A:325:ALA:O	1:A:328:LEU:HB2	2.18	0.43
1:H:331:HIS:ND1	1:H:332:PRO:HD2	2.33	0.43
1:K:270:LEU:O	1:K:271:ALA:HB2	2.18	0.43
1:A:234:CYS:HA	1:A:254:LEU:O	2.17	0.43
1:H:240:ALA:O	1:H:244:ASN:HB2	2.19	0.43
1:J:241:THR:HG23	1:J:242:PRO:HD2	2.00	0.43
1:C:210:THR:HG22	1:C:215:ARG:N	2.24	0.43
1:I:216:CYS:SG	1:I:355:MET:CE	3.07	0.43
1:H:117:VAL:HA	1:H:120:GLU:HB2	2.00	0.43
1:I:156:ILE:HG23	1:I:181:ALA:CB	2.47	0.43
1:E:333:LYS:HE2	1:E:445:ILE:CG2	2.48	0.43
1:C:345:HIS:CE1	1:C:347:GLU:HG2	2.53	0.43
1:C:439:LEU:C	1:C:441:ALA:N	2.71	0.43
1:G:260:THR:CG2	1:G:270:LEU:HD22	2.48	0.43
1:A:192:LEU:HG	1:A:196:LEU:HD23	2.00	0.43
1:H:94:GLU:O	1:H:95:LEU:C	2.57	0.43
1:E:133:LEU:CD1	1:E:285:ARG:HD3	2.48	0.43
1:H:192:LEU:HG	1:H:196:LEU:HD23	2.01	0.43
1:D:127:GLU:OE2	1:D:257:HIS:NE2	2.52	0.43
1:L:117:VAL:HG23	1:L:118:VAL:N	2.34	0.43
1:D:135:MET:CE	1:D:141:ALA:HA	2.43	0.43
1:H:64:ALA:O	1:H:122:LYS:HE2	2.19	0.43
1:H:156:ILE:CG2	1:H:181:ALA:HB2	2.48	0.43
1:L:203:LEU:HB2	1:L:232:LEU:HB2	2.01	0.43
1:J:219:ILE:HG21	1:J:250:LEU:HB2	2.00	0.43
1:L:421:LEU:HD12	1:L:422:VAL:H	1.82	0.43
1:J:143:THR:HG23	1:J:169:PHE:CE1	2.53	0.43
1:J:324:MET:HG2	1:J:431:PHE:CE1	2.53	0.43
1:C:260:THR:CG2	1:C:270:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:339:TYR:CD1	1:I:362:VAL:HG22	2.54	0.43
1:H:196:LEU:HD13	1:H:196:LEU:HA	1.82	0.43
1:G:129:ALA:HB2	1:G:248:LEU:CD1	2.47	0.43
1:C:323:ARG:O	1:C:327:ILE:HG13	2.19	0.43
1:C:240:ALA:O	1:C:241:THR:CB	2.56	0.43
1:C:211:ASN:HA	1:C:212:PRO:HA	1.87	0.43
1:E:146:LEU:O	1:E:150:VAL:HG23	2.18	0.43
1:A:209:PRO:HG3	1:A:355:MET:HE1	2.00	0.43
1:D:209:PRO:HG3	1:D:355:MET:HE1	2.01	0.43
1:F:156:ILE:CG2	1:F:181:ALA:HB2	2.48	0.43
1:D:113:ASN:O	1:D:117:VAL:HG13	2.19	0.43
1:F:87:TYR:OH	1:F:113:ASN:HA	2.18	0.43
1:G:261:LYS:O	1:G:265:GLY:HA2	2.19	0.43
1:B:373:THR:OG1	1:B:420:ASN:HA	2.18	0.43
1:J:320:THR:HG23	1:J:431:PHE:HD1	1.84	0.43
1:F:270:LEU:HD23	1:F:270:LEU:N	2.34	0.43
1:B:150:VAL:HB	1:B:179:ILE:HD13	2.01	0.43
1:L:204:PHE:CE2	1:L:222:VAL:HG11	2.53	0.43
1:L:322:LEU:O	1:L:325:ALA:HB3	2.19	0.43
1:B:244:ASN:O	1:B:245:GLN:HB3	2.19	0.43
1:A:159:THR:HA	1:A:184:ILE:O	2.19	0.43
1:G:389:PHE:HB2	1:G:425:SER:OG	2.18	0.43
1:I:187:ALA:O	1:I:189:VAL:N	2.51	0.43
1:J:343:GLN:HB3	1:J:343:GLN:HE21	1.56	0.43
1:E:119:LEU:HG	1:E:134:LEU:HD11	2.00	0.43
1:G:376:PHE:CE1	1:G:442:LEU:HG	2.54	0.43
1:I:256:LEU:HB2	1:I:274:ILE:HG12	2.00	0.43
1:A:58:GLY:HA3	1:A:311:HIS:CD2	2.54	0.43
1:F:82:VAL:HG12	1:F:84:THR:HG22	2.01	0.43
1:I:258:SER:C	1:I:260:THR:N	2.72	0.43
1:G:426:PHE:HE1	1:G:438:ILE:HD11	1.84	0.43
1:G:121:GLU:O	1:G:124:SER:HB2	2.19	0.43
1:L:103:ARG:HG2	1:L:104:ALA:N	2.34	0.43
1:L:74:THR:C	1:L:76:ALA:H	2.22	0.43
1:G:103:ARG:HG2	1:G:104:ALA:N	2.34	0.43
1:J:211:ASN:HA	1:J:212:PRO:HA	1.88	0.43
1:E:209:PRO:HD3	1:E:240:ALA:HB2	2.00	0.43
1:E:311:HIS:CD2	1:E:312:LEU:HD23	2.54	0.43
1:C:156:ILE:CG2	1:C:181:ALA:HB2	2.49	0.43
1:L:443:ASP:C	1:L:445:ILE:N	2.72	0.43
1:E:159:THR:HA	1:E:184:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HA	1:A:80:PRO:HD3	1.90	0.43
1:A:269:VAL:C	1:A:270:LEU:HD23	2.39	0.43
1:A:336:HIS:HB3	1:A:365:GLU:HG3	2.00	0.43
1:F:196:LEU:HD12	1:F:229:LYS:HB2	2.00	0.43
1:D:260:THR:CG2	1:D:270:LEU:HD22	2.49	0.43
1:L:196:LEU:HD12	1:L:229:LYS:HB2	2.01	0.43
1:G:167:ARG:NH1	1:G:167:ARG:HG2	2.33	0.43
1:B:139:MET:HB3	1:D:290:ILE:O	2.19	0.43
1:B:103:ARG:HG2	1:B:104:ALA:N	2.34	0.43
1:L:94:GLU:O	1:L:97:ASP:HB2	2.18	0.43
1:L:248:LEU:HA	1:L:248:LEU:HD23	1.87	0.43
1:J:243:LEU:CD1	1:J:311:HIS:HA	2.49	0.43
1:C:87:TYR:HA	1:D:75:ASP:O	2.18	0.43
1:E:310:LEU:O	1:E:314:VAL:HG23	2.18	0.43
1:E:370:LEU:HD23	1:E:419:ASP:CB	2.46	0.43
1:G:204:PHE:CE2	1:G:222:VAL:HG11	2.54	0.43
1:F:386:ALA:HB1	1:F:387:PRO:CD	2.49	0.43
1:B:217:VAL:CG1	1:B:222:VAL:HG21	2.49	0.43
1:F:258:SER:O	1:F:260:THR:N	2.52	0.43
1:E:192:LEU:HD21	1:E:222:VAL:HG13	2.01	0.43
1:E:384:TYR:CZ	1:H:67:ARG:HD2	2.53	0.43
1:G:234:CYS:HA	1:G:254:LEU:O	2.19	0.43
1:C:160:THR:HG23	1:C:184:ILE:O	2.19	0.43
1:D:259:ALA:HB3	1:D:271:ALA:HB3	2.00	0.43
1:F:312:LEU:HD23	1:F:312:LEU:N	2.34	0.43
1:G:211:ASN:HB2	1:G:239:PHE:HE2	1.83	0.42
1:D:138:GLY:O	1:D:141:ALA:HB3	2.19	0.42
1:K:265:GLY:HA3	1:K:313:ARG:NH1	2.34	0.42
1:G:373:THR:OG1	1:G:420:ASN:HA	2.19	0.42
1:L:206:THR:O	1:L:235:ILE:HA	2.19	0.42
1:E:187:ALA:O	1:E:189:VAL:HG23	2.19	0.42
1:D:270:LEU:N	1:D:270:LEU:HD23	2.33	0.42
1:A:320:THR:O	1:A:324:MET:HB2	2.17	0.42
1:C:164:ARG:HD3	1:C:404:TYR:CE2	2.54	0.42
1:C:262:PHE:CE1	1:C:390:GLY:HA2	2.54	0.42
1:K:416:GLY:O	1:K:418:MET:HG2	2.19	0.42
1:J:187:ALA:O	1:J:189:VAL:N	2.52	0.42
1:H:243:LEU:CD1	1:H:311:HIS:HA	2.50	0.42
1:K:243:LEU:CD1	1:K:311:HIS:HA	2.50	0.42
1:C:185:ASP:OD1	1:C:215:ARG:NH2	2.52	0.42
1:K:211:ASN:HB2	1:K:239:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASP:HB3	1:B:210:THR:OG1	2.19	0.42
1:A:439:LEU:HA	1:A:442:LEU:HD12	2.01	0.42
1:B:60:VAL:CG1	1:B:64:ALA:HB2	2.49	0.42
1:G:260:THR:HG23	1:G:270:LEU:HD22	2.01	0.42
1:A:160:THR:HG23	1:A:184:ILE:O	2.19	0.42
1:J:291:LEU:HD22	1:L:143:THR:HG21	2.00	0.42
1:A:291:LEU:HD22	1:C:143:THR:HG21	2.01	0.42
1:C:140:CYS:O	1:C:144:VAL:HG23	2.19	0.42
1:D:158:THR:HA	1:D:205:PHE:O	2.19	0.42
1:D:64:ALA:O	1:D:122:LYS:HE2	2.19	0.42
1:D:60:VAL:HG12	1:D:64:ALA:HB2	2.01	0.42
1:J:211:ASN:HB2	1:J:239:PHE:HE2	1.83	0.42
1:J:174:LEU:N	1:J:175:PRO:CD	2.83	0.42
1:H:215:ARG:HD2	1:H:347:GLU:OE2	2.19	0.42
1:C:87:TYR:OH	1:C:113:ASN:HA	2.19	0.42
1:A:398:GLN:O	1:A:399:PRO:C	2.58	0.42
1:E:206:THR:O	1:E:235:ILE:HA	2.19	0.42
1:K:398:GLN:O	1:K:401:ILE:N	2.51	0.42
1:L:165:LYS:HA	1:L:168:ILE:HD12	2.01	0.42
1:J:106:PHE:O	1:J:108:TYR:N	2.52	0.42
1:A:117:VAL:O	1:A:121:GLU:HG3	2.19	0.42
1:J:164:ARG:O	1:J:167:ARG:HB3	2.19	0.42
1:I:160:THR:HG23	1:I:184:ILE:O	2.19	0.42
1:A:50:TYR:OH	1:A:68:LEU:HB2	2.19	0.42
1:J:95:LEU:O	1:J:95:LEU:HD12	2.18	0.42
1:L:238:THR:HB	2:L:511:HEN:H2A2	2.00	0.42
1:K:58:GLY:HA3	1:K:311:HIS:CD2	2.55	0.42
1:C:243:LEU:CD1	1:C:311:HIS:HA	2.49	0.42
1:B:345:HIS:HE1	1:B:347:GLU:HG2	1.83	0.42
1:C:63:HIS:CD2	1:C:67:ARG:HD3	2.54	0.42
1:H:110:ARG:HD3	1:H:292:GLY:CA	2.50	0.42
1:K:377:VAL:HG23	1:K:378:ASP:N	2.34	0.42
1:I:135:MET:HE1	1:I:141:ALA:HA	2.01	0.42
1:I:135:MET:HE1	1:I:274:ILE:HD12	2.02	0.42
1:H:259:ALA:HA	1:H:263:LEU:HB2	2.01	0.42
1:K:72:ILE:O	1:K:72:ILE:HG12	2.18	0.42
1:F:117:VAL:HG23	1:F:118:VAL:N	2.35	0.42
1:J:173:ILE:O	1:J:176:LYS:HB2	2.18	0.42
1:B:217:VAL:HG13	1:B:222:VAL:HG21	2.02	0.42
1:J:428:VAL:HG13	1:J:428:VAL:O	2.20	0.42
1:D:331:HIS:CG	1:D:332:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:TYR:O	1:B:164:ARG:C	2.58	0.42
1:F:163:TYR:O	1:F:164:ARG:C	2.58	0.42
1:K:150:VAL:HB	1:K:179:ILE:HD13	2.01	0.42
1:L:234:CYS:HA	1:L:254:LEU:O	2.19	0.42
1:I:238:THR:HB	2:I:508:HEN:H2A2	2.01	0.42
1:J:126:LEU:HA	1:J:126:LEU:HD23	1.80	0.42
1:F:126:LEU:HD23	1:F:126:LEU:HA	1.82	0.42
1:L:242:PRO:HD3	1:L:257:HIS:CE1	2.54	0.42
1:A:211:ASN:ND2	1:A:212:PRO:N	2.67	0.42
1:C:250:LEU:CD1	1:C:354:GLN:HB2	2.50	0.42
1:B:313:ARG:O	1:B:317:GLN:HG3	2.20	0.42
1:L:123:ILE:HD13	1:L:273:CYS:SG	2.60	0.42
1:I:389:PHE:HB2	1:I:425:SER:HB2	2.02	0.42
1:D:322:LEU:O	1:D:325:ALA:HB3	2.20	0.42
1:K:321:ALA:HB2	1:K:360:GLY:HA2	2.01	0.42
1:E:346:PRO:HB2	1:E:347:GLU:OE2	2.20	0.42
1:A:209:PRO:HD3	1:A:240:ALA:HB2	2.02	0.42
1:A:313:ARG:O	1:A:317:GLN:HG3	2.19	0.42
1:G:146:LEU:O	1:G:150:VAL:HG23	2.20	0.42
1:A:373:THR:OG1	1:A:420:ASN:HA	2.19	0.42
1:B:173:ILE:O	1:B:176:LYS:HB2	2.20	0.42
1:K:63:HIS:HD2	1:K:67:ARG:HD3	1.83	0.42
1:D:394:SER:C	1:D:395:ILE:HG13	2.38	0.42
1:J:82:VAL:HG12	1:J:84:THR:HG22	2.00	0.42
1:J:72:ILE:O	1:J:72:ILE:HG12	2.20	0.42
1:K:106:PHE:O	1:K:107:GLU:HB3	2.19	0.42
1:H:163:TYR:O	1:H:164:ARG:C	2.58	0.42
1:G:192:LEU:HG	1:G:196:LEU:HD23	2.02	0.42
1:J:331:HIS:HB3	1:J:334:VAL:HG23	2.01	0.42
1:J:394:SER:HB2	1:J:429:GLU:OE2	2.19	0.42
1:E:150:VAL:CG1	1:E:179:ILE:HD13	2.49	0.42
1:E:141:ALA:O	1:E:142:SER:C	2.58	0.42
1:E:156:ILE:HG23	1:E:181:ALA:CB	2.50	0.42
1:G:63:HIS:CD2	1:G:67:ARG:HD3	2.55	0.42
1:A:133:LEU:CD1	1:A:285:ARG:HD3	2.50	0.42
1:B:173:ILE:C	1:B:175:PRO:HD2	2.39	0.42
1:J:277:PRO:HG2	1:J:280:LEU:HB2	2.01	0.42
1:E:438:ILE:O	1:E:442:LEU:HD12	2.20	0.42
1:I:141:ALA:HB1	1:I:274:ILE:HD11	2.02	0.42
1:G:269:VAL:C	1:G:270:LEU:HD23	2.40	0.42
1:A:223:SER:HA	1:A:233:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:VAL:O	1:E:61:ALA:C	2.57	0.42
1:I:60:VAL:HG13	1:I:64:ALA:HB2	2.01	0.42
1:E:211:ASN:HA	1:E:212:PRO:HA	1.82	0.42
1:L:345:HIS:HE1	1:L:347:GLU:HG2	1.82	0.42
1:H:172:THR:O	1:H:175:PRO:HG2	2.20	0.42
1:E:174:LEU:N	1:E:175:PRO:CD	2.80	0.42
1:D:339:TYR:CD1	1:D:362:VAL:HG22	2.55	0.42
1:K:156:ILE:O	1:K:181:ALA:HA	2.20	0.42
1:K:156:ILE:HG23	1:K:181:ALA:CB	2.50	0.42
1:K:156:ILE:CG2	1:K:181:ALA:HB2	2.50	0.42
1:G:72:ILE:HG23	1:G:72:ILE:O	2.20	0.42
1:I:242:PRO:HD3	1:I:257:HIS:CE1	2.55	0.42
1:A:83:ASN:O	1:B:78:THR:OG1	2.33	0.42
1:E:60:VAL:CG1	1:E:64:ALA:HB2	2.50	0.42
1:B:243:LEU:CD1	1:B:311:HIS:HA	2.50	0.42
1:C:60:VAL:O	1:C:64:ALA:N	2.51	0.42
1:J:60:VAL:CG1	1:J:64:ALA:HB2	2.50	0.42
1:A:156:ILE:HG13	1:A:203:LEU:HD23	2.00	0.42
1:D:145:MET:HE1	1:D:146:LEU:HD23	2.01	0.42
1:F:146:LEU:O	1:F:150:VAL:HG23	2.19	0.42
1:L:217:VAL:HG13	1:L:222:VAL:HG21	2.02	0.42
1:I:374:ALA:O	1:I:377:VAL:HG22	2.20	0.42
1:G:94:GLU:O	1:G:97:ASP:HB2	2.20	0.42
1:D:196:LEU:HD12	1:D:229:LYS:HB2	2.02	0.42
1:K:234:CYS:HA	1:K:254:LEU:O	2.20	0.42
1:I:126:LEU:HD23	1:I:126:LEU:HA	1.78	0.42
1:B:242:PRO:HD3	1:B:257:HIS:CE1	2.54	0.41
1:J:421:LEU:HD12	1:J:422:VAL:H	1.85	0.41
1:H:110:ARG:HD3	1:H:292:GLY:HA2	2.01	0.41
1:K:398:GLN:O	1:K:399:PRO:C	2.58	0.41
1:F:196:LEU:HD13	1:F:196:LEU:HA	1.81	0.41
1:G:205:PHE:HE1	1:G:256:LEU:HD21	1.85	0.41
1:J:192:LEU:HG	1:J:196:LEU:HD23	2.02	0.41
1:L:324:MET:HG2	1:L:431:PHE:CE1	2.55	0.41
1:J:206:THR:O	1:J:235:ILE:HA	2.20	0.41
1:K:52:SER:OG	1:K:53:PHE:N	2.53	0.41
1:F:60:VAL:O	1:F:61:ALA:C	2.57	0.41
1:F:60:VAL:O	1:F:62:ILE:N	2.54	0.41
1:G:428:VAL:HG13	1:G:428:VAL:O	2.20	0.41
1:C:383:PRO:HA	1:C:394:SER:O	2.20	0.41
1:H:207:GLU:OE1	2:H:507:HEN:H2A3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ASP:HB3	1:F:210:THR:OG1	2.20	0.41
1:A:208:SER:HA	1:A:209:PRO:C	2.39	0.41
1:F:268:ASP:HB2	1:H:83:ASN:O	2.20	0.41
1:B:331:HIS:CG	1:B:332:PRO:HD2	2.55	0.41
1:A:339:TYR:CD1	1:A:362:VAL:HG22	2.55	0.41
1:A:398:GLN:O	1:A:400:ALA:N	2.53	0.41
1:E:280:LEU:HD23	1:E:280:LEU:HA	1.91	0.41
1:G:366:VAL:O	1:G:420:ASN:HB3	2.21	0.41
1:J:442:LEU:C	1:J:444:SER:N	2.74	0.41
1:A:428:VAL:HG12	1:D:62:ILE:HD11	2.03	0.41
1:K:270:LEU:N	1:K:270:LEU:HD23	2.34	0.41
1:J:238:THR:HB	2:J:509:HEN:H2A2	2.02	0.41
1:D:187:ALA:O	1:D:189:VAL:N	2.53	0.41
1:G:207:GLU:CB	1:G:236:ASP:HB3	2.45	0.41
1:D:209:PRO:HA	1:D:215:ARG:O	2.20	0.41
1:D:211:ASN:HB2	1:D:239:PHE:HE2	1.85	0.41
1:F:219:ILE:HB	1:F:250:LEU:HD12	2.01	0.41
1:B:369:ASP:O	1:B:370:LEU:C	2.59	0.41
1:C:72:ILE:HG23	1:C:72:ILE:O	2.20	0.41
1:E:159:THR:HG23	1:E:206:THR:HB	2.01	0.41
1:D:278:LEU:O	1:D:280:LEU:N	2.53	0.41
1:L:196:LEU:HD13	1:L:196:LEU:HA	1.82	0.41
1:A:73:VAL:O	1:A:74:THR:HG23	2.20	0.41
1:I:383:PRO:HB3	1:I:394:SER:HB3	2.03	0.41
1:L:428:VAL:HG13	1:L:428:VAL:O	2.20	0.41
1:C:170:ILE:HG23	1:C:174:LEU:HD12	2.01	0.41
1:I:145:MET:HG2	1:I:149:LEU:HD12	2.03	0.41
1:A:335:ARG:HE	1:A:335:ARG:HB2	1.71	0.41
1:K:79:THR:HA	1:K:80:PRO:HD3	1.89	0.41
1:K:208:SER:HA	1:K:209:PRO:C	2.41	0.41
1:E:336:HIS:O	1:E:364:PHE:HB2	2.20	0.41
1:K:260:THR:CG2	1:K:270:LEU:HD22	2.51	0.41
1:H:89:PHE:CD2	1:H:95:LEU:HA	2.55	0.41
1:H:196:LEU:HD12	1:H:229:LYS:HB2	2.01	0.41
1:A:121:GLU:O	1:A:124:SER:HB2	2.20	0.41
1:F:393:GLU:OE2	1:G:308:LYS:HD2	2.21	0.41
1:B:238:THR:HB	2:B:501:HEN:H2A2	2.00	0.41
1:C:145:MET:HG2	1:C:149:LEU:HD12	2.02	0.41
1:F:208:SER:HA	1:F:209:PRO:C	2.39	0.41
1:A:60:VAL:O	1:A:61:ALA:C	2.58	0.41
1:H:347:GLU:CB	1:H:350:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:THR:HG22	1:B:215:ARG:N	2.24	0.41
1:D:210:THR:CG2	1:D:215:ARG:H	2.29	0.41
1:I:83:ASN:O	1:K:268:ASP:HB2	2.20	0.41
1:D:82:VAL:HG12	1:D:84:THR:HG22	2.01	0.41
1:C:331:HIS:CG	1:C:332:PRO:HD2	2.56	0.41
1:A:420:ASN:O	1:A:422:VAL:HG23	2.21	0.41
1:K:114:PRO:O	1:K:117:VAL:HG22	2.20	0.41
1:H:260:THR:CG2	1:H:270:LEU:HD22	2.49	0.41
1:H:94:GLU:O	1:H:97:ASP:HB2	2.20	0.41
1:E:290:ILE:O	1:G:139:MET:HB3	2.20	0.41
1:C:82:VAL:HG22	1:D:80:PRO:HB3	2.02	0.41
1:J:158:THR:HA	1:J:205:PHE:O	2.20	0.41
1:H:296:ASN:OD1	1:H:298:ASN:HB2	2.21	0.41
1:F:60:VAL:CG1	1:F:64:ALA:HB2	2.50	0.41
1:J:58:GLY:HA3	1:J:311:HIS:CD2	2.55	0.41
1:J:382:ILE:HB	1:J:383:PRO:HD3	2.03	0.41
1:K:243:LEU:HD12	1:K:314:VAL:HG21	2.02	0.41
1:A:60:VAL:HG12	1:A:64:ALA:HB2	2.02	0.41
1:I:345:HIS:HE1	1:I:347:GLU:HG2	1.85	0.41
1:K:135:MET:HE2	1:K:274:ILE:HD12	2.01	0.41
1:E:343:GLN:HE21	1:E:343:GLN:HB3	1.63	0.41
1:J:373:THR:OG1	1:J:420:ASN:HA	2.20	0.41
1:F:140:CYS:HB2	1:H:292:GLY:O	2.20	0.41
1:F:141:ALA:HB1	1:F:274:ILE:HD11	2.01	0.41
1:L:336:HIS:HB3	1:L:365:GLU:HG3	2.01	0.41
1:K:163:TYR:O	1:K:164:ARG:C	2.59	0.41
1:J:163:TYR:O	1:J:164:ARG:C	2.59	0.41
1:D:262:PHE:CE1	1:D:390:GLY:HA2	2.55	0.41
1:F:94:GLU:O	1:F:97:ASP:HB2	2.21	0.41
1:L:106:PHE:O	1:L:108:TYR:N	2.54	0.41
1:L:394:SER:HB2	1:L:429:GLU:OE2	2.19	0.41
1:B:187:ALA:O	1:B:189:VAL:N	2.54	0.41
1:A:64:ALA:O	1:A:122:LYS:HE2	2.21	0.41
1:G:60:VAL:O	1:G:64:ALA:N	2.46	0.41
1:J:170:ILE:HA	1:J:174:LEU:CD1	2.40	0.41
1:H:345:HIS:HA	1:H:346:PRO:HD3	1.95	0.41
1:L:57:ASP:HB3	1:L:243:LEU:CD2	2.50	0.41
1:A:57:ASP:HB3	1:A:243:LEU:CD2	2.51	0.41
1:E:243:LEU:HD12	1:E:314:VAL:HG21	2.03	0.41
1:K:174:LEU:N	1:K:175:PRO:CD	2.82	0.41
1:A:259:ALA:HA	1:A:263:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:ILE:CG2	1:G:181:ALA:HB2	2.51	0.41
1:J:63:HIS:CD2	1:J:67:ARG:HD3	2.56	0.41
1:C:331:HIS:ND1	1:C:332:PRO:HD2	2.35	0.41
1:I:376:PHE:HB2	1:I:445:ILE:HD12	2.03	0.41
1:C:343:GLN:HE21	1:C:343:GLN:HB3	1.57	0.41
1:F:135:MET:HE2	1:F:141:ALA:HA	2.02	0.41
1:C:141:ALA:HB1	1:C:274:ILE:HD11	2.02	0.41
1:K:217:VAL:O	1:K:219:ILE:N	2.52	0.41
1:C:140:CYS:O	1:C:143:THR:HB	2.21	0.41
1:H:119:LEU:HD21	1:H:303:ILE:HG21	2.01	0.41
1:D:50:TYR:HB3	1:D:51:ALA:H	1.68	0.41
1:H:159:THR:HG23	1:H:206:THR:HB	2.02	0.41
1:F:85:SER:OG	1:H:267:ASN:HA	2.21	0.41
1:L:305:ARG:O	1:L:308:LYS:HB2	2.21	0.41
1:A:383:PRO:HB2	1:A:396:VAL:CG2	2.35	0.41
1:B:206:THR:OG1	1:B:207:GLU:N	2.54	0.41
1:F:348:HIS:O	1:F:352:LYS:HB2	2.20	0.41
1:G:261:LYS:HB2	1:G:262:PHE:H	1.70	0.41
1:I:320:THR:HG23	1:I:431:PHE:HD1	1.85	0.41
1:J:438:ILE:O	1:J:441:ALA:HB3	2.21	0.41
1:I:72:ILE:HG23	1:I:72:ILE:O	2.20	0.41
1:H:138:GLY:O	1:H:141:ALA:HB3	2.20	0.41
1:G:158:THR:HA	1:G:205:PHE:O	2.21	0.41
1:K:258:SER:C	1:K:260:THR:N	2.74	0.41
1:I:258:SER:C	1:I:260:THR:H	2.23	0.41
1:C:143:THR:HG23	1:C:169:PHE:CE1	2.56	0.41
2:I:508:HEN:P	1:K:110:ARG:HH21	2.43	0.41
1:J:331:HIS:CG	1:J:332:PRO:HD2	2.55	0.41
1:L:260:THR:CG2	1:L:270:LEU:HD22	2.50	0.41
1:K:194:LEU:O	1:K:198:GLN:HG3	2.21	0.41
1:B:389:PHE:HB2	1:B:425:SER:HB2	2.03	0.41
1:G:106:PHE:O	1:G:107:GLU:HB3	2.21	0.41
1:D:240:ALA:O	1:D:244:ASN:HB2	2.20	0.41
1:J:382:ILE:HB	1:J:383:PRO:CD	2.51	0.41
1:G:211:ASN:HD22	1:G:212:PRO:N	2.19	0.41
1:K:145:MET:HE2	1:K:146:LEU:HA	2.01	0.41
1:K:211:ASN:HA	1:K:212:PRO:HA	1.89	0.41
1:B:211:ASN:HA	1:B:212:PRO:HA	1.84	0.41
1:B:135:MET:CE	1:B:141:ALA:HA	2.51	0.41
1:L:156:ILE:HG23	1:L:181:ALA:CB	2.51	0.41
1:F:343:GLN:HB3	1:F:343:GLN:HE21	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:343:GLN:HE21	1:H:343:GLN:HB3	1.54	0.41
1:F:281:VAL:HG13	1:F:282:SER:N	2.35	0.41
1:D:174:LEU:N	1:D:175:PRO:CD	2.84	0.41
1:J:261:LYS:HB3	1:J:389:PHE:O	2.21	0.41
1:B:143:THR:HG23	1:B:169:PHE:CE1	2.56	0.41
1:C:192:LEU:HG	1:C:196:LEU:HD23	2.03	0.41
1:L:173:ILE:O	1:L:176:LYS:HB2	2.21	0.41
1:A:397:ASP:OD1	1:A:399:PRO:HD3	2.21	0.41
1:E:155:HIS:ND1	1:E:180:THR:O	2.54	0.41
1:L:280:LEU:HD23	1:L:280:LEU:HA	1.95	0.41
1:B:67:ARG:HD2	1:C:384:TYR:CZ	2.56	0.41
1:A:187:ALA:O	1:A:189:VAL:HG23	2.21	0.41
1:J:143:THR:HG21	1:L:291:LEU:HD22	2.03	0.41
1:F:365:GLU:HB3	1:F:420:ASN:HB2	2.02	0.41
1:F:420:ASN:O	1:F:422:VAL:HG23	2.21	0.41
1:E:204:PHE:CE2	1:E:222:VAL:HG11	2.56	0.41
1:F:145:MET:HE1	1:F:146:LEU:HD23	2.02	0.41
1:I:291:LEU:O	1:K:140:CYS:HA	2.21	0.41
1:K:248:LEU:HD23	1:K:248:LEU:HA	1.92	0.41
1:B:443:ASP:C	1:B:445:ILE:N	2.74	0.41
1:B:103:ARG:HG2	1:B:104:ALA:H	1.85	0.41
1:E:114:PRO:O	1:E:117:VAL:HG22	2.21	0.41
1:E:302:LEU:HA	1:E:302:LEU:HD23	1.94	0.41
1:H:208:SER:HA	1:H:209:PRO:C	2.41	0.41
1:I:110:ARG:HH21	2:K:510:HEN:P	2.43	0.41
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.74	0.41
1:A:383:PRO:HA	1:A:394:SER:O	2.21	0.41
1:A:62:ILE:O	1:A:122:LYS:NZ	2.54	0.41
1:A:243:LEU:HD12	1:A:314:VAL:HG21	2.03	0.41
1:J:113:ASN:OD1	1:J:115:THR:HG22	2.21	0.41
1:J:278:LEU:O	1:J:280:LEU:N	2.54	0.41
1:G:442:LEU:HD23	1:G:445:ILE:HD12	2.03	0.41
1:B:270:LEU:HD23	1:B:270:LEU:N	2.36	0.41
1:H:106:PHE:O	1:H:108:TYR:N	2.54	0.41
1:I:160:THR:HG22	1:I:183:VAL:HG12	2.03	0.41
1:L:389:PHE:HB2	1:L:425:SER:OG	2.21	0.41
1:F:103:ARG:HG2	1:F:104:ALA:N	2.36	0.41
1:L:312:LEU:HD23	1:L:312:LEU:N	2.36	0.41
1:D:376:PHE:HB2	1:D:445:ILE:CD1	2.38	0.40
1:J:127:GLU:OE2	1:J:242:PRO:HB3	2.21	0.40
1:B:268:ASP:CB	1:D:83:ASN:O	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:350:ILE:O	1:I:354:GLN:HG2	2.21	0.40
1:A:211:ASN:HA	1:A:212:PRO:HA	1.83	0.40
1:J:113:ASN:O	1:J:117:VAL:HG13	2.21	0.40
1:H:335:ARG:HE	1:H:335:ARG:HB2	1.58	0.40
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.87	0.40
1:C:420:ASN:O	1:C:422:VAL:HG23	2.21	0.40
1:C:196:LEU:HA	1:C:196:LEU:HD13	1.85	0.40
1:H:386:ALA:HB1	1:H:387:PRO:CD	2.51	0.40
1:A:56:SER:OG	1:D:430:ASP:HB2	2.20	0.40
1:K:377:VAL:CG2	1:K:378:ASP:N	2.84	0.40
1:L:287:LEU:HD12	1:L:287:LEU:O	2.20	0.40
1:A:92:THR:OG1	1:C:378:ASP:OD1	2.36	0.40
1:H:331:HIS:CE1	1:H:333:LYS:HB2	2.56	0.40
1:B:223:SER:HA	1:B:233:VAL:HG21	2.02	0.40
1:J:411:ASP:O	1:J:414:LYS:HB2	2.21	0.40
1:F:137:SER:O	1:F:138:GLY:C	2.60	0.40
1:I:240:ALA:O	1:I:244:ASN:HB2	2.21	0.40
1:F:57:ASP:HB3	1:F:243:LEU:CD2	2.51	0.40
1:L:211:ASN:HB2	1:L:239:PHE:HE2	1.85	0.40
1:F:83:ASN:O	1:H:268:ASP:CB	2.70	0.40
1:K:119:LEU:HD12	1:K:119:LEU:O	2.21	0.40
1:B:117:VAL:O	1:B:121:GLU:HG3	2.21	0.40
1:I:170:ILE:HG23	1:I:174:LEU:HD12	2.02	0.40
1:J:160:THR:HG23	1:J:184:ILE:O	2.21	0.40
1:K:339:TYR:CD1	1:K:362:VAL:HG22	2.55	0.40
1:C:258:SER:C	1:C:260:THR:N	2.74	0.40
1:J:72:ILE:HD13	1:J:80:PRO:HG2	2.03	0.40
1:G:87:TYR:CE1	1:G:106:PHE:HB2	2.56	0.40
1:I:382:ILE:HD12	1:I:437:ASP:HB2	2.03	0.40
1:E:322:LEU:O	1:E:325:ALA:HB3	2.21	0.40
1:D:60:VAL:O	1:D:61:ALA:C	2.60	0.40
1:F:211:ASN:HA	1:F:212:PRO:HA	1.87	0.40
1:F:345:HIS:HA	1:F:346:PRO:HD3	1.93	0.40
1:D:132:THR:HG22	1:D:133:LEU:N	2.36	0.40
2:A:500:HEN:OG2	1:C:111:TYR:HE2	2.03	0.40
1:E:141:ALA:HB1	1:E:274:ILE:HD11	2.02	0.40
1:A:277:PRO:O	1:A:281:VAL:HG12	2.21	0.40
1:C:72:ILE:HD13	1:C:80:PRO:HG2	2.02	0.40
1:C:336:HIS:HB3	1:C:365:GLU:HG3	2.04	0.40
1:E:260:THR:CG2	1:E:270:LEU:HD22	2.50	0.40
1:J:398:GLN:O	1:J:399:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:MET:HG2	1:D:110:ARG:NH2	2.37	0.40
1:B:73:VAL:O	1:B:74:THR:HG23	2.21	0.40
1:L:187:ALA:O	1:L:189:VAL:N	2.55	0.40
1:I:94:GLU:O	1:I:97:ASP:HB2	2.22	0.40
1:B:377:VAL:CG2	1:B:378:ASP:N	2.84	0.40
1:K:364:PHE:CD2	1:K:364:PHE:O	2.74	0.40
1:J:99:LYS:HD3	1:J:99:LYS:HA	1.90	0.40
1:L:156:ILE:HG13	1:L:203:LEU:HD23	2.02	0.40
1:G:203:LEU:HB2	1:G:232:LEU:HB2	2.02	0.40
1:C:79:THR:HA	1:C:80:PRO:HD3	1.93	0.40
1:I:376:PHE:CE1	1:I:442:LEU:HG	2.56	0.40
1:H:439:LEU:C	1:H:441:ALA:N	2.75	0.40
1:E:439:LEU:C	1:E:441:ALA:N	2.74	0.40
1:C:377:VAL:HG23	1:C:378:ASP:N	2.37	0.40
1:C:91:LYS:HG3	1:C:94:GLU:HG3	2.03	0.40
1:E:62:ILE:HD11	1:H:428:VAL:HG12	2.03	0.40
1:A:320:THR:HG23	1:A:431:PHE:HD1	1.86	0.40
1:C:160:THR:HG22	1:C:183:VAL:HG12	2.03	0.40
1:E:262:PHE:CE1	1:E:390:GLY:HA2	2.56	0.40
1:A:163:TYR:O	1:A:164:ARG:C	2.60	0.40
1:H:160:THR:HG22	1:H:183:VAL:HG12	2.03	0.40
1:E:408:SER:OG	1:E:411:ASP:HB2	2.21	0.40
1:B:117:VAL:HA	1:B:120:GLU:HB2	2.03	0.40
1:I:287:LEU:O	1:I:287:LEU:HD12	2.22	0.40
1:A:82:VAL:HG21	1:A:114:PRO:HG2	2.02	0.40
1:G:377:VAL:HG23	1:G:378:ASP:N	2.37	0.40
1:C:258:SER:C	1:C:260:THR:H	2.25	0.40
1:D:160:THR:HG22	1:D:183:VAL:HG12	2.03	0.40
1:G:305:ARG:O	1:G:308:LYS:HB2	2.21	0.40
1:D:262:PHE:O	1:D:263:LEU:C	2.60	0.40
1:L:382:ILE:HD12	1:L:437:ASP:HB2	2.04	0.40
1:C:259:ALA:HA	1:C:263:LEU:HB2	2.04	0.40
1:E:416:GLY:O	1:E:418:MET:HG2	2.20	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	394/445 (88%)	322 (82%)	64 (16%)	8 (2%)	9	48
1	B	394/445 (88%)	320 (81%)	63 (16%)	11 (3%)	6	37
1	C	394/445 (88%)	324 (82%)	56 (14%)	14 (4%)	4	30
1	D	394/445 (88%)	331 (84%)	55 (14%)	8 (2%)	9	48
1	E	394/445 (88%)	327 (83%)	56 (14%)	11 (3%)	6	37
1	F	394/445 (88%)	316 (80%)	69 (18%)	9 (2%)	8	44
1	G	394/445 (88%)	332 (84%)	54 (14%)	8 (2%)	9	48
1	H	394/445 (88%)	327 (83%)	61 (16%)	6 (2%)	13	55
1	I	394/445 (88%)	329 (84%)	52 (13%)	13 (3%)	5	32
1	J	394/445 (88%)	328 (83%)	59 (15%)	7 (2%)	11	51
1	K	394/445 (88%)	325 (82%)	57 (14%)	12 (3%)	5	35
1	L	394/445 (88%)	325 (82%)	60 (15%)	9 (2%)	8	44
All	All	4728/5340 (88%)	3906 (83%)	706 (15%)	116 (2%)	7	41

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ASP
1	B	188	ASP
1	C	188	ASP
1	D	164	ARG
1	D	188	ASP
1	E	188	ASP
1	F	188	ASP
1	G	188	ASP
1	H	188	ASP
1	I	188	ASP
1	J	188	ASP
1	K	188	ASP

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Mol	Chain	Res	Type
1	L	188	ASP
1	A	164	ARG
1	B	164	ARG
1	B	444	SER
1	C	164	ARG
1	C	265	GLY
1	D	279	LYS
1	D	442	LEU
1	E	164	ARG
1	E	370	LEU
1	F	164	ARG
1	G	164	ARG
1	H	164	ARG
1	I	164	ARG
1	J	164	ARG
1	K	164	ARG
1	K	265	GLY
1	K	279	LYS
1	L	164	ARG
1	C	61	ALA
1	C	279	LYS
1	E	261	LYS
1	F	279	LYS
1	G	265	GLY
1	G	444	SER
1	H	259	ALA
1	I	61	ALA
1	J	279	LYS
1	A	279	LYS
1	B	53	PHE
1	B	241	THR
1	B	259	ALA
1	B	416	GLY
1	C	320	THR
1	C	442	LEU
1	D	107	GLU
1	E	141	ALA
1	E	218	ASP
1	E	294	ALA
1	E	416	GLY
1	E	417	ILE
1	F	107	GLU

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Mol	Chain	Res	Type
1	F	241	THR
1	F	259	ALA
1	H	442	LEU
1	I	218	ASP
1	I	259	ALA
1	I	321	ALA
1	J	107	GLU
1	K	61	ALA
1	K	241	THR
1	L	107	GLU
1	L	370	LEU
1	A	218	ASP
1	A	241	THR
1	A	370	LEU
1	A	399	PRO
1	B	107	GLU
1	B	279	LYS
1	B	370	LEU
1	C	107	GLU
1	C	198	GLN
1	C	241	THR
1	C	319	SER
1	C	370	LEU
1	D	370	LEU
1	E	241	THR
1	H	241	THR
1	I	241	THR
1	I	279	LYS
1	I	370	LEU
1	J	53	PHE
1	J	241	THR
1	K	107	GLU
1	K	259	ALA
1	L	241	THR
1	L	320	THR
1	L	442	LEU
1	A	416	GLY
1	D	241	THR
1	D	416	GLY
1	G	321	ALA
1	G	370	LEU
1	I	265	GLY

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Mol	Chain	Res	Type
1	J	416	GLY
1	K	387	PRO
1	L	399	PRO
1	F	399	PRO
1	G	241	THR
1	L	416	GLY
1	G	219	ILE
1	H	399	PRO
1	I	417	ILE
1	K	417	ILE
1	F	416	GLY
1	I	416	GLY
1	K	399	PRO
1	K	427	GLY
1	B	399	PRO
1	C	399	PRO
1	C	416	GLY
1	E	387	PRO
1	F	417	ILE
1	I	73	VAL

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	327/364 (90%)	278 (85%)	49 (15%)	3	17
1	B	327/364 (90%)	283 (86%)	44 (14%)	5	22
1	C	327/364 (90%)	275 (84%)	52 (16%)	3	14
1	D	327/364 (90%)	279 (85%)	48 (15%)	4	18
1	E	327/364 (90%)	276 (84%)	51 (16%)	3	15
1	F	327/364 (90%)	274 (84%)	53 (16%)	3	14
1	G	327/364 (90%)	282 (86%)	45 (14%)	4	21
1	H	327/364 (90%)	279 (85%)	48 (15%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	327/364 (90%)	284 (87%)	43 (13%)	5	24
1	J	327/364 (90%)	281 (86%)	46 (14%)	4	20
1	K	327/364 (90%)	279 (85%)	48 (15%)	4	18
1	L	327/364 (90%)	283 (86%)	44 (14%)	5	22
All	All	3924/4368 (90%)	3353 (85%)	571 (15%)	4	19

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	56	SER
1	A	70	ARG
1	A	91	LYS
1	A	93	SER
1	A	101	LYS
1	A	115	THR
1	A	134	LEU
1	A	135	MET
1	A	142	SER
1	A	145	MET
1	A	156	ILE
1	A	161	ASP
1	A	162	CYS
1	A	165	LYS
1	A	177	MET
1	A	180	THR
1	A	196	LEU
1	A	199	LYS
1	A	200	LYS
1	A	203	LEU
1	A	210	THR
1	A	211	ASN
1	A	214	LEU
1	A	273	CYS
1	A	275	SER
1	A	278	LEU
1	A	303	ILE
1	A	311	HIS
1	A	315	GLN
1	A	335	ARG
1	A	343	GLN

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Mol	Chain	Res	Type
1	A	344	SER
1	A	347	GLU
1	A	352	LYS
1	A	370	LEU
1	A	394	SER
1	A	396	VAL
1	A	397	ASP
1	A	402	MET
1	A	403	SER
1	A	410	SER
1	A	414	LYS
1	A	420	ASN
1	A	423	ARG
1	A	428	VAL
1	A	430	ASP
1	A	443	ASP
1	A	445	ILE
1	B	52	SER
1	B	56	SER
1	B	70	ARG
1	B	79	THR
1	B	93	SER
1	B	101	LYS
1	B	115	THR
1	B	134	LEU
1	B	135	MET
1	B	142	SER
1	B	145	MET
1	B	156	ILE
1	B	161	ASP
1	B	165	LYS
1	B	177	MET
1	B	180	THR
1	B	196	LEU
1	B	199	LYS
1	B	200	LYS
1	B	203	LEU
1	B	210	THR
1	B	211	ASN
1	B	214	LEU
1	B	273	CYS
1	B	275	SER

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Mol	Chain	Res	Type
1	B	279	LYS
1	B	303	ILE
1	B	311	HIS
1	B	315	GLN
1	B	335	ARG
1	B	343	GLN
1	B	344	SER
1	B	347	GLU
1	B	352	LYS
1	B	353	LYS
1	B	370	LEU
1	B	396	VAL
1	B	402	MET
1	B	403	SER
1	B	410	SER
1	B	414	LYS
1	B	420	ASN
1	B	430	ASP
1	B	444	SER
1	C	56	SER
1	C	70	ARG
1	C	91	LYS
1	C	93	SER
1	C	100	GLU
1	C	101	LYS
1	C	115	THR
1	C	131	SER
1	C	134	LEU
1	C	135	MET
1	C	142	SER
1	C	145	MET
1	C	156	ILE
1	C	161	ASP
1	C	165	LYS
1	C	177	MET
1	C	180	THR
1	C	196	LEU
1	C	199	LYS
1	C	200	LYS
1	C	203	LEU
1	C	210	THR
1	C	211	ASN

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Mol	Chain	Res	Type
1	C	214	LEU
1	C	223	SER
1	C	224	LYS
1	C	273	CYS
1	C	275	SER
1	C	278	LEU
1	C	279	LYS
1	C	303	ILE
1	C	311	HIS
1	C	315	GLN
1	C	335	ARG
1	C	343	GLN
1	C	344	SER
1	C	347	GLU
1	C	352	LYS
1	C	353	LYS
1	C	370	LEU
1	C	394	SER
1	C	396	VAL
1	C	397	ASP
1	C	402	MET
1	C	403	SER
1	C	410	SER
1	C	414	LYS
1	C	420	ASN
1	C	423	ARG
1	C	428	VAL
1	C	442	LEU
1	C	444	SER
1	D	70	ARG
1	D	91	LYS
1	D	93	SER
1	D	101	LYS
1	D	115	THR
1	D	134	LEU
1	D	135	MET
1	D	137	SER
1	D	142	SER
1	D	145	MET
1	D	156	ILE
1	D	161	ASP
1	D	165	LYS

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Mol	Chain	Res	Type
1	D	177	MET
1	D	180	THR
1	D	196	LEU
1	D	199	LYS
1	D	200	LYS
1	D	203	LEU
1	D	210	THR
1	D	211	ASN
1	D	214	LEU
1	D	223	SER
1	D	273	CYS
1	D	275	SER
1	D	278	LEU
1	D	279	LYS
1	D	303	ILE
1	D	311	HIS
1	D	315	GLN
1	D	335	ARG
1	D	343	GLN
1	D	344	SER
1	D	347	GLU
1	D	352	LYS
1	D	353	LYS
1	D	370	LEU
1	D	394	SER
1	D	396	VAL
1	D	397	ASP
1	D	402	MET
1	D	403	SER
1	D	410	SER
1	D	414	LYS
1	D	420	ASN
1	D	423	ARG
1	D	428	VAL
1	D	430	ASP
1	E	55	ASN
1	E	70	ARG
1	E	91	LYS
1	E	93	SER
1	E	101	LYS
1	E	115	THR
1	E	134	LEU

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Mol	Chain	Res	Type
1	E	135	MET
1	E	142	SER
1	E	145	MET
1	E	156	ILE
1	E	161	ASP
1	E	162	CYS
1	E	165	LYS
1	E	177	MET
1	E	180	THR
1	E	196	LEU
1	E	199	LYS
1	E	200	LYS
1	E	203	LEU
1	E	210	THR
1	E	211	ASN
1	E	214	LEU
1	E	223	SER
1	E	273	CYS
1	E	275	SER
1	E	279	LYS
1	E	303	ILE
1	E	305	ARG
1	E	311	HIS
1	E	312	LEU
1	E	315	GLN
1	E	335	ARG
1	E	343	GLN
1	E	344	SER
1	E	347	GLU
1	E	352	LYS
1	E	353	LYS
1	E	370	LEU
1	E	394	SER
1	E	396	VAL
1	E	397	ASP
1	E	402	MET
1	E	403	SER
1	E	410	SER
1	E	414	LYS
1	E	420	ASN
1	E	423	ARG
1	E	430	ASP

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Mol	Chain	Res	Type
1	E	443	ASP
1	E	444	SER
1	F	54	LEU
1	F	55	ASN
1	F	56	SER
1	F	70	ARG
1	F	93	SER
1	F	101	LYS
1	F	115	THR
1	F	131	SER
1	F	134	LEU
1	F	135	MET
1	F	137	SER
1	F	142	SER
1	F	145	MET
1	F	156	ILE
1	F	161	ASP
1	F	162	CYS
1	F	165	LYS
1	F	177	MET
1	F	180	THR
1	F	196	LEU
1	F	199	LYS
1	F	200	LYS
1	F	203	LEU
1	F	210	THR
1	F	211	ASN
1	F	214	LEU
1	F	223	SER
1	F	224	LYS
1	F	270	LEU
1	F	273	CYS
1	F	275	SER
1	F	278	LEU
1	F	279	LYS
1	F	285	ARG
1	F	303	ILE
1	F	311	HIS
1	F	335	ARG
1	F	343	GLN
1	F	344	SER
1	F	347	GLU

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Mol	Chain	Res	Type
1	F	352	LYS
1	F	353	LYS
1	F	370	LEU
1	F	396	VAL
1	F	397	ASP
1	F	402	MET
1	F	403	SER
1	F	410	SER
1	F	414	LYS
1	F	420	ASN
1	F	428	VAL
1	F	430	ASP
1	F	443	ASP
1	G	56	SER
1	G	70	ARG
1	G	93	SER
1	G	101	LYS
1	G	115	THR
1	G	131	SER
1	G	134	LEU
1	G	142	SER
1	G	145	MET
1	G	150	VAL
1	G	161	ASP
1	G	162	CYS
1	G	165	LYS
1	G	177	MET
1	G	180	THR
1	G	196	LEU
1	G	199	LYS
1	G	200	LYS
1	G	203	LEU
1	G	210	THR
1	G	211	ASN
1	G	214	LEU
1	G	223	SER
1	G	273	CYS
1	G	275	SER
1	G	278	LEU
1	G	303	ILE
1	G	311	HIS
1	G	315	GLN

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Mol	Chain	Res	Type
1	G	335	ARG
1	G	343	GLN
1	G	344	SER
1	G	347	GLU
1	G	352	LYS
1	G	353	LYS
1	G	370	LEU
1	G	396	VAL
1	G	402	MET
1	G	403	SER
1	G	410	SER
1	G	420	ASN
1	G	428	VAL
1	G	430	ASP
1	G	443	ASP
1	G	444	SER
1	H	56	SER
1	H	70	ARG
1	H	74	THR
1	H	91	LYS
1	H	93	SER
1	H	101	LYS
1	H	115	THR
1	H	134	LEU
1	H	135	MET
1	H	142	SER
1	H	156	ILE
1	H	161	ASP
1	H	162	CYS
1	H	165	LYS
1	H	177	MET
1	H	180	THR
1	H	196	LEU
1	H	199	LYS
1	H	200	LYS
1	H	203	LEU
1	H	210	THR
1	H	211	ASN
1	H	214	LEU
1	H	224	LYS
1	H	273	CYS
1	H	275	SER

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Mol	Chain	Res	Type
1	H	278	LEU
1	H	279	LYS
1	H	303	ILE
1	H	311	HIS
1	H	315	GLN
1	H	335	ARG
1	H	343	GLN
1	H	344	SER
1	H	347	GLU
1	H	352	LYS
1	H	353	LYS
1	H	394	SER
1	H	396	VAL
1	H	402	MET
1	H	403	SER
1	H	410	SER
1	H	414	LYS
1	H	420	ASN
1	H	423	ARG
1	H	430	ASP
1	H	443	ASP
1	H	445	ILE
1	I	70	ARG
1	I	91	LYS
1	I	93	SER
1	I	101	LYS
1	I	115	THR
1	I	131	SER
1	I	134	LEU
1	I	135	MET
1	I	142	SER
1	I	145	MET
1	I	156	ILE
1	I	161	ASP
1	I	165	LYS
1	I	177	MET
1	I	180	THR
1	I	196	LEU
1	I	199	LYS
1	I	200	LYS
1	I	203	LEU
1	I	210	THR

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Mol	Chain	Res	Type
1	I	211	ASN
1	I	214	LEU
1	I	223	SER
1	I	273	CYS
1	I	275	SER
1	I	278	LEU
1	I	303	ILE
1	I	311	HIS
1	I	315	GLN
1	I	335	ARG
1	I	343	GLN
1	I	344	SER
1	I	347	GLU
1	I	352	LYS
1	I	370	LEU
1	I	396	VAL
1	I	402	MET
1	I	403	SER
1	I	410	SER
1	I	414	LYS
1	I	420	ASN
1	I	428	VAL
1	I	430	ASP
1	J	56	SER
1	J	70	ARG
1	J	91	LYS
1	J	93	SER
1	J	101	LYS
1	J	115	THR
1	J	131	SER
1	J	134	LEU
1	J	135	MET
1	J	142	SER
1	J	145	MET
1	J	161	ASP
1	J	165	LYS
1	J	177	MET
1	J	180	THR
1	J	196	LEU
1	J	199	LYS
1	J	200	LYS
1	J	203	LEU

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Mol	Chain	Res	Type
1	J	210	THR
1	J	211	ASN
1	J	214	LEU
1	J	223	SER
1	J	273	CYS
1	J	275	SER
1	J	278	LEU
1	J	279	LYS
1	J	303	ILE
1	J	311	HIS
1	J	315	GLN
1	J	335	ARG
1	J	343	GLN
1	J	344	SER
1	J	347	GLU
1	J	352	LYS
1	J	353	LYS
1	J	370	LEU
1	J	394	SER
1	J	396	VAL
1	J	402	MET
1	J	403	SER
1	J	410	SER
1	J	414	LYS
1	J	420	ASN
1	J	428	VAL
1	J	430	ASP
1	K	70	ARG
1	K	93	SER
1	K	101	LYS
1	K	115	THR
1	K	131	SER
1	K	134	LEU
1	K	135	MET
1	K	142	SER
1	K	145	MET
1	K	161	ASP
1	K	162	CYS
1	K	165	LYS
1	K	177	MET
1	K	180	THR
1	K	196	LEU

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Mol	Chain	Res	Type
1	K	199	LYS
1	K	200	LYS
1	K	203	LEU
1	K	210	THR
1	K	211	ASN
1	K	214	LEU
1	K	223	SER
1	K	256	LEU
1	K	273	CYS
1	K	275	SER
1	K	278	LEU
1	K	303	ILE
1	K	305	ARG
1	K	311	HIS
1	K	315	GLN
1	K	335	ARG
1	K	343	GLN
1	K	344	SER
1	K	347	GLU
1	K	352	LYS
1	K	353	LYS
1	K	370	LEU
1	K	394	SER
1	K	396	VAL
1	K	402	MET
1	K	403	SER
1	K	410	SER
1	K	414	LYS
1	K	420	ASN
1	K	428	VAL
1	K	443	ASP
1	K	444	SER
1	K	445	ILE
1	L	70	ARG
1	L	91	LYS
1	L	93	SER
1	L	100	GLU
1	L	101	LYS
1	L	115	THR
1	L	134	LEU
1	L	135	MET
1	L	142	SER

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Mol	Chain	Res	Type
1	L	145	MET
1	L	156	ILE
1	L	161	ASP
1	L	162	CYS
1	L	165	LYS
1	L	177	MET
1	L	180	THR
1	L	196	LEU
1	L	199	LYS
1	L	200	LYS
1	L	203	LEU
1	L	210	THR
1	L	211	ASN
1	L	214	LEU
1	L	273	CYS
1	L	275	SER
1	L	303	ILE
1	L	311	HIS
1	L	315	GLN
1	L	335	ARG
1	L	343	GLN
1	L	344	SER
1	L	347	GLU
1	L	370	LEU
1	L	394	SER
1	L	396	VAL
1	L	397	ASP
1	L	402	MET
1	L	403	SER
1	L	410	SER
1	L	420	ASN
1	L	423	ARG
1	L	428	VAL
1	L	430	ASP
1	L	443	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	63	HIS
1	A	211	ASN

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Mol	Chain	Res	Type
1	A	343	GLN
1	B	63	HIS
1	B	211	ASN
1	B	343	GLN
1	C	211	ASN
1	C	343	GLN
1	C	420	ASN
1	D	63	HIS
1	D	211	ASN
1	D	343	GLN
1	E	63	HIS
1	E	211	ASN
1	E	343	GLN
1	F	55	ASN
1	F	63	HIS
1	F	211	ASN
1	F	343	GLN
1	G	63	HIS
1	G	211	ASN
1	G	343	GLN
1	H	63	HIS
1	H	211	ASN
1	H	343	GLN
1	I	55	ASN
1	I	63	HIS
1	I	211	ASN
1	I	343	GLN
1	I	420	ASN
1	J	63	HIS
1	J	211	ASN
1	J	343	GLN
1	K	63	HIS
1	K	211	ASN
1	K	343	GLN
1	L	63	HIS
1	L	211	ASN
1	L	343	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEN	A	500	-	25,27,27	3.01	12 (48%)	29,39,39	2.08	10 (34%)
2	HEN	B	501	-	25,27,27	2.92	11 (44%)	29,39,39	1.96	9 (31%)
2	HEN	C	502	-	25,27,27	2.87	13 (52%)	29,39,39	2.01	11 (37%)
2	HEN	D	503	-	25,27,27	3.00	12 (48%)	29,39,39	1.93	11 (37%)
2	HEN	E	504	-	25,27,27	3.52	13 (52%)	29,39,39	2.19	10 (34%)
2	HEN	F	505	-	25,27,27	2.92	12 (48%)	29,39,39	2.00	10 (34%)
2	HEN	G	506	-	25,27,27	2.88	12 (48%)	29,39,39	1.95	8 (27%)
2	HEN	H	507	-	25,27,27	3.02	12 (48%)	29,39,39	2.00	9 (31%)
2	HEN	I	508	-	25,27,27	2.90	13 (52%)	29,39,39	2.02	9 (31%)
2	HEN	J	509	-	25,27,27	3.22	13 (52%)	29,39,39	2.06	9 (31%)
2	HEN	K	510	-	25,27,27	3.07	13 (52%)	29,39,39	1.99	8 (27%)
2	HEN	L	511	-	25,27,27	2.95	13 (52%)	29,39,39	1.96	11 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEN	A	500	-	-	2/17/22/22	0/1/1/1
2	HEN	B	501	-	-	2/17/22/22	0/1/1/1
2	HEN	C	502	-	-	2/17/22/22	0/1/1/1
2	HEN	D	503	-	-	2/17/22/22	0/1/1/1
2	HEN	E	504	-	-	2/17/22/22	0/1/1/1
2	HEN	F	505	-	-	2/17/22/22	0/1/1/1
2	HEN	G	506	-	-	2/17/22/22	0/1/1/1
2	HEN	H	507	-	-	2/17/22/22	0/1/1/1
2	HEN	I	508	-	-	2/17/22/22	0/1/1/1
2	HEN	J	509	-	-	2/17/22/22	0/1/1/1
2	HEN	K	510	-	-	2/17/22/22	0/1/1/1
2	HEN	L	511	-	-	2/17/22/22	0/1/1/1

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	HEN	C4A-N4A	-5.63	1.38	1.46
2	A	500	HEN	C4A-N4A	-5.25	1.38	1.46
2	F	505	HEN	C4A-N4A	-5.14	1.38	1.46
2	D	503	HEN	CAI-N4A	-4.88	1.21	1.30
2	L	511	HEN	C4A-N4A	-4.84	1.39	1.46
2	G	506	HEN	C4A-N4A	-4.74	1.39	1.46
2	H	507	HEN	C4A-N4A	-4.57	1.39	1.46
2	J	509	HEN	C4A-N4A	-4.53	1.39	1.46
2	F	505	HEN	CAI-N4A	-4.52	1.22	1.30
2	A	500	HEN	CAI-N4A	-4.47	1.22	1.30
2	L	511	HEN	CAI-N4A	-4.36	1.22	1.30
2	C	502	HEN	C4A-N4A	-4.35	1.40	1.46
2	B	501	HEN	C4A-N4A	-4.35	1.40	1.46
2	I	508	HEN	C4A-N4A	-4.24	1.40	1.46
2	C	502	HEN	CAI-N4A	-4.15	1.23	1.30
2	E	504	HEN	C4A-N4A	-4.09	1.40	1.46
2	K	510	HEN	C4A-N4A	-3.94	1.40	1.46
2	G	506	HEN	CAI-N4A	-3.94	1.23	1.30
2	B	501	HEN	CAI-N4A	-3.90	1.23	1.30
2	H	507	HEN	CAI-N4A	-3.82	1.23	1.30
2	J	509	HEN	CAI-N4A	-3.77	1.23	1.30
2	K	510	HEN	CAI-N4A	-3.72	1.23	1.30
2	I	508	HEN	CAI-N4A	-3.42	1.24	1.30
2	E	504	HEN	CAI-N4A	-3.26	1.24	1.30
2	E	504	HEN	PG-OG2	-2.97	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	509	HEN	PG-OG2	-2.87	1.47	1.54
2	H	507	HEN	O3-C3	-2.74	1.30	1.37
2	J	509	HEN	O3-C3	-2.63	1.30	1.37
2	D	503	HEN	O3-C3	-2.57	1.31	1.37
2	C	502	HEN	O3-C3	-2.51	1.31	1.37
2	H	507	HEN	PG-OG2	-2.50	1.48	1.54
2	A	500	HEN	PG-OG2	-2.50	1.48	1.54
2	G	506	HEN	O3-C3	-2.49	1.31	1.37
2	L	511	HEN	O3-C3	-2.48	1.31	1.37
2	B	501	HEN	O3-C3	-2.45	1.31	1.37
2	I	508	HEN	PG-OG2	-2.39	1.49	1.54
2	G	506	HEN	PG-OG2	-2.35	1.49	1.54
2	F	505	HEN	PG-OG2	-2.35	1.49	1.54
2	K	510	HEN	PG-OG2	-2.35	1.49	1.54
2	A	500	HEN	O3-C3	-2.26	1.31	1.37
2	I	508	HEN	O3-C3	-2.26	1.31	1.37
2	K	510	HEN	O3-C3	-2.25	1.31	1.37
2	F	505	HEN	O3-C3	-2.25	1.31	1.37
2	D	503	HEN	PG-OG2	-2.24	1.49	1.54
2	L	511	HEN	PG-OG2	-2.17	1.49	1.54
2	C	502	HEN	PG-OG2	-2.11	1.49	1.54
2	E	504	HEN	O3-C3	-2.09	1.32	1.37
2	F	505	HEN	CBC-CAI	2.00	1.55	1.52
2	I	508	HEN	C4A-C4	2.02	1.55	1.51
2	G	506	HEN	CBC-CAI	2.02	1.55	1.52
2	I	508	HEN	CBC-CAI	2.09	1.55	1.52
2	L	511	HEN	C4A-C4	2.15	1.55	1.51
2	J	509	HEN	C4A-C4	2.18	1.55	1.51
2	C	502	HEN	C4A-C4	2.18	1.55	1.51
2	A	500	HEN	CBC-CAI	2.20	1.55	1.52
2	D	503	HEN	C3-C2	2.32	1.42	1.40
2	L	511	HEN	CBC-CAI	2.34	1.56	1.52
2	B	501	HEN	CBC-CAI	2.37	1.56	1.52
2	B	501	HEN	PG-OG1	2.38	1.60	1.54
2	D	503	HEN	CBC-CAI	2.42	1.56	1.52
2	K	510	HEN	C4A-C4	2.44	1.56	1.51
2	H	507	HEN	CBC-CAI	2.45	1.56	1.52
2	C	502	HEN	PG-OG1	2.65	1.61	1.54
2	K	510	HEN	CBC-CAI	2.66	1.56	1.52
2	K	510	HEN	PG-OG1	2.66	1.61	1.54
2	F	505	HEN	PG-OG1	2.68	1.61	1.54
2	L	511	HEN	PG-OG1	2.70	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	508	HEN	PG-OG1	2.75	1.61	1.54
2	G	506	HEN	PG-OG1	2.76	1.61	1.54
2	L	511	HEN	C3-C2	2.77	1.42	1.40
2	E	504	HEN	C4A-C4	2.78	1.56	1.51
2	D	503	HEN	PG-OG1	2.79	1.61	1.54
2	C	502	HEN	C3-C2	2.83	1.42	1.40
2	E	504	HEN	CBC-CAI	2.90	1.56	1.52
2	C	502	HEN	CBC-CAI	2.93	1.57	1.52
2	A	500	HEN	PG-OG1	2.96	1.62	1.54
2	H	507	HEN	PG-OG1	3.02	1.62	1.54
2	A	500	HEN	CBI-CAI	3.02	1.50	1.45
2	J	509	HEN	PG-OG1	3.04	1.62	1.54
2	J	509	HEN	CBC-CAI	3.05	1.57	1.52
2	J	509	HEN	C2-N1	3.13	1.40	1.34
2	I	508	HEN	CBI-CAI	3.15	1.51	1.45
2	B	501	HEN	C3-C2	3.16	1.43	1.40
2	C	502	HEN	CBI-CAI	3.19	1.51	1.45
2	F	505	HEN	CBI-CAI	3.22	1.51	1.45
2	E	504	HEN	C2-N1	3.23	1.40	1.34
2	A	500	HEN	C2-N1	3.24	1.40	1.34
2	H	507	HEN	C3-C2	3.25	1.43	1.40
2	F	505	HEN	C3-C2	3.25	1.43	1.40
2	G	506	HEN	C3-C2	3.28	1.43	1.40
2	E	504	HEN	PG-OG1	3.31	1.63	1.54
2	K	510	HEN	C2-N1	3.36	1.41	1.34
2	F	505	HEN	C2-N1	3.38	1.41	1.34
2	D	503	HEN	CBI-CAI	3.39	1.51	1.45
2	L	511	HEN	C2-N1	3.40	1.41	1.34
2	B	501	HEN	C2-N1	3.43	1.41	1.34
2	G	506	HEN	C2-N1	3.44	1.41	1.34
2	H	507	HEN	CBI-CAI	3.46	1.51	1.45
2	I	508	HEN	C2-N1	3.47	1.41	1.34
2	H	507	HEN	C2-N1	3.47	1.41	1.34
2	C	502	HEN	C2-N1	3.53	1.41	1.34
2	K	510	HEN	C3-C2	3.53	1.43	1.40
2	D	503	HEN	C2-N1	3.56	1.41	1.34
2	G	506	HEN	CBI-CAI	3.61	1.51	1.45
2	L	511	HEN	CBI-CAI	3.63	1.51	1.45
2	F	505	HEN	C3-C4	3.89	1.46	1.40
2	B	501	HEN	CBI-CAI	3.90	1.52	1.45
2	G	506	HEN	C3-C4	3.99	1.46	1.40
2	J	509	HEN	CBI-CAI	4.16	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	509	HEN	C3-C2	4.19	1.43	1.40
2	L	511	HEN	C3-C4	4.28	1.46	1.40
2	E	504	HEN	CBI-CAI	4.28	1.52	1.45
2	K	510	HEN	CBI-CAI	4.37	1.53	1.45
2	A	500	HEN	C3-C2	4.41	1.43	1.40
2	C	502	HEN	C3-C4	4.46	1.47	1.40
2	I	508	HEN	C3-C2	4.49	1.43	1.40
2	B	501	HEN	C3-C4	4.50	1.47	1.40
2	H	507	HEN	C3-C4	4.54	1.47	1.40
2	D	503	HEN	C3-C4	4.58	1.47	1.40
2	K	510	HEN	C3-C4	4.78	1.47	1.40
2	I	508	HEN	C3-C4	4.96	1.47	1.40
2	A	500	HEN	PG-CEI	5.08	1.86	1.79
2	A	500	HEN	C3-C4	5.43	1.48	1.40
2	I	508	HEN	PG-CEI	5.44	1.87	1.79
2	J	509	HEN	C3-C4	5.58	1.48	1.40
2	C	502	HEN	PG-CEI	5.83	1.87	1.79
2	G	506	HEN	C5-C4	5.99	1.49	1.40
2	D	503	HEN	PG-CEI	6.04	1.88	1.79
2	J	509	HEN	C5-C4	6.07	1.49	1.40
2	H	507	HEN	C5-C4	6.09	1.49	1.40
2	F	505	HEN	C5-C4	6.21	1.49	1.40
2	L	511	HEN	PG-CEI	6.23	1.88	1.79
2	B	501	HEN	C5-C4	6.24	1.49	1.40
2	E	504	HEN	C3-C4	6.30	1.49	1.40
2	D	503	HEN	C5-C4	6.39	1.49	1.40
2	C	502	HEN	C5-C4	6.45	1.49	1.40
2	G	506	HEN	PG-CEI	6.47	1.88	1.79
2	A	500	HEN	C5-C4	6.47	1.49	1.40
2	K	510	HEN	C5-C4	6.63	1.49	1.40
2	L	511	HEN	C5-C4	6.64	1.49	1.40
2	F	505	HEN	PG-CEI	6.65	1.88	1.79
2	B	501	HEN	PG-CEI	6.66	1.88	1.79
2	E	504	HEN	C5-C4	6.67	1.49	1.40
2	I	508	HEN	C5-C4	6.81	1.50	1.40
2	K	510	HEN	PG-CEI	7.12	1.89	1.79
2	E	504	HEN	C3-C2	7.18	1.45	1.40
2	H	507	HEN	PG-CEI	7.30	1.89	1.79
2	J	509	HEN	PG-CEI	7.60	1.90	1.79
2	E	504	HEN	PG-CEI	7.80	1.90	1.79

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	HEN	C5-C6-N1	-3.31	118.11	123.86
2	B	501	HEN	C5-C6-N1	-3.26	118.21	123.86
2	G	506	HEN	C5-C6-N1	-3.25	118.23	123.86
2	F	505	HEN	C5-C6-N1	-3.24	118.24	123.86
2	K	510	HEN	C5-C6-N1	-3.23	118.25	123.86
2	L	511	HEN	C5-C6-N1	-3.18	118.33	123.86
2	I	508	HEN	C5-C6-N1	-3.17	118.36	123.86
2	J	509	HEN	C5-C6-N1	-3.16	118.37	123.86
2	D	503	HEN	C5-C6-N1	-3.16	118.38	123.86
2	H	507	HEN	C5-C6-N1	-3.13	118.43	123.86
2	H	507	HEN	CGI-CBI-CAI	-3.11	116.23	124.10
2	A	500	HEN	C5-C6-N1	-3.10	118.48	123.86
2	L	511	HEN	CGI-CBI-CAI	-3.02	116.46	124.10
2	C	502	HEN	CGI-CBI-CAI	-2.98	116.56	124.10
2	E	504	HEN	C5-C6-N1	-2.98	118.68	123.86
2	A	500	HEN	CGI-CBI-CAI	-2.76	117.14	124.10
2	D	503	HEN	CGI-CBI-CAI	-2.70	117.27	124.10
2	F	505	HEN	CGI-CBI-CAI	-2.70	117.28	124.10
2	E	504	HEN	OG1-PG-OG3	-2.60	105.74	112.40
2	H	507	HEN	OG1-PG-OG3	-2.53	105.92	112.40
2	J	509	HEN	OG1-PG-OG3	-2.48	106.06	112.40
2	J	509	HEN	CGI-CBI-CAI	-2.41	118.02	124.10
2	A	500	HEN	OG3-PG-CEI	-2.39	105.13	111.05
2	F	505	HEN	OG1-PG-OG3	-2.36	106.37	112.40
2	K	510	HEN	OG1-PG-OG3	-2.33	106.44	112.40
2	E	504	HEN	CGI-CBI-CAI	-2.28	118.35	124.10
2	I	508	HEN	CGI-CBI-CAI	-2.21	118.51	124.10
2	D	503	HEN	OG1-PG-OG3	-2.21	106.76	112.40
2	I	508	HEN	OG1-PG-OG3	-2.19	106.79	112.40
2	D	503	HEN	OG3-PG-CEI	-2.14	105.75	111.05
2	H	507	HEN	C3-C2-N1	-2.12	117.68	120.61
2	C	502	HEN	OG3-PG-CEI	-2.11	105.81	111.05
2	G	506	HEN	OG1-PG-OG3	-2.09	107.05	112.40
2	C	502	HEN	OG1-PG-OG3	-2.09	107.06	112.40
2	F	505	HEN	C3-C2-N1	-2.08	117.74	120.61
2	G	506	HEN	C3-C2-N1	-2.06	117.77	120.61
2	D	503	HEN	C3-C2-N1	-2.04	117.80	120.61
2	B	501	HEN	OG3-PG-CEI	-2.04	106.00	111.05
2	L	511	HEN	C3-C2-N1	-2.04	117.80	120.61
2	A	500	HEN	OG1-PG-OG3	-2.04	107.20	112.40
2	B	501	HEN	C3-C2-N1	-2.02	117.83	120.61
2	B	501	HEN	OG1-PG-OG3	-2.01	107.25	112.40
2	L	511	HEN	OG3-PG-CEI	-2.01	106.06	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	511	HEN	OG1-PG-OG3	-2.01	107.27	112.40
2	C	502	HEN	C3-C2-N1	-2.00	117.84	120.61
2	C	502	HEN	OG2-PG-OG3	2.00	117.53	112.40
2	L	511	HEN	C4A-C4-C5	2.01	122.60	119.56
2	A	500	HEN	OP3-P-OP1	2.02	115.09	107.38
2	K	510	HEN	OG1-PG-CEI	2.05	111.63	107.04
2	D	503	HEN	OG2-PG-OG3	2.06	117.67	112.40
2	L	511	HEN	OP3-P-OP1	2.06	115.22	107.38
2	D	503	HEN	C6-C5-C4	2.06	119.63	118.09
2	E	504	HEN	O3-C3-C4	2.06	124.26	118.11
2	J	509	HEN	OP3-P-OP1	2.07	115.25	107.38
2	I	508	HEN	OG2-PG-OG3	2.07	117.70	112.40
2	F	505	HEN	OG1-PG-CEI	2.08	111.69	107.04
2	B	501	HEN	OP3-P-OP1	2.10	115.39	107.38
2	D	503	HEN	OP3-P-OP1	2.11	115.42	107.38
2	G	506	HEN	OP3-P-OP1	2.11	115.42	107.38
2	F	505	HEN	OP3-P-OP1	2.14	115.51	107.38
2	K	510	HEN	OP3-P-OP1	2.18	115.67	107.38
2	C	502	HEN	OP3-P-OP1	2.19	115.71	107.38
2	E	504	HEN	OP3-P-OP1	2.20	115.76	107.38
2	I	508	HEN	OP3-P-OP1	2.20	115.77	107.38
2	A	500	HEN	OG2-PG-OG3	2.25	118.16	112.40
2	F	505	HEN	C6-C5-C4	2.37	119.86	118.09
2	H	507	HEN	C6-C5-C4	2.39	119.87	118.09
2	L	511	HEN	C6-C5-C4	2.40	119.88	118.09
2	J	509	HEN	OG1-PG-CEI	2.61	112.89	107.04
2	G	506	HEN	C6-C5-C4	2.61	120.04	118.09
2	H	507	HEN	OG1-PG-CEI	2.67	113.03	107.04
2	A	500	HEN	C6-C5-C4	2.69	120.10	118.09
2	B	501	HEN	C6-C5-C4	2.73	120.13	118.09
2	C	502	HEN	C6-C5-C4	2.79	120.17	118.09
2	D	503	HEN	C4-C4A-N4A	2.80	125.15	113.97
2	L	511	HEN	C4-C4A-N4A	2.83	125.26	113.97
2	I	508	HEN	C6-C5-C4	2.84	120.21	118.09
2	K	510	HEN	C6-C5-C4	2.91	120.26	118.09
2	J	509	HEN	C6-C5-C4	3.07	120.38	118.09
2	F	505	HEN	C4-C4A-N4A	3.07	126.21	113.97
2	E	504	HEN	OG1-PG-CEI	3.22	114.26	107.04
2	C	502	HEN	C4-C4A-N4A	3.27	127.00	113.97
2	B	501	HEN	C4-C4A-N4A	3.30	127.15	113.97
2	G	506	HEN	C4-C4A-N4A	3.32	127.20	113.97
2	H	507	HEN	C4-C4A-N4A	3.34	127.30	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	509	HEN	C4-C4A-N4A	3.35	127.34	113.97
2	E	504	HEN	C6-C5-C4	3.41	120.64	118.09
2	K	510	HEN	C4-C4A-N4A	3.49	127.87	113.97
2	H	507	HEN	C6-N1-C2	3.57	126.56	119.28
2	G	506	HEN	C6-N1-C2	3.61	126.64	119.28
2	E	504	HEN	C6-N1-C2	3.62	126.66	119.28
2	C	502	HEN	C6-N1-C2	3.65	126.72	119.28
2	L	511	HEN	C6-N1-C2	3.66	126.75	119.28
2	D	503	HEN	C6-N1-C2	3.68	126.79	119.28
2	B	501	HEN	C6-N1-C2	3.68	126.79	119.28
2	F	505	HEN	C6-N1-C2	3.69	126.80	119.28
2	J	509	HEN	C6-N1-C2	3.69	126.81	119.28
2	K	510	HEN	C6-N1-C2	3.70	126.82	119.28
2	A	500	HEN	C4-C4A-N4A	3.70	128.72	113.97
2	I	508	HEN	C6-N1-C2	3.71	126.85	119.28
2	I	508	HEN	C4-C4A-N4A	3.72	128.79	113.97
2	A	500	HEN	C6-N1-C2	3.76	126.96	119.28
2	E	504	HEN	C4-C4A-N4A	4.02	130.02	113.97
2	D	503	HEN	C2A-C2-C3	4.95	127.01	121.04
2	H	507	HEN	C2A-C2-C3	5.05	127.13	121.04
2	C	502	HEN	C2A-C2-C3	5.06	127.14	121.04
2	L	511	HEN	C2A-C2-C3	5.11	127.20	121.04
2	B	501	HEN	C2A-C2-C3	5.16	127.27	121.04
2	K	510	HEN	C2A-C2-C3	5.21	127.32	121.04
2	G	506	HEN	C2A-C2-C3	5.25	127.38	121.04
2	F	505	HEN	C2A-C2-C3	5.29	127.42	121.04
2	I	508	HEN	C2A-C2-C3	5.45	127.61	121.04
2	A	500	HEN	C2A-C2-C3	5.50	127.67	121.04
2	J	509	HEN	C2A-C2-C3	5.51	127.69	121.04
2	E	504	HEN	C2A-C2-C3	5.73	127.95	121.04

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEN	C5-C4-C4A-N4A
2	E	504	HEN	C5-C4-C4A-N4A
2	J	509	HEN	C5-C4-C4A-N4A
2	E	504	HEN	C3-C4-C4A-N4A
2	A	500	HEN	C3-C4-C4A-N4A
2	J	509	HEN	C3-C4-C4A-N4A
2	H	507	HEN	C5-C4-C4A-N4A

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Mol	Chain	Res	Type	Atoms
2	D	503	HEN	C5-C4-C4A-N4A
2	I	508	HEN	C5-C4-C4A-N4A
2	D	503	HEN	C3-C4-C4A-N4A
2	H	507	HEN	C3-C4-C4A-N4A
2	I	508	HEN	C3-C4-C4A-N4A
2	F	505	HEN	C5-C4-C4A-N4A
2	G	506	HEN	C5-C4-C4A-N4A
2	B	501	HEN	C5-C4-C4A-N4A
2	F	505	HEN	C3-C4-C4A-N4A
2	C	502	HEN	C5-C4-C4A-N4A
2	C	502	HEN	C3-C4-C4A-N4A
2	L	511	HEN	C5-C4-C4A-N4A
2	K	510	HEN	C5-C4-C4A-N4A
2	K	510	HEN	C3-C4-C4A-N4A
2	G	506	HEN	C3-C4-C4A-N4A
2	L	511	HEN	C3-C4-C4A-N4A
2	B	501	HEN	C3-C4-C4A-N4A

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEN	3	0
2	B	501	HEN	1	0
2	D	503	HEN	2	0
2	E	504	HEN	1	0
2	F	505	HEN	1	0
2	G	506	HEN	1	0
2	H	507	HEN	2	0
2	I	508	HEN	2	0
2	J	509	HEN	1	0
2	K	510	HEN	1	0
2	L	511	HEN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.