



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

PDB ID : 1MTO
Title : Crystal structure of a Phosphofructokinase mutant from *Bacillus stearothermophilus* bound with fructose-6-phosphate
Authors : Riley-Lovingshimer, M.R.; Ronning, D.R.; Sacchettini, J.C.; Reinhart, G.D.
Deposited on : 2002-09-21
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

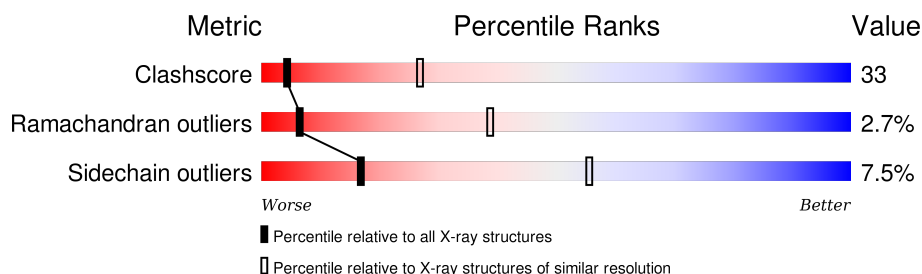
1 Overall quality at a glance

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	319	
1	B	319	
1	C	319	
1	D	319	
1	E	319	
1	F	319	
1	G	319	

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Mol	Chain	Length	Quality of chain
1	H	319	<div><div></div><div>46%</div><div>50%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19328 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 6-phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	B	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	C	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	D	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	E	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	F	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	G	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			
1	H	319	Total	C	N	O	S	0	0	0
			2400	1499	436	457	8			

There are 16 discrepancies between the modelled and reference sequences:

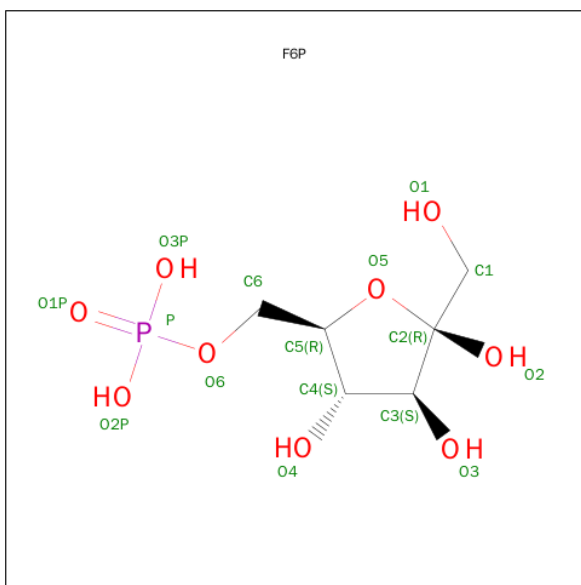
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	TRP	TYR	ENGINEERED	UNP P00512
A	179	TYR	TRP	ENGINEERED	UNP P00512
B	164	TRP	TYR	ENGINEERED	UNP P00512
B	179	TYR	TRP	ENGINEERED	UNP P00512
C	164	TRP	TYR	ENGINEERED	UNP P00512
C	179	TYR	TRP	ENGINEERED	UNP P00512
D	164	TRP	TYR	ENGINEERED	UNP P00512
D	179	TYR	TRP	ENGINEERED	UNP P00512
E	164	TRP	TYR	ENGINEERED	UNP P00512
E	179	TYR	TRP	ENGINEERED	UNP P00512
F	164	TRP	TYR	ENGINEERED	UNP P00512
F	179	TYR	TRP	ENGINEERED	UNP P00512
G	164	TRP	TYR	ENGINEERED	UNP P00512

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Chain	Residue	Modelled	Actual	Comment	Reference
G	179	TYR	TRP	ENGINEERED	UNP P00512
H	164	TRP	TYR	ENGINEERED	UNP P00512
H	179	TYR	TRP	ENGINEERED	UNP P00512

- Molecule 2 is SUGAR (FRUCTOSE-6-PHOSPHATE) (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).



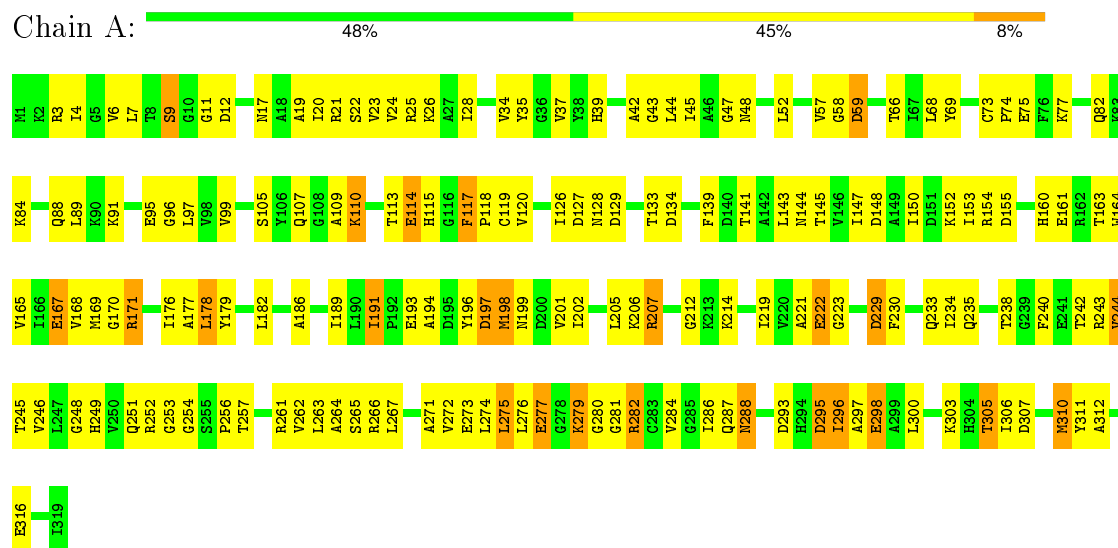
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	F	1	Total	C	O	P	0	0
			16	6	9	1		
2	E	1	Total	C	O	P	0	0
			16	6	9	1		
2	H	1	Total	C	O	P	0	0
			16	6	9	1		
2	G	1	Total	C	O	P	0	0
			16	6	9	1		

3 Residue-property plots

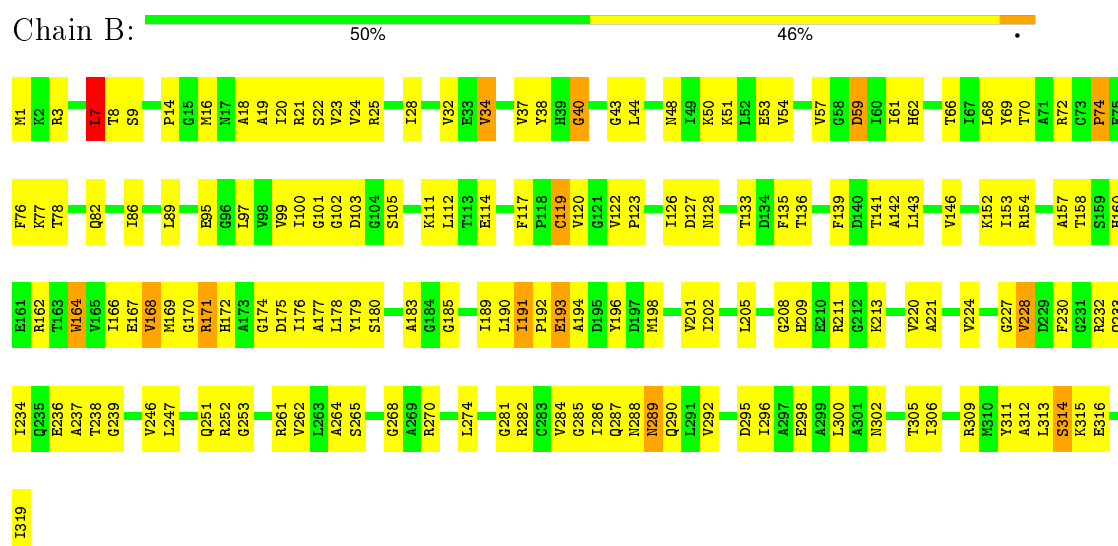
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

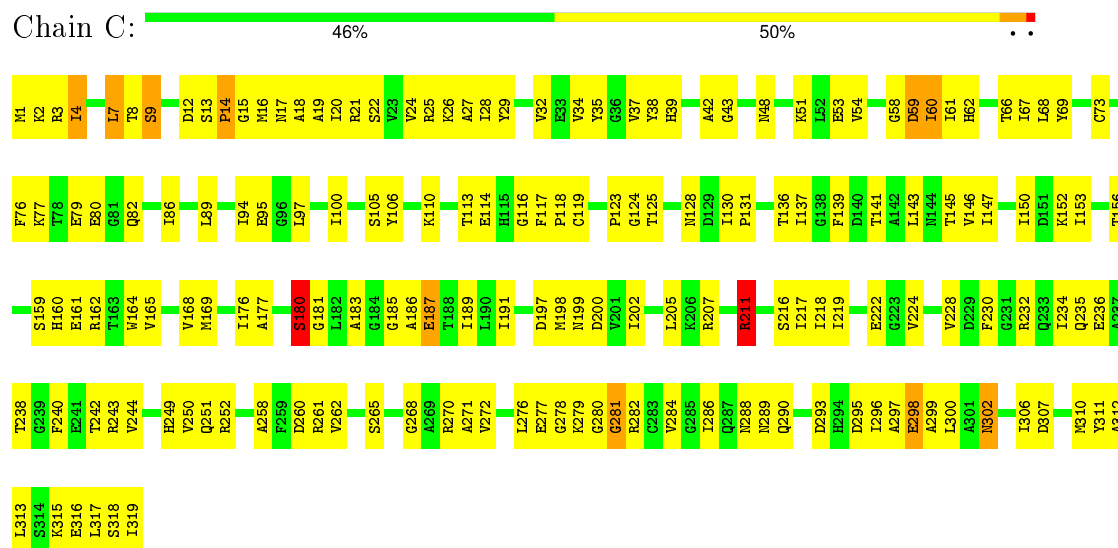
- Molecule 1: 6-phosphofructokinase



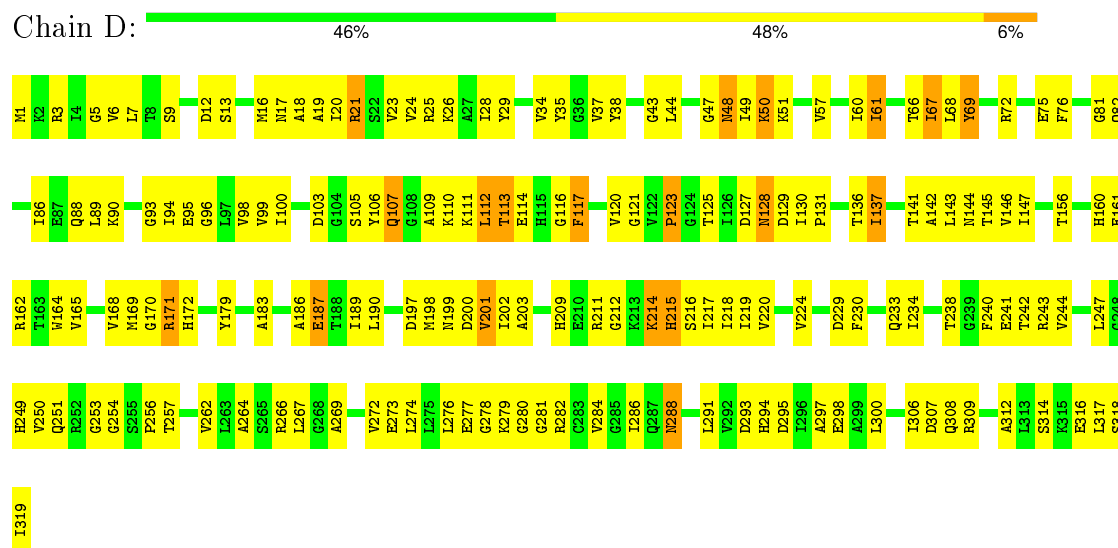
- Molecule 1: 6-phosphofructokinase



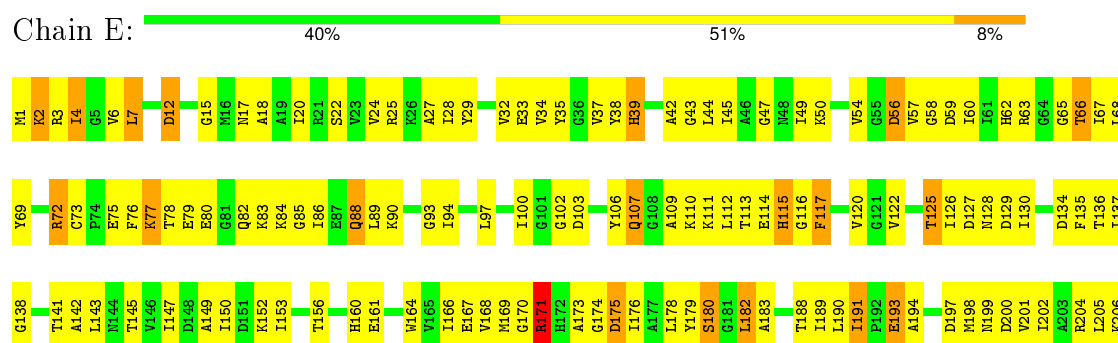
- Molecule 1: 6-phosphofructokinase

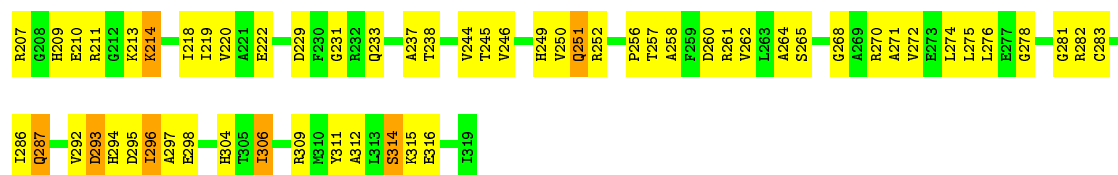


- Molecule 1: 6-phosphofructokinase



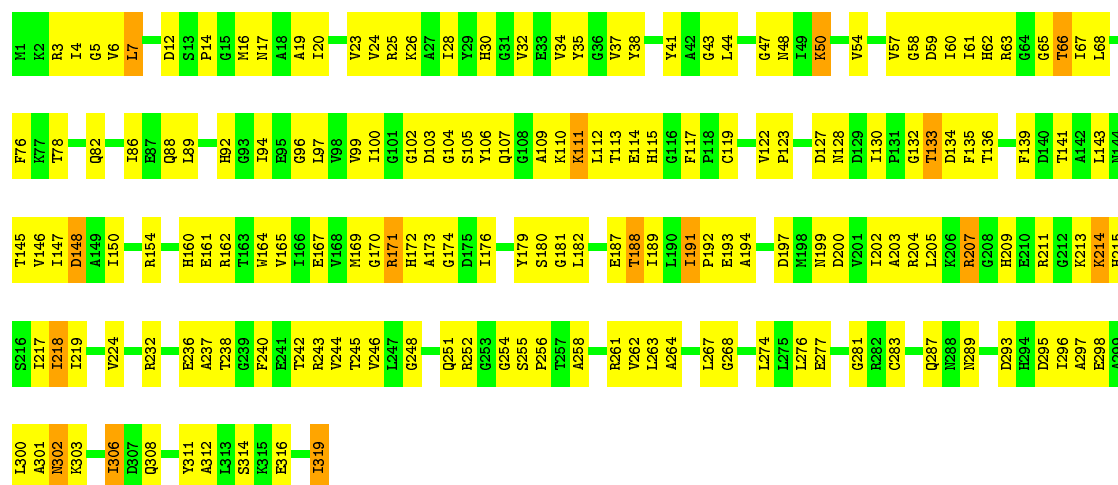
- Molecule 1: 6-phosphofructokinase





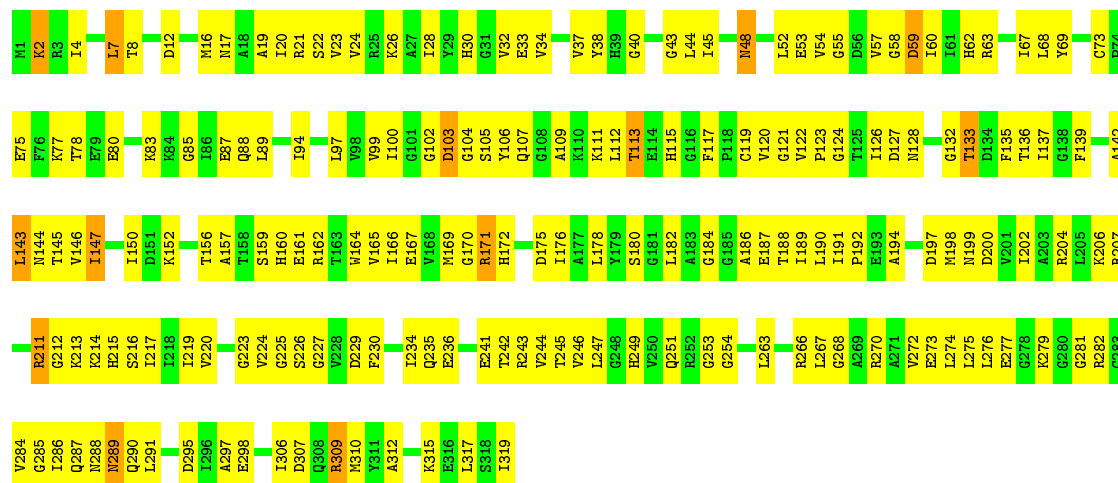
• Molecule 1: 6-phosphofructokinase

Chain F: 46% 50% 5%



• Molecule 1: 6-phosphofructokinase

Chain G: 41% 55% 4%



• Molecule 1: 6-phosphofructokinase

Chain H: 46% 50% 4%



C73	I153	V228	A299
F80	R154	D229	R304
I86	D155	F230	T305
E87	T156	G231	I306
Q88	H160	R232	R309
L89	E161	Q233	M310
K90	W164	T234	Y311
	V165	Q235	A312
G93	I166	T242	L313
I94	E167	R243	S314
F95	W168	V244	K315
G96	M169	T245	E316
L97	G170	V246	L317
V98	R171	L247	S318
Y99	H172	G248	I319
I100	A173	H249	
G101	G174	V250	
S105	D175	Q251	
A109	A177	R252	
K110	L178	G253	
K111	Y179	G254	
L112		S255	
L113	A183	P256	
	G184	T257	
F117	E187	A258	
P118	L190	R261	
C119	I191	V262	
V120	P192		
G121	E193	L267	
V122		G268	
I126	M198	A269	
D127	W199	R270	
H128	D200	A271	
P131	V201	V272	
G132	I202	E273	
T133	A203	L274	
D134	R207	L275	
F135	E210	L276	
T136	R211	G280	
	G212	G281	
F139	K213	R282	
D140	K214	G283	
T141	H215	V284	
A142	S216	I286	
L143	I217	Q287	
H144	I218	V288	
T145	I219	H289	
V146	V220	Q290	
I147		L291	
D148		V292	
A149	V224	D293	
I150	G225	H294	
D151	S226	D295	
K152	G227	I296	
		A297	
		E298	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.68Å 106.87Å 119.59Å 90.00° 113.98° 90.00°	Depositor
Resolution (Å)	29.84 – 3.20	Depositor
% Data completeness (in resolution range)	86.7 (29.84-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19328	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F6P

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	0.35	0/2436	0.60	0/3282
1	B	0.38	0/2436	0.63	1/3282 (0.0%)
1	C	0.35	0/2436	0.60	0/3282
1	D	0.38	0/2436	0.62	0/3282
1	E	0.37	0/2436	0.62	0/3282
1	F	0.37	0/2436	0.61	0/3282
1	G	0.39	0/2436	0.62	0/3282
1	H	0.37	0/2436	0.62	0/3282
All	All	0.37	0/19488	0.62	1/26256 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2400	0	2417	172	0
1	B	2400	0	2417	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2400	0	2417	151	0
1	D	2400	0	2417	170	0
1	E	2400	0	2417	184	0
1	F	2400	0	2417	180	0
1	G	2400	0	2417	180	0
1	H	2400	0	2417	169	0
2	A	16	0	11	1	0
2	B	16	0	11	0	0
2	C	16	0	11	1	0
2	D	16	0	11	0	0
2	E	16	0	11	0	0
2	F	16	0	11	2	0
2	G	16	0	11	1	0
2	H	16	0	11	3	0
All	All	19328	0	19424	1274	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 33.

All (1274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HH12	1:A:293:ASP:HB3	1.04	1.11
1:H:171:ARG:HG3	1:H:172:HIS:H	1.19	1.06
1:F:14:PRO:HG2	1:F:141:THR:HG21	1.38	1.03
1:A:24:VAL:HG21	1:A:57:VAL:HG11	1.45	0.98
1:D:123:PRO:HB2	1:D:136:THR:HG22	1.45	0.96
1:F:171:ARG:HG3	1:F:172:HIS:H	1.28	0.95
1:G:164:TRP:HZ3	1:G:245:THR:HG1	1.06	0.95
1:A:145:THR:HG23	1:B:152:LYS:NZ	1.81	0.94
1:G:190:LEU:HD12	1:G:220:VAL:HG22	1.47	0.94
1:A:3:ARG:HD3	1:A:35:TYR:HE2	1.30	0.94
1:D:187:GLU:HG3	1:D:216:SER:HB3	1.49	0.94
1:A:282:ARG:NH1	1:A:293:ASP:HB3	1.86	0.90
1:A:165:VAL:HB	1:A:244:VAL:HG12	1.51	0.89
1:C:8:THR:HG22	1:C:100:ILE:HB	1.55	0.89
1:A:145:THR:HG23	1:B:152:LYS:HZ2	1.38	0.88
1:G:171:ARG:HG3	1:G:172:HIS:H	1.38	0.88
1:D:24:VAL:HA	1:D:34:VAL:HG11	1.57	0.87
1:B:171:ARG:HG3	1:B:172:HIS:H	1.38	0.87
1:D:230:PHE:O	1:D:234:ILE:HG12	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:LEU:HD21	1:F:179:TYR:HB3	1.58	0.85
1:C:123:PRO:HB2	1:C:136:THR:HG22	1.57	0.85
1:E:17:ASN:HD21	1:E:67:ILE:HG23	1.39	0.85
1:G:24:VAL:HG13	1:G:34:VAL:HG21	1.60	0.84
1:B:126:ILE:O	1:B:176:ILE:HD11	1.77	0.84
1:D:123:PRO:O	1:D:137:ILE:HG12	1.77	0.83
1:H:147:ILE:HA	1:H:150:ILE:HD13	1.58	0.83
1:E:7:LEU:HB3	1:E:37:VAL:HB	1.61	0.83
1:F:7:LEU:HD11	1:F:99:VAL:HG22	1.61	0.82
1:H:169:MET:HG3	1:H:251:GLN:NE2	1.95	0.82
1:H:211:ARG:HH12	1:H:319:ILE:HG22	1.45	0.82
1:E:249:HIS:HB2	1:F:164:TRP:CH2	2.16	0.81
1:G:19:ALA:O	1:G:23:VAL:HG23	1.81	0.80
1:H:171:ARG:HG3	1:H:172:HIS:N	1.96	0.80
1:E:78:THR:HG22	1:E:80:GLU:H	1.45	0.80
1:E:167:GLU:HB3	1:E:246:VAL:HG13	1.64	0.80
1:D:82:GLN:O	1:D:86:ILE:HG12	1.80	0.80
1:C:187:GLU:HG3	1:C:216:SER:HB3	1.64	0.79
1:F:161:GLU:HG2	1:F:214:LYS:HG3	1.63	0.79
1:D:75:GLU:H	1:D:75:GLU:CD	1.85	0.79
1:G:142:ALA:O	1:G:146:VAL:HG23	1.83	0.79
1:B:24:VAL:O	1:B:28:ILE:HG12	1.83	0.78
1:H:86:ILE:HA	1:H:89:LEU:HD12	1.64	0.78
1:H:7:LEU:HB3	1:H:37:VAL:HB	1.65	0.78
1:D:186:ALA:HB3	1:D:189:ILE:HD11	1.66	0.78
1:E:113:THR:HG21	1:E:281:GLY:HA2	1.65	0.78
1:D:68:LEU:O	1:D:69:TYR:HB2	1.82	0.78
1:E:72:ARG:H	1:E:72:ARG:HD2	1.49	0.77
1:F:232:ARG:O	1:F:236:GLU:HG3	1.83	0.77
1:E:204:ARG:HH22	1:E:315:LYS:HD2	1.50	0.77
1:D:171:ARG:HG3	1:D:172:HIS:H	1.49	0.77
1:D:37:VAL:HG22	1:D:49:ILE:HD12	1.66	0.77
1:F:14:PRO:HG2	1:F:141:THR:CG2	2.14	0.77
1:F:19:ALA:HB2	1:F:264:ALA:HB1	1.67	0.77
1:B:198:MET:HG2	1:B:233:GLN:NE2	2.00	0.77
1:E:72:ARG:HH11	1:E:72:ARG:H	1.30	0.76
1:B:208:GLY:HA3	1:B:213:LYS:HZ3	1.48	0.76
1:F:14:PRO:CG	1:F:141:THR:HG21	2.15	0.76
1:C:123:PRO:O	1:C:137:ILE:HG12	1.84	0.76
1:H:187:GLU:HG3	1:H:216:SER:HB2	1.67	0.76
1:E:176:ILE:O	1:E:180:SER:HB3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:LEU:HD13	1:G:117:PHE:CE2	2.20	0.76
1:B:24:VAL:HG21	1:B:57:VAL:HG11	1.68	0.75
1:D:247:LEU:HB2	1:D:251:GLN:HE21	1.51	0.75
1:E:141:THR:HA	1:E:257:THR:HG23	1.69	0.75
1:C:7:LEU:HD12	1:C:97:LEU:HD11	1.69	0.75
1:D:295:ASP:HB3	1:D:298:GLU:HG2	1.67	0.74
1:G:152:LYS:O	1:H:253:GLY:HA3	1.87	0.74
1:D:144:ASN:HA	1:D:147:ILE:HG12	1.69	0.74
1:D:38:TYR:O	1:D:43:GLY:HA3	1.87	0.74
1:A:207:ARG:HB3	1:A:207:ARG:HH11	1.50	0.74
1:C:281:GLY:O	1:C:296:ILE:HG13	1.86	0.74
1:H:7:LEU:HD12	1:H:97:LEU:HD11	1.69	0.74
1:D:143:LEU:HD11	1:D:179:TYR:HB2	1.69	0.74
1:E:191:ILE:HD13	1:E:191:ILE:H	1.53	0.74
1:C:4:ILE:HD11	1:C:34:VAL:HG22	1.67	0.74
1:A:24:VAL:HG13	1:A:34:VAL:HG21	1.67	0.74
1:G:253:GLY:HA3	1:H:152:LYS:O	1.87	0.74
1:G:166:ILE:HD12	1:G:219:ILE:HD11	1.68	0.74
1:G:7:LEU:HB3	1:G:37:VAL:HB	1.70	0.74
1:H:198:MET:O	1:H:202:ILE:HG12	1.87	0.74
1:G:123:PRO:O	1:G:137:ILE:HG12	1.87	0.74
1:C:58:GLY:O	1:C:59:ASP:HB3	1.86	0.74
1:G:235:GLN:HB2	1:G:242:THR:HB	1.68	0.74
1:A:74:PRO:HD2	1:A:75:GLU:OE1	1.87	0.74
1:E:24:VAL:HB	1:E:57:VAL:HG11	1.71	0.73
1:G:167:GLU:HB3	1:G:246:VAL:HG13	1.69	0.73
1:D:106:TYR:O	1:D:109:ALA:HB3	1.89	0.73
1:B:82:GLN:HE22	1:B:111:LYS:HG3	1.53	0.73
1:E:79:GLU:O	1:E:83:LYS:HG3	1.88	0.73
1:D:187:GLU:HG3	1:D:216:SER:CB	2.18	0.73
1:A:128:ASN:HB2	1:A:139:PHE:CD2	2.23	0.73
1:A:141:THR:HA	1:A:257:THR:HG23	1.70	0.73
1:E:249:HIS:HB2	1:F:164:TRP:HH2	1.54	0.72
1:A:95:GLU:O	1:A:118:PRO:HD2	1.88	0.72
1:F:169:MET:HG3	1:F:251:GLN:NE2	2.04	0.72
1:B:89:LEU:HD13	1:B:117:PHE:CE2	2.24	0.72
1:G:191:ILE:HD12	1:G:194:ALA:H	1.55	0.72
1:C:20:ILE:HD13	1:C:68:LEU:HG	1.72	0.72
1:B:176:ILE:O	1:B:180:SER:HB3	1.87	0.72
1:D:21:ARG:HH12	1:D:25:ARG:NH1	1.87	0.72
1:F:134:ASP:OD2	1:F:287:GLN:HA	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:HG21	1:A:281:GLY:HA2	1.71	0.72
1:G:178:LEU:HD22	1:G:306:ILE:HD13	1.72	0.72
1:A:152:LYS:O	1:A:155:ASP:HB2	1.90	0.72
1:C:296:ILE:O	1:C:300:LEU:HD23	1.90	0.71
1:G:200:ASP:O	1:G:204:ARG:HG3	1.89	0.71
1:A:7:LEU:HD21	1:A:99:VAL:HG22	1.72	0.71
1:C:312:ALA:O	1:C:316:GLU:HG3	1.89	0.71
1:E:72:ARG:HH11	1:E:72:ARG:N	1.89	0.71
1:D:295:ASP:OD2	1:D:297:ALA:HB3	1.90	0.71
1:A:7:LEU:HB3	1:A:37:VAL:HB	1.73	0.71
1:F:302:ASN:HD22	1:F:303:LYS:H	1.36	0.71
1:A:198:MET:HE3	1:A:201:VAL:HG21	1.71	0.70
1:G:254:GLY:CA	1:H:152:LYS:HD3	2.20	0.70
1:E:258:ALA:HB2	1:G:147:ILE:HD13	1.73	0.70
1:G:128:ASN:HB2	1:G:139:PHE:CD2	2.25	0.70
1:A:282:ARG:HH12	1:A:293:ASP:CB	1.94	0.69
1:A:24:VAL:CG2	1:A:57:VAL:HG11	2.22	0.69
1:A:126:ILE:O	1:A:176:ILE:HD11	1.92	0.69
1:H:13:SER:O	1:H:16:MET:HG3	1.91	0.69
1:C:86:ILE:HA	1:C:89:LEU:HD12	1.74	0.69
1:F:143:LEU:HD11	1:F:179:TYR:HB2	1.73	0.69
1:A:161:GLU:OE1	1:A:214:LYS:HD2	1.93	0.69
1:E:77:LYS:NZ	1:E:77:LYS:HB3	2.07	0.69
1:F:164:TRP:HZ3	1:F:245:THR:HG1	1.39	0.69
1:G:7:LEU:HD23	1:G:40:GLY:HA2	1.73	0.69
1:F:47:GLY:HA3	1:F:88:GLN:NE2	2.07	0.69
1:A:44:LEU:HD11	1:A:89:LEU:HG	1.75	0.69
1:B:169:MET:HG3	1:B:251:GLN:NE2	2.08	0.69
1:G:83:LYS:O	1:G:87:GLU:HG2	1.93	0.69
1:G:161:GLU:HA	1:G:215:HIS:HB3	1.73	0.68
1:C:160:HIS:O	1:C:162:ARG:HG3	1.94	0.68
1:B:128:ASN:HB2	1:B:139:PHE:CD2	2.29	0.68
1:B:8:THR:HG22	1:B:100:ILE:HB	1.76	0.68
1:G:38:TYR:HA	1:G:68:LEU:O	1.92	0.68
1:B:143:LEU:HD21	1:B:179:TYR:HB3	1.73	0.68
1:F:171:ARG:HG3	1:F:172:HIS:N	2.06	0.68
1:E:103:ASP:HA	1:E:106:TYR:HB2	1.76	0.68
1:B:208:GLY:CA	1:B:213:LYS:HZ3	2.05	0.68
1:F:174:GLY:HA3	1:F:191:ILE:HB	1.75	0.68
1:B:82:GLN:O	1:B:86:ILE:HG13	1.94	0.68
1:B:16:MET:O	1:B:20:ILE:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:VAL:O	1:A:266:ARG:HG3	1.94	0.67
1:G:7:LEU:HD11	1:G:99:VAL:HG22	1.75	0.67
1:E:190:LEU:HD12	1:E:220:VAL:HG22	1.77	0.67
1:G:225:GLY:HA3	1:G:230:PHE:CE1	2.29	0.67
1:E:214:LYS:H	1:E:214:LYS:HD3	1.59	0.67
1:B:281:GLY:O	1:B:296:ILE:HG13	1.94	0.67
1:E:17:ASN:ND2	1:E:67:ILE:HG23	2.10	0.67
1:F:164:TRP:HZ3	1:F:245:THR:CB	2.06	0.67
1:A:191:ILE:HD11	1:A:194:ALA:HB3	1.76	0.67
1:C:232:ARG:O	1:C:236:GLU:HG3	1.95	0.67
1:F:26:LYS:HE2	1:F:30:HIS:NE2	2.09	0.67
1:A:58:GLY:O	1:A:59:ASP:HB3	1.93	0.67
1:B:7:LEU:CD1	1:B:99:VAL:HG22	2.25	0.67
1:D:276:LEU:C	1:D:278:GLY:H	1.96	0.67
1:E:141:THR:HA	1:E:257:THR:CG2	2.25	0.66
1:A:4:ILE:O	1:A:34:VAL:HA	1.95	0.66
1:G:268:GLY:O	1:G:272:VAL:HG23	1.95	0.66
1:E:258:ALA:O	1:E:262:VAL:HG23	1.94	0.66
1:F:191:ILE:HG12	1:F:193:GLU:H	1.60	0.66
1:E:207:ARG:HH11	1:E:207:ARG:HB3	1.60	0.66
1:A:24:VAL:HB	1:A:57:VAL:HG21	1.78	0.66
1:E:147:ILE:HG21	1:E:183:ALA:HB3	1.75	0.66
1:C:14:PRO:CB	1:C:141:THR:HG21	2.25	0.66
1:C:160:HIS:HE1	1:D:12:ASP:H	1.41	0.66
1:G:249:HIS:HB2	1:H:164:TRP:CH2	2.29	0.66
1:E:143:LEU:HD21	1:E:179:TYR:HB3	1.77	0.66
1:E:141:THR:OG1	1:E:256:PRO:HA	1.96	0.66
1:F:298:GLU:O	1:F:301:ALA:HB3	1.95	0.66
1:F:161:GLU:HB3	1:F:214:LYS:HB2	1.78	0.66
1:F:277:GLU:HG2	1:F:277:GLU:O	1.95	0.66
1:D:288:ASN:HD22	1:D:288:ASN:N	1.92	0.66
1:B:171:ARG:HG3	1:B:172:HIS:N	2.10	0.66
1:E:44:LEU:HD11	1:E:89:LEU:HD21	1.76	0.66
1:E:152:LYS:NZ	1:F:145:THR:HG23	2.11	0.66
1:D:24:VAL:O	1:D:28:ILE:HG12	1.97	0.65
1:G:249:HIS:HB2	1:H:164:TRP:HH2	1.61	0.65
1:C:186:ALA:HB2	1:C:219:ILE:HD13	1.77	0.65
1:G:225:GLY:HA3	1:G:230:PHE:HE1	1.61	0.65
1:G:211:ARG:HH21	1:G:213:LYS:HE2	1.60	0.65
1:D:5:GLY:HA2	1:D:35:TYR:O	1.97	0.65
1:D:307:ASP:OD2	1:D:309:ARG:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:ASP:OD2	1:G:199:ASN:HB2	1.97	0.65
1:B:20:ILE:HD12	1:B:68:LEU:HD12	1.78	0.64
1:C:207:ARG:HH11	1:C:211:ARG:HE	1.44	0.64
1:C:211:ARG:CB	1:C:211:ARG:HH11	2.10	0.64
1:G:295:ASP:HB3	1:G:298:GLU:HG3	1.78	0.64
1:F:193:GLU:HB3	1:F:306:ILE:HD12	1.79	0.64
1:H:25:ARG:HG3	1:H:25:ARG:HH11	1.62	0.64
1:A:23:VAL:HG13	1:A:272:VAL:CG2	2.27	0.64
1:B:202:ILE:HD13	1:B:237:ALA:CB	2.28	0.64
1:D:19:ALA:HB2	1:D:264:ALA:HB1	1.78	0.64
1:F:165:VAL:HB	1:F:244:VAL:HG22	1.80	0.64
1:H:5:GLY:O	1:H:97:LEU:HD12	1.98	0.64
1:C:160:HIS:CE1	1:D:12:ASP:H	2.16	0.64
1:G:169:MET:HG3	1:G:251:GLN:NE2	2.13	0.64
1:F:316:GLU:O	1:F:319:ILE:HD11	1.97	0.64
1:F:128:ASN:HB2	1:F:139:PHE:CD2	2.33	0.63
1:A:89:LEU:HD13	1:A:117:PHE:CE2	2.33	0.63
1:C:12:ASP:H	1:D:160:HIS:HE1	1.46	0.63
1:B:22:SER:HB2	1:B:265:SER:HA	1.81	0.63
1:F:24:VAL:HG11	1:F:57:VAL:HG11	1.79	0.63
1:G:143:LEU:O	1:G:147:ILE:HG23	1.99	0.63
1:G:147:ILE:HA	1:G:150:ILE:HD13	1.80	0.63
1:G:78:THR:HG22	1:G:80:GLU:H	1.62	0.63
1:A:145:THR:HG23	1:B:152:LYS:HZ3	1.63	0.63
1:A:165:VAL:HB	1:A:244:VAL:CG1	2.28	0.63
1:D:269:ALA:O	1:D:273:GLU:HG3	1.98	0.63
1:A:113:THR:C	1:A:115:HIS:H	2.02	0.63
1:B:51:LYS:HE3	1:B:53:GLU:OE1	1.98	0.63
1:E:306:ILE:HD13	1:E:306:ILE:H	1.63	0.63
1:E:189:ILE:HD12	1:E:189:ILE:N	2.13	0.62
1:A:182:LEU:HD23	1:C:262:VAL:HG13	1.81	0.62
1:A:77:LYS:NZ	1:A:77:LYS:HB2	2.12	0.62
1:D:21:ARG:NH1	1:D:25:ARG:NH1	2.47	0.62
1:G:126:ILE:O	1:G:176:ILE:HD11	1.99	0.62
1:F:191:ILE:HD12	1:F:311:TYR:CE2	2.34	0.62
1:F:312:ALA:O	1:F:316:GLU:HG3	1.99	0.62
1:E:17:ASN:ND2	1:E:67:ILE:HG12	2.13	0.62
1:B:128:ASN:OD1	1:B:135:PHE:HA	1.99	0.62
1:H:171:ARG:CG	1:H:172:HIS:H	2.04	0.62
1:D:123:PRO:CB	1:D:136:THR:HG22	2.23	0.62
1:A:282:ARG:HB3	1:A:282:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:MET:HE3	1:D:249:HIS:HA	1.82	0.62
1:A:134:ASP:OD2	1:A:287:GLN:HA	2.00	0.62
1:A:24:VAL:O	1:A:28:ILE:HG12	2.00	0.62
1:D:137:ILE:HD11	1:D:267:LEU:HD12	1.81	0.62
1:F:97:LEU:HB3	1:F:119:CYS:SG	2.40	0.62
1:A:113:THR:HG23	1:A:119:CYS:HB2	1.81	0.61
1:E:207:ARG:NH1	1:E:207:ARG:HB3	2.15	0.61
1:C:198:MET:O	1:C:202:ILE:HG12	1.99	0.61
1:E:84:LYS:O	1:E:88:GLN:HB2	2.00	0.61
1:A:118:PRO:HB3	1:A:280:GLY:HA3	1.81	0.61
1:F:112:LEU:O	1:F:117:PHE:HB2	1.99	0.61
1:G:99:VAL:CG1	1:G:105:SER:HB3	2.31	0.61
1:F:302:ASN:ND2	1:F:303:LYS:H	1.99	0.61
1:E:63:ARG:HH12	1:H:62:HIS:HE1	1.46	0.61
1:B:78:THR:O	1:B:82:GLN:HG3	2.01	0.61
1:E:166:ILE:HD13	1:E:245:THR:HB	1.83	0.61
1:D:37:VAL:HG22	1:D:49:ILE:CD1	2.31	0.61
1:H:19:ALA:O	1:H:23:VAL:HG23	2.01	0.61
1:E:114:GLU:C	1:E:116:GLY:H	2.03	0.61
1:D:186:ALA:HB3	1:D:189:ILE:CD1	2.30	0.61
1:F:169:MET:SD	2:F:1005:F6P:H11	2.41	0.61
1:F:143:LEU:HD11	1:F:179:TYR:CB	2.31	0.61
1:G:211:ARG:HG2	1:G:211:ARG:HH11	1.65	0.61
1:E:229:ASP:O	1:E:233:GLN:HG3	2.01	0.61
1:B:287:GLN:OE1	1:B:292:VAL:HG21	2.00	0.61
1:H:211:ARG:NH1	1:H:319:ILE:HG22	2.16	0.61
1:E:45:ILE:HD11	1:E:76:PHE:HD1	1.66	0.61
1:D:13:SER:O	1:D:16:MET:HG3	2.00	0.60
1:A:139:PHE:CE2	1:A:176:ILE:HD13	2.36	0.60
1:D:61:ILE:O	1:D:61:ILE:HG12	2.00	0.60
1:G:52:LEU:HD11	1:G:68:LEU:HD21	1.83	0.60
1:H:249:HIS:C	1:H:251:GLN:H	2.02	0.60
1:E:207:ARG:CB	1:E:207:ARG:HH11	2.14	0.60
1:C:152:LYS:HD3	1:D:254:GLY:HA3	1.83	0.60
1:F:192:PRO:HG3	1:F:224:VAL:HG23	1.82	0.60
1:H:21:ARG:HA	1:H:57:VAL:HB	1.81	0.60
1:D:113:THR:HG21	1:D:281:GLY:HA2	1.83	0.60
1:D:76:PHE:HZ	1:D:112:LEU:HD21	1.67	0.60
1:D:82:GLN:OE1	1:D:111:LYS:HB3	2.00	0.60
1:D:21:ARG:HE	1:D:61:ILE:HB	1.67	0.60
1:G:211:ARG:NH2	1:G:213:LYS:HE2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:GLY:HA3	1:H:88:GLN:OE1	2.01	0.60
1:E:282:ARG:HD2	1:E:294:HIS:O	2.02	0.60
1:F:207:ARG:HH22	1:F:319:ILE:HG22	1.67	0.60
1:F:164:TRP:HZ3	1:F:245:THR:OG1	1.85	0.60
1:G:124:GLY:HA2	1:G:137:ILE:HB	1.83	0.60
1:G:2:LYS:NZ	1:G:2:LYS:HB3	2.16	0.60
1:A:253:GLY:HA3	1:B:152:LYS:O	2.01	0.60
1:D:171:ARG:CG	1:D:172:HIS:H	2.14	0.60
1:F:296:ILE:HG22	1:F:300:LEU:HD12	1.84	0.60
1:H:145:THR:HG21	1:H:250:VAL:O	2.02	0.60
1:E:102:GLY:HA2	1:E:130:ILE:HD11	1.82	0.60
1:B:120:VAL:HA	1:B:282:ARG:O	2.01	0.60
1:H:128:ASN:HD21	1:H:135:PHE:HA	1.66	0.60
1:E:125:THR:OG1	1:E:126:ILE:N	2.35	0.59
1:C:21:ARG:HB2	1:C:60:ILE:HD11	1.83	0.59
1:D:16:MET:O	1:D:20:ILE:HG12	2.02	0.59
1:D:127:ASP:OD1	1:D:170:GLY:HA2	2.02	0.59
1:E:78:THR:HG22	1:E:80:GLU:N	2.15	0.59
1:E:86:ILE:HG23	1:E:117:PHE:CE1	2.38	0.59
1:F:5:GLY:HA2	1:F:35:TYR:O	2.03	0.59
1:C:77:LYS:HB2	1:C:77:LYS:NZ	2.18	0.59
1:A:118:PRO:HA	1:A:280:GLY:O	2.01	0.59
1:G:128:ASN:OD1	1:G:135:PHE:HA	2.03	0.59
1:E:156:THR:HA	1:F:12:ASP:OD2	2.03	0.59
1:F:106:TYR:O	1:F:109:ALA:HB3	2.03	0.59
1:E:137:ILE:CD1	1:E:264:ALA:HA	2.32	0.59
1:D:89:LEU:HD13	1:D:117:PHE:CE2	2.38	0.59
1:A:198:MET:HG2	1:A:233:GLN:NE2	2.17	0.59
1:E:171:ARG:N	1:E:222:GLU:OE2	2.34	0.59
1:C:9:SER:OG	1:C:105:SER:HB3	2.03	0.59
1:A:39:HIS:O	1:A:42:ALA:HB3	2.03	0.59
1:G:202:ILE:O	1:G:206:LYS:HG3	2.03	0.59
1:B:7:LEU:HD11	1:B:99:VAL:HG22	1.83	0.59
1:E:80:GLU:O	1:E:84:LYS:HG3	2.02	0.58
1:F:164:TRP:HZ3	1:F:245:THR:HB	1.67	0.58
1:A:191:ILE:H	1:A:191:ILE:HD13	1.67	0.58
1:D:142:ALA:O	1:D:146:VAL:HG23	2.03	0.58
1:C:252:ARG:HD3	2:C:1004:F6P:O2	2.02	0.58
1:E:182:LEU:HD13	1:E:182:LEU:O	2.02	0.58
1:A:152:LYS:O	1:B:253:GLY:HA3	2.04	0.58
1:E:3:ARG:HD3	1:E:35:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:309:ARG:NH2	1:H:316:GLU:OE1	2.35	0.58
1:F:7:LEU:CD1	1:F:99:VAL:HG22	2.33	0.58
1:D:19:ALA:O	1:D:23:VAL:HG23	2.02	0.58
1:B:168:VAL:HG23	1:B:169:MET:N	2.19	0.58
1:H:38:TYR:N	1:H:38:TYR:CD2	2.71	0.58
1:D:89:LEU:HD22	1:D:94:ILE:HG21	1.85	0.58
1:F:38:TYR:O	1:F:43:GLY:HA3	2.04	0.58
1:B:176:ILE:O	1:B:180:SER:CB	2.51	0.58
1:H:113:THR:HA	1:H:117:PHE:O	2.04	0.58
1:C:7:LEU:HB3	1:C:37:VAL:HB	1.85	0.58
1:C:202:ILE:HG23	1:C:238:THR:CG2	2.33	0.58
1:D:161:GLU:OE2	1:D:214:LYS:HD2	2.04	0.58
1:F:274:LEU:HD21	1:F:293:ASP:CB	2.34	0.58
1:B:232:ARG:O	1:B:236:GLU:HG3	2.03	0.57
1:D:312:ALA:O	1:D:316:GLU:HG3	2.04	0.57
1:G:146:VAL:HG12	1:G:150:ILE:CD1	2.34	0.57
1:E:112:LEU:O	1:E:117:PHE:HB2	2.04	0.57
1:A:4:ILE:O	1:A:4:ILE:HG13	2.04	0.57
1:A:3:ARG:HD3	1:A:35:TYR:CE2	2.23	0.57
1:F:28:ILE:HD12	1:F:54:VAL:HB	1.85	0.57
1:E:270:ARG:CZ	1:E:274:LEU:HD11	2.34	0.57
1:B:213:LYS:O	1:B:213:LYS:HG3	2.03	0.57
1:G:266:ARG:HB3	1:G:291:LEU:HD11	1.86	0.57
1:F:202:ILE:HD13	1:F:237:ALA:CB	2.34	0.57
1:F:202:ILE:HD13	1:F:237:ALA:HB1	1.86	0.57
1:F:242:THR:O	1:F:243:ARG:NH2	2.36	0.57
1:E:38:TYR:O	1:E:39:HIS:HB2	2.05	0.57
1:F:146:VAL:C	1:F:148:ASP:H	2.07	0.57
1:A:45:ILE:HD12	1:A:73:CYS:SG	2.44	0.57
1:E:161:GLU:OE1	1:E:214:LYS:HG3	2.04	0.57
1:C:24:VAL:O	1:C:28:ILE:HG12	2.05	0.57
1:C:296:ILE:HG22	1:C:296:ILE:O	2.04	0.57
1:C:67:ILE:HD12	1:C:68:LEU:N	2.20	0.57
1:C:153:ILE:O	1:C:156:THR:HG22	2.03	0.57
1:B:142:ALA:O	1:B:146:VAL:HG23	2.05	0.57
1:A:303:LYS:HB2	1:A:303:LYS:NZ	2.20	0.57
1:E:29:TYR:HB2	1:G:319:ILE:HD11	1.85	0.57
1:E:191:ILE:HD13	1:E:191:ILE:N	2.20	0.57
1:E:24:VAL:O	1:E:28:ILE:HG12	2.04	0.57
1:F:302:ASN:HD22	1:F:303:LYS:N	2.03	0.57
1:D:168:VAL:HA	1:D:251:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:HE	1:C:54:VAL:CG2	2.17	0.57
1:H:200:ASP:O	1:H:203:ALA:HB3	2.04	0.57
1:A:89:LEU:HB3	1:A:117:PHE:CZ	2.39	0.56
1:F:295:ASP:OD2	1:F:297:ALA:HB3	2.05	0.56
1:E:42:ALA:HB2	1:E:73:CYS:HB2	1.85	0.56
1:E:312:ALA:O	1:E:316:GLU:HG3	2.04	0.56
1:E:120:VAL:HG13	1:E:282:ARG:O	2.05	0.56
1:D:113:THR:HG21	1:D:281:GLY:CA	2.35	0.56
1:B:8:THR:HA	1:B:100:ILE:O	2.05	0.56
1:E:272:VAL:O	1:E:276:LEU:HG	2.04	0.56
1:A:160:HIS:NE2	1:B:252:ARG:NH2	2.52	0.56
1:E:12:ASP:OD2	1:E:65:GLY:HA2	2.05	0.56
1:G:211:ARG:NH2	1:G:213:LYS:HG2	2.20	0.56
1:E:311:TYR:O	1:E:314:SER:HB3	2.04	0.56
1:H:21:ARG:NH1	1:H:61:ILE:HD12	2.18	0.56
1:F:205:LEU:O	1:F:209:HIS:HB2	2.05	0.56
1:F:23:VAL:HG22	1:F:268:GLY:O	2.05	0.56
1:D:21:ARG:HE	1:D:61:ILE:HD12	1.71	0.56
1:F:113:THR:C	1:F:115:HIS:H	2.09	0.56
1:H:150:ILE:HD12	1:H:150:ILE:H	1.70	0.56
1:A:306:ILE:O	1:A:306:ILE:HD12	2.06	0.56
1:C:181:GLY:HA3	1:C:189:ILE:HD11	1.88	0.56
1:E:276:LEU:C	1:E:278:GLY:H	2.08	0.56
1:G:78:THR:HG22	1:G:80:GLU:HG2	1.87	0.56
1:E:153:ILE:HG13	1:E:166:ILE:HD11	1.86	0.56
1:H:312:ALA:O	1:H:316:GLU:HG3	2.05	0.56
1:E:15:GLY:O	1:E:18:ALA:HB3	2.05	0.56
1:G:190:LEU:HD12	1:G:220:VAL:CG2	2.29	0.56
1:A:242:THR:HG22	1:A:243:ARG:N	2.20	0.56
1:H:249:HIS:C	1:H:251:GLN:N	2.59	0.56
1:C:156:THR:HA	1:D:12:ASP:OD1	2.06	0.56
1:E:103:ASP:O	1:E:107:GLN:HG2	2.06	0.56
1:F:193:GLU:CB	1:F:306:ILE:HD12	2.36	0.56
1:H:174:GLY:HA3	1:H:191:ILE:HB	1.87	0.56
1:C:276:LEU:C	1:C:278:GLY:H	2.09	0.56
1:C:14:PRO:HD3	1:C:252:ARG:O	2.07	0.55
1:B:208:GLY:HA3	1:B:213:LYS:NZ	2.20	0.55
1:G:198:MET:O	1:G:202:ILE:HG12	2.05	0.55
1:F:57:VAL:O	1:F:57:VAL:HG23	2.07	0.55
1:H:42:ALA:HB2	1:H:73:CYS:HB2	1.88	0.55
1:E:62:HIS:HE1	1:H:63:ARG:HH12	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASN:HA	1:D:147:ILE:CG1	2.35	0.55
1:G:32:VAL:HG21	1:G:276:LEU:HD21	1.87	0.55
1:D:128:ASN:HA	1:D:136:THR:OG1	2.06	0.55
1:D:68:LEU:O	1:D:69:TYR:CB	2.54	0.55
1:E:205:LEU:HD21	1:E:218:ILE:HD11	1.88	0.55
1:C:145:THR:HG21	1:C:250:VAL:O	2.07	0.55
1:H:131:PRO:HB2	1:H:299:ALA:O	2.07	0.55
1:B:193:GLU:HG2	1:B:306:ILE:HG23	1.89	0.55
1:D:17:ASN:OD1	1:D:67:ILE:HG23	2.05	0.55
1:D:197:ASP:OD2	1:D:199:ASN:HB2	2.07	0.55
1:A:34:VAL:HG23	1:A:52:LEU:HB2	1.88	0.55
1:D:141:THR:HA	1:D:257:THR:HG23	1.88	0.55
1:G:7:LEU:CD1	1:G:97:LEU:HD21	2.37	0.55
1:C:310:MET:O	1:C:313:LEU:HB3	2.07	0.55
1:H:38:TYR:HD2	1:H:38:TYR:N	2.05	0.55
1:C:143:LEU:O	1:C:147:ILE:HG23	2.06	0.55
1:D:318:SER:C	1:D:319:ILE:HG13	2.25	0.55
1:A:19:ALA:HA	1:A:264:ALA:O	2.07	0.55
1:A:143:LEU:HD11	1:A:179:TYR:HB3	1.87	0.55
1:E:128:ASN:HA	1:E:136:THR:CG2	2.37	0.55
1:F:161:GLU:CG	1:F:214:LYS:HG3	2.33	0.55
1:H:86:ILE:O	1:H:89:LEU:HB2	2.07	0.55
1:E:189:ILE:HD13	1:E:314:SER:OG	2.06	0.55
1:A:196:TYR:O	1:A:197:ASP:HB2	2.06	0.55
1:H:120:VAL:HA	1:H:282:ARG:O	2.06	0.55
1:G:12:ASP:OD1	1:H:156:THR:HA	2.06	0.55
1:D:198:MET:HE3	1:D:201:VAL:HB	1.89	0.55
1:F:311:TYR:O	1:F:314:SER:HB3	2.06	0.55
1:G:156:THR:HA	1:H:12:ASP:OD2	2.07	0.55
1:A:248:GLY:O	1:A:251:GLN:HG3	2.06	0.55
1:D:103:ASP:HB3	1:D:130:ILE:HD12	1.88	0.55
1:A:110:LYS:HE3	1:A:114:GLU:CD	2.26	0.55
1:E:141:THR:CA	1:E:257:THR:HG23	2.36	0.55
1:E:63:ARG:HH12	1:H:62:HIS:CE1	2.24	0.55
1:D:1:MET:HA	1:D:95:GLU:OE1	2.07	0.55
1:B:72:ARG:HG2	1:B:72:ARG:HH11	1.72	0.55
1:B:143:LEU:HD11	1:B:180:SER:N	2.21	0.54
1:D:3:ARG:HD2	1:D:93:GLY:O	2.08	0.54
1:B:123:PRO:HB2	1:B:136:THR:HG22	1.89	0.54
1:E:12:ASP:HB2	1:E:66:THR:HG22	1.88	0.54
1:B:178:LEU:HD22	1:B:306:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:CB	1:A:246:VAL:HG22	2.37	0.54
1:B:25:ARG:NH1	1:D:317:LEU:O	2.39	0.54
1:A:120:VAL:HA	1:A:282:ARG:O	2.07	0.54
1:F:16:MET:O	1:F:20:ILE:HG12	2.07	0.54
1:E:68:LEU:O	1:E:69:TYR:HB2	2.06	0.54
1:B:24:VAL:CG2	1:B:57:VAL:HG11	2.36	0.54
1:G:122:VAL:HG13	1:G:267:LEU:HB3	1.89	0.54
1:F:89:LEU:HD13	1:F:117:PHE:CE2	2.43	0.54
1:G:212:GLY:O	1:G:214:LYS:HE3	2.07	0.54
1:H:258:ALA:O	1:H:262:VAL:HG23	2.07	0.54
1:G:119:CYS:O	1:G:281:GLY:N	2.34	0.54
1:C:4:ILE:H	1:C:4:ILE:HD13	1.73	0.54
1:C:25:ARG:HE	1:C:54:VAL:HG23	1.71	0.54
1:D:7:LEU:HD12	1:D:7:LEU:C	2.27	0.54
1:D:266:ARG:HE	1:D:291:LEU:HD11	1.72	0.54
1:G:120:VAL:HA	1:G:282:ARG:O	2.08	0.54
1:G:273:GLU:O	1:G:277:GLU:HG3	2.08	0.54
1:A:262:VAL:HG23	1:C:183:ALA:HB2	1.89	0.54
1:F:128:ASN:HA	1:F:136:THR:OG1	2.08	0.54
1:F:263:LEU:HD12	1:F:267:LEU:HG	1.90	0.54
1:B:153:ILE:HG21	1:B:166:ILE:HD11	1.89	0.54
1:E:82:GLN:OE1	1:E:111:LYS:HB3	2.07	0.54
1:B:82:GLN:HE22	1:B:111:LYS:CG	2.19	0.54
1:H:272:VAL:O	1:H:276:LEU:HG	2.08	0.54
1:H:35:TYR:HA	1:H:51:LYS:HA	1.89	0.54
1:G:73:CYS:C	1:G:75:GLU:H	2.10	0.54
1:D:114:GLU:C	1:D:116:GLY:H	2.11	0.54
1:H:24:VAL:HG22	1:H:34:VAL:HG11	1.90	0.54
1:G:211:ARG:HH22	1:G:213:LYS:HG2	1.73	0.54
1:A:249:HIS:CD2	1:B:164:TRP:HH2	2.26	0.54
1:H:169:MET:HE1	2:H:1007:F6P:H61	1.90	0.53
1:A:254:GLY:HA2	1:B:152:LYS:HG2	1.90	0.53
1:A:59:ASP:O	1:A:59:ASP:OD1	2.27	0.53
1:G:295:ASP:OD2	1:G:297:ALA:HB3	2.08	0.53
1:G:45:ILE:HG22	1:G:85:GLY:N	2.24	0.53
1:F:141:THR:OG1	1:F:256:PRO:HA	2.08	0.53
1:H:41:TYR:HE2	1:H:105:SER:HA	1.73	0.53
1:E:107:GLN:HE21	1:E:107:GLN:HA	1.73	0.53
1:H:80:GLU:CD	1:H:80:GLU:H	2.11	0.53
1:A:221:ALA:O	1:A:223:GLY:N	2.41	0.53
1:F:171:ARG:CG	1:F:172:HIS:H	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:ILE:O	1:G:180:SER:HB2	2.09	0.53
1:F:191:ILE:HG12	1:F:193:GLU:N	2.23	0.53
1:E:128:ASN:HA	1:E:136:THR:HG23	1.89	0.53
1:B:289:ASN:O	1:B:290:GLN:HG3	2.09	0.53
1:D:171:ARG:HG3	1:D:172:HIS:N	2.20	0.53
1:A:197:ASP:OD2	1:A:199:ASN:HB2	2.09	0.53
1:C:280:GLY:O	1:C:282:ARG:N	2.41	0.53
1:G:171:ARG:CG	1:G:172:HIS:H	2.14	0.53
1:G:24:VAL:O	1:G:28:ILE:HG13	2.09	0.53
1:E:3:ARG:HD2	1:E:93:GLY:O	2.08	0.53
1:G:17:ASN:OD1	1:G:67:ILE:HG23	2.09	0.53
1:B:127:ASP:OD1	1:B:170:GLY:HA2	2.09	0.53
1:B:20:ILE:O	1:B:24:VAL:HG23	2.08	0.53
1:C:27:ALA:HB3	1:C:34:VAL:HG21	1.91	0.53
1:C:59:ASP:O	1:C:59:ASP:CG	2.46	0.53
1:E:152:LYS:HZ2	1:F:145:THR:HG23	1.72	0.53
1:C:168:VAL:O	1:C:222:GLU:HB3	2.09	0.53
1:H:169:MET:HG3	1:H:251:GLN:HE22	1.71	0.53
1:H:32:VAL:HG21	1:H:276:LEU:HD21	1.91	0.53
1:A:37:VAL:HG21	1:A:97:LEU:HD11	1.91	0.53
1:C:202:ILE:HG23	1:C:238:THR:HG22	1.90	0.53
1:D:198:MET:O	1:D:202:ILE:HG12	2.09	0.53
1:H:190:LEU:HD12	1:H:220:VAL:HG22	1.91	0.53
1:A:186:ALA:HB2	1:A:219:ILE:HD13	1.91	0.53
1:B:22:SER:OG	1:B:265:SER:O	2.24	0.53
1:F:19:ALA:O	1:F:23:VAL:HG23	2.09	0.53
1:H:164:TRP:HZ3	1:H:245:THR:HB	1.74	0.53
1:E:49:ILE:O	1:E:50:LYS:HD3	2.09	0.53
1:C:288:ASN:O	1:C:290:GLN:HG2	2.08	0.53
1:H:89:LEU:HD13	1:H:117:PHE:CE2	2.44	0.52
1:E:191:ILE:HD11	1:E:194:ALA:HB3	1.90	0.52
1:D:288:ASN:ND2	1:D:288:ASN:N	2.57	0.52
1:A:277:GLU:HB3	1:A:279:LYS:CE	2.38	0.52
1:B:171:ARG:CG	1:B:172:HIS:H	2.09	0.52
1:B:24:VAL:HA	1:B:34:VAL:HG21	1.92	0.52
1:C:306:ILE:C	1:C:306:ILE:HD12	2.30	0.52
1:G:146:VAL:HG13	1:G:247:LEU:CD1	2.39	0.52
1:D:129:ASP:OD2	1:D:171:ARG:HD2	2.09	0.52
1:G:267:LEU:HD22	1:G:284:VAL:HG23	1.92	0.52
1:F:306:ILE:HD11	1:F:308:GLN:NE2	2.24	0.52
1:C:272:VAL:O	1:C:276:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:GLY:O	1:H:214:LYS:N	2.41	0.52
1:B:174:GLY:HA3	1:B:191:ILE:HB	1.90	0.52
1:G:286:ILE:HD11	1:G:289:ASN:HA	1.90	0.52
1:H:154:ARG:NH2	1:H:184:GLY:O	2.32	0.52
1:A:282:ARG:CB	1:A:282:ARG:HH11	2.22	0.52
1:H:280:GLY:O	1:H:282:ARG:HG2	2.08	0.52
1:H:146:VAL:O	1:H:149:ALA:HB3	2.09	0.52
1:D:215:HIS:O	1:D:215:HIS:ND1	2.42	0.52
1:G:146:VAL:HG12	1:G:150:ILE:HD11	1.92	0.52
1:H:25:ARG:HG3	1:H:25:ARG:NH1	2.24	0.52
1:G:88:GLN:HA	1:G:88:GLN:OE1	2.09	0.52
1:B:192:PRO:O	1:B:194:ALA:N	2.43	0.52
1:A:165:VAL:CB	1:A:244:VAL:HG12	2.34	0.52
1:F:20:ILE:O	1:F:24:VAL:HG23	2.09	0.52
1:A:205:LEU:CD1	1:A:234:ILE:HD12	2.38	0.52
1:H:191:ILE:HD12	1:H:193:GLU:HB2	1.92	0.52
1:D:197:ASP:C	1:D:199:ASN:H	2.11	0.52
1:D:145:THR:HG21	1:D:250:VAL:O	2.10	0.52
1:B:190:LEU:HD12	1:B:220:VAL:HG22	1.90	0.52
1:B:313:LEU:O	1:B:315:LYS:N	2.43	0.52
1:E:295:ASP:HB3	1:E:298:GLU:HB3	1.92	0.52
1:F:6:VAL:HG13	1:F:68:LEU:HD11	1.91	0.52
1:A:169:MET:HG3	1:A:251:GLN:NE2	2.25	0.52
1:F:58:GLY:O	1:F:59:ASP:HB3	2.10	0.52
1:D:162:ARG:HD3	1:D:241:GLU:HG3	1.91	0.52
1:H:267:LEU:HD22	1:H:285:GLY:H	1.75	0.52
1:E:113:THR:HG21	1:E:281:GLY:CA	2.36	0.52
1:F:100:ILE:HG12	1:F:122:VAL:HB	1.91	0.52
1:A:150:ILE:HD12	1:A:219:ILE:HD11	1.92	0.52
1:G:254:GLY:N	1:H:152:LYS:HD3	2.25	0.51
1:G:123:PRO:HD3	1:G:284:VAL:O	2.09	0.51
1:A:17:ASN:HA	1:A:20:ILE:HD12	1.92	0.51
1:A:9:SER:HB3	1:A:105:SER:OG	2.09	0.51
1:B:175:ASP:OD2	1:B:306:ILE:HG22	2.10	0.51
1:D:75:GLU:N	1:D:75:GLU:CD	2.60	0.51
1:G:68:LEU:O	1:G:69:TYR:HB2	2.10	0.51
1:G:188:THR:C	1:G:189:ILE:HD12	2.30	0.51
1:A:274:LEU:HD21	1:A:293:ASP:OD2	2.11	0.51
1:H:211:ARG:HH12	1:H:319:ILE:CG2	2.21	0.51
1:C:17:ASN:HD21	1:C:67:ILE:HG13	1.76	0.51
1:F:41:TYR:C	1:F:43:GLY:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ASN:OD1	1:F:67:ILE:HG23	2.11	0.51
1:D:47:GLY:HA3	1:D:88:GLN:NE2	2.26	0.51
1:E:268:GLY:O	1:E:271:ALA:HB3	2.11	0.51
1:G:164:TRP:HH2	1:H:249:HIS:CG	2.27	0.51
1:G:157:ALA:O	1:G:161:GLU:N	2.43	0.51
1:H:38:TYR:O	1:H:43:GLY:HA3	2.11	0.51
1:G:53:GLU:O	1:G:55:GLY:N	2.43	0.51
1:D:44:LEU:HD11	1:D:89:LEU:HG	1.92	0.51
1:H:112:LEU:O	1:H:117:PHE:HB3	2.11	0.51
1:A:23:VAL:HG13	1:A:272:VAL:HG22	1.93	0.51
1:A:129:ASP:OD1	1:A:171:ARG:HD2	2.11	0.51
1:G:164:TRP:HH2	1:H:249:HIS:ND1	2.09	0.51
1:E:7:LEU:HD13	1:E:7:LEU:N	2.25	0.51
1:C:160:HIS:O	1:C:161:GLU:C	2.48	0.51
1:H:45:ILE:C	1:H:47:GLY:H	2.13	0.51
1:B:153:ILE:O	1:B:157:ALA:HB2	2.09	0.51
1:D:107:GLN:O	1:D:110:LYS:N	2.43	0.51
1:B:230:PHE:O	1:B:234:ILE:HD13	2.09	0.51
1:H:228:VAL:N	1:H:244:VAL:HG11	2.26	0.51
1:B:160:HIS:HB2	1:B:162:ARG:HG3	1.93	0.51
1:B:198:MET:O	1:B:202:ILE:HG13	2.10	0.51
1:F:24:VAL:HA	1:F:34:VAL:HG21	1.92	0.51
1:D:286:ILE:O	1:D:286:ILE:HG23	2.11	0.51
1:H:169:MET:HG3	1:H:251:GLN:CD	2.30	0.51
1:C:230:PHE:O	1:C:234:ILE:HG13	2.11	0.51
1:E:202:ILE:HG21	1:E:237:ALA:HB1	1.93	0.51
1:D:3:ARG:HG2	1:D:94:ILE:HD13	1.92	0.51
1:F:248:GLY:O	1:F:251:GLN:HG3	2.10	0.51
1:C:181:GLY:HA3	1:C:189:ILE:CD1	2.41	0.51
1:C:211:ARG:HH11	1:C:211:ARG:HB2	1.75	0.51
1:H:25:ARG:HE	1:H:54:VAL:HG22	1.75	0.51
1:G:58:GLY:O	1:G:59:ASP:HB3	2.11	0.51
1:H:126:ILE:HG13	1:H:127:ASP:N	2.25	0.51
1:A:21:ARG:NH2	1:A:25:ARG:HH12	2.09	0.51
1:D:49:ILE:HG22	1:D:50:LYS:N	2.26	0.51
1:D:88:GLN:HA	1:D:88:GLN:OE1	2.11	0.51
1:E:59:ASP:CG	1:E:59:ASP:O	2.48	0.51
1:B:193:GLU:H	1:B:193:GLU:CD	2.15	0.50
1:F:181:GLY:HA3	1:F:189:ILE:HG12	1.91	0.50
1:F:146:VAL:C	1:F:148:ASP:N	2.63	0.50
1:A:243:ARG:HH21	1:A:243:ARG:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ARG:NH1	1:B:213:LYS:HD3	2.26	0.50
1:G:226:SER:O	1:G:229:ASP:N	2.45	0.50
1:A:305:THR:HG22	1:A:306:ILE:H	1.74	0.50
1:B:7:LEU:C	1:B:7:LEU:HD22	2.31	0.50
1:F:76:PHE:HZ	1:F:112:LEU:HG	1.76	0.50
1:D:229:ASP:O	1:D:233:GLN:HB2	2.11	0.50
1:E:129:ASP:HB3	1:E:173:ALA:HB2	1.93	0.50
1:C:268:GLY:O	1:C:271:ALA:HB3	2.10	0.50
1:D:211:ARG:HH11	1:D:211:ARG:HB2	1.76	0.50
1:C:106:TYR:HD2	1:C:296:ILE:HG23	1.76	0.50
1:G:169:MET:HG3	1:G:251:GLN:CD	2.31	0.50
1:E:168:VAL:O	1:E:222:GLU:HB3	2.10	0.50
1:G:270:ARG:HD2	1:G:273:GLU:OE2	2.10	0.50
1:C:168:VAL:HG21	1:C:177:ALA:HA	1.93	0.50
1:H:133:THR:HB	1:H:285:GLY:HA3	1.93	0.50
1:F:102:GLY:HA2	1:F:130:ILE:HD11	1.93	0.50
1:A:84:LYS:O	1:A:88:GLN:HG2	2.10	0.50
1:G:102:GLY:O	1:G:105:SER:N	2.42	0.50
1:H:164:TRP:HZ3	1:H:245:THR:HG1	1.57	0.50
1:E:89:LEU:HD13	1:E:117:PHE:CE2	2.45	0.50
1:D:26:LYS:HE2	1:D:273:GLU:HG2	1.93	0.50
1:B:74:PRO:O	1:B:77:LYS:HB2	2.11	0.50
1:C:249:HIS:C	1:C:251:GLN:N	2.64	0.50
1:G:7:LEU:HD11	1:G:97:LEU:HD21	1.94	0.50
1:H:128:ASN:HD22	1:H:136:THR:HG23	1.75	0.50
1:B:38:TYR:O	1:B:43:GLY:HA3	2.11	0.50
1:D:113:THR:HA	1:D:117:PHE:O	2.11	0.50
1:D:276:LEU:C	1:D:278:GLY:N	2.64	0.50
1:D:75:GLU:O	1:D:81:GLY:HA3	2.12	0.50
1:E:160:HIS:HE1	1:F:12:ASP:H	1.60	0.50
1:G:187:GLU:CG	1:G:216:SER:OG	2.60	0.50
1:C:26:LYS:O	1:C:29:TYR:HB3	2.12	0.50
1:E:258:ALA:HB2	1:G:147:ILE:HG21	1.93	0.50
1:G:128:ASN:HA	1:G:136:THR:OG1	2.11	0.50
1:F:12:ASP:HA	1:F:16:MET:SD	2.52	0.50
1:F:25:ARG:HD2	1:H:317:LEU:O	2.12	0.50
1:F:97:LEU:HD23	1:F:119:CYS:SG	2.52	0.50
1:A:163:THR:HG21	1:A:234:ILE:HG21	1.94	0.50
1:H:9:SER:O	1:H:101:GLY:HA3	2.12	0.50
1:D:35:TYR:HB2	1:D:94:ILE:HD11	1.93	0.49
1:F:147:ILE:HA	1:F:150:ILE:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:CG	1:A:282:ARG:HH11	2.25	0.49
1:A:141:THR:HA	1:A:257:THR:CG2	2.42	0.49
1:E:86:ILE:O	1:E:90:LYS:HG3	2.12	0.49
1:F:63:ARG:HH12	1:G:62:HIS:HE1	1.58	0.49
1:A:171:ARG:HB2	1:A:171:ARG:HH11	1.77	0.49
1:F:7:LEU:HD13	1:F:7:LEU:O	2.12	0.49
1:G:7:LEU:CD1	1:G:99:VAL:HG22	2.42	0.49
1:E:143:LEU:HD11	1:E:179:TYR:HB2	1.94	0.49
1:F:203:ALA:O	1:F:207:ARG:HB2	2.11	0.49
1:H:24:VAL:HA	1:H:34:VAL:HG21	1.94	0.49
1:F:35:TYR:CB	1:F:94:ILE:HD11	2.42	0.49
1:D:7:LEU:HD11	1:D:99:VAL:HG13	1.93	0.49
1:B:38:TYR:CE2	1:B:50:LYS:HE3	2.47	0.49
1:C:197:ASP:OD2	1:C:199:ASN:HB2	2.11	0.49
1:C:205:LEU:HD21	1:C:218:ILE:HD11	1.95	0.49
1:E:120:VAL:HA	1:E:282:ARG:O	2.13	0.49
1:C:4:ILE:CD1	1:C:34:VAL:HG22	2.41	0.49
1:B:261:ARG:HD2	1:D:183:ALA:O	2.12	0.49
1:C:2:LYS:C	1:C:32:VAL:HG13	2.33	0.49
1:F:258:ALA:O	1:F:262:VAL:HG23	2.13	0.49
1:A:202:ILE:HD11	1:A:234:ILE:HD13	1.94	0.49
1:G:286:ILE:HG23	1:G:286:ILE:O	2.12	0.49
1:B:18:ALA:HB3	1:B:264:ALA:CB	2.42	0.49
1:G:202:ILE:CD1	1:G:234:ILE:HG12	2.42	0.49
1:E:106:TYR:O	1:E:109:ALA:HB3	2.13	0.49
1:A:26:LYS:NZ	1:A:273:GLU:OE2	2.46	0.49
1:B:23:VAL:HG22	1:B:268:GLY:O	2.12	0.49
1:A:107:GLN:C	1:A:109:ALA:H	2.16	0.49
1:E:134:ASP:OD2	1:E:287:GLN:HA	2.12	0.49
1:G:167:GLU:CB	1:G:246:VAL:HG13	2.39	0.49
1:C:21:ARG:NH2	1:C:25:ARG:HH12	2.10	0.49
1:A:167:GLU:HB2	1:A:246:VAL:HG22	1.95	0.49
1:E:2:LYS:NZ	1:E:2:LYS:HB2	2.27	0.49
1:C:51:LYS:HE2	1:C:53:GLU:OE1	2.13	0.49
1:E:62:HIS:HE1	1:H:63:ARG:NH1	2.10	0.49
1:E:178:LEU:HA	1:E:189:ILE:HG21	1.95	0.49
1:H:294:HIS:HB2	1:H:299:ALA:HB2	1.94	0.49
1:G:127:ASP:OD1	1:G:170:GLY:HA2	2.12	0.49
1:D:144:ASN:OD1	1:D:147:ILE:HD11	2.13	0.49
1:C:318:SER:O	1:C:319:ILE:C	2.51	0.49
1:B:68:LEU:O	1:B:69:TYR:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASP:H	1:B:160:HIS:CE1	2.31	0.48
1:B:189:ILE:N	1:B:189:ILE:HD12	2.28	0.48
1:H:169:MET:CE	2:H:1007:F6P:H61	2.43	0.48
1:G:263:LEU:HG	1:G:267:LEU:HD12	1.93	0.48
1:H:139:PHE:O	1:H:143:LEU:HB2	2.12	0.48
1:H:3:ARG:NH1	1:H:35:TYR:CE2	2.81	0.48
1:B:319:ILE:HD12	1:D:29:TYR:HD2	1.78	0.48
1:A:178:LEU:HA	1:A:189:ILE:HG21	1.95	0.48
1:C:12:ASP:H	1:D:160:HIS:CE1	2.30	0.48
1:C:14:PRO:HB3	1:C:141:THR:HG21	1.93	0.48
1:E:128:ASN:OD1	1:E:135:PHE:HA	2.13	0.48
1:A:295:ASP:HB2	1:A:298:GLU:HG2	1.95	0.48
1:G:152:LYS:HA	1:H:254:GLY:H	1.79	0.48
1:C:152:LYS:O	1:D:253:GLY:HA3	2.13	0.48
1:F:188:THR:OG1	1:F:204:ARG:NH2	2.47	0.48
1:D:24:VAL:CB	1:D:57:VAL:HG11	2.43	0.48
1:C:249:HIS:HD2	1:C:252:ARG:NH1	2.11	0.48
1:E:281:GLY:C	1:E:282:ARG:HG2	2.33	0.48
1:A:229:ASP:O	1:A:233:GLN:HG3	2.14	0.48
1:E:77:LYS:HZ3	1:E:77:LYS:HB3	1.75	0.48
1:E:206:LYS:HG3	1:E:238:THR:HG22	1.95	0.48
1:E:58:GLY:O	1:E:59:ASP:HB3	2.12	0.48
1:G:182:LEU:CD2	1:G:310:MET:HE2	2.43	0.48
1:G:21:ARG:HG2	1:G:21:ARG:HH11	1.78	0.48
1:F:261:ARG:HB2	1:H:183:ALA:HB1	1.94	0.48
1:D:187:GLU:HG2	1:D:217:ILE:H	1.78	0.48
1:A:279:LYS:HD3	1:A:279:LYS:H	1.79	0.48
1:E:25:ARG:HB3	1:G:317:LEU:HD22	1.94	0.48
1:B:111:LYS:HA	1:B:111:LYS:HE2	1.95	0.48
1:B:99:VAL:CG1	1:B:105:SER:HB3	2.43	0.48
1:E:188:THR:HG22	1:E:218:ILE:HG23	1.95	0.48
1:D:280:GLY:O	1:D:282:ARG:HG2	2.14	0.48
1:E:231:GLY:HA3	1:E:244:VAL:CG2	2.44	0.48
1:D:218:ILE:HD12	1:D:218:ILE:N	2.28	0.48
1:D:224:VAL:O	1:D:224:VAL:HG12	2.14	0.48
1:E:27:ALA:HB3	1:E:34:VAL:CG2	2.44	0.48
1:A:110:LYS:HD3	1:A:297:ALA:HB2	1.94	0.48
1:B:62:HIS:HB3	1:B:261:ARG:NH1	2.29	0.48
1:B:76:PHE:HZ	1:B:112:LEU:HG	1.77	0.48
1:H:8:THR:HG23	1:H:20:ILE:HD11	1.95	0.48
1:B:25:ARG:HD3	1:B:54:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ILE:O	1:A:300:LEU:HB2	2.14	0.48
1:D:24:VAL:HB	1:D:57:VAL:HG11	1.96	0.48
1:F:161:GLU:HA	1:F:215:HIS:HB3	1.95	0.48
1:E:276:LEU:C	1:E:278:GLY:N	2.66	0.48
1:G:166:ILE:HD12	1:G:219:ILE:CD1	2.41	0.47
1:F:191:ILE:HD13	1:F:191:ILE:H	1.79	0.47
1:C:217:ILE:HG22	1:C:219:ILE:CD1	2.44	0.47
1:E:160:HIS:CE1	1:F:12:ASP:H	2.32	0.47
1:G:160:HIS:HE1	1:H:12:ASP:OD1	1.97	0.47
1:A:263:LEU:HD12	1:A:267:LEU:HG	1.96	0.47
1:A:286:ILE:O	1:A:286:ILE:HG23	2.14	0.47
1:D:121:GLY:O	1:D:284:VAL:HG22	2.14	0.47
1:C:124:GLY:HA2	1:C:137:ILE:HB	1.94	0.47
1:F:7:LEU:HB3	1:F:37:VAL:HB	1.95	0.47
1:B:211:ARG:CZ	1:B:213:LYS:HD3	2.43	0.47
1:C:17:ASN:O	1:C:18:ALA:C	2.53	0.47
1:F:128:ASN:OD1	1:F:135:PHE:HA	2.13	0.47
1:A:261:ARG:NH1	1:C:147:ILE:HD12	2.29	0.47
1:H:160:HIS:O	1:H:161:GLU:HB2	2.15	0.47
1:B:153:ILE:HD13	1:B:166:ILE:CD1	2.44	0.47
1:C:113:THR:HA	1:C:117:PHE:O	2.14	0.47
1:C:191:ILE:C	1:C:224:VAL:HG11	2.35	0.47
1:C:27:ALA:HB3	1:C:34:VAL:CG2	2.44	0.47
1:G:254:GLY:HA3	1:H:152:LYS:HD3	1.95	0.47
1:F:193:GLU:HG2	1:F:306:ILE:HG23	1.96	0.47
1:C:306:ILE:HD12	1:C:307:ASP:C	2.33	0.47
1:D:215:HIS:ND1	1:D:215:HIS:C	2.67	0.47
1:G:288:ASN:O	1:G:290:GLN:HG3	2.14	0.47
1:D:23:VAL:CG1	1:D:98:VAL:HG21	2.44	0.47
1:A:266:ARG:HD2	1:C:310:MET:CE	2.44	0.47
1:H:25:ARG:HE	1:H:54:VAL:CG2	2.27	0.47
1:E:292:VAL:O	1:E:293:ASP:HB3	2.14	0.47
1:A:133:THR:O	1:A:133:THR:HG23	2.15	0.47
1:B:70:THR:HG23	1:B:70:THR:O	2.15	0.47
1:F:143:LEU:HD21	1:F:179:TYR:CB	2.38	0.47
1:E:72:ARG:N	1:E:72:ARG:HD2	2.25	0.47
1:H:94:ILE:HG22	1:H:96:GLY:O	2.13	0.47
1:D:242:THR:HG22	1:D:243:ARG:N	2.28	0.47
1:A:96:GLY:HA3	1:A:275:LEU:HD13	1.96	0.47
1:D:24:VAL:HG21	1:D:57:VAL:HG11	1.96	0.47
1:F:164:TRP:CZ3	1:F:245:THR:OG1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HD11	1:B:89:LEU:HG	1.95	0.47
1:D:21:ARG:NE	1:D:61:ILE:HB	2.27	0.47
1:A:59:ASP:O	1:A:59:ASP:CG	2.52	0.47
1:B:7:LEU:HB3	1:B:37:VAL:HB	1.96	0.47
1:E:160:HIS:CE1	1:F:252:ARG:NH2	2.83	0.47
1:F:281:GLY:O	1:F:296:ILE:HG13	2.14	0.47
1:H:51:LYS:HE2	1:H:53:GLU:CD	2.35	0.47
1:E:202:ILE:HG23	1:E:238:THR:HG23	1.96	0.47
1:A:300:LEU:O	1:A:300:LEU:HD23	2.15	0.47
1:A:22:SER:HA	1:C:317:LEU:HD22	1.96	0.47
1:C:146:VAL:HG12	1:C:150:ILE:HD13	1.97	0.47
1:H:218:ILE:N	1:H:218:ILE:HD12	2.30	0.47
1:B:9:SER:O	1:B:101:GLY:HA3	2.15	0.47
1:F:110:LYS:HD2	1:F:297:ALA:HB2	1.96	0.47
1:G:12:ASP:OD2	1:H:160:HIS:HE1	1.98	0.47
1:E:295:ASP:O	1:E:296:ILE:C	2.53	0.47
1:F:197:ASP:HB3	1:F:200:ASP:HB2	1.96	0.47
1:B:176:ILE:O	1:B:176:ILE:HG22	2.15	0.47
1:B:168:VAL:HG22	1:B:221:ALA:HA	1.96	0.47
1:A:143:LEU:HD11	1:A:179:TYR:CB	2.44	0.47
1:C:110:LYS:HG2	1:C:114:GLU:OE2	2.14	0.47
1:D:9:SER:HB3	1:D:105:SER:HB3	1.97	0.47
1:B:59:ASP:CG	1:B:59:ASP:O	2.52	0.47
1:A:120:VAL:HG11	1:A:271:ALA:HB1	1.97	0.47
1:F:62:HIS:HA	1:F:261:ARG:NH2	2.30	0.47
1:G:99:VAL:HG12	1:G:105:SER:HB3	1.96	0.47
1:A:191:ILE:HD12	1:A:311:TYR:CE2	2.50	0.47
1:B:7:LEU:HD23	1:B:40:GLY:HA2	1.96	0.47
1:G:16:MET:O	1:G:20:ILE:HG12	2.15	0.47
1:A:168:VAL:O	1:A:222:GLU:HB3	2.14	0.47
1:A:274:LEU:C	1:A:276:LEU:H	2.17	0.46
1:G:242:THR:CG2	1:G:243:ARG:N	2.78	0.46
1:E:24:VAL:HA	1:E:34:VAL:HG21	1.97	0.46
1:H:8:THR:CG2	1:H:20:ILE:HD11	2.45	0.46
1:B:288:ASN:HB3	1:D:288:ASN:HB3	1.96	0.46
1:C:228:VAL:HA	1:C:244:VAL:HG11	1.97	0.46
1:E:4:ILE:HG21	1:E:275:LEU:HD23	1.97	0.46
1:C:302:ASN:HD22	1:C:302:ASN:HA	1.53	0.46
1:D:112:LEU:O	1:D:117:PHE:HB2	2.15	0.46
1:H:198:MET:HG2	1:H:233:GLN:NE2	2.30	0.46
1:C:82:GLN:O	1:C:86:ILE:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ARG:NH1	1:C:211:ARG:HH21	2.13	0.46
1:A:147:ILE:C	1:A:147:ILE:HD12	2.36	0.46
1:C:8:THR:HB	1:C:16:MET:HE1	1.97	0.46
1:E:17:ASN:OD1	1:E:65:GLY:O	2.33	0.46
1:D:49:ILE:O	1:D:50:LYS:NZ	2.48	0.46
1:B:208:GLY:CA	1:B:213:LYS:NZ	2.78	0.46
1:D:143:LEU:HD11	1:D:179:TYR:CB	2.42	0.46
1:H:26:LYS:HE3	1:H:30:HIS:NE2	2.30	0.46
1:A:12:ASP:OD1	1:B:160:HIS:HE1	1.98	0.46
1:E:32:VAL:HG12	1:E:33:GLU:N	2.30	0.46
1:B:238:THR:OG1	1:B:239:GLY:N	2.47	0.46
1:D:165:VAL:HB	1:D:244:VAL:HG22	1.98	0.46
1:H:256:PRO:HG2	1:H:261:ARG:HG2	1.97	0.46
1:B:167:GLU:CB	1:B:246:VAL:HG22	2.45	0.46
1:B:270:ARG:NH1	1:B:274:LEU:HD21	2.30	0.46
1:C:252:ARG:HG3	1:C:252:ARG:HH11	1.80	0.46
1:A:193:GLU:HG2	1:A:306:ILE:HG13	1.97	0.46
1:C:3:ARG:HD3	1:C:35:TYR:CZ	2.50	0.46
1:C:38:TYR:O	1:C:43:GLY:HA3	2.15	0.46
1:G:75:GLU:C	1:G:77:LYS:H	2.19	0.46
1:A:221:ALA:C	1:A:223:GLY:N	2.69	0.46
1:A:221:ALA:C	1:A:223:GLY:H	2.18	0.46
1:F:6:VAL:HG13	1:F:6:VAL:O	2.15	0.46
1:A:177:ALA:O	1:A:178:LEU:C	2.53	0.46
1:G:165:VAL:HB	1:G:244:VAL:HG22	1.96	0.46
1:D:306:ILE:HD11	1:D:308:GLN:NE2	2.30	0.46
1:D:48:ASN:O	1:D:49:ILE:HD13	2.16	0.46
1:C:38:TYR:CE1	1:C:68:LEU:HA	2.50	0.46
1:H:164:TRP:HZ3	1:H:245:THR:CB	2.29	0.46
1:C:186:ALA:CB	1:C:219:ILE:HD13	2.45	0.46
1:A:230:PHE:O	1:A:234:ILE:HG12	2.16	0.46
1:A:277:GLU:HB3	1:A:279:LYS:HE2	1.97	0.46
1:G:58:GLY:O	1:G:59:ASP:CB	2.63	0.46
1:A:68:LEU:O	1:A:69:TYR:HB2	2.15	0.46
1:F:61:ILE:HG23	1:F:62:HIS:N	2.29	0.46
1:B:22:SER:CB	1:B:265:SER:HA	2.46	0.46
1:F:127:ASP:OD2	2:F:1005:F6P:H3	2.15	0.46
1:B:185:GLY:HA2	1:D:21:ARG:NH2	2.31	0.46
1:F:76:PHE:HZ	1:F:112:LEU:CG	2.29	0.46
1:D:197:ASP:C	1:D:199:ASN:N	2.69	0.46
1:C:280:GLY:C	1:C:282:ARG:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TYR:CD1	1:C:94:ILE:HD11	2.51	0.46
1:B:111:LYS:O	1:B:114:GLU:N	2.49	0.46
1:G:207:ARG:HG2	1:G:207:ARG:NH1	2.30	0.46
1:F:88:GLN:HA	1:F:88:GLN:OE1	2.16	0.46
1:E:114:GLU:C	1:E:116:GLY:N	2.67	0.46
1:F:209:HIS:C	1:F:211:ARG:H	2.18	0.46
1:D:162:ARG:NH1	1:D:162:ARG:HG3	2.31	0.46
1:H:231:GLY:HA3	1:H:244:VAL:HG22	1.98	0.46
1:F:103:ASP:OD1	1:F:104:GLY:N	2.49	0.46
1:C:197:ASP:OD1	1:C:199:ASN:ND2	2.48	0.46
1:H:178:LEU:HD22	1:H:306:ILE:HD13	1.97	0.46
1:G:312:ALA:O	1:G:315:LYS:HB2	2.15	0.46
1:F:127:ASP:OD1	1:F:170:GLY:HA2	2.15	0.46
1:F:150:ILE:CD1	1:F:219:ILE:HD11	2.46	0.46
1:F:82:GLN:OE1	1:F:111:LYS:HB3	2.16	0.46
1:G:307:ASP:C	1:G:307:ASP:OD2	2.54	0.46
1:D:144:ASN:HD22	1:D:257:THR:HG21	1.81	0.45
1:D:141:THR:HG21	1:D:256:PRO:HA	1.97	0.45
1:E:77:LYS:HB3	1:E:77:LYS:HZ2	1.79	0.45
1:E:44:LEU:O	1:E:47:GLY:N	2.48	0.45
1:H:128:ASN:HB2	1:H:139:PHE:CD2	2.51	0.45
1:G:113:THR:C	1:G:115:HIS:H	2.18	0.45
1:B:14:PRO:CB	1:B:141:THR:HG21	2.45	0.45
1:B:154:ARG:HG3	1:B:154:ARG:HH11	1.82	0.45
1:C:295:ASP:HB3	1:C:298:GLU:HG2	1.99	0.45
1:A:238:THR:C	1:A:240:PHE:H	2.18	0.45
1:E:44:LEU:HD11	1:E:89:LEU:CD2	2.43	0.45
1:B:312:ALA:O	1:B:315:LYS:HB2	2.17	0.45
1:D:76:PHE:CZ	1:D:112:LEU:HD21	2.50	0.45
1:H:45:ILE:O	1:H:88:GLN:HG3	2.17	0.45
1:F:41:TYR:O	1:F:44:LEU:N	2.49	0.45
1:A:202:ILE:O	1:A:206:LYS:HG3	2.16	0.45
1:A:242:THR:CG2	1:A:243:ARG:N	2.79	0.45
1:E:201:VAL:HG12	1:E:205:LEU:HD12	1.98	0.45
1:A:196:TYR:HD1	1:A:196:TYR:H	1.63	0.45
1:G:187:GLU:HG2	1:G:216:SER:OG	2.17	0.45
1:C:197:ASP:O	1:C:200:ASP:N	2.48	0.45
1:G:309:ARG:O	1:G:312:ALA:HB3	2.17	0.45
1:C:295:ASP:C	1:C:297:ALA:H	2.19	0.45
1:H:310:MET:O	1:H:313:LEU:HB3	2.16	0.45
1:D:189:ILE:HG13	1:D:219:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:LYS:HG2	1:H:254:GLY:CA	2.47	0.45
1:C:297:ALA:O	1:C:299:ALA:N	2.50	0.45
1:G:99:VAL:O	1:G:121:GLY:HA2	2.16	0.45
1:F:191:ILE:HD11	1:F:194:ALA:HB3	1.97	0.45
1:H:62:HIS:HB3	1:H:261:ARG:NH1	2.31	0.45
1:G:113:THR:HG21	1:G:281:GLY:HA3	1.99	0.45
1:H:226:SER:OG	1:H:228:VAL:HG23	2.16	0.45
1:G:274:LEU:HD22	1:G:279:LYS:HD3	1.99	0.45
1:C:187:GLU:CG	1:C:216:SER:HB3	2.40	0.45
1:H:89:LEU:HD13	1:H:117:PHE:CZ	2.51	0.45
1:H:21:ARG:NH1	1:H:21:ARG:HG2	2.30	0.45
1:A:303:LYS:NZ	1:A:303:LYS:CB	2.79	0.45
1:F:78:THR:O	1:F:82:GLN:HG3	2.16	0.45
1:E:209:HIS:C	1:E:211:ARG:H	2.20	0.45
1:H:207:ARG:O	1:H:210:GLU:HG2	2.16	0.45
1:F:123:PRO:HB2	1:F:136:THR:HG22	1.99	0.45
1:B:189:ILE:HD13	1:B:314:SER:OG	2.17	0.45
1:F:32:VAL:HG21	1:F:276:LEU:HD21	1.99	0.45
1:C:187:GLU:HG3	1:C:216:SER:CB	2.40	0.45
1:B:89:LEU:HD13	1:B:117:PHE:CZ	2.52	0.45
1:F:238:THR:HB	1:F:240:PHE:CE1	2.51	0.45
1:F:187:GLU:OE1	1:F:213:LYS:HD3	2.16	0.45
1:C:139:PHE:CZ	1:C:143:LEU:HD22	2.52	0.45
1:D:125:THR:HG21	1:D:130:ILE:HG12	1.98	0.45
1:B:18:ALA:HB3	1:B:264:ALA:HB3	1.98	0.45
1:F:289:ASN:ND2	1:H:134:ASP:OD2	2.50	0.45
1:G:133:THR:HB	1:G:285:GLY:HA3	1.99	0.45
1:E:39:HIS:HB2	1:E:43:GLY:HA3	1.98	0.45
1:G:176:ILE:O	1:G:180:SER:CB	2.65	0.45
1:G:226:SER:O	1:G:227:GLY:C	2.55	0.45
1:G:26:LYS:HE2	1:G:273:GLU:HG3	1.99	0.45
1:F:4:ILE:HG22	1:F:96:GLY:HA3	1.99	0.45
1:C:15:GLY:HA3	1:C:137:ILE:CG2	2.47	0.45
1:G:99:VAL:HG11	1:G:105:SER:HB3	1.99	0.45
1:C:25:ARG:NE	1:C:54:VAL:HG23	2.32	0.45
1:D:306:ILE:C	1:D:306:ILE:HD12	2.37	0.45
1:C:270:ARG:HG3	1:C:284:VAL:HG11	1.99	0.45
1:H:252:ARG:HD3	2:H:1007:F6P:O2	2.17	0.44
1:C:14:PRO:HB2	1:C:141:THR:HG21	1.96	0.44
1:F:99:VAL:CG1	1:F:105:SER:HB3	2.47	0.44
1:B:198:MET:HG2	1:B:233:GLN:HE21	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ILE:HG13	1:E:54:VAL:HG22	1.98	0.44
1:C:86:ILE:HD12	1:C:86:ILE:N	2.32	0.44
1:E:143:LEU:HD12	1:E:143:LEU:HA	1.81	0.44
1:F:107:GLN:C	1:F:109:ALA:N	2.70	0.44
1:F:38:TYR:HE2	1:F:50:LYS:HB2	1.82	0.44
1:C:42:ALA:HB2	1:C:73:CYS:HB2	1.98	0.44
1:E:45:ILE:N	1:E:45:ILE:HD13	2.32	0.44
1:G:2:LYS:HB3	1:G:2:LYS:HZ3	1.80	0.44
1:F:114:GLU:O	1:F:115:HIS:CD2	2.70	0.44
1:C:249:HIS:C	1:C:251:GLN:H	2.20	0.44
1:D:23:VAL:HG11	1:D:98:VAL:HG21	2.00	0.44
1:E:62:HIS:O	1:E:256:PRO:HD2	2.17	0.44
1:A:75:GLU:H	1:A:75:GLU:CD	2.21	0.44
1:A:7:LEU:HD21	1:A:99:VAL:CG2	2.45	0.44
1:A:44:LEU:HD11	1:A:89:LEU:CG	2.45	0.44
1:H:112:LEU:O	1:H:117:PHE:CB	2.65	0.44
1:E:256:PRO:HG2	1:E:261:ARG:HG2	1.98	0.44
1:G:234:ILE:C	1:G:236:GLU:N	2.71	0.44
1:A:89:LEU:HD13	1:A:117:PHE:CZ	2.51	0.44
1:H:295:ASP:OD2	1:H:297:ALA:HB3	2.18	0.44
1:H:231:GLY:HA3	1:H:244:VAL:CG2	2.47	0.44
1:C:114:GLU:C	1:C:116:GLY:H	2.21	0.44
1:C:235:GLN:HG3	1:C:240:PHE:O	2.17	0.44
1:F:3:ARG:NH1	1:F:92:HIS:O	2.50	0.44
1:G:132:GLY:HA2	1:G:287:GLN:HE22	1.82	0.44
1:C:286:ILE:HG23	1:C:286:ILE:O	2.17	0.44
1:A:154:ARG:O	1:A:154:ARG:HG2	2.17	0.44
1:H:44:LEU:HD11	1:H:89:LEU:CD2	2.47	0.44
1:H:28:ILE:C	1:H:30:HIS:N	2.71	0.44
1:D:1:MET:HE1	1:D:96:GLY:HA3	2.00	0.44
1:C:146:VAL:HG12	1:C:150:ILE:CD1	2.47	0.44
1:F:111:LYS:HE3	1:F:111:LYS:N	2.33	0.44
1:C:95:GLU:O	1:C:118:PRO:HD2	2.18	0.44
1:E:175:ASP:OD2	1:E:304:HIS:NE2	2.51	0.44
1:G:106:TYR:O	1:G:109:ALA:HB3	2.17	0.44
1:A:82:GLN:NE2	1:A:115:HIS:CE1	2.85	0.44
1:G:21:ARG:HG2	1:G:21:ARG:NH1	2.33	0.44
1:H:287:GLN:HB2	1:H:292:VAL:HG21	1.98	0.44
1:E:38:TYR:CD1	1:E:68:LEU:HA	2.53	0.44
1:C:7:LEU:C	1:C:7:LEU:HD22	2.38	0.44
1:D:21:ARG:HH12	1:D:25:ARG:HH12	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:HD3	1:C:54:VAL:HG23	1.99	0.44
1:D:130:ILE:HA	1:D:131:PRO:HD3	1.78	0.44
1:C:306:ILE:HD12	1:C:307:ASP:N	2.32	0.44
1:G:187:GLU:HG3	1:G:216:SER:OG	2.17	0.44
1:C:242:THR:O	1:C:243:ARG:NH2	2.41	0.44
1:G:171:ARG:O	1:G:223:GLY:HA3	2.18	0.44
1:E:110:LYS:O	1:E:113:THR:N	2.50	0.44
1:A:198:MET:HE3	1:A:201:VAL:CG2	2.46	0.44
1:A:193:GLU:HG2	1:A:306:ILE:CG1	2.47	0.44
1:H:35:TYR:HB2	1:H:94:ILE:HD12	1.99	0.44
1:H:270:ARG:HG3	1:H:284:VAL:CG1	2.48	0.44
1:G:186:ALA:HB3	1:G:189:ILE:HD11	1.99	0.44
1:A:312:ALA:O	1:A:316:GLU:HG3	2.17	0.44
1:G:171:ARG:HG3	1:G:172:HIS:N	2.19	0.44
1:H:7:LEU:HD22	1:H:7:LEU:C	2.39	0.44
1:A:113:THR:C	1:A:115:HIS:N	2.69	0.44
1:G:204:ARG:O	1:G:207:ARG:N	2.50	0.44
1:C:152:LYS:HA	1:D:254:GLY:N	2.32	0.44
1:A:263:LEU:HD11	1:A:267:LEU:HD11	1.99	0.44
1:F:132:GLY:O	1:F:133:THR:HB	2.18	0.44
1:E:22:SER:HB2	1:E:265:SER:HA	1.99	0.44
1:D:190:LEU:HD12	1:D:220:VAL:HG22	2.00	0.44
1:E:78:THR:O	1:E:82:GLN:HG3	2.18	0.43
1:C:17:ASN:C	1:C:19:ALA:N	2.70	0.43
1:F:302:ASN:ND2	1:F:303:LYS:N	2.61	0.43
1:G:126:ILE:O	1:G:139:PHE:HD2	2.01	0.43
1:G:230:PHE:HD1	1:G:230:PHE:H	1.65	0.43
1:H:24:VAL:HG21	1:H:57:VAL:HG11	1.99	0.43
1:D:262:VAL:O	1:D:266:ARG:HG3	2.18	0.43
1:E:49:ILE:HG21	1:E:94:ILE:HD11	1.99	0.43
1:C:165:VAL:HG22	1:C:218:ILE:HB	2.00	0.43
1:E:174:GLY:N	1:E:193:GLU:OE2	2.51	0.43
1:H:282:ARG:HD2	1:H:295:ASP:HA	2.01	0.43
1:H:270:ARG:HG3	1:H:284:VAL:HG12	2.00	0.43
1:F:60:ILE:HD13	1:F:67:ILE:HD13	2.00	0.43
1:B:133:THR:HB	1:B:285:GLY:HA3	1.99	0.43
1:G:171:ARG:HB3	2:G:1008:F6P:O4	2.18	0.43
1:D:111:LYS:O	1:D:112:LEU:C	2.56	0.43
1:E:62:HIS:CE1	1:H:63:ARG:HH12	2.34	0.43
1:D:144:ASN:CA	1:D:147:ILE:HG12	2.45	0.43
1:F:100:ILE:HA	1:F:122:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:LYS:HE3	1:G:30:HIS:CD2	2.53	0.43
1:H:93:GLY:O	1:H:94:ILE:C	2.57	0.43
1:C:176:ILE:O	1:C:180:SER:HB2	2.18	0.43
1:A:6:VAL:HG13	1:A:68:LEU:HD11	2.01	0.43
1:E:250:VAL:C	1:E:252:ARG:H	2.22	0.43
1:E:85:GLY:O	1:E:89:LEU:HG	2.18	0.43
1:F:107:GLN:O	1:F:109:ALA:N	2.51	0.43
1:D:212:GLY:C	1:D:214:LYS:H	2.22	0.43
1:E:198:MET:O	1:E:201:VAL:HB	2.18	0.43
1:H:161:GLU:HB3	1:H:214:LYS:HB2	2.00	0.43
1:G:162:ARG:NE	1:G:241:GLU:OE2	2.51	0.43
1:H:235:GLN:HB2	1:H:242:THR:HB	2.00	0.43
1:B:224:VAL:O	1:B:224:VAL:HG13	2.19	0.43
1:E:286:ILE:O	1:E:286:ILE:HG23	2.19	0.43
1:C:252:ARG:HG3	1:C:252:ARG:NH1	2.34	0.43
1:G:38:TYR:O	1:G:43:GLY:HA3	2.18	0.43
1:H:25:ARG:O	1:H:28:ILE:N	2.49	0.43
1:H:286:ILE:HD11	1:H:289:ASN:HA	2.01	0.43
1:E:249:HIS:CD2	1:F:164:TRP:HZ2	2.36	0.43
1:G:23:VAL:HG13	1:G:272:VAL:HG22	2.01	0.43
1:F:162:ARG:O	1:F:215:HIS:HB2	2.18	0.43
1:G:89:LEU:HD23	1:G:94:ILE:HG13	2.00	0.43
1:H:100:ILE:HG12	1:H:122:VAL:HB	2.00	0.43
1:C:150:ILE:HD12	1:C:150:ILE:N	2.34	0.43
1:F:164:TRP:CZ3	1:F:245:THR:HB	2.51	0.43
1:G:7:LEU:HD12	1:G:97:LEU:HD21	2.01	0.43
1:H:16:MET:HE2	1:H:100:ILE:O	2.19	0.43
1:F:306:ILE:H	1:F:306:ILE:HD13	1.83	0.43
1:E:147:ILE:HG21	1:E:183:ALA:CB	2.45	0.43
1:F:107:GLN:C	1:F:109:ALA:H	2.22	0.43
1:G:162:ARG:NH2	1:G:241:GLU:OE2	2.51	0.43
1:B:97:LEU:HD23	1:B:119:CYS:SG	2.58	0.43
1:G:8:THR:HG22	1:G:100:ILE:HB	2.00	0.43
1:E:107:GLN:NE2	1:E:107:GLN:HA	2.34	0.43
1:E:126:ILE:HG13	1:E:127:ASP:N	2.34	0.43
1:F:283:CYS:O	1:F:293:ASP:HA	2.19	0.43
1:H:193:GLU:OE1	1:H:193:GLU:N	2.52	0.43
1:A:252:ARG:HH11	1:A:252:ARG:HG3	1.84	0.43
1:C:311:TYR:CE1	1:C:315:LYS:HE3	2.53	0.43
1:B:205:LEU:O	1:B:209:HIS:HB2	2.19	0.43
1:C:62:HIS:HB3	1:C:261:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:ARG:NH1	1:H:319:ILE:O	2.52	0.43
1:H:143:LEU:HD11	1:H:179:TYR:HB2	2.00	0.43
1:B:146:VAL:HG13	1:B:247:LEU:HD11	2.01	0.43
1:G:44:LEU:O	1:G:88:GLN:HG3	2.18	0.43
1:B:302:ASN:HD22	1:B:302:ASN:N	2.16	0.43
1:D:5:GLY:O	1:D:98:VAL:N	2.51	0.43
1:C:77:LYS:HB2	1:C:77:LYS:HZ2	1.81	0.43
1:D:7:LEU:O	1:D:7:LEU:HD12	2.19	0.43
1:E:138:GLY:HA2	1:E:260:ASP:OD2	2.19	0.43
1:C:13:SER:O	1:C:14:PRO:C	2.57	0.42
1:A:110:LYS:O	1:A:114:GLU:HG3	2.18	0.42
1:G:282:ARG:HG2	1:G:282:ARG:HH11	1.84	0.42
1:F:62:HIS:HA	1:F:261:ARG:CZ	2.49	0.42
1:B:170:GLY:O	1:B:171:ARG:C	2.58	0.42
1:H:44:LEU:HD11	1:H:89:LEU:HD21	2.01	0.42
1:B:198:MET:HE3	1:B:201:VAL:HB	2.01	0.42
1:D:21:ARG:NE	1:D:61:ILE:HD12	2.34	0.42
1:A:43:GLY:C	1:A:45:ILE:N	2.69	0.42
1:H:35:TYR:CZ	1:H:51:LYS:HB2	2.54	0.42
1:A:252:ARG:HD3	2:A:1002:F6P:O2	2.19	0.42
1:F:32:VAL:HG21	1:F:276:LEU:CD2	2.50	0.42
1:C:39:HIS:O	1:C:42:ALA:HB3	2.18	0.42
1:A:21:ARG:HA	1:A:57:VAL:HB	2.02	0.42
1:B:128:ASN:ND2	1:B:175:ASP:OD1	2.41	0.42
1:D:113:THR:O	1:D:116:GLY:N	2.52	0.42
1:B:21:ARG:HA	1:B:57:VAL:HB	2.01	0.42
1:G:80:GLU:O	1:G:83:LYS:HG2	2.18	0.42
1:E:63:ARG:NH1	1:H:62:HIS:HE1	2.15	0.42
1:F:202:ILE:HG23	1:F:238:THR:CG2	2.49	0.42
1:G:113:THR:HG21	1:G:281:GLY:CA	2.49	0.42
1:G:53:GLU:C	1:G:55:GLY:N	2.73	0.42
1:G:216:SER:OG	1:G:217:ILE:N	2.52	0.42
1:E:20:ILE:HD11	1:E:100:ILE:HD13	2.01	0.42
1:E:191:ILE:CD1	1:E:191:ILE:N	2.81	0.42
1:F:295:ASP:O	1:F:296:ILE:C	2.57	0.42
1:D:200:ASP:O	1:D:201:VAL:C	2.58	0.42
1:B:19:ALA:O	1:B:23:VAL:HG23	2.19	0.42
1:A:307:ASP:O	1:A:310:MET:N	2.43	0.42
1:D:50:LYS:NZ	1:D:50:LYS:HB2	2.34	0.42
1:G:226:SER:H	1:G:230:PHE:HE1	1.68	0.42
1:H:247:LEU:O	1:H:250:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HB3	1:A:170:GLY:H	1.70	0.42
1:B:190:LEU:HD22	1:B:196:TYR:CG	2.54	0.42
1:E:252:ARG:NH2	1:F:160:HIS:CE1	2.88	0.42
1:D:21:ARG:HH11	1:D:21:ARG:CG	2.33	0.42
1:F:41:TYR:C	1:F:43:GLY:H	2.23	0.42
1:G:32:VAL:HG12	1:G:33:GLU:N	2.34	0.42
1:B:284:VAL:O	1:B:284:VAL:HG23	2.20	0.42
1:F:188:THR:HB	1:F:218:ILE:HG13	2.01	0.42
1:F:176:ILE:O	1:F:180:SER:HB2	2.19	0.42
1:H:167:GLU:HB3	1:H:246:VAL:HG13	2.02	0.42
1:F:167:GLU:HB3	1:F:246:VAL:HG13	2.02	0.42
1:A:274:LEU:C	1:A:276:LEU:N	2.73	0.42
1:H:171:ARG:CG	1:H:172:HIS:N	2.67	0.42
1:D:234:ILE:O	1:D:238:THR:HG23	2.20	0.42
1:E:7:LEU:HD12	1:E:97:LEU:HD11	2.01	0.42
1:H:113:THR:HG21	1:H:281:GLY:N	2.35	0.42
1:E:152:LYS:HG2	1:F:254:GLY:CA	2.50	0.42
1:C:21:ARG:CD	1:C:61:ILE:HB	2.48	0.42
1:B:300:LEU:HA	1:B:300:LEU:HD23	1.90	0.42
1:C:169:MET:HE1	1:C:249:HIS:HA	2.02	0.42
1:F:319:ILE:N	1:F:319:ILE:HD12	2.35	0.42
1:A:252:ARG:NH2	1:B:160:HIS:CE1	2.88	0.42
1:H:175:ASP:O	1:H:176:ILE:C	2.58	0.42
1:A:191:ILE:HG12	1:A:193:GLU:H	1.84	0.42
1:E:147:ILE:C	1:E:147:ILE:HD12	2.40	0.42
1:E:149:ALA:O	1:E:152:LYS:HB2	2.20	0.42
1:C:146:VAL:HG11	1:C:180:SER:OG	2.20	0.42
1:E:6:VAL:CG2	1:E:100:ILE:HD11	2.49	0.42
1:E:197:ASP:O	1:E:200:ASP:N	2.52	0.42
1:H:269:ALA:O	1:H:273:GLU:HG3	2.19	0.42
1:G:4:ILE:O	1:G:34:VAL:HA	2.20	0.42
1:D:111:LYS:O	1:D:113:THR:N	2.53	0.42
1:A:139:PHE:HE2	1:A:176:ILE:HD13	1.84	0.42
1:C:181:GLY:O	1:C:185:GLY:N	2.43	0.42
1:F:181:GLY:HA2	1:F:219:ILE:HG13	2.01	0.42
1:H:141:THR:CG2	1:H:256:PRO:HA	2.50	0.42
1:B:232:ARG:HD2	1:H:243:ARG:NH2	2.35	0.42
1:A:43:GLY:O	1:A:47:GLY:N	2.45	0.42
1:B:227:GLY:O	1:B:228:VAL:C	2.59	0.42
1:H:128:ASN:HA	1:H:136:THR:CG2	2.50	0.41
1:E:171:ARG:HB2	1:E:171:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:ARG:HH12	1:F:213:LYS:HE2	1.84	0.41
1:F:63:ARG:HH12	1:G:62:HIS:CE1	2.37	0.41
1:H:134:ASP:OD1	1:H:287:GLN:HA	2.20	0.41
1:H:99:VAL:HG21	1:H:109:ALA:HB2	2.02	0.41
1:F:262:VAL:HG22	1:H:183:ALA:HB2	2.02	0.41
1:B:139:PHE:CE1	1:B:143:LEU:HD22	2.55	0.41
1:H:16:MET:O	1:H:20:ILE:HG12	2.20	0.41
1:F:20:ILE:HD13	1:F:100:ILE:HD12	2.02	0.41
1:D:200:ASP:O	1:D:203:ALA:HB3	2.20	0.41
1:H:53:GLU:OE2	1:H:53:GLU:HA	2.20	0.41
1:E:142:ALA:O	1:E:145:THR:N	2.53	0.41
1:G:102:GLY:O	1:G:104:GLY:N	2.52	0.41
1:B:86:ILE:O	1:B:86:ILE:HG22	2.19	0.41
1:A:82:GLN:NE2	1:A:115:HIS:ND1	2.69	0.41
1:H:128:ASN:O	1:H:304:HIS:CE1	2.73	0.41
1:A:252:ARG:HG3	1:A:252:ARG:NH1	2.35	0.41
1:E:249:HIS:CB	1:F:164:TRP:CH2	2.96	0.41
1:E:39:HIS:CE1	1:F:161:GLU:OE2	2.73	0.41
1:A:306:ILE:C	1:A:306:ILE:HD12	2.40	0.41
1:G:211:ARG:NH1	1:G:211:ARG:HG2	2.34	0.41
1:F:147:ILE:HD12	1:H:261:ARG:CZ	2.51	0.41
1:H:21:ARG:HH11	1:H:21:ARG:HG2	1.85	0.41
1:F:243:ARG:HG2	1:F:243:ARG:HH21	1.85	0.41
1:A:127:ASP:OD1	1:A:170:GLY:HA2	2.20	0.41
1:B:123:PRO:HD3	1:B:284:VAL:O	2.21	0.41
1:E:295:ASP:O	1:E:297:ALA:N	2.54	0.41
1:E:100:ILE:HA	1:E:122:VAL:O	2.19	0.41
1:E:199:ASN:O	1:E:200:ASP:C	2.58	0.41
1:A:153:ILE:HD11	1:A:245:THR:HG21	2.02	0.41
1:E:150:ILE:HD11	1:E:219:ILE:HD11	2.02	0.41
1:F:65:GLY:C	1:F:66:THR:HG22	2.40	0.41
1:B:176:ILE:CG2	1:B:176:ILE:O	2.69	0.41
1:B:82:GLN:NE2	1:B:111:LYS:HG3	2.29	0.41
1:A:191:ILE:N	1:A:191:ILE:HD13	2.35	0.41
1:B:9:SER:HB3	1:B:105:SER:OG	2.20	0.41
1:E:86:ILE:HD11	1:E:115:HIS:HB2	2.02	0.41
1:F:146:VAL:O	1:F:148:ASP:N	2.53	0.41
1:A:163:THR:O	1:A:242:THR:HG23	2.19	0.41
1:H:161:GLU:HA	1:H:215:HIS:HB3	2.03	0.41
1:H:267:LEU:HD22	1:H:284:VAL:HB	2.03	0.41
1:D:211:ARG:NH1	1:D:211:ARG:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:SER:HB2	1:C:265:SER:HA	2.03	0.41
1:G:112:LEU:HA	1:G:112:LEU:HD12	1.96	0.41
1:A:145:THR:CG2	1:B:152:LYS:HZ3	2.33	0.41
1:D:23:VAL:HA	1:D:272:VAL:HG21	2.03	0.41
1:G:146:VAL:O	1:G:150:ILE:HD12	2.21	0.41
1:D:141:THR:HA	1:D:257:THR:CG2	2.50	0.41
1:F:173:ALA:HA	1:F:193:GLU:OE2	2.19	0.41
1:B:7:LEU:CB	1:B:37:VAL:HB	2.51	0.41
1:D:120:VAL:HA	1:D:282:ARG:O	2.19	0.41
1:H:98:VAL:HG23	1:H:275:LEU:HD11	2.02	0.41
1:E:75:GLU:HG2	1:E:75:GLU:H	1.73	0.41
1:E:12:ASP:H	1:F:160:HIS:HE1	1.67	0.41
1:D:141:THR:CG2	1:D:256:PRO:HA	2.51	0.41
1:G:207:ARG:HH11	1:G:207:ARG:HG2	1.86	0.41
1:E:137:ILE:HD13	1:E:264:ALA:HA	2.02	0.41
1:E:56:ASP:C	1:E:58:GLY:H	2.24	0.41
1:C:242:THR:HG22	1:C:243:ARG:N	2.35	0.41
1:E:250:VAL:HG23	1:E:251:GLN:N	2.36	0.41
1:H:150:ILE:HD12	1:H:150:ILE:N	2.34	0.41
1:E:258:ALA:CB	1:G:147:ILE:HD13	2.47	0.41
1:G:150:ILE:HG21	1:G:184:GLY:CA	2.51	0.41
1:B:28:ILE:HD13	1:B:32:VAL:O	2.21	0.41
1:B:100:ILE:HG12	1:B:122:VAL:HB	2.02	0.41
1:E:137:ILE:HD11	1:E:264:ALA:HA	2.02	0.41
1:G:75:GLU:C	1:G:77:LYS:N	2.74	0.41
1:A:11:GLY:HA2	1:B:160:HIS:NE2	2.36	0.41
1:G:159:SER:OG	1:H:66:THR:HG22	2.21	0.41
1:A:288:ASN:HD22	1:A:288:ASN:HA	1.55	0.41
1:D:24:VAL:CG2	1:D:57:VAL:HG11	2.50	0.41
1:D:272:VAL:O	1:D:276:LEU:HG	2.21	0.41
1:H:113:THR:HG21	1:H:281:GLY:HA3	2.03	0.41
1:D:67:ILE:HG13	1:D:68:LEU:N	2.36	0.41
1:G:103:ASP:O	1:G:104:GLY:C	2.58	0.41
1:G:191:ILE:C	1:G:224:VAL:HG21	2.41	0.41
1:B:185:GLY:HA2	1:D:21:ARG:HH21	1.84	0.41
1:C:189:ILE:HD13	1:C:219:ILE:HB	2.01	0.41
1:C:211:ARG:NH1	1:C:211:ARG:HB2	2.36	0.41
1:E:114:GLU:O	1:E:116:GLY:N	2.54	0.41
1:E:171:ARG:HB2	1:E:171:ARG:HH11	1.86	0.41
1:D:198:MET:HE1	1:D:201:VAL:HG11	2.02	0.41
1:B:153:ILE:O	1:B:153:ILE:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LEU:HD22	1:B:196:TYR:CD2	2.55	0.41
1:H:284:VAL:HG23	1:H:285:GLY:H	1.86	0.41
1:G:144:ASN:O	1:G:145:THR:C	2.59	0.41
1:H:41:TYR:O	1:H:44:LEU:HB3	2.21	0.41
1:F:207:ARG:HH11	1:F:207:ARG:HG3	1.86	0.41
1:A:77:LYS:HZ3	1:A:77:LYS:HB2	1.86	0.41
1:H:270:ARG:HD3	1:H:270:ARG:O	2.21	0.41
1:H:126:ILE:O	1:H:176:ILE:HD11	2.20	0.41
1:A:22:SER:HB2	1:A:265:SER:HA	2.03	0.41
1:D:300:LEU:HD23	1:D:300:LEU:HA	1.93	0.41
1:C:252:ARG:NH2	1:D:160:HIS:CE1	2.89	0.40
1:F:26:LYS:HE2	1:F:30:HIS:CD2	2.56	0.40
1:B:102:GLY:O	1:B:105:SER:HB2	2.21	0.40
1:C:276:LEU:C	1:C:278:GLY:N	2.74	0.40
1:H:120:VAL:HG11	1:H:271:ALA:HA	2.03	0.40
1:G:22:SER:O	1:G:26:LYS:HB3	2.21	0.40
1:E:283:CYS:O	1:E:293:ASP:HA	2.22	0.40
1:D:274:LEU:HD22	1:D:279:LYS:HG3	2.04	0.40
1:B:1:MET:HA	1:B:95:GLU:OE1	2.21	0.40
1:F:154:ARG:HA	1:F:217:ILE:HD11	2.02	0.40
1:F:255:SER:OG	1:F:261:ARG:NH2	2.53	0.40
1:C:13:SER:O	1:C:15:GLY:N	2.54	0.40
1:B:180:SER:O	1:B:183:ALA:HB3	2.21	0.40
1:D:18:ALA:O	1:D:21:ARG:HB3	2.20	0.40
1:A:198:MET:HA	1:A:198:MET:CE	2.51	0.40
1:A:198:MET:HG2	1:A:233:GLN:HE22	1.85	0.40
1:D:26:LYS:HE2	1:D:273:GLU:CG	2.51	0.40
1:A:43:GLY:C	1:A:45:ILE:H	2.25	0.40
1:F:103:ASP:N	1:F:130:ILE:CD1	2.84	0.40
1:B:262:VAL:HG23	1:D:183:ALA:HB2	2.04	0.40
1:D:282:ARG:HB3	1:D:294:HIS:O	2.22	0.40
1:G:60:ILE:HA	1:G:63:ARG:HG3	2.04	0.40
1:G:275:LEU:HA	1:G:275:LEU:HD23	1.89	0.40
1:B:21:ARG:O	1:B:22:SER:C	2.59	0.40
1:E:281:GLY:O	1:E:282:ARG:HG2	2.21	0.40
1:D:20:ILE:HD12	1:D:68:LEU:HD12	2.03	0.40
1:C:27:ALA:CB	1:C:34:VAL:CG2	3.00	0.40
1:G:7:LEU:C	1:G:7:LEU:HD22	2.40	0.40
1:C:17:ASN:ND2	1:C:67:ILE:HG13	2.37	0.40
1:F:243:ARG:HG2	1:F:243:ARG:NH2	2.36	0.40
1:F:209:HIS:C	1:F:211:ARG:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ILE:HA	1:F:63:ARG:HG2	2.04	0.40
1:B:189:ILE:O	1:B:311:TYR:HE2	2.04	0.40
1:C:130:ILE:HA	1:C:131:PRO:HD3	1.89	0.40
1:C:1:MET:HA	1:C:1:MET:HE2	2.02	0.40
1:G:111:LYS:HB3	1:G:111:LYS:NZ	2.36	0.40
1:E:169:MET:HB3	1:E:170:GLY:H	1.70	0.40
1:F:256:PRO:HG2	1:F:261:ARG:HE	1.86	0.40
1:B:175:ASP:C	1:B:177:ALA:N	2.75	0.40
1:D:35:TYR:CE1	1:D:51:LYS:HB2	2.56	0.40
1:D:6:VAL:HA	1:D:98:VAL:HB	2.03	0.40
1:E:176:ILE:HG22	1:E:176:ILE:O	2.22	0.40
1:A:23:VAL:HA	1:A:272:VAL:HG21	2.03	0.40
1:A:256:PRO:HG2	1:A:261:ARG:HE	1.85	0.40
1:C:280:GLY:C	1:C:282:ARG:N	2.74	0.40
1:G:106:TYR:O	1:G:107:GLN:C	2.60	0.40
1:G:60:ILE:O	1:G:63:ARG:N	2.46	0.40
1:B:61:ILE:O	1:B:61:ILE:HG12	2.21	0.40
1:F:171:ARG:CG	1:F:172:HIS:N	2.73	0.40
1:A:254:GLY:CA	1:B:152:LYS:HG2	2.50	0.40
1:D:20:ILE:HD13	1:D:100:ILE:HD12	2.03	0.40
1:C:17:ASN:O	1:C:19:ALA:N	2.55	0.40
1:G:204:ARG:C	1:G:206:LYS:N	2.74	0.40
1:A:233:GLN:HE21	1:A:233:GLN:HB3	1.63	0.40
1:C:186:ALA:HB3	1:C:189:ILE:HD11	2.04	0.40
1:B:295:ASP:HB3	1:B:298:GLU:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	317/319 (99%)	275 (87%)	34 (11%)	8 (2%)	7 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	317/319 (99%)	263 (83%)	47 (15%)	7 (2%)	8	45
1	C	317/319 (99%)	254 (80%)	52 (16%)	11 (4%)	4	31
1	D	317/319 (99%)	268 (84%)	37 (12%)	12 (4%)	4	28
1	E	317/319 (99%)	270 (85%)	35 (11%)	12 (4%)	4	28
1	F	317/319 (99%)	281 (89%)	34 (11%)	2 (1%)	30	75
1	G	317/319 (99%)	263 (83%)	46 (14%)	8 (2%)	7	41
1	H	317/319 (99%)	261 (82%)	48 (15%)	8 (2%)	7	41
All	All	2536/2552 (99%)	2135 (84%)	333 (13%)	68 (3%)	6	39

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	GLU
1	C	279	LYS
1	G	211	ARG
1	H	171	ARG
1	H	213	LYS
1	H	284	VAL
1	A	197	ASP
1	B	168	VAL
1	B	171	ARG
1	B	314	SER
1	C	180	SER
1	C	281	GLY
1	C	298	GLU
1	D	137	ILE
1	D	214	LYS
1	E	175	ASP
1	E	193	GLU
1	E	213	LYS
1	F	133	THR
1	G	48	ASN
1	H	40	GLY
1	A	91	LYS
1	A	222	GLU
1	A	235	GLN
1	C	59	ASP
1	C	76	PHE
1	C	211	ARG
1	C	258	ALA

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Mol	Chain	Res	Type
1	D	107	GLN
1	D	171	ARG
1	D	277	GLU
1	E	107	GLN
1	E	251	GLN
1	G	54	VAL
1	G	103	ASP
1	H	175	ASP
1	D	60	ILE
1	D	69	TYR
1	D	90	LYS
1	D	112	LEU
1	D	201	VAL
1	E	115	HIS
1	E	171	ARG
1	E	210	GLU
1	E	293	ASP
1	E	296	ILE
1	F	171	ARG
1	G	59	ASP
1	G	171	ARG
1	A	114	GLU
1	A	178	LEU
1	C	14	PRO
1	C	69	TYR
1	C	79	GLU
1	D	123	PRO
1	E	39	HIS
1	E	60	ILE
1	A	212	GLY
1	B	40	GLY
1	H	224	VAL
1	H	297	ALA
1	D	61	ILE
1	G	57	VAL
1	G	192	PRO
1	H	60	ILE
1	A	296	ILE
1	B	74	PRO
1	B	228	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	247/247 (100%)	221 (90%)	26 (10%)	8	35
1	B	247/247 (100%)	231 (94%)	16 (6%)	21	61
1	C	247/247 (100%)	227 (92%)	20 (8%)	15	51
1	D	247/247 (100%)	229 (93%)	18 (7%)	17	57
1	E	247/247 (100%)	225 (91%)	22 (9%)	12	44
1	F	247/247 (100%)	230 (93%)	17 (7%)	19	59
1	G	247/247 (100%)	237 (96%)	10 (4%)	38	77
1	H	247/247 (100%)	228 (92%)	19 (8%)	16	54
All	All	1976/1976 (100%)	1828 (92%)	148 (8%)	17	55

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	48	ASN
1	A	59	ASP
1	A	66	THR
1	A	110	LYS
1	A	117	PHE
1	A	144	ASN
1	A	148	ASP
1	A	164	TRP
1	A	167	GLU
1	A	171	ARG
1	A	191	ILE
1	A	198	MET
1	A	207	ARG
1	A	229	ASP
1	A	244	VAL
1	A	275	LEU
1	A	277	GLU
1	A	279	LYS

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Mol	Chain	Res	Type
1	A	282	ARG
1	A	284	VAL
1	A	288	ASN
1	A	295	ASP
1	A	298	GLU
1	A	305	THR
1	A	310	MET
1	B	3	ARG
1	B	7	LEU
1	B	34	VAL
1	B	48	ASN
1	B	59	ASP
1	B	66	THR
1	B	103	ASP
1	B	119	CYS
1	B	158	THR
1	B	164	TRP
1	B	191	ILE
1	B	286	ILE
1	B	289	ASN
1	B	305	THR
1	B	309	ARG
1	B	316	GLU
1	C	4	ILE
1	C	7	LEU
1	C	9	SER
1	C	48	ASN
1	C	60	ILE
1	C	66	THR
1	C	80	GLU
1	C	119	CYS
1	C	125	THR
1	C	128	ASN
1	C	159	SER
1	C	164	TRP
1	C	180	SER
1	C	187	GLU
1	C	211	ARG
1	C	260	ASP
1	C	277	GLU
1	C	289	ASN
1	C	293	ASP

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Mol	Chain	Res	Type
1	C	302	ASN
1	D	21	ARG
1	D	48	ASN
1	D	50	LYS
1	D	66	THR
1	D	67	ILE
1	D	72	ARG
1	D	113	THR
1	D	117	PHE
1	D	128	ASN
1	D	156	THR
1	D	164	TRP
1	D	187	GLU
1	D	209	HIS
1	D	215	HIS
1	D	240	PHE
1	D	288	ASN
1	D	293	ASP
1	D	314	SER
1	E	1	MET
1	E	2	LYS
1	E	4	ILE
1	E	7	LEU
1	E	12	ASP
1	E	56	ASP
1	E	66	THR
1	E	72	ARG
1	E	77	LYS
1	E	88	GLN
1	E	117	PHE
1	E	125	THR
1	E	164	TRP
1	E	171	ARG
1	E	180	SER
1	E	182	LEU
1	E	191	ILE
1	E	214	LYS
1	E	287	GLN
1	E	306	ILE
1	E	309	ARG
1	E	314	SER
1	F	7	LEU

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Mol	Chain	Res	Type
1	F	48	ASN
1	F	50	LYS
1	F	66	THR
1	F	86	ILE
1	F	111	LYS
1	F	148	ASP
1	F	182	LEU
1	F	188	THR
1	F	191	ILE
1	F	199	ASN
1	F	207	ARG
1	F	214	LYS
1	F	218	ILE
1	F	302	ASN
1	F	306	ILE
1	F	319	ILE
1	G	2	LYS
1	G	7	LEU
1	G	48	ASN
1	G	113	THR
1	G	133	THR
1	G	143	LEU
1	G	147	ILE
1	G	175	ASP
1	G	289	ASN
1	G	309	ARG
1	H	4	ILE
1	H	7	LEU
1	H	38	TYR
1	H	48	ASN
1	H	80	GLU
1	H	90	LYS
1	H	95	GLU
1	H	110	LYS
1	H	119	CYS
1	H	128	ASN
1	H	165	VAL
1	H	175	ASP
1	H	214	LYS
1	H	228	VAL
1	H	229	ASP
1	H	290	GLN

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Mol	Chain	Res	Type
1	H	305	THR
1	H	309	ARG
1	H	314	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	48	ASN
1	A	82	GLN
1	A	144	ASN
1	A	233	GLN
1	A	288	ASN
1	A	302	ASN
1	B	82	GLN
1	B	160	HIS
1	B	233	GLN
1	B	251	GLN
1	B	289	ASN
1	B	302	ASN
1	C	17	ASN
1	C	39	HIS
1	C	48	ASN
1	C	128	ASN
1	C	160	HIS
1	C	199	ASN
1	C	233	GLN
1	C	235	GLN
1	C	251	GLN
1	C	289	ASN
1	C	302	ASN
1	D	39	HIS
1	D	107	GLN
1	D	128	ASN
1	D	160	HIS
1	D	251	GLN
1	D	288	ASN
1	D	294	HIS
1	D	308	GLN
1	E	17	ASN
1	E	39	HIS
1	E	48	ASN

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Mol	Chain	Res	Type
1	E	62	HIS
1	E	107	GLN
1	E	160	HIS
1	E	288	ASN
1	F	39	HIS
1	F	48	ASN
1	F	62	HIS
1	F	115	HIS
1	F	160	HIS
1	F	199	ASN
1	F	233	GLN
1	F	287	GLN
1	F	288	ASN
1	F	302	ASN
1	F	308	GLN
1	G	39	HIS
1	G	62	HIS
1	G	160	HIS
1	G	287	GLN
1	G	288	ASN
1	G	289	ASN
1	G	290	GLN
1	G	302	ASN
1	H	39	HIS
1	H	48	ASN
1	H	62	HIS
1	H	82	GLN
1	H	128	ASN
1	H	160	HIS
1	H	233	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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	F6P	A	1002	-	15,16,16	1.04	0	16,25,25	0.83	0
2	F6P	B	1001	-	15,16,16	1.06	0	16,25,25	0.89	0
2	F6P	C	1004	-	15,16,16	1.01	0	16,25,25	0.90	0
2	F6P	D	1003	-	15,16,16	1.07	1 (6%)	16,25,25	0.81	0
2	F6P	E	1006	-	15,16,16	1.10	1 (6%)	16,25,25	0.89	0
2	F6P	F	1005	-	15,16,16	1.07	1 (6%)	16,25,25	0.97	0
2	F6P	G	1008	-	15,16,16	1.02	1 (6%)	16,25,25	0.89	0
2	F6P	H	1007	-	15,16,16	0.95	0	16,25,25	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F6P	A	1002	-	-	0/9/28/28	0/1/1/1
2	F6P	B	1001	-	-	0/9/28/28	0/1/1/1
2	F6P	C	1004	-	-	0/9/28/28	0/1/1/1
2	F6P	D	1003	-	-	0/9/28/28	0/1/1/1
2	F6P	E	1006	-	-	0/9/28/28	0/1/1/1
2	F6P	F	1005	-	-	0/9/28/28	0/1/1/1
2	F6P	G	1008	-	-	0/9/28/28	0/1/1/1
2	F6P	H	1007	-	-	0/9/28/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1003	F6P	O5-C2	-2.63	1.39	1.43
2	G	1008	F6P	O5-C2	-2.44	1.39	1.43
2	F	1005	F6P	O5-C2	-2.36	1.39	1.43
2	E	1006	F6P	C1-C2	2.30	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	F6P	1	0
2	C	1004	F6P	1	0
2	F	1005	F6P	2	0
2	G	1008	F6P	1	0
2	H	1007	F6P	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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