



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:24 PM UTC

PDB ID : 1MTO / pdb_00001mto
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

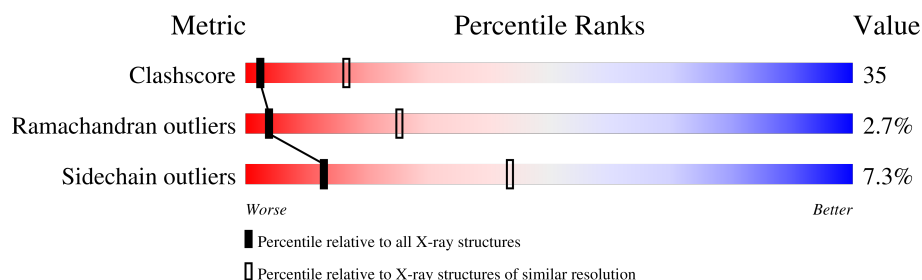
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	319	45% 46% 8%
1	B	319	46% 48% 5%
1	C	319	45% 50% . .
1	D	319	43% 49% 7%
1	E	319	38% 52% 9% .
1	F	319	42% 52% 5%
1	G	319	39% 54% 7%
1	H	319	45% 50% 5%

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:

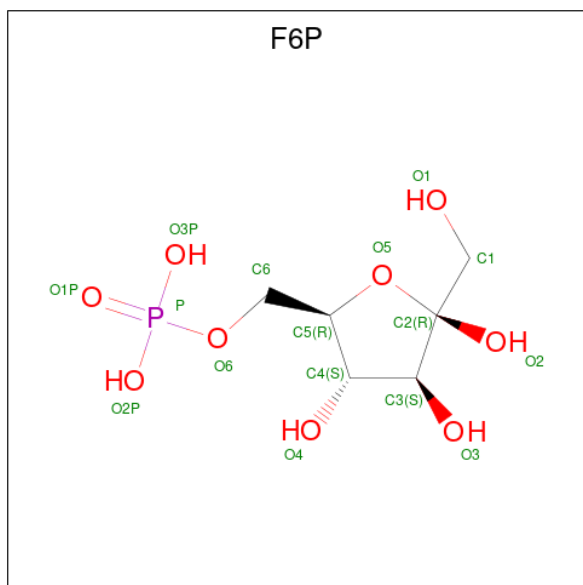
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	TRP	TYR	engineered mutation	UNP P00512
A	179	TYR	TRP	engineered mutation	UNP P00512
B	164	TRP	TYR	engineered mutation	UNP P00512
B	179	TYR	TRP	engineered mutation	UNP P00512
C	164	TRP	TYR	engineered mutation	UNP P00512
C	179	TYR	TRP	engineered mutation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

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

- Molecule 2 is 6-O-phosphono-beta-D-fructofuranose (CCD ID: F6P) (formula: $C_6H_{13}O_9P$).



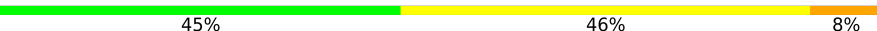
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		
2	E	1	Total	C	O	P	0	0
			16	6	9	1		
2	F	1	Total	C	O	P	0	0
			16	6	9	1		
2	G	1	Total	C	O	P	0	0
			16	6	9	1		
2	H	1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

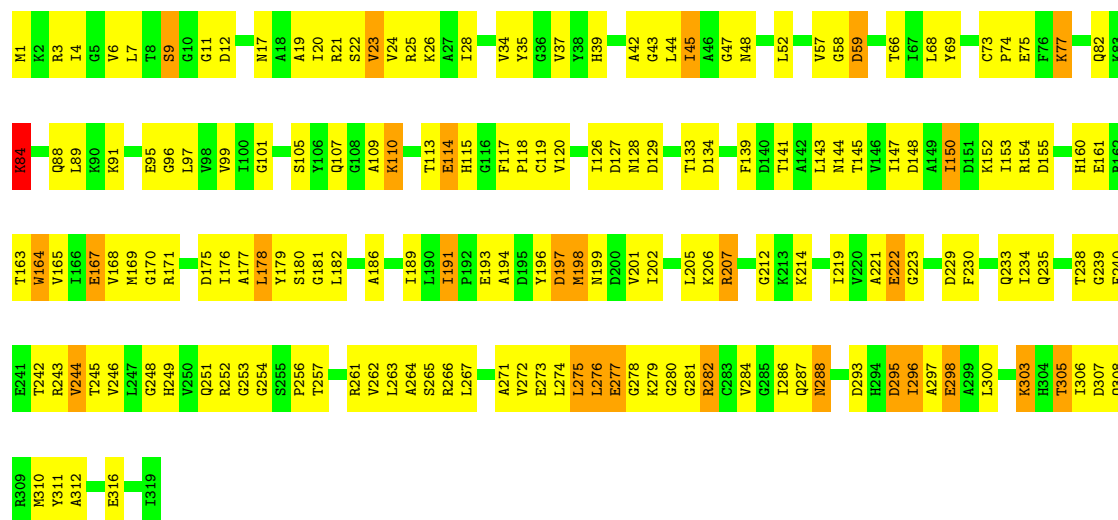
3 Residue-property plots

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

Note EDS was not executed.

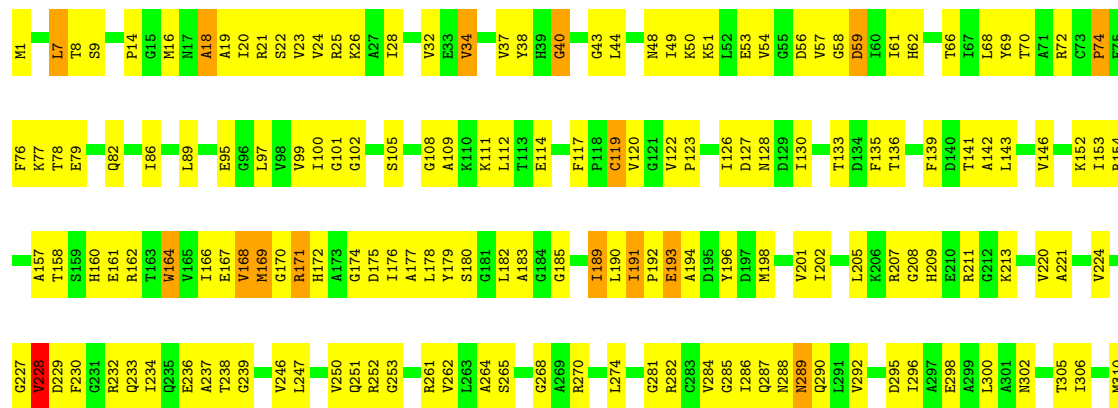
• Molecule 1: 6-phosphofructokinase

Chain A: 

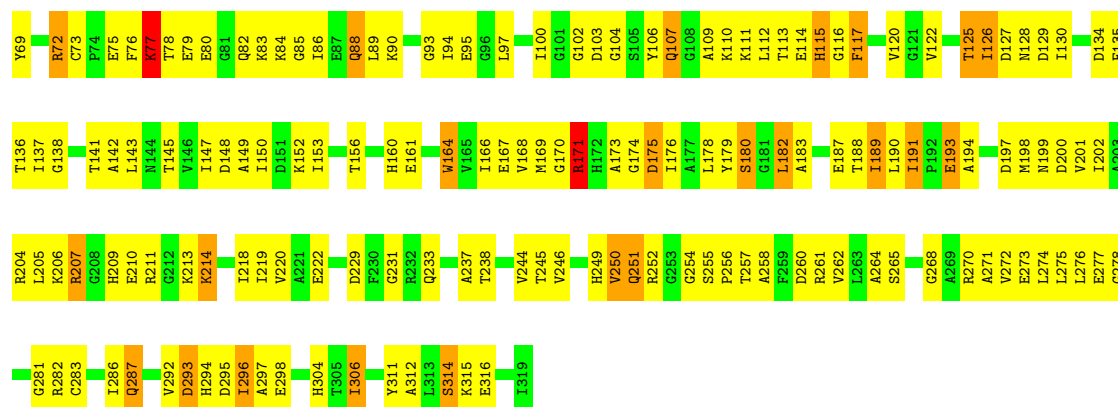


• Molecule 1: 6-phosphofructokinase

Chain B: 

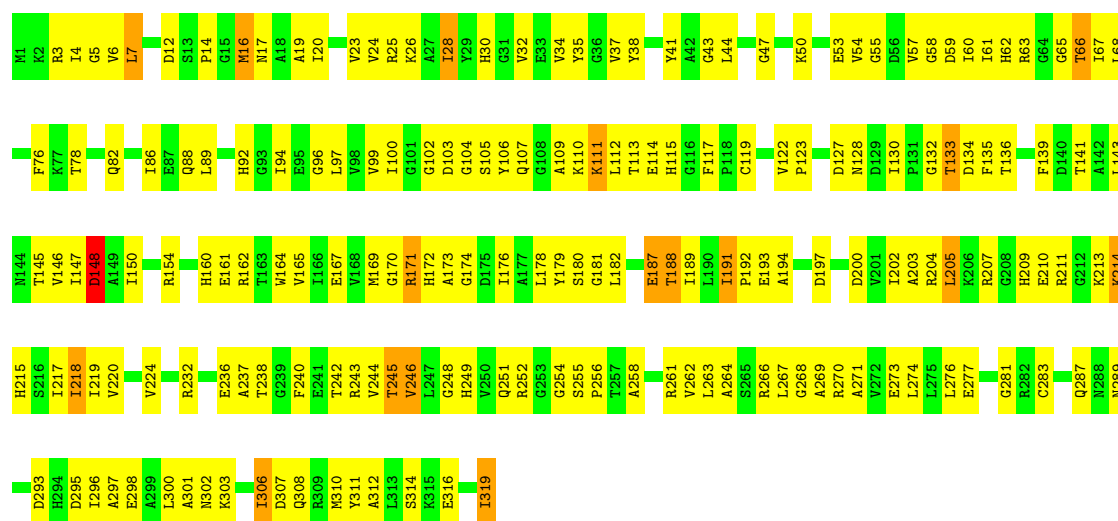






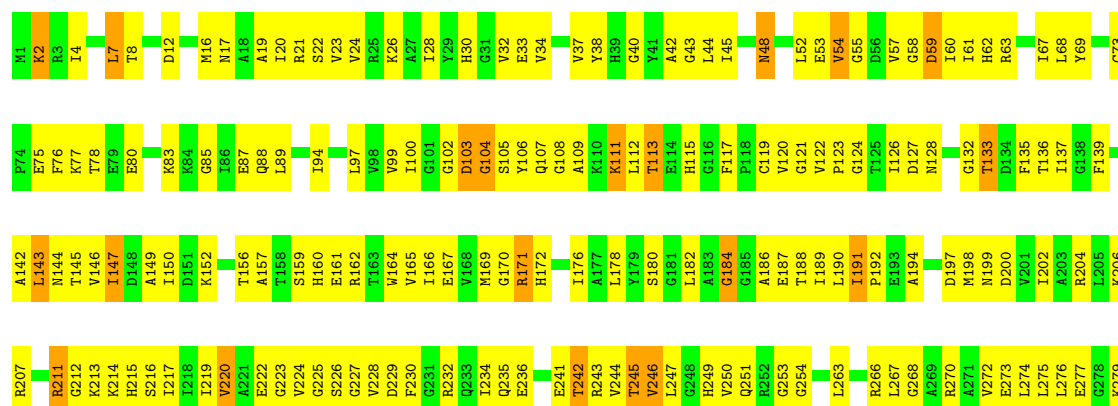
• Molecule 1: 6-phosphofructokinase

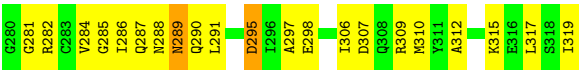
Chain F: 42% 52% 5%



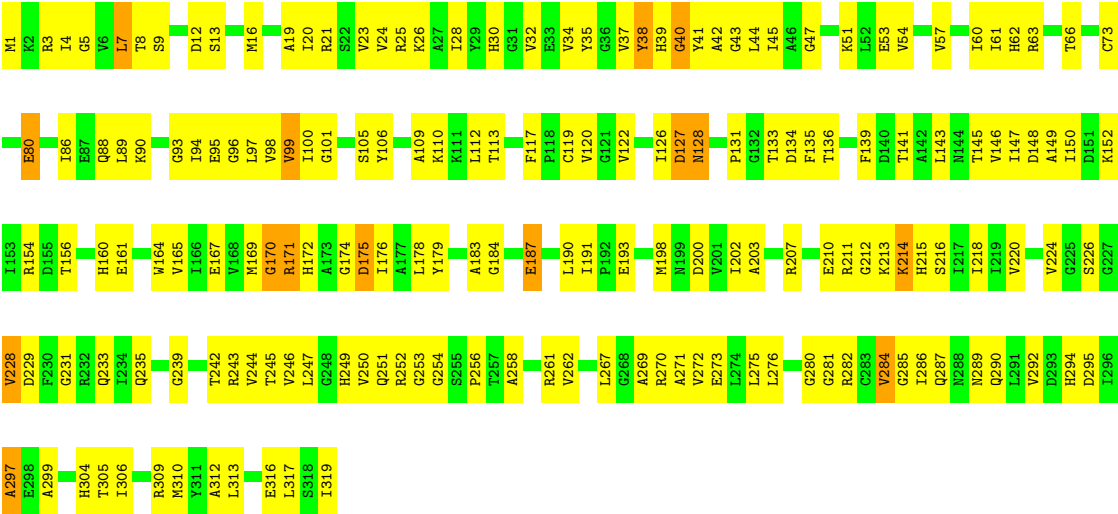
• Molecule 1: 6-phosphofructokinase

Chain G: 39% 54% 7%





● Molecule 1: 6-phosphofructokinase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	0.45	0/2436	0.92	8/3282 (0.2%)
1	B	0.50	0/2436	0.97	7/3282 (0.2%)
1	C	0.46	0/2436	0.92	1/3282 (0.0%)
1	D	0.49	0/2436	0.96	11/3282 (0.3%)
1	E	0.46	0/2436	0.98	11/3282 (0.3%)
1	F	0.48	0/2436	0.94	5/3282 (0.2%)
1	G	0.48	0/2436	0.95	7/3282 (0.2%)
1	H	0.47	0/2436	0.92	4/3282 (0.1%)
All	All	0.47	0/19488	0.95	54/26256 (0.2%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	VAL	N-CA-C	-9.45	100.71	113.00
1	B	130	ILE	N-CA-C	-8.26	101.34	109.02
1	A	84	LYS	N-CA-C	-7.14	104.54	113.18
1	B	18	ALA	N-CA-C	-6.90	103.69	111.07
1	D	221	ALA	N-CA-C	-6.86	100.13	110.28
1	D	250	VAL	N-CA-C	-6.72	103.93	113.07
1	E	126	ILE	N-CA-C	-6.70	106.49	112.12
1	E	277	GLU	N-CA-C	-6.70	105.22	113.19
1	H	148	ASP	N-CA-C	-6.56	103.97	112.23
1	D	20	ILE	N-CA-C	-6.40	104.27	110.42
1	F	220	VAL	N-CA-C	6.35	117.02	107.75
1	E	148	ASP	N-CA-C	-6.29	104.52	111.82
1	G	184	GLY	N-CA-C	-6.21	107.18	115.32
1	E	255	SER	CA-C-N	6.18	126.09	119.85
1	E	255	SER	C-N-CA	6.18	126.09	119.85
1	A	239	GLY	N-CA-C	-5.99	107.81	115.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	170	GLY	N-CA-C	-5.96	106.20	115.67
1	E	254	GLY	N-CA-C	5.94	119.67	112.48
1	G	250	VAL	N-CA-C	-5.94	103.67	111.09
1	E	104	GLY	N-CA-C	-5.91	105.64	112.50
1	G	104	GLY	N-CA-C	-5.83	105.58	112.64
1	B	311	TYR	N-CA-C	-5.82	104.94	111.28
1	E	77	LYS	N-CA-C	-5.80	106.04	113.01
1	A	276	LEU	N-CA-C	-5.80	106.13	113.43
1	B	56	ASP	N-CA-C	5.80	117.60	111.28
1	D	163	THR	N-CA-C	-5.71	101.19	110.20
1	G	220	VAL	N-CA-C	5.61	115.67	107.37
1	H	239	GLY	N-CA-C	-5.60	107.92	115.36
1	D	271	ALA	N-CA-C	-5.58	105.12	111.14
1	D	109	ALA	N-CA-C	-5.57	105.11	111.07
1	D	253	GLY	N-CA-C	5.55	120.53	112.60
1	A	150	ILE	N-CA-C	-5.53	104.98	110.62
1	A	45	ILE	N-CA-C	-5.48	106.85	111.56
1	F	210	GLU	N-CA-C	-5.43	106.72	113.19
1	A	23	VAL	N-CA-C	-5.38	105.84	110.74
1	B	164	TRP	N-CA-C	5.38	118.33	109.72
1	F	16	MET	N-CA-C	-5.35	105.35	111.07
1	A	101	GLY	N-CA-C	5.34	118.06	110.74
1	D	128	ASN	N-CA-C	-5.32	105.43	112.24
1	H	127	ASP	N-CA-C	5.26	117.69	111.33
1	D	34	VAL	N-CA-C	5.24	115.50	108.17
1	E	164	TRP	N-CA-C	5.23	117.34	109.23
1	G	42	ALA	N-CA-C	-5.19	105.27	111.03
1	E	250	VAL	N-CA-C	-5.16	105.51	110.72
1	B	58	GLY	N-CA-C	-5.15	105.16	112.37
1	E	95	GLU	N-CA-C	5.15	118.34	111.75
1	B	49	ILE	N-CA-C	5.12	115.34	107.77
1	A	164	TRP	N-CA-C	5.09	117.87	109.72
1	F	249	HIS	N-CA-C	5.08	119.24	113.19
1	G	295	ASP	N-CA-C	-5.08	102.12	109.59
1	D	130	ILE	CA-C-N	5.04	125.48	120.14
1	D	130	ILE	C-N-CA	5.04	125.48	120.14
1	F	148	ASP	N-CA-C	-5.02	106.32	112.90
1	G	76	PHE	N-CA-C	-5.01	107.23	113.19

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	2400	0	2417	181	0
1	B	2400	0	2417	164	0
1	C	2400	0	2417	162	0
1	D	2400	0	2417	185	0
1	E	2400	0	2417	191	0
1	F	2400	0	2417	191	0
1	G	2400	0	2417	191	0
1	H	2400	0	2417	181	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	4	0
All	All	19328	0	19424	1361	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 35.

All (1361) 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: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:G:190:LEU:HD12	1:G:220:VAL:HG22	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:266:ARG:HD2	1:C:310:MET:HE3	1.55	0.88
1:G:171:ARG:HG3	1:G:172:HIS:H	1.38	0.88
1:B:208:GLY:HA3	1:B:213:LYS:HZ3	1.39	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
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:F:143:LEU:HD21	1:F:179:TYR:HB3	1.58	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:D:75:GLU:CD	1:D:75:GLU:H	1.85	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:E:78:THR:HG22	1:E:80:GLU:H	1.45	0.80
1:H:171:ARG:HG3	1:H:172:HIS:N	1.96	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: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:D:171:ARG:HG3	1:D:172:HIS:H	1.49	0.77
1:E:204:ARG:HH22	1:E:315:LYS:HD2	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:VAL:HG22	1:D:49:ILE:HD12	1.66	0.77
1:B:198:MET:HG2	1:B:233:GLN:NE2	2.00	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:E:72:ARG:H	1:E:72:ARG:HH11	1.30	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
1:H:16:MET:HE2	1:H:100:ILE:HG22	1.67	0.76
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:C:7:LEU:HD12	1:C:97:LEU:HD11	1.69	0.75
1:E:141:THR:HA	1:E:257:THR:HG23	1.69	0.75
1:D:38:TYR:O	1:D:43:GLY:HA3	1.87	0.74
1:D:144:ASN:HA	1:D:147:ILE:HG12	1.69	0.74
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: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:D:143:LEU:HD11	1:D:179:TYR:HB2	1.69	0.74
1:H:7:LEU:HD12	1:H:97:LEU:HD11	1.69	0.74
1:C:4:ILE:HD11	1:C:34:VAL:HG22	1.67	0.74
1:E:191:ILE:H	1:E:191:ILE:HD13	1.53	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:7:LEU:HB3	1:G:37:VAL:HB	1.70	0.74
1:G:166:ILE:HD12	1:G:219:ILE:HD11	1.68	0.74
1:H:198:MET:O	1:H:202:ILE:HG12	1.87	0.74
1:C:58:GLY:O	1:C:59:ASP:HB3	1.86	0.74
1:G:123:PRO:O	1:G:137:ILE:HG12	1.87	0.74
1:A:74:PRO:HD2	1:A:75:GLU:OE1	1.87	0.74
1:G:235:GLN:HB2	1:G:242:THR:HB	1.68	0.74
1:E:24:VAL:HB	1:E:57:VAL:HG11	1.71	0.73
1:D:276:LEU:C	1:D:278:GLY:H	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:20:ILE:HD13	1:C:68:LEU:HG	1.72	0.72
1:G:191:ILE:HD12	1:G:194:ALA:H	1.55	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:A:113:THR:HG21	1:A:281:GLY:HA2	1.71	0.72
1:F:134:ASP:OD2	1:F:287:GLN:HA	1.90	0.72
1:A:152:LYS:O	1:A:155:ASP:HB2	1.90	0.72
1:G:178:LEU:HD22	1:G:306:ILE:HD13	1.72	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: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: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:A:282:ARG:HH12	1:A:293:ASP:CB	1.94	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: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:143:LEU:HD11	1:F:179:TYR:HB2	1.73	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:F:47:GLY:HA3	1:F:88:GLN:NE2	2.07	0.69
1:G:7:LEU:HD23	1:G:40:GLY:HA2	1.73	0.69
1:B:208:GLY:CA	1:B:213:LYS:HZ3	2.06	0.69
1:G:83:LYS:O	1:G:87:GLU:HG2	1.93	0.69
1:C:160:HIS:O	1:C:162:ARG:HG3	1.94	0.68
1:G:161:GLU:HA	1:G:215:HIS:HB3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:THR:HG22	1:B:100:ILE:HB	1.76	0.68
1:B:128:ASN:HB2	1:B:139:PHE:CD2	2.29	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: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
1:A:262:VAL:O	1:A:266:ARG:HG3	1.94	0.67
1:E:190:LEU:HD12	1:E:220:VAL:HG22	1.77	0.67
1:G:7:LEU:HD11	1:G:99:VAL:HG22	1.75	0.67
1:G:225:GLY:HA3	1:G:230:PHE:CE1	2.29	0.67
1:B:281:GLY:O	1:B:296:ILE:HG13	1.94	0.67
1:E:214:LYS:H	1:E:214:LYS:HD3	1.59	0.67
1:A:191:ILE:HD11	1:A:194:ALA:HB3	1.76	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: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: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:E:207:ARG:HH11	1:E:207:ARG:HB3	1.60	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:G:268:GLY:O	1:G:272:VAL:HG23	1.95	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:E:143:LEU:HD21	1:E:179:TYR:HB3	1.77	0.66
1:G:249:HIS:HB2	1:H:164:TRP:CH2	2.29	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:O	1:F:277:GLU:HG2	1.95	0.66
1:A:113:THR:C	1:A:115:HIS:H	2.02	0.66
1:D:288:ASN:N	1:D:288:ASN:HD22	1.92	0.66
1:E:114:GLU:C	1:E:116:GLY:H	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:249:HIS:C	1:H:251:GLN:H	2.02	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
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:F:316:GLU:O	1:F:319:ILE:HD11	1.97	0.64
1:G:169:MET:HG3	1:G:251:GLN:NE2	2.13	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:78:THR:HG22	1:G:80:GLU:H	1.62	0.63
1:G:147:ILE:HA	1:G:150:ILE:HD13	1.80	0.63
1:A:198:MET:HE3	1:A:198:MET:HA	1.80	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: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:A:77:LYS:HB2	1:A:77:LYS:NZ	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HD23	1:C:262:VAL:HG13	1.81	0.62
1:E:189:ILE:HD12	1:E:189:ILE:N	2.13	0.62
1:D:21:ARG:NH1	1:D:25:ARG:NH1	2.47	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:G:126:ILE:O	1:G:176:ILE:HD11	1.99	0.62
1:B:128:ASN:OD1	1:B:135:PHE:HA	1.99	0.62
1:E:17:ASN:ND2	1:E:67:ILE:HG12	2.13	0.62
1:D:123:PRO:CB	1:D:136:THR:HG22	2.23	0.62
1:H:171:ARG:CG	1:H:172:HIS:H	2.04	0.62
1:A:134:ASP:OD2	1:A:287:GLN:HA	2.00	0.62
1:A:282:ARG:HB3	1:A:282:ARG:HH11	1.63	0.62
1:D:169:MET:HE3	1:D:248:GLY:O	1.99	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:C:198:MET:O	1:C:202:ILE:HG12	1.99	0.61
1:E:207:ARG:HB3	1:E:207:ARG:NH1	2.15	0.61
1:A:118:PRO:HB3	1:A:280:GLY:HA3	1.81	0.61
1:E:84:LYS:O	1:E:88:GLN:HB2	2.00	0.61
1:F:112:LEU:O	1:F:117:PHE:HB2	1.99	0.61
1:E:63:ARG:HH12	1:H:62:HIS:HE1	1.46	0.61
1:F:302:ASN:ND2	1:F:303:LYS:H	1.99	0.61
1:G:99:VAL:CG1	1:G:105:SER:HB3	2.31	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:A:198:MET:HE3	1:A:201:VAL:HB	1.83	0.61
1:D:37:VAL:HG22	1:D:49:ILE:CD1	2.31	0.61
1:F:164:TRP:HZ3	1:F:245:THR:HG1	1.48	0.61
1:H:19:ALA:O	1:H:23:VAL:HG23	2.01	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:B:287:GLN:OE1	1:B:292:VAL:HG21	2.00	0.61
1:E:229:ASP:O	1:E:233:GLN:HG3	2.01	0.61
1:F:143:LEU:HD11	1:F:179:TYR:CB	2.31	0.61
1:G:211:ARG:HH11	1:G:211:ARG:HG2	1.65	0.61
1:D:1:MET:HE1	1:D:96:GLY:HA3	1.82	0.61
1:E:45:ILE:HD11	1:E:76:PHE:HD1	1.66	0.61
1:H:211:ARG:NH1	1:H:319:ILE:HG22	2.16	0.61
1:A:139:PHE:CE2	1:A:176:ILE:HD13	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:SER:O	1:D:16:MET:HG3	2.00	0.60
1:D:61:ILE:HG12	1:D:61:ILE:O	2.00	0.60
1:G:52:LEU:HD11	1:G:68:LEU:HD21	1.83	0.60
1:C:152:LYS:HD3	1:D:254:GLY:HA3	1.83	0.60
1:E:207:ARG:HH11	1:E:207:ARG:CB	2.14	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:21:ARG:HE	1:D:61:ILE:HB	1.67	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:113:THR:HG21	1:D:281:GLY:HA2	1.83	0.60
1:E:276:LEU:C	1:E:278:GLY:H	2.08	0.60
1:G:211:ARG:NH2	1:G:213:LYS:HE2	2.15	0.60
1:H:47:GLY:HA3	1:H:88:GLN:OE1	2.01	0.60
1:C:276:LEU:C	1:C:278:GLY:H	2.09	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:2:LYS:NZ	1:G:2:LYS:HB3	2.16	0.60
1:G:124:GLY:HA2	1:G:137:ILE:HB	1.83	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:B:120:VAL:HA	1:B:282:ARG:O	2.01	0.60
1:E:102:GLY:HA2	1:E:130:ILE:HD11	1.82	0.60
1:H:145:THR:HG21	1:H:250:VAL:O	2.02	0.60
1:F:113:THR:C	1:F:115:HIS:H	2.09	0.60
1:H:128:ASN:HD21	1:H:135:PHE:HA	1.66	0.60
1:A:110:LYS:HE3	1:A:114:GLU:CD	2.26	0.59
1:F:146:VAL:C	1:F:148:ASP:H	2.07	0.59
1:C:21:ARG:HB2	1:C:60:ILE:HD11	1.83	0.59
1:D:318:SER:C	1:D:319:ILE:HG13	2.25	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:C:77:LYS:HB2	1:C:77:LYS:NZ	2.18	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:A:118:PRO:HA	1:A:280:GLY:O	2.01	0.59
1:E:137:ILE:CD1	1:E:264:ALA:HA	2.32	0.59
1:E:156:THR:HA	1:F:12:ASP:OD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:TYR:O	1:F:109:ALA:HB3	2.03	0.59
1:G:73:CYS:C	1:G:75:GLU:H	2.10	0.59
1:G:128:ASN:OD1	1:G:135:PHE:HA	2.03	0.59
1:A:198:MET:HG2	1:A:233:GLN:NE2	2.17	0.59
1:C:9:SER:OG	1:C:105:SER:HB3	2.03	0.59
1:D:89:LEU:HD13	1:D:117:PHE:CE2	2.38	0.59
1:E:171:ARG:N	1:E:222:GLU:OE2	2.34	0.59
1:A:39:HIS:O	1:A:42:ALA:HB3	2.03	0.59
1:D:7:LEU:HD12	1:D:7:LEU:C	2.27	0.59
1:B:7:LEU:HD11	1:B:99:VAL:HG22	1.83	0.59
1:G:202:ILE:O	1:G:206:LYS:HG3	2.03	0.59
1:E:80:GLU:O	1:E:84:LYS:HG3	2.02	0.58
1:A:191:ILE:HD13	1:A:191:ILE:H	1.67	0.58
1:D:142:ALA:O	1:D:146:VAL:HG23	2.03	0.58
1:F:164:TRP:HZ3	1:F:245:THR:HB	1.67	0.58
1:C:252:ARG:HD3	2:C:1004:F6P:O2	2.02	0.58
1:D:114:GLU:C	1:D:116:GLY:H	2.11	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
1:H:309:ARG:NH2	1:H:316:GLU:OE1	2.35	0.58
1:D:19:ALA:O	1:D:23:VAL:HG23	2.02	0.58
1:F:7:LEU:CD1	1:F:99:VAL:HG22	2.33	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:H:80:GLU:H	1:H:80:GLU:CD	2.11	0.58
1:F:38:TYR:O	1:F:43:GLY:HA3	2.04	0.58
1:F:266:ARG:HD2	1:H:310:MET:HE3	1.84	0.58
1:B:176:ILE:O	1:B:180:SER:CB	2.51	0.58
1:B:182:LEU:HD22	1:B:310:MET:HE3	1.86	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:H:113:THR:HA	1:H:117:PHE:O	2.04	0.58
1:B:232:ARG:O	1:B:236:GLU:HG3	2.03	0.57
1:C:59:ASP:CG	1:C:59:ASP:O	2.46	0.57
1:D:312:ALA:O	1:D:316:GLU:HG3	2.04	0.57
1:E:112:LEU:O	1:E:117:PHE:HB2	2.04	0.57
1:G:146:VAL:HG12	1:G:150:ILE:CD1	2.34	0.57
1:A:3:ARG:HD3	1:A:35:TYR:CE2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:O	1:A:4:ILE:HG13	2.04	0.57
1:B:168:VAL:HG23	1:B:169:MET:N	2.19	0.57
1:E:270:ARG:CZ	1:E:274:LEU:HD11	2.34	0.57
1:F:28:ILE:HD12	1:F:54:VAL:HB	1.85	0.57
1:B:213:LYS:O	1:B:213:LYS:HG3	2.03	0.57
1:F:202:ILE:HD13	1:F:237:ALA:HB1	1.86	0.57
1:F:202:ILE:HD13	1:F:237:ALA:CB	2.34	0.57
1:F:242:THR:O	1:F:243:ARG:NH2	2.36	0.57
1:G:266:ARG:HB3	1:G:291:LEU:HD11	1.86	0.57
1:H:249:HIS:C	1:H:251:GLN:N	2.59	0.57
1:A:45:ILE:HD12	1:A:73:CYS:SG	2.44	0.57
1:E:38:TYR:O	1:E:39:HIS:HB2	2.05	0.57
1:E:125:THR:OG1	1:E:126:ILE:N	2.35	0.57
1:C:24:VAL:O	1:C:28:ILE:HG12	2.05	0.57
1:C:306:ILE:C	1:C:306:ILE:HD12	2.30	0.57
1:E:161:GLU:OE1	1:E:214:LYS:HG3	2.04	0.57
1:A:303:LYS:HB2	1:A:303:LYS:NZ	2.20	0.57
1:B:142:ALA:O	1:B:146:VAL:HG23	2.05	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:C:296:ILE:O	1:C:296:ILE:HG22	2.04	0.57
1:E:29:TYR:HB2	1:G:319:ILE:HD11	1.85	0.57
1:F:146:VAL:C	1:F:148:ASP:N	2.63	0.57
1:E:24:VAL:O	1:E:28:ILE:HG12	2.04	0.57
1:E:191:ILE:HD13	1:E:191:ILE:N	2.20	0.57
1:F:302:ASN:HD22	1:F:303:LYS:N	2.03	0.57
1:G:198:MET:HA	1:G:198:MET:HE2	1.86	0.57
1:C:25:ARG:HE	1:C:54:VAL:CG2	2.17	0.57
1:D:168:VAL:HA	1:D:251:GLN:HE22	1.70	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: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:F:295:ASP:OD2	1:F:297:ALA:HB3	2.05	0.56
1:E:120:VAL:HG13	1:E:282:ARG:O	2.05	0.56
1:B:8:THR:HA	1:B:100:ILE:O	2.05	0.56
1:D:113:THR:HG21	1:D:281:GLY:CA	2.35	0.56
1:D:197:ASP:C	1:D:199:ASN:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:TYR:O	1:E:314:SER:HB3	2.04	0.56
1:F:205:LEU:O	1:F:209:HIS:HB2	2.05	0.56
1:G:188:THR:C	1:G:189:ILE:HD12	2.30	0.56
1:G:211:ARG:NH2	1:G:213:LYS:HG2	2.20	0.56
1:H:21:ARG:NH1	1:H:61:ILE:HD12	2.18	0.56
1:D:21:ARG:HE	1:D:61:ILE:HD12	1.71	0.56
1:F:23:VAL:HG22	1:F:268:GLY:O	2.05	0.56
1:A:306:ILE:HD12	1:A:306:ILE:O	2.06	0.56
1:C:181:GLY:HA3	1:C:189:ILE:HD11	1.88	0.56
1:H:150:ILE:HD12	1:H:150:ILE:H	1.70	0.56
1:E:15:GLY:O	1:E:18:ALA:HB3	2.05	0.56
1:E:153:ILE:HG13	1:E:166:ILE:HD11	1.86	0.56
1:G:78:THR:HG22	1:G:80:GLU:HG2	1.87	0.56
1:H:312:ALA:O	1:H:316:GLU:HG3	2.05	0.56
1:A:242:THR:HG22	1:A:243:ARG:N	2.20	0.56
1:C:160:HIS:O	1:C:161:GLU:C	2.48	0.56
1:G:190:LEU:HD12	1:G:220:VAL:CG2	2.29	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:45:ILE:C	1:H:47:GLY:H	2.13	0.56
1:H:174:GLY:HA3	1:H:191:ILE:HB	1.87	0.56
1:C:14:PRO:HD3	1:C:252:ARG:O	2.07	0.55
1:F:57:VAL:HG23	1:F:57:VAL:O	2.07	0.55
1:G:198:MET:O	1:G:202:ILE:HG12	2.05	0.55
1:H:42:ALA:HB2	1:H:73:CYS:HB2	1.88	0.55
1:H:169:MET:HG3	1:H:251:GLN:CD	2.30	0.55
1:D:144:ASN:HA	1:D:147:ILE:CG1	2.35	0.55
1:E:59:ASP:O	1:E:59:ASP:CG	2.48	0.55
1:E:62:HIS:HE1	1:H:63:ARG:HH12	1.53	0.55
1:G:32:VAL:HG21	1:G:276:LEU:HD21	1.87	0.55
1:C:145:THR:HG21	1:C:250:VAL:O	2.07	0.55
1:D:68:LEU:O	1:D:69:TYR:CB	2.54	0.55
1:D:128:ASN:HA	1:D:136:THR:OG1	2.06	0.55
1:E:205:LEU:HD21	1:E:218:ILE:HD11	1.88	0.55
1:H:131:PRO:HB2	1:H:299:ALA:O	2.07	0.55
1:B:7:LEU:C	1:B:7:LEU:HD22	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:O	1:C:147:ILE:HG23	2.06	0.55
1:C:310:MET:O	1:C:313:LEU:HB3	2.07	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:G:169:MET:HG3	1:G:251:GLN:CD	2.31	0.55
1:H:38:TYR:N	1:H:38:TYR:HD2	2.05	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:41:TYR:C	1:F:43:GLY:N	2.63	0.55
1:A:196:TYR:O	1:A:197:ASP:HB2	2.06	0.55
1:E:189:ILE:HD13	1:E:314:SER:OG	2.06	0.55
1:F:161:GLU:CG	1:F:214:LYS:HG3	2.33	0.55
1:G:12:ASP:OD1	1:H:156:THR:HA	2.06	0.55
1:H:86:ILE:O	1:H:89:LEU:HB2	2.07	0.55
1:H:120:VAL:HA	1:H:282:ARG:O	2.06	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: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:B:72:ARG:HG2	1:B:72:ARG:HH11	1.72	0.55
1:D:1:MET:HA	1:D:95:GLU:OE1	2.07	0.55
1:E:63:ARG:HH12	1:H:62:HIS:CE1	2.24	0.55
1:E:141:THR:CA	1:E:257:THR:HG23	2.36	0.55
1:B:123:PRO:HB2	1:B:136:THR:HG22	1.89	0.54
1:B:143:LEU:HD11	1:B:180:SER:N	2.21	0.54
1:B:169:MET:HE3	1:B:251:GLN:HB2	1.89	0.54
1:B:193:GLU:CD	1:B:193:GLU:H	2.15	0.54
1:D:3:ARG:HD2	1:D:93:GLY:O	2.08	0.54
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:B:178:LEU:HD22	1:B:306:ILE:HD12	1.88	0.54
1:E:12:ASP:HB2	1:E:66:THR:HG22	1.88	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:B:24:VAL:CG2	1:B:57:VAL:HG11	2.36	0.54
1:E:68:LEU:O	1:E:69:TYR:HB2	2.06	0.54
1:F:89:LEU:HD13	1:F:117:PHE:CE2	2.43	0.54
1:G:119:CYS:O	1:G:281:GLY:N	2.34	0.54
1:G:122:VAL:HG13	1:G:267:LEU:HB3	1.89	0.54
1:G:212:GLY:O	1:G:214:LYS:HE3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:258:ALA:O	1:H:262:VAL:HG23	2.07	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:266:ARG:HE	1:D:291:LEU:HD11	1.72	0.54
1:C:2:LYS:C	1:C:32:VAL:HG13	2.33	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:B:153:ILE:HG21	1:B:166:ILE:HD11	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:82:GLN:HE22	1:B:111:LYS:CG	2.19	0.54
1:E:82:GLN:OE1	1:E:111:LYS:HB3	2.07	0.54
1:H:35:TYR:HA	1:H:51:LYS:HA	1.89	0.54
1:H:272:VAL:O	1:H:276:LEU:HG	2.08	0.54
1:H:24:VAL:HG22	1:H:34:VAL:HG11	1.90	0.54
1:A:179:TYR:CE1	1:A:310:MET:HE1	2.43	0.54
1:A:249:HIS:CD2	1:B:164:TRP:HH2	2.26	0.54
1:G:211:ARG:HH22	1:G:213:LYS:HG2	1.73	0.54
1:A:59:ASP:OD1	1:A:59:ASP:O	2.27	0.53
1:A:254:GLY:HA2	1:B:152:LYS:HG2	1.90	0.53
1:G:45:ILE:HG22	1:G:85:GLY:N	2.24	0.53
1:G:295:ASP:OD2	1:G:297:ALA:HB3	2.08	0.53
1:A:221:ALA:O	1:A:223:GLY:N	2.41	0.53
1:C:318:SER:O	1:C:319:ILE:C	2.51	0.53
1:E:107:GLN:HE21	1:E:107:GLN:HA	1.73	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:B:289:ASN:O	1:B:290:GLN:HG3	2.09	0.53
1:E:128:ASN:HA	1:E:136:THR:HG23	1.89	0.53
1:F:171:ARG:CG	1:F:172:HIS:H	2.05	0.53
1:F:191:ILE:HG12	1:F:193:GLU:N	2.23	0.53
1:G:176:ILE:O	1:G:180:SER:HB2	2.09	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:D:171:ARG:HG3	1:D:172:HIS:N	2.20	0.53
1:G:171:ARG:CG	1:G:172:HIS:H	2.14	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:G:24:VAL:O	1:G:28:ILE:HG13	2.09	0.53
1:B:20:ILE:O	1:B:24:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASP:OD1	1:B:170:GLY:HA2	2.09	0.53
1:C:27:ALA:HB3	1:C:34:VAL:HG21	1.91	0.53
1:C:168:VAL:O	1:C:222:GLU:HB3	2.09	0.53
1:E:152:LYS:HZ2	1:F:145:THR:HG23	1.72	0.53
1:E:281:GLY:C	1:E:282:ARG:HG2	2.33	0.53
1:H:32:VAL:HG21	1:H:276:LEU:HD21	1.91	0.53
1:H:169:MET:HG3	1:H:251:GLN:HE22	1.71	0.53
1:A:37:VAL:HG21	1:A:97:LEU:HD11	1.91	0.53
1:A:186:ALA:HB2	1:A:219:ILE:HD13	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:B:22:SER:OG	1:B:265:SER:O	2.24	0.53
1:C:288:ASN:O	1:C:290:GLN:HG2	2.08	0.53
1:E:49:ILE:O	1:E:50:LYS:HD3	2.09	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:A:277:GLU:HB3	1:A:279:LYS:CE	2.38	0.52
1:E:191:ILE:HD11	1:E:194:ALA:HB3	1.90	0.52
1:H:89:LEU:HD13	1:H:117:PHE:CE2	2.44	0.52
1:B:24:VAL:HA	1:B:34:VAL:HG21	1.92	0.52
1:B:171:ARG:CG	1:B:172:HIS:H	2.09	0.52
1:A:107:GLN:C	1:A:109:ALA:H	2.16	0.52
1:B:174:GLY:HA3	1:B:191:ILE:HB	1.90	0.52
1:C:272:VAL:O	1:C:276:LEU:HG	2.10	0.52
1:D:129:ASP:OD2	1:D:171:ARG:HD2	2.09	0.52
1:F:306:ILE:HD11	1:F:308:GLN:NE2	2.24	0.52
1:G:146:VAL:HG13	1:G:247:LEU:CD1	2.39	0.52
1:G:267:LEU:HD22	1:G:284:VAL:HG23	1.92	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:H:212:GLY:O	1:H:214:LYS:N	2.41	0.52
1:A:282:ARG:HH11	1:A:282:ARG:CB	2.22	0.52
1:C:191:ILE:C	1:C:224:VAL:HG11	2.35	0.52
1:D:215:HIS:O	1:D:215:HIS:ND1	2.42	0.52
1:E:276:LEU:C	1:E:278:GLY:N	2.66	0.52
1:H:146:VAL:O	1:H:149:ALA:HB3	2.09	0.52
1:H:280:GLY:O	1:H:282:ARG:HG2	2.08	0.52
1:B:192:PRO:O	1:B:194:ALA:N	2.43	0.52
1:C:17:ASN:O	1:C:18:ALA:C	2.53	0.52
1:D:169:MET:HE3	1:D:248:GLY:C	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:GLN:HA	1:G:88:GLN:OE1	2.09	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:A:165:VAL:CB	1:A:244:VAL:HG12	2.34	0.52
1:A:205:LEU:CD1	1:A:234:ILE:HD12	2.38	0.52
1:D:145:THR:HG21	1:D:250:VAL:O	2.10	0.52
1:D:215:HIS:ND1	1:D:215:HIS:C	2.67	0.52
1:F:20:ILE:O	1:F:24:VAL:HG23	2.09	0.52
1:F:179:TYR:CZ	1:F:310:MET:HE1	2.45	0.52
1:H:191:ILE:HD12	1:H:193:GLU:HB2	1.92	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:59:ASP:O	1:A:59:ASP:CG	2.52	0.52
1:A:169:MET:HG3	1:A:251:GLN:NE2	2.25	0.52
1:C:306:ILE:HD12	1:C:307:ASP:C	2.33	0.52
1:D:162:ARG:HD3	1:D:241:GLU:HG3	1.91	0.52
1:F:58:GLY:O	1:F:59:ASP:HB3	2.10	0.52
1:H:267:LEU:HD22	1:H:285:GLY:H	1.75	0.52
1:A:150:ILE:HD12	1:A:219:ILE:HD11	1.92	0.52
1:D:276:LEU:C	1:D:278:GLY:N	2.64	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:H:51:LYS:HE2	1:H:53:GLU:CD	2.35	0.52
1:A:9:SER:HB3	1:A:105:SER:OG	2.09	0.51
1:A:17:ASN:HA	1:A:20:ILE:HD12	1.92	0.51
1:E:295:ASP:O	1:E:296:ILE:C	2.53	0.51
1:G:123:PRO:HD3	1:G:284:VAL:O	2.09	0.51
1:G:254:GLY:N	1:H:152:LYS:HD3	2.25	0.51
1:B:59:ASP:CG	1:B:59:ASP:O	2.52	0.51
1:B:175:ASP:OD2	1:B:306:ILE:HG22	2.10	0.51
1:G:68:LEU:O	1:G:69:TYR:HB2	2.10	0.51
1:A:274:LEU:HD21	1:A:293:ASP:OD2	2.11	0.51
1:C:17:ASN:HD21	1:C:67:ILE:HG13	1.76	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:F:17:ASN:OD1	1:F:67:ILE:HG23	2.11	0.51
1:H:211:ARG:HH12	1:H:319:ILE:CG2	2.21	0.51
1:A:274:LEU:C	1:A:276:LEU:H	2.17	0.51
1:D:198:MET:HE1	1:D:201:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:GLU:O	1:G:55:GLY:N	2.43	0.51
1:G:157:ALA:O	1:G:161:GLU:N	2.43	0.51
1:G:164:TRP:HH2	1:H:249:HIS:CG	2.27	0.51
1:H:38:TYR:O	1:H:43:GLY:HA3	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:A:147:ILE:C	1:A:147:ILE:HD12	2.36	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:B:153:ILE:O	1:B:157:ALA:HB2	2.09	0.51
1:B:160:HIS:HB2	1:B:162:ARG:HG3	1.93	0.51
1:B:230:PHE:O	1:B:234:ILE:HD13	2.09	0.51
1:D:107:GLN:O	1:D:110:LYS:N	2.43	0.51
1:E:7:LEU:HD13	1:E:7:LEU:N	2.25	0.51
1:G:164:TRP:HH2	1:H:249:HIS:ND1	2.09	0.51
1:H:228:VAL:N	1:H:244:VAL:HG11	2.26	0.51
1:B:198:MET:O	1:B:202:ILE:HG13	2.10	0.51
1:D:286:ILE:HG23	1:D:286:ILE:O	2.11	0.51
1:E:114:GLU:C	1:E:116:GLY:N	2.67	0.51
1:F:24:VAL:HA	1:F:34:VAL:HG21	1.92	0.51
1:A:177:ALA:O	1:A:178:LEU:C	2.53	0.51
1:A:221:ALA:C	1:A:223:GLY:H	2.18	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:A:221:ALA:C	1:A:223:GLY:N	2.69	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:C:280:GLY:C	1:C:282:ARG:H	2.19	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:G:58:GLY:O	1:G:59:ASP:HB3	2.11	0.51
1:H:25:ARG:HE	1:H:54:VAL:HG22	1.75	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:A:243:ARG:HG2	1:A:243:ARG:HH21	1.76	0.50
1:F:181:GLY:HA3	1:F:189:ILE:HG12	1.91	0.50
1:A:305:THR:HG22	1:A:306:ILE:H	1.74	0.50
1:B:211:ARG:NH1	1:B:213:LYS:HD3	2.26	0.50
1:C:268:GLY:O	1:C:271:ALA:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ASP:C	1:D:199:ASN:N	2.69	0.50
1:D:211:ARG:HH11	1:D:211:ARG:HB2	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:F:76:PHE:HZ	1:F:112:LEU:HG	1.76	0.50
1:G:226:SER:O	1:G:229:ASP:N	2.45	0.50
1:A:84:LYS:O	1:A:88:GLN:HG2	2.10	0.50
1:C:106:TYR:HD2	1:C:296:ILE:HG23	1.76	0.50
1:C:168:VAL:HG21	1:C:177:ALA:HA	1.93	0.50
1:C:249:HIS:C	1:C:251:GLN:N	2.64	0.50
1:E:168:VAL:O	1:E:222:GLU:HB3	2.10	0.50
1:F:102:GLY:HA2	1:F:130:ILE:HD11	1.93	0.50
1:F:209:HIS:C	1:F:211:ARG:H	2.18	0.50
1:G:75:GLU:C	1:G:77:LYS:H	2.19	0.50
1:G:270:ARG:HD2	1:G:273:GLU:OE2	2.10	0.50
1:G:307:ASP:OD2	1:G:307:ASP:C	2.54	0.50
1:H:133:THR:HB	1:H:285:GLY:HA3	1.93	0.50
1:B:74:PRO:O	1:B:77:LYS:HB2	2.11	0.50
1:D:26:LYS:HE2	1:D:273:GLU:HG2	1.93	0.50
1:E:89:LEU:HD13	1:E:117:PHE:CE2	2.45	0.50
1:G:102:GLY:O	1:G:105:SER:N	2.42	0.50
1:G:113:THR:C	1:G:115:HIS:H	2.18	0.50
1:B:38:TYR:O	1:B:43:GLY:HA3	2.11	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:A:238:THR:C	1:A:240:PHE:H	2.18	0.50
1:C:26:LYS:O	1:C:29:TYR:HB3	2.12	0.50
1:D:75:GLU:O	1:D:81:GLY:HA3	2.12	0.50
1:D:113:THR:HA	1:D:117:PHE:O	2.11	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:295:ASP:C	1:C:297:ALA:H	2.19	0.50
1:E:258:ALA:HB2	1:G:147:ILE:HG21	1.93	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:G:128:ASN:HA	1:G:136:THR:OG1	2.11	0.50
1:A:113:THR:C	1:A:115:HIS:N	2.69	0.50
1:A:163:THR:HG21	1:A:234:ILE:HG21	1.94	0.50
1:F:97:LEU:HD23	1:F:119:CYS:SG	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:HIS:C	1:E:211:ARG:H	2.20	0.49
1:F:147:ILE:HA	1:F:150:ILE:CG1	2.42	0.49
1:A:141:THR:HA	1:A:257:THR:CG2	2.42	0.49
1:A:171:ARG:HH11	1:A:171:ARG:HB2	1.77	0.49
1:A:282:ARG:HH11	1:A:282:ARG:CG	2.25	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: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:D:7:LEU:HD11	1:D:99:VAL:HG13	1.93	0.49
1:E:143:LEU:HD11	1:E:179:TYR:HB2	1.94	0.49
1:F:7:LEU:HD13	1:F:7:LEU:O	2.12	0.49
1:F:35:TYR:CB	1:F:94:ILE:HD11	2.42	0.49
1:F:203:ALA:O	1:F:207:ARG:HB2	2.11	0.49
1:G:7:LEU:CD1	1:G:99:VAL:HG22	2.42	0.49
1:G:226:SER:O	1:G:227:GLY:C	2.55	0.49
1:H:24:VAL:HA	1:H:34:VAL:HG21	1.94	0.49
1:B:261:ARG:HD2	1:D:183:ALA:O	2.12	0.49
1:C:4:ILE:CD1	1:C:34:VAL:HG22	2.41	0.49
1:D:306:ILE:C	1:D:306:ILE:HD12	2.37	0.49
1:E:120:VAL:HA	1:E:282:ARG:O	2.13	0.49
1:A:202:ILE:HD11	1:A:234:ILE:HD13	1.94	0.49
1:B:18:ALA:HB3	1:B:264:ALA:CB	2.42	0.49
1:F:258:ALA:O	1:F:262:VAL:HG23	2.13	0.49
1:G:286:ILE:HG23	1:G:286:ILE:O	2.12	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:E:106:TYR:O	1:E:109:ALA:HB3	2.13	0.49
1:F:107:GLN:C	1:F:109:ALA:N	2.70	0.49
1:G:202:ILE:CD1	1:G:234:ILE:HG12	2.42	0.49
1:A:75:GLU:H	1:A:75:GLU:CD	2.21	0.49
1:B:208:GLY:HA3	1:B:213:LYS:NZ	2.20	0.49
1:E:134:ASP:OD2	1:E:287:GLN:HA	2.12	0.49
1:A:167:GLU:HB2	1:A:246:VAL:HG22	1.95	0.49
1:C:21:ARG:NH2	1:C:25:ARG:HH12	2.10	0.49
1:C:51:LYS:HE2	1:C:53:GLU:OE1	2.13	0.49
1:C:114:GLU:C	1:C:116:GLY:H	2.21	0.49
1:C:249:HIS:C	1:C:251:GLN:H	2.20	0.49
1:E:2:LYS:HB2	1:E:2:LYS:NZ	2.27	0.49
1:G:167:GLU:CB	1:G:246:VAL:HG13	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:127:ASP:OD1	1:G:170:GLY:HA2	2.12	0.49
1:H:294:HIS:HB2	1:H:299:ALA:HB2	1.94	0.49
1:D:144:ASN:OD1	1:D:147:ILE:HD11	2.13	0.49
1:D:198:MET:HE3	1:D:201:VAL:HB	1.95	0.49
1:A:12:ASP:H	1:B:160:HIS:CE1	2.31	0.48
1:B:68:LEU:O	1:B:69:TYR:HB2	2.13	0.48
1:B:189:ILE:HD12	1:B:189:ILE:N	2.28	0.48
1:C:7:LEU:C	1:C:7:LEU:HD22	2.38	0.48
1:A:178:LEU:HA	1:A:189:ILE:HG21	1.95	0.48
1:B:319:ILE:HD12	1:D:29:TYR:HD2	1.78	0.48
1:G:263:LEU:HG	1:G:267:LEU:HD12	1.93	0.48
1:H:3:ARG:NH1	1:H:35:TYR:CE2	2.81	0.48
1:H:139:PHE:O	1:H:143:LEU:HB2	2.12	0.48
1:H:169:MET:CE	2:H:1007:F6P:H61	2.43	0.48
1:A:295:ASP:HB2	1:A:298:GLU:HG2	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:H:7:LEU:C	1:H:7:LEU:HD22	2.39	0.48
1:H:28:ILE:C	1:H:30:HIS:N	2.71	0.48
1:C:17:ASN:C	1:C:19:ALA:N	2.70	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:G:152:LYS:HA	1:H:254:GLY:H	1.79	0.48
1:A:229:ASP:O	1:A:233:GLN:HG3	2.14	0.48
1:C:249:HIS:HD2	1:C:252:ARG:NH1	2.11	0.48
1:D:24:VAL:CB	1:D:57:VAL:HG11	2.43	0.48
1:E:58:GLY:O	1:E:59:ASP:HB3	2.12	0.48
1:E:77:LYS:HB3	1:E:77:LYS:HZ3	1.75	0.48
1:E:206:LYS:HG3	1:E:238:THR:HG22	1.95	0.48
1:G:21:ARG:HH11	1:G:21:ARG:HG2	1.78	0.48
1:A:279:LYS:H	1:A:279:LYS:HD3	1.79	0.48
1:D:111:LYS:O	1:D:112:LEU:C	2.56	0.48
1:D:187:GLU:HG2	1:D:217:ILE:H	1.78	0.48
1:D:212:GLY:C	1:D:214:LYS:H	2.22	0.48
1:E:25:ARG:HB3	1:G:317:LEU:HD22	1.94	0.48
1:F:261:ARG:HB2	1:H:183:ALA:HB1	1.94	0.48
1:H:93:GLY:O	1:H:94:ILE:C	2.57	0.48
1:B:99:VAL:CG1	1:B:105:SER:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:HE2	1:B:111:LYS:HA	1.95	0.48
1:D:218:ILE:N	1:D:218:ILE:HD12	2.28	0.48
1:D:224:VAL:HG12	1:D:224:VAL:O	2.14	0.48
1:D:280:GLY:O	1:D:282:ARG:HG2	2.14	0.48
1:E:188:THR:HG22	1:E:218:ILE:HG23	1.95	0.48
1:E:231:GLY:HA3	1:E:244:VAL:CG2	2.44	0.48
1:E:250:VAL:C	1:E:252:ARG:H	2.22	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:E:27:ALA:HB3	1:E:34:VAL:CG2	2.44	0.48
1:A:296:ILE:O	1:A:300:LEU:HB2	2.14	0.48
1:B:25:ARG:HD3	1:B:54:VAL:HG23	1.96	0.48
1:H:8:THR:HG23	1:H:20:ILE:HD11	1.95	0.48
1:A:198:MET:HE3	1:A:201:VAL:CB	2.43	0.48
1:D:24:VAL:HB	1:D:57:VAL:HG11	1.96	0.48
1:F:107:GLN:C	1:F:109:ALA:H	2.22	0.48
1:F:161:GLU:HA	1:F:215:HIS:HB3	1.95	0.48
1:G:166:ILE:HD12	1:G:219:ILE:CD1	2.41	0.47
1:A:263:LEU:HD12	1:A:267:LEU:HG	1.96	0.47
1:A:286:ILE:HG23	1:A:286:ILE:O	2.14	0.47
1:C:217:ILE:HG22	1:C:219:ILE:CD1	2.44	0.47
1:D:121:GLY:O	1:D:284:VAL:HG22	2.14	0.47
1:D:288:ASN:N	1:D:288:ASN:ND2	2.57	0.47
1:E:160:HIS:CE1	1:F:12:ASP:H	2.32	0.47
1:F:191:ILE:HD13	1:F:191:ILE:H	1.79	0.47
1:G:160:HIS:HE1	1:H:12:ASP:OD1	1.97	0.47
1:A:261:ARG:NH1	1:C:147:ILE:HD12	2.29	0.47
1:B:153:ILE:HD13	1:B:166:ILE:CD1	2.44	0.47
1:B:211:ARG:CZ	1:B:213:LYS:HD3	2.43	0.47
1:C:13:SER:O	1:C:14:PRO:C	2.57	0.47
1:C:113:THR:HA	1:C:117:PHE:O	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:F:128:ASN:OD1	1:F:135:PHE:HA	2.13	0.47
1:H:160:HIS:O	1:H:161:GLU:HB2	2.15	0.47
1:A:43:GLY:C	1:A:45:ILE:N	2.69	0.47
1:C:27:ALA:HB3	1:C:34:VAL:CG2	2.44	0.47
1:F:193:GLU:HG2	1:F:306:ILE:HG23	1.96	0.47
1:G:254:GLY:HA3	1:H:152:LYS:HD3	1.95	0.47
1:G:288:ASN:O	1:G:290:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:HG23	1:A:133:THR:O	2.15	0.47
1:B:70:THR:HG23	1:B:70:THR:O	2.15	0.47
1:D:23:VAL:CG1	1:D:98:VAL:HG21	2.44	0.47
1:E:292:VAL:O	1:E:293:ASP:HB3	2.14	0.47
1:H:25:ARG:HE	1:H:54:VAL:CG2	2.27	0.47
1:A:96:GLY:HA3	1:A:275:LEU:HD13	1.96	0.47
1:D:242:THR:HG22	1:D:243:ARG:N	2.28	0.47
1:E:72:ARG:HD2	1:E:72:ARG:N	2.25	0.47
1:F:143:LEU:HD21	1:F:179:TYR:CB	2.38	0.47
1:G:53:GLU:C	1:G:55:GLY:N	2.73	0.47
1:H:94:ILE:HG22	1:H:96:GLY:O	2.13	0.47
1:A:22:SER:HA	1:C:317:LEU:HD22	1.96	0.47
1:A:300:LEU:HD23	1:A:300:LEU:O	2.15	0.47
1:B:7:LEU:HB3	1:B:37:VAL:HB	1.96	0.47
1:B:44:LEU:HD11	1:B:89:LEU:HG	1.95	0.47
1:C:146:VAL:HG12	1:C:150:ILE:HD13	1.97	0.47
1:D:21:ARG:NE	1:D:61:ILE:HB	2.27	0.47
1:D:24:VAL:HG21	1:D:57:VAL:HG11	1.96	0.47
1:D:200:ASP:O	1:D:201:VAL:C	2.58	0.47
1:E:160:HIS:CE1	1:F:252:ARG:NH2	2.83	0.47
1:E:202:ILE:HG23	1:E:238:THR:HG23	1.96	0.47
1:F:164:TRP:CZ3	1:F:245:THR:OG1	2.62	0.47
1:F:281:GLY:O	1:F:296:ILE:HG13	2.14	0.47
1:F:295:ASP:O	1:F:296:ILE:C	2.57	0.47
1:H:218:ILE:HD12	1:H:218:ILE:N	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:F:197:ASP:HB3	1:F:200:ASP:HB2	1.96	0.47
1:G:12:ASP:OD2	1:H:160:HIS:HE1	1.98	0.47
1:A:143:LEU:HD11	1:A:179:TYR:CB	2.44	0.47
1:A:274:LEU:C	1:A:276:LEU:N	2.73	0.47
1:B:168:VAL:HG22	1:B:221:ALA:HA	1.96	0.47
1:B:176:ILE:O	1:B:176:ILE:HG22	2.15	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:A:120:VAL:HG11	1:A:271:ALA:HB1	1.97	0.47
1:A:168:VAL:O	1:A:222:GLU:HB3	2.14	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:F:62:HIS:HA	1:F:261:ARG:NH2	2.30	0.47
1:G:16:MET:O	1:G:20:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:VAL:HG12	1:G:105:SER:HB3	1.96	0.47
1:H:175:ASP:O	1:H:176:ILE:C	2.58	0.47
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:C:302:ASN:HD22	1:C:302:ASN:HA	1.53	0.46
1:E:4:ILE:HG21	1:E:275:LEU:HD23	1.97	0.46
1:E:24:VAL:HA	1:E:34:VAL:HG21	1.97	0.46
1:E:147:ILE:HD12	1:E:147:ILE:C	2.40	0.46
1:G:242:THR:CG2	1:G:243:ARG:N	2.78	0.46
1:H:8:THR:CG2	1:H:20:ILE:HD11	2.45	0.46
1:B:227:GLY:O	1:B:228:VAL:C	2.59	0.46
1:C:82:GLN:O	1:C:86:ILE:HD13	2.15	0.46
1:C:207:ARG:NH1	1:C:211:ARG:HH21	2.13	0.46
1:D:112:LEU:O	1:D:117:PHE:HB2	2.15	0.46
1:F:41:TYR:C	1:F:43:GLY:H	2.23	0.46
1:H:198:MET:HG2	1:H:233:GLN:NE2	2.30	0.46
1:A:12:ASP:OD1	1:B:160:HIS:HE1	1.98	0.46
1:B:208:GLY:CA	1:B:213:LYS:NZ	2.78	0.46
1:B:238:THR:OG1	1:B:239:GLY:N	2.47	0.46
1:C:169:MET:HE3	1:C:248:GLY:O	2.15	0.46
1:D:49:ILE:O	1:D:50:LYS:NZ	2.48	0.46
1:D:143:LEU:HD11	1:D:179:TYR:CB	2.42	0.46
1:D:165:VAL:HB	1:D:244:VAL:HG22	1.98	0.46
1:E:17:ASN:OD1	1:E:65:GLY:O	2.33	0.46
1:E:32:VAL:HG12	1:E:33:GLU:N	2.30	0.46
1:H:26:LYS:HE3	1:H:30:HIS:NE2	2.30	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:H:256:PRO:HG2	1:H:261:ARG:HG2	1.97	0.46
1:A:193:GLU:HG2	1:A:306:ILE:HG13	1.97	0.46
1:B:170:GLY:O	1:B:171:ARG:C	2.58	0.46
1:C:3:ARG:HD3	1:C:35:TYR:CZ	2.50	0.46
1:C:252:ARG:HG3	1:C:252:ARG:HH11	1.80	0.46
1:C:38:TYR:O	1:C:43:GLY:HA3	2.15	0.46
1:D:306:ILE:HD11	1:D:308:GLN:NE2	2.30	0.46
1:E:199:ASN:O	1:E:200:ASP:C	2.58	0.46
1:F:6:VAL:HG13	1:F:6:VAL:O	2.15	0.46
1:G:165:VAL:HB	1:G:244:VAL:HG22	1.96	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:A:306:ILE:HD12	1:A:306:ILE:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:CE1	1:C:68:LEU:HA	2.50	0.46
1:C:186:ALA:CB	1:C:219:ILE:HD13	2.45	0.46
1:D:48:ASN:O	1:D:49:ILE:HD13	2.16	0.46
1:D:182:LEU:HD23	1:D:310:MET:HE3	1.97	0.46
1:F:65:GLY:C	1:F:66:THR:HG22	2.40	0.46
1:G:58:GLY:O	1:G:59:ASP:CB	2.63	0.46
1:G:75:GLU:C	1:G:77:LYS:N	2.74	0.46
1:H:164:TRP:HZ3	1:H:245:THR:CB	2.29	0.46
1:H:169:MET:HE2	2:H:1007:F6P:H4	1.97	0.46
1:B:22:SER:CB	1:B:265:SER:HA	2.46	0.46
1:B:185:GLY:HA2	1:D:21:ARG:NH2	2.31	0.46
1:C:35:TYR:CD1	1:C:94:ILE:HD11	2.51	0.46
1:D:1:MET:HE2	1:D:4:ILE:HG22	1.98	0.46
1:F:61:ILE:HG23	1:F:62:HIS:N	2.29	0.46
1:F:76:PHE:HZ	1:F:112:LEU:CG	2.29	0.46
1:F:127:ASP:OD2	2:F:1005:F6P:H3	2.15	0.46
1:B:111:LYS:O	1:B:114:GLU:N	2.49	0.46
1:C:1:MET:HE2	1:C:1:MET:HA	1.97	0.46
1:C:197:ASP:OD1	1:C:199:ASN:ND2	2.48	0.46
1:D:162:ARG:HG3	1:D:162:ARG:NH1	2.31	0.46
1:E:56:ASP:C	1:E:58:GLY:H	2.24	0.46
1:F:88:GLN:OE1	1:F:88:GLN:HA	2.16	0.46
1:F:103:ASP:OD1	1:F:104:GLY:N	2.49	0.46
1:G:207:ARG:NH1	1:G:207:ARG:HG2	2.30	0.46
1:G:312:ALA:O	1:G:315:LYS:HB2	2.15	0.46
1:H:178:LEU:HD22	1:H:306:ILE:HD13	1.97	0.46
1:H:231:GLY:HA3	1:H:244:VAL:HG22	1.98	0.46
1:F:82:GLN:OE1	1:F:111:LYS:HB3	2.16	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:B:14:PRO:CB	1:B:141:THR:HG21	2.45	0.45
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.82	0.45
1:C:276:LEU:C	1:C:278:GLY:N	2.74	0.45
1:C:295:ASP:HB3	1:C:298:GLU:HG2	1.99	0.45
1:D:141:THR:HG21	1:D:256:PRO:HA	1.97	0.45
1:D:144:ASN:HD22	1:D:257:THR:HG21	1.81	0.45
1:E:44:LEU:O	1:E:47:GLY:N	2.48	0.45
1:E:77:LYS:HB3	1:E:77:LYS:HZ2	1.79	0.45
1:G:144:ASN:O	1:G:145:THR:C	2.59	0.45
1:G:191:ILE:C	1:G:224:VAL:HG21	2.41	0.45
1:H:128:ASN:HB2	1:H:139:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ALA:O	1:B:315:LYS:HB2	2.17	0.45
1:E:44:LEU:HD11	1:E:89:LEU:CD2	2.43	0.45
1:G:103:ASP:O	1:G:104:GLY:C	2.58	0.45
1:A:196:TYR:H	1:A:196:TYR:HD1	1.63	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:C:197:ASP:O	1:C:200:ASP:N	2.48	0.45
1:D:76:PHE:CZ	1:D:112:LEU:HD21	2.50	0.45
1:E:201:VAL:HG12	1:E:205:LEU:HD12	1.98	0.45
1:F:41:TYR:O	1:F:44:LEU:N	2.49	0.45
1:G:7:LEU:C	1:G:7:LEU:HD22	2.40	0.45
1:G:187:GLU:HG2	1:G:216:SER:OG	2.17	0.45
1:G:309:ARG:O	1:G:312:ALA:HB3	2.17	0.45
1:H:45:ILE:O	1:H:88:GLN:HG3	2.17	0.45
1:H:310:MET:O	1:H:313:LEU:HB3	2.16	0.45
1:A:43:GLY:C	1:A:45:ILE:H	2.25	0.45
1:C:297:ALA:O	1:C:299:ALA:N	2.50	0.45
1:D:189:ILE:HG13	1:D:219:ILE:HB	1.99	0.45
1:G:152:LYS:HG2	1:H:254:GLY:CA	2.47	0.45
1:F:191:ILE:HD11	1:F:194:ALA:HB3	1.97	0.45
1:G:99:VAL:O	1:G:121:GLY:HA2	2.16	0.45
1:G:113:THR:HG21	1:G:281:GLY:HA3	1.99	0.45
1:G:274:LEU:HD22	1:G:279:LYS:HD3	1.99	0.45
1:H:62:HIS:HB3	1:H:261:ARG:NH1	2.31	0.45
1:H:226:SER:OG	1:H:228:VAL:HG23	2.16	0.45
1:A:303:LYS:NZ	1:A:303:LYS:CB	2.79	0.45
1:B:21:ARG:O	1:B:22:SER:C	2.59	0.45
1:C:187:GLU:CG	1:C:216:SER:HB3	2.40	0.45
1:C:280:GLY:C	1:C:282:ARG:N	2.74	0.45
1:F:78:THR:O	1:F:82:GLN:HG3	2.16	0.45
1:G:106:TYR:O	1:G:107:GLN:C	2.60	0.45
1:H:21:ARG:NH1	1:H:21:ARG:HG2	2.30	0.45
1:H:89:LEU:HD13	1:H:117:PHE:CZ	2.51	0.45
1:H:207:ARG:O	1:H:210:GLU:HG2	2.16	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:F:123:PRO:HB2	1:F:136:THR:HG22	1.99	0.45
1:F:209:HIS:C	1:F:211:ARG:N	2.75	0.45
1:B:18:ALA:HB3	1:B:264:ALA:HB3	1.98	0.45
1:B:89:LEU:HD13	1:B:117:PHE:CZ	2.52	0.45
1:C:139:PHE:CZ	1:C:143:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLU:HG3	1:C:216:SER:CB	2.40	0.45
1:D:125:THR:HG21	1:D:130:ILE:HG12	1.98	0.45
1:F:187:GLU:OE1	1:F:213:LYS:HD3	2.16	0.45
1:F:238:THR:HB	1:F:240:PHE:CE1	2.51	0.45
1:F:289:ASN:ND2	1:H:134:ASP:OD2	2.50	0.45
1:G:113:THR:C	1:G:115:HIS:N	2.75	0.45
1:G:133:THR:HB	1:G:285:GLY:HA3	1.99	0.45
1:B:310:MET:HE2	1:B:310:MET:HB3	1.81	0.45
1:E:39:HIS:HB2	1:E:43:GLY:HA3	1.98	0.45
1:F:4:ILE:HG22	1:F:96:GLY:HA3	1.99	0.45
1:G:26:LYS:HE2	1:G:273:GLU:HG3	1.99	0.45
1:G:176:ILE:O	1:G:180:SER:CB	2.65	0.45
1:H:169:MET:HE2	2:H:1007:F6P:H61	1.99	0.45
1:C:15:GLY:HA3	1:C:137:ILE:CG2	2.47	0.45
1:C:25:ARG:NE	1:C:54:VAL:HG23	2.32	0.45
1:C:270:ARG:HG3	1:C:284:VAL:HG11	1.99	0.45
1:G:99:VAL:HG11	1:G:105:SER:HB3	1.99	0.45
1:G:204:ARG:C	1:G:206:LYS:N	2.74	0.45
1:B:198:MET:HG2	1:B:233:GLN:HE21	1.79	0.44
1:C:14:PRO:HB2	1:C:141:THR:HG21	1.96	0.44
1:C:42:ALA:HB2	1:C:73:CYS:HB2	1.98	0.44
1:C:86:ILE:HD12	1:C:86:ILE:N	2.32	0.44
1:E:28:ILE:HG13	1:E:54:VAL:HG22	1.98	0.44
1:E:143:LEU:HA	1:E:143:LEU:HD12	1.81	0.44
1:F:38:TYR:HE2	1:F:50:LYS:HB2	1.82	0.44
1:F:99:VAL:CG1	1:F:105:SER:HB3	2.47	0.44
1:G:73:CYS:C	1:G:75:GLU:N	2.75	0.44
1:G:234:ILE:C	1:G:236:GLU:N	2.71	0.44
1:H:24:VAL:O	1:H:25:ARG:C	2.60	0.44
1:H:252:ARG:HD3	2:H:1007:F6P:O2	2.17	0.44
1:C:258:ALA:O	1:C:259:PHE:C	2.60	0.44
1:E:45:ILE:N	1:E:45:ILE:HD13	2.32	0.44
1:F:114:GLU:O	1:F:115:HIS:CD2	2.70	0.44
1:G:2:LYS:HB3	1:G:2:LYS:HZ3	1.80	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:A:68:LEU:O	1:A:69:TYR:HB2	2.15	0.44
1:C:144:ASN:O	1:C:145:THR:C	2.60	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:G:182:LEU:HD23	1:G:310:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:HIS:O	1:H:40:GLY:C	2.59	0.44
1:A:89:LEU:HD13	1:A:117:PHE:CZ	2.51	0.44
1:A:154:ARG:HG2	1:A:154:ARG:O	2.17	0.44
1:B:250:VAL:C	1:B:252:ARG:H	2.25	0.44
1:C:235:GLN:HG3	1:C:240:PHE:O	2.17	0.44
1:C:286:ILE:O	1:C:286:ILE:HG23	2.17	0.44
1:E:256:PRO:HG2	1:E:261:ARG:HG2	1.98	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:H:112:LEU:O	1:H:117:PHE:CB	2.65	0.44
1:H:231:GLY:HA3	1:H:244:VAL:CG2	2.47	0.44
1:H:295:ASP:OD2	1:H:297:ALA:HB3	2.18	0.44
1:C:95:GLU:O	1:C:118:PRO:HD2	2.18	0.44
1:C:146:VAL:HG12	1:C:150:ILE:CD1	2.47	0.44
1:E:175:ASP:OD2	1:E:304:HIS:NE2	2.51	0.44
1:F:111:LYS:N	1:F:111:LYS:HE3	2.33	0.44
1:G:106:TYR:O	1:G:109:ALA:HB3	2.17	0.44
1:H:28:ILE:C	1:H:30:HIS:H	2.26	0.44
1:H:44:LEU:HD11	1:H:89:LEU:CD2	2.47	0.44
1:A:82:GLN:NE2	1:A:115:HIS:CE1	2.85	0.44
1:C:77:LYS:HB2	1:C:77:LYS:HZ2	1.80	0.44
1:G:21:ARG:HG2	1:G:21:ARG:NH1	2.33	0.44
1:H:281:GLY:C	1:H:282:ARG:HG2	2.43	0.44
1:H:287:GLN:HB2	1:H:292:VAL:HG21	1.98	0.44
1:C:25:ARG:HD3	1:C:54:VAL:HG23	1.99	0.44
1:C:242:THR:O	1:C:243:ARG:NH2	2.41	0.44
1:C:306:ILE:HD12	1:C:307:ASP:N	2.32	0.44
1:D:21:ARG:HH12	1:D:25:ARG:HH12	1.59	0.44
1:D:130:ILE:HA	1:D:131:PRO:HD3	1.78	0.44
1:E:38:TYR:CD1	1:E:68:LEU:HA	2.53	0.44
1:G:187:GLU:HG3	1:G:216:SER:OG	2.17	0.44
1:H:1:MET:HE3	1:H:275:LEU:O	2.18	0.44
1:A:193:GLU:HG2	1:A:306:ILE:CG1	2.47	0.44
1:A:312:ALA:O	1:A:316:GLU:HG3	2.17	0.44
1:C:295:ASP:C	1:C:297:ALA:N	2.74	0.44
1:E:110:LYS:O	1:E:113:THR:N	2.50	0.44
1:G:171:ARG:O	1:G:223:GLY:HA3	2.18	0.44
1:G:186:ALA:HB3	1:G:189:ILE:HD11	1.99	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:A:263:LEU:HD11	1:A:267:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:HA	1:D:254:GLY:N	2.32	0.44
1:D:190:LEU:HD12	1:D:220:VAL:HG22	2.00	0.44
1:E:22:SER:HB2	1:E:265:SER:HA	1.99	0.44
1:F:132:GLY:O	1:F:133:THR:HB	2.18	0.44
1:G:171:ARG:HG3	1:G:172:HIS:N	2.19	0.44
1:G:204:ARG:O	1:G:207:ARG:N	2.50	0.44
1:C:165:VAL:HG22	1:C:218:ILE:HB	2.00	0.43
1:D:208:GLY:C	1:D:210:GLU:N	2.74	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:E:78:THR:O	1:E:82:GLN:HG3	2.18	0.43
1:E:174:GLY:N	1:E:193:GLU:OE2	2.51	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:H	1:G:230:PHE:HD1	1.65	0.43
1:H:24:VAL:HG21	1:H:57:VAL:HG11	1.99	0.43
1:B:133:THR:HB	1:B:285:GLY:HA3	1.99	0.43
1:B:198:MET:HE3	1:B:201:VAL:HB	2.00	0.43
1:F:60:ILE:HD13	1:F:67:ILE:HD13	2.00	0.43
1:H:270:ARG:HG3	1:H:284:VAL:HG12	2.00	0.43
1:H:282:ARG:HD2	1:H:295:ASP:HA	2.01	0.43
1:A:6:VAL:HG13	1:A:68:LEU:HD11	2.01	0.43
1:C:176:ILE:O	1:C:180:SER:HB2	2.18	0.43
1:D:89:LEU:C	1:D:91:LYS:H	2.26	0.43
1:D:144:ASN:CA	1:D:147:ILE:HG12	2.45	0.43
1:D:211:ARG:C	1:D:213:LYS:H	2.27	0.43
1:E:62:HIS:CE1	1:H:63:ARG:HH12	2.34	0.43
1:F:100:ILE:HA	1:F:122:VAL:O	2.18	0.43
1:G:26:LYS:HE3	1:G:30:HIS:CD2	2.53	0.43
1:G:171:ARG:HB3	2:G:1008:F6P:O4	2.18	0.43
1:B:224:VAL:O	1:B:224:VAL:HG13	2.19	0.43
1:E:85:GLY:O	1:E:89:LEU:HG	2.18	0.43
1:E:198:MET:O	1:E:201:VAL:HB	2.18	0.43
1:E:286:ILE:HG23	1:E:286:ILE:O	2.19	0.43
1:F:107:GLN:O	1:F:109:ALA:N	2.51	0.43
1:F:179:TYR:CE2	1:F:310:MET:HE1	2.53	0.43
1:G:162:ARG:NE	1:G:241:GLU:OE2	2.51	0.43
1:H:161:GLU:HB3	1:H:214:LYS:HB2	2.00	0.43
1:H:235:GLN:HB2	1:H:242:THR:HB	2.00	0.43
1:A:179:TYR:CD1	1:A:310:MET:HE1	2.53	0.43
1:C:252:ARG:NH1	1:C:252:ARG:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:GLU:C	1:D:318:SER:H	2.26	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:C:150:ILE:HD12	1:C:150:ILE:N	2.34	0.43
1:E:249:HIS:CD2	1:F:164:TRP:HZ2	2.36	0.43
1:F:162:ARG:O	1:F:215:HIS:HB2	2.18	0.43
1:G:23:VAL:HG13	1:G:272:VAL:HG22	2.01	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:B:97:LEU:HD23	1:B:119:CYS:SG	2.58	0.43
1:E:147:ILE:HG21	1:E:183:ALA:CB	2.45	0.43
1:F:164:TRP:CZ3	1:F:245:THR:HB	2.51	0.43
1:F:306:ILE:HD13	1:F:306:ILE:H	1.83	0.43
1:G:7:LEU:HD12	1:G:97:LEU:HD21	2.01	0.43
1:G:8:THR:HG22	1:G:100:ILE:HB	2.00	0.43
1:G:162:ARG:NH2	1:G:241:GLU:OE2	2.51	0.43
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.84	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
1:C:311:TYR:CE1	1:C:315:LYS:HE3	2.53	0.43
1:E:107:GLN:HA	1:E:107:GLN:NE2	2.34	0.43
1:F:283:CYS:O	1:F:293:ASP:HA	2.19	0.43
1:H:193:GLU:N	1:H:193:GLU:OE1	2.52	0.43
1:A:180:SER:O	1:A:181:GLY:C	2.58	0.43
1:B:146:VAL:HG13	1:B:247:LEU:HD11	2.01	0.43
1:B:207:ARG:C	1:B:209:HIS:N	2.76	0.43
1:B:302:ASN:N	1:B:302:ASN:HD22	2.16	0.43
1:E:126:ILE:HG13	1:E:127:ASP:N	2.34	0.43
1:G:44:LEU:O	1:G:88:GLN:HG3	2.18	0.43
1:H:143:LEU:HD11	1:H:179:TYR:HB2	2.00	0.43
1:H:211:ARG:NH1	1:H:319:ILE:O	2.52	0.43
1:D:5:GLY:O	1:D:98:VAL:N	2.51	0.43
1:D:7:LEU:HD12	1:D:7:LEU:O	2.19	0.43
1:E:138:GLY:HA2	1:E:260:ASP:OD2	2.19	0.43
1:F:204:ARG:O	1:F:205:LEU:C	2.61	0.43
1:G:53:GLU:O	1:G:54:VAL:C	2.62	0.43
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:A:252:ARG:HD3	2:A:1002:F6P:O2	2.19	0.42
1:C:39:HIS:O	1:C:42:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ARG:NE	1:D:61:ILE:HD12	2.34	0.42
1:D:318:SER:C	1:D:319:ILE:CG1	2.90	0.42
1:F:32:VAL:HG21	1:F:276:LEU:CD2	2.50	0.42
1:F:62:HIS:HA	1:F:261:ARG:CZ	2.49	0.42
1:G:197:ASP:O	1:G:198:MET:C	2.61	0.42
1:H:35:TYR:CZ	1:H:51:LYS:HB2	2.54	0.42
1:H:44:LEU:HD11	1:H:89:LEU:HD21	2.01	0.42
1:A:21:ARG:HA	1:A:57:VAL:HB	2.02	0.42
1:B:21:ARG:HA	1:B:57:VAL:HB	2.01	0.42
1:B:128:ASN:ND2	1:B:175:ASP:OD1	2.41	0.42
1:B:175:ASP:C	1:B:177:ALA:N	2.75	0.42
1:C:24:VAL:O	1:C:25:ARG:C	2.63	0.42
1:D:106:TYR:O	1:D:107:GLN:C	2.62	0.42
1:D:113:THR:O	1:D:116:GLY:N	2.52	0.42
1:E:20:ILE:HD11	1:E:100:ILE:HD13	2.01	0.42
1:E:63:ARG:NH1	1:H:62:HIS:HE1	2.15	0.42
1:F:113:THR:C	1:F:115:HIS:N	2.76	0.42
1:F:202:ILE:HG23	1:F:238:THR:CG2	2.49	0.42
1:G:80:GLU:O	1:G:83:LYS:HG2	2.18	0.42
1:G:113:THR:HG21	1:G:281:GLY:CA	2.49	0.42
1:G:216:SER:OG	1:G:217:ILE:N	2.52	0.42
1:A:307:ASP:O	1:A:310:MET:N	2.43	0.42
1:B:19:ALA:O	1:B:23:VAL:HG23	2.19	0.42
1:E:191:ILE:N	1:E:191:ILE:CD1	2.81	0.42
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: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
1:B:284:VAL:O	1:B:284:VAL:HG23	2.20	0.42
1:B:312:ALA:O	1:B:313:LEU:C	2.61	0.42
1:B:313:LEU:C	1:B:315:LYS:N	2.78	0.42
1:C:8:THR:HB	1:C:16:MET:HE1	2.02	0.42
1:C:257:THR:O	1:C:258:ALA:C	2.62	0.42
1:C:297:ALA:C	1:C:299:ALA:N	2.77	0.42
1:D:21:ARG:HH11	1:D:21:ARG:CG	2.33	0.42
1:E:252:ARG:NH2	1:F:160:HIS:CE1	2.88	0.42
1:F:167:GLU:HB3	1:F:246:VAL:HG13	2.02	0.42
1:F:176:ILE:O	1:F:180:SER:HB2	2.19	0.42
1:F:188:THR:HB	1:F:218:ILE:HG13	2.01	0.42
1:G:32:VAL:HG12	1:G:33:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:GLU:HB3	1:H:246:VAL:HG13	2.02	0.42
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.90	0.42
1:C:21:ARG:CD	1:C:61:ILE:HB	2.48	0.42
1:C:307:ASP:C	1:C:307:ASP:OD2	2.62	0.42
1:D:60:ILE:C	1:D:62:HIS:H	2.28	0.42
1:D:208:GLY:C	1:D:210:GLU:H	2.28	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:E:152:LYS:HG2	1:F:254:GLY:CA	2.50	0.42
1:H:25:ARG:O	1:H:26:LYS:C	2.62	0.42
1:H:113:THR:HG21	1:H:281:GLY:N	2.35	0.42
1:H:171:ARG:CG	1:H:172:HIS:N	2.67	0.42
1:A:252:ARG:NH2	1:B:160:HIS:CE1	2.88	0.42
1:E:142:ALA:O	1:E:143:LEU:C	2.62	0.42
1:F:319:ILE:N	1:F:319:ILE:HD12	2.35	0.42
1:A:191:ILE:HG12	1:A:193:GLU:H	1.84	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:149:ALA:O	1:E:152:LYS:HB2	2.20	0.42
1:E:197:ASP:O	1:E:200:ASP:N	2.52	0.42
1:G:108:GLY:O	1:G:109:ALA:C	2.62	0.42
1:H:269:ALA:O	1:H:273:GLU:HG3	2.19	0.42
1:A:43:GLY:O	1:A:47:GLY:N	2.45	0.42
1:A:139:PHE:HE2	1:A:176:ILE:HD13	1.84	0.42
1:B:232:ARG:HD2	1:H:243:ARG:NH2	2.35	0.42
1:C:181:GLY:O	1:C:185:GLY:N	2.43	0.42
1:D:3:ARG:HD2	1:D:93:GLY:C	2.45	0.42
1:D:111:LYS:O	1:D:113:THR:N	2.53	0.42
1:F:181:GLY:HA2	1:F:219:ILE:HG13	2.01	0.42
1:G:4:ILE:O	1:G:34:VAL:HA	2.20	0.42
1:H:141:THR:CG2	1:H:256:PRO:HA	2.50	0.42
1:A:307:ASP:O	1:A:308:GLN:C	2.63	0.41
1:D:107:GLN:C	1:D:109:ALA:N	2.77	0.41
1:E:171:ARG:NH1	1:E:171:ARG:HB2	2.35	0.41
1:F:63:ARG:HH12	1:G:62:HIS:CE1	2.37	0.41
1:F:211:ARG:HH12	1:F:213:LYS:HE2	1.84	0.41
1:H:99:VAL:HG21	1:H:109:ALA:HB2	2.02	0.41
1:H:128:ASN:HA	1:H:136:THR:CG2	2.50	0.41
1:H:134:ASP:OD1	1:H:287:GLN:HA	2.20	0.41
1:B:139:PHE:CE1	1:B:143:LEU:HD22	2.55	0.41
1:D:200:ASP:O	1:D:203:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ALA:O	1:E:145:THR:N	2.53	0.41
1:F:20:ILE:HD13	1:F:100:ILE:HD12	2.02	0.41
1:F:262:VAL:HG22	1:H:183:ALA:HB2	2.02	0.41
1:H:16:MET:O	1:H:20:ILE:HG12	2.20	0.41
1:H:53:GLU:HA	1:H:53:GLU:OE2	2.20	0.41
1:A:1:MET:HE2	1:A:95:GLU:HB3	2.01	0.41
1:A:82:GLN:NE2	1:A:115:HIS:ND1	2.69	0.41
1:A:252:ARG:HG3	1:A:252:ARG:NH1	2.35	0.41
1:B:78:THR:O	1:B:79:GLU:C	2.63	0.41
1:B:86:ILE:O	1:B:86:ILE:HG22	2.19	0.41
1:F:273:GLU:O	1:F:274:LEU:C	2.63	0.41
1:G:60:ILE:O	1:G:61:ILE:C	2.63	0.41
1:G:102:GLY:O	1:G:104:GLY:N	2.52	0.41
1:H:105:SER:O	1:H:106:TYR:C	2.63	0.41
1:H:128:ASN:O	1:H:304:HIS:CE1	2.73	0.41
1:A:127:ASP:OD1	1:A:170:GLY:HA2	2.20	0.41
1:A:153:ILE:HD11	1:A:245:THR:HG21	2.02	0.41
1:B:123:PRO:HD3	1:B:284:VAL:O	2.21	0.41
1:E:39:HIS:CE1	1:F:161:GLU:OE2	2.73	0.41
1:E:100:ILE:HA	1:E:122:VAL:O	2.19	0.41
1:E:110:LYS:O	1:E:111:LYS:C	2.63	0.41
1:E:150:ILE:HD11	1:E:219:ILE:HD11	2.02	0.41
1:E:249:HIS:CB	1:F:164:TRP:CH2	2.96	0.41
1:E:271:ALA:C	1:E:273:GLU:N	2.78	0.41
1:E:295:ASP:O	1:E:297:ALA:N	2.54	0.41
1:F:147:ILE:HD12	1:H:261:ARG:CZ	2.51	0.41
1:F:243:ARG:HH21	1:F:243:ARG:HG2	1.85	0.41
1:G:211:ARG:HG2	1:G:211:ARG:NH1	2.34	0.41
1:H:21:ARG:HG2	1:H:21:ARG:HH11	1.85	0.41
1:H:170:GLY:O	1:H:171:ARG:C	2.63	0.41
1:H:295:ASP:C	1:H:297:ALA:N	2.76	0.41
1:A:163:THR:O	1:A:242:THR:HG23	2.19	0.41
1:A:191:ILE:HD13	1:A:191:ILE:N	2.35	0.41
1:A:206:LYS:O	1:A:207:ARG:C	2.63	0.41
1:B:9:SER:HB3	1:B:105:SER:OG	2.20	0.41
1:B:82:GLN:NE2	1:B:111:LYS:HG3	2.29	0.41
1:B:176:ILE:O	1:B:176:ILE:CG2	2.69	0.41
1:B:207:ARG:C	1:B:209:HIS:H	2.27	0.41
1:C:16:MET:HE3	1:C:100:ILE:HG22	2.02	0.41
1:C:22:SER:HB2	1:C:265:SER:HA	2.03	0.41
1:D:211:ARG:HB2	1:D:211:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ALA:O	1:E:28:ILE:C	2.63	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:F:270:ARG:O	1:F:271:ALA:C	2.62	0.41
1:G:112:LEU:HD12	1:G:112:LEU:HA	1.96	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:A:145:THR:CG2	1:B:152:LYS:HZ3	2.33	0.41
1:B:7:LEU:CB	1:B:37:VAL:HB	2.51	0.41
1:D:23:VAL:HA	1:D:272:VAL:HG21	2.03	0.41
1:D:120:VAL:HA	1:D:282:ARG:O	2.19	0.41
1:D:141:THR:HA	1:D:257:THR:CG2	2.50	0.41
1:E:75:GLU:H	1:E:75:GLU:HG2	1.73	0.41
1:E:89:LEU:O	1:E:90:LYS:C	2.64	0.41
1:F:173:ALA:HA	1:F:193:GLU:OE2	2.19	0.41
1:F:307:ASP:OD2	1:F:307:ASP:C	2.63	0.41
1:G:146:VAL:O	1:G:150:ILE:HD12	2.21	0.41
1:G:232:ARG:C	1:G:234:ILE:N	2.78	0.41
1:H:98:VAL:HG23	1:H:275:LEU:HD11	2.02	0.41
1:C:114:GLU:C	1:C:116:GLY:N	2.79	0.41
1:C:242:THR:HG22	1:C:243:ARG:N	2.35	0.41
1:D:141:THR:CG2	1:D:256:PRO:HA	2.51	0.41
1:E:12:ASP:H	1:F:160:HIS:HE1	1.67	0.41
1:E:137:ILE:HD13	1:E:264:ALA:HA	2.02	0.41
1:F:53:GLU:C	1:F:55:GLY:N	2.76	0.41
1:G:207:ARG:HG2	1:G:207:ARG:HH11	1.86	0.41
1:A:11:GLY:HA2	1:B:160:HIS:NE2	2.36	0.41
1:A:288:ASN:HD22	1:A:288:ASN:HA	1.55	0.41
1:B:25:ARG:O	1:B:26:LYS:C	2.64	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:D:249:HIS:C	1:D:251:GLN:N	2.78	0.41
1:E:137:ILE:HD11	1:E:264:ALA:HA	2.02	0.41
1:E:182:LEU:HD13	1:E:182:LEU:C	2.46	0.41
1:E:250:VAL:HG23	1:E:251:GLN:N	2.36	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:G:159:SER:OG	1:H:66:THR:HG22	2.21	0.41
1:G:222:GLU:C	1:G:224:VAL:H	2.29	0.41
1:H:150:ILE:HD12	1:H:150:ILE:N	2.34	0.41
1:A:77:LYS:HB2	1:A:77:LYS:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:HD22	1:A:175:ASP:CG	2.29	0.41
1:B:185:GLY:HA2	1:D:21:ARG:HH21	1.84	0.41
1:B:190:LEU:HD22	1:B:196:TYR:CD2	2.55	0.41
1:B:246:VAL:O	1:B:247:LEU:C	2.64	0.41
1:C:189:ILE:HD13	1:C:219:ILE:HB	2.01	0.41
1:C:211:ARG:HB2	1:C:211:ARG:NH1	2.36	0.41
1:D:24:VAL:CG2	1:D:57:VAL:HG11	2.50	0.41
1:D:67:ILE:HG13	1:D:68:LEU:N	2.36	0.41
1:D:272:VAL:O	1:D:276:LEU:HG	2.21	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:F:269:ALA:O	1:F:270:ARG:C	2.62	0.41
1:G:149:ALA:O	1:G:150:ILE:C	2.64	0.41
1:H:113:THR:HG21	1:H:281:GLY:HA3	2.03	0.41
1:H:284:VAL:HG23	1:H:285:GLY:H	1.86	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:F:178:LEU:HG	1:F:310:MET:HE2	2.01	0.41
1:F:207:ARG:HG3	1:F:207:ARG:HH11	1.86	0.41
1:H:41:TYR:O	1:H:44:LEU:HB3	2.21	0.41
1:H:126:ILE:O	1:H:176:ILE:HD11	2.20	0.41
1:H:270:ARG:HD3	1:H:270:ARG:O	2.21	0.41
1:B:1:MET:HA	1:B:95:GLU:OE1	2.21	0.40
1:B:102:GLY:O	1:B:105:SER:HB2	2.21	0.40
1:C:169:MET:HE3	1:C:248:GLY:C	2.46	0.40
1:C:252:ARG:NH2	1:D:160:HIS:CE1	2.89	0.40
1:D:274:LEU:HD22	1:D:279:LYS:HG3	2.04	0.40
1:E:283:CYS:O	1:E:293:ASP:HA	2.22	0.40
1:F:26:LYS:HE2	1:F:30:HIS:CD2	2.56	0.40
1:F:154:ARG:HA	1:F:217:ILE:HD11	2.02	0.40
1:G:22:SER:O	1:G:26:LYS:HB3	2.21	0.40
1:H:120:VAL:HG11	1:H:271:ALA:HA	2.03	0.40
1:A:198:MET:HG2	1:A:233:GLN:HE22	1.85	0.40
1:B:108:GLY:O	1:B:109:ALA:C	2.64	0.40
1:B:180:SER:O	1:B:183:ALA:HB3	2.21	0.40
1:B:262:VAL:HG23	1:D:183:ALA:HB2	2.04	0.40
1:C:13:SER:O	1:C:15:GLY:N	2.54	0.40
1:C:66:THR:C	1:C:68:LEU:N	2.79	0.40
1:D:18:ALA:O	1:D:21:ARG:HB3	2.20	0.40
1:D:26:LYS:HE2	1:D:273:GLU:CG	2.51	0.40
1:D:282:ARG:HB3	1:D:294:HIS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ASP:N	1:F:130:ILE:CD1	2.84	0.40
1:F:255:SER:OG	1:F:261:ARG:NH2	2.53	0.40
1:G:60:ILE:HA	1:G:63:ARG:HG3	2.04	0.40
1:G:275:LEU:HD23	1:G:275:LEU:HA	1.89	0.40
1:H:306:ILE:C	1:H:306:ILE:HD12	2.46	0.40
1:B:189:ILE:O	1:B:311:TYR:HE2	2.04	0.40
1:C:17:ASN:ND2	1:C:67:ILE:HG13	2.37	0.40
1:C:27:ALA:CB	1:C:34:VAL:CG2	3.00	0.40
1:C:130:ILE:HA	1:C:131:PRO:HD3	1.89	0.40
1:D:20:ILE:HD12	1:D:68:LEU:HD12	2.03	0.40
1:D:249:HIS:C	1:D:251:GLN:H	2.28	0.40
1:E:169:MET:HB3	1:E:170:GLY:H	1.70	0.40
1:E:193:GLU:H	1:E:193:GLU:CD	2.29	0.40
1:E:281:GLY:O	1:E:282:ARG:HG2	2.21	0.40
1:F:60:ILE:HA	1:F:63:ARG:HG2	2.04	0.40
1:F:243:ARG:NH2	1:F:243:ARG:HG2	2.36	0.40
1:G:111:LYS:HB3	1:G:111:LYS:NZ	2.36	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:B:61:ILE:O	1:B:61:ILE:HG12	2.21	0.40
1:D:6:VAL:HA	1:D:98:VAL:HB	2.03	0.40
1:D:35:TYR:CE1	1:D:51:LYS:HB2	2.56	0.40
1:E:176:ILE:O	1:E:176:ILE:HG22	2.22	0.40
1:F:256:PRO:HG2	1:F:261:ARG:HE	1.86	0.40
1:G:60:ILE:O	1:G:63:ARG:N	2.46	0.40
1:G:234:ILE:C	1:G:236:GLU:H	2.28	0.40
1:H:175:ASP:CG	1:H:304:HIS:HE2	2.29	0.40
1:A:193:GLU:N	1:A:193:GLU:CD	2.80	0.40
1:A:233:GLN:HE21	1:A:233:GLN:HB3	1.63	0.40
1:A:254:GLY:CA	1:B:152:LYS:HG2	2.50	0.40
1:A:276:LEU:C	1:A:278:GLY:H	2.29	0.40
1:B:229:ASP:O	1:B:230:PHE:C	2.65	0.40
1:B:295:ASP:HB3	1:B:298:GLU:HG2	2.04	0.40
1:C:17:ASN:O	1:C:19:ALA:N	2.55	0.40
1:C:186:ALA:HB3	1:C:189:ILE:HD11	2.04	0.40
1:D:20:ILE:HD13	1:D:100:ILE:HD12	2.03	0.40
1:D:75:GLU:CD	1:D:75:GLU:N	2.60	0.40
1:F:171:ARG:CG	1:F:172:HIS:N	2.73	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	317/319 (99%)	275 (87%)	34 (11%)	8 (2%)	4	27
1	B	317/319 (99%)	263 (83%)	47 (15%)	7 (2%)	5	29
1	C	317/319 (99%)	254 (80%)	52 (16%)	11 (4%)	3	20
1	D	317/319 (99%)	268 (84%)	37 (12%)	12 (4%)	2	18
1	E	317/319 (99%)	270 (85%)	35 (11%)	12 (4%)	2	18
1	F	317/319 (99%)	281 (89%)	34 (11%)	2 (1%)	21	56
1	G	317/319 (99%)	263 (83%)	46 (14%)	8 (2%)	4	27
1	H	317/319 (99%)	261 (82%)	48 (15%)	8 (2%)	4	27
All	All	2536/2552 (99%)	2135 (84%)	333 (13%)	68 (3%)	4	25

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	223 (90%)	24 (10%)	8	32
1	B	247/247 (100%)	231 (94%)	16 (6%)	15	47
1	C	247/247 (100%)	227 (92%)	20 (8%)	11	39
1	D	247/247 (100%)	234 (95%)	13 (5%)	20	53
1	E	247/247 (100%)	223 (90%)	24 (10%)	8	32
1	F	247/247 (100%)	230 (93%)	17 (7%)	14	45
1	G	247/247 (100%)	233 (94%)	14 (6%)	18	51
1	H	247/247 (100%)	230 (93%)	17 (7%)	14	45
All	All	1976/1976 (100%)	1831 (93%)	145 (7%)	13	43

All (145) 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	77	LYS
1	A	84	LYS

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Mol	Chain	Res	Type
1	A	110	LYS
1	A	144	ASN
1	A	148	ASP
1	A	164	TRP
1	A	167	GLU
1	A	191	ILE
1	A	198	MET
1	A	207	ARG
1	A	244	VAL
1	A	275	LEU
1	A	277	GLU
1	A	282	ARG
1	A	284	VAL
1	A	288	ASN
1	A	295	ASP
1	A	298	GLU
1	A	303	LYS
1	A	305	THR
1	B	7	LEU
1	B	34	VAL
1	B	48	ASN
1	B	59	ASP
1	B	66	THR
1	B	119	CYS
1	B	158	THR
1	B	161	GLU
1	B	169	MET
1	B	189	ILE
1	B	191	ILE
1	B	228	VAL
1	B	286	ILE
1	B	289	ASN
1	B	305	THR
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	63	ARG
1	C	66	THR
1	C	77	LYS

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Mol	Chain	Res	Type
1	C	80	GLU
1	C	119	CYS
1	C	125	THR
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	302	ASN
1	D	2	LYS
1	D	21	ARG
1	D	34	VAL
1	D	48	ASN
1	D	50	LYS
1	D	66	THR
1	D	67	ILE
1	D	113	THR
1	D	156	THR
1	D	187	GLU
1	D	209	HIS
1	D	288	ASN
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	45	ILE
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	187	GLU

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Mol	Chain	Res	Type
1	E	189	ILE
1	E	191	ILE
1	E	207	ARG
1	E	214	LYS
1	E	287	GLN
1	E	306	ILE
1	E	314	SER
1	F	7	LEU
1	F	28	ILE
1	F	66	THR
1	F	86	ILE
1	F	111	LYS
1	F	148	ASP
1	F	182	LEU
1	F	187	GLU
1	F	188	THR
1	F	191	ILE
1	F	205	LEU
1	F	214	LYS
1	F	218	ILE
1	F	245	THR
1	F	246	VAL
1	F	306	ILE
1	F	319	ILE
1	G	2	LYS
1	G	7	LEU
1	G	48	ASN
1	G	111	LYS
1	G	113	THR
1	G	133	THR
1	G	143	LEU
1	G	147	ILE
1	G	191	ILE
1	G	228	VAL
1	G	242	THR
1	G	245	THR
1	G	246	VAL
1	G	289	ASN
1	H	4	ILE
1	H	7	LEU
1	H	38	TYR
1	H	80	GLU

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Mol	Chain	Res	Type
1	H	90	LYS
1	H	95	GLU
1	H	99	VAL
1	H	110	LYS
1	H	119	CYS
1	H	128	ASN
1	H	165	VAL
1	H	187	GLU
1	H	214	LYS
1	H	228	VAL
1	H	229	ASP
1	H	290	GLN
1	H	305	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	48	ASN
1	A	82	GLN
1	A	88	GLN
1	A	144	ASN
1	A	199	ASN
1	A	233	GLN
1	A	251	GLN
1	A	288	ASN
1	A	290	GLN
1	A	302	ASN
1	B	82	GLN
1	B	92	HIS
1	B	160	HIS
1	B	251	GLN
1	B	289	ASN
1	B	290	GLN
1	B	302	ASN
1	C	17	ASN
1	C	48	ASN
1	C	128	ASN
1	C	199	ASN
1	C	235	GLN
1	C	251	GLN
1	C	289	ASN

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Mol	Chain	Res	Type
1	C	302	ASN
1	D	107	GLN
1	D	160	HIS
1	D	209	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
1	E	62	HIS
1	E	92	HIS
1	E	107	GLN
1	E	144	ASN
1	E	160	HIS
1	E	288	ASN
1	F	48	ASN
1	F	62	HIS
1	F	115	HIS
1	F	160	HIS
1	F	199	ASN
1	F	209	HIS
1	F	233	GLN
1	F	287	GLN
1	F	288	ASN
1	F	290	GLN
1	F	302	ASN
1	F	308	GLN
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

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Mol	Chain	Res	Type
1	H	233	GLN
1	H	287	GLN
1	H	288	ASN
1	H	302	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	1008	-	15,16,16	1.05	1 (6%)	16,25,25	0.94	0
2	F6P	E	1006	-	15,16,16	1.06	0	16,25,25	0.95	0
2	F6P	D	1003	-	15,16,16	1.09	1 (6%)	16,25,25	0.87	0
2	F6P	A	1002	-	15,16,16	1.03	0	16,25,25	0.89	0
2	F6P	C	1004	-	15,16,16	1.04	0	16,25,25	0.96	0
2	F6P	H	1007	-	15,16,16	0.98	0	16,25,25	0.99	1 (6%)
2	F6P	B	1001	-	15,16,16	1.07	0	16,25,25	0.94	0
2	F6P	F	1005	-	15,16,16	1.09	1 (6%)	16,25,25	1.04	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	G	1008	-	-	3/9/28/28	0/1/1/1
2	F6P	E	1006	-	-	3/9/28/28	0/1/1/1
2	F6P	D	1003	-	-	2/9/28/28	0/1/1/1
2	F6P	A	1002	-	-	1/9/28/28	0/1/1/1
2	F6P	C	1004	-	-	0/9/28/28	0/1/1/1
2	F6P	H	1007	-	-	3/9/28/28	0/1/1/1
2	F6P	B	1001	-	-	2/9/28/28	0/1/1/1
2	F6P	F	1005	-	-	0/9/28/28	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1003	F6P	O5-C2	-2.77	1.39	1.43
2	G	1008	F6P	O5-C2	-2.58	1.39	1.43
2	F	1005	F6P	O5-C2	-2.51	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1007	F6P	O6-P-O1P	2.08	112.07	106.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	F6P	O5-C5-C6-O6
2	D	1003	F6P	O5-C5-C6-O6
2	E	1006	F6P	O5-C5-C6-O6
2	B	1001	F6P	C4-C5-C6-O6
2	D	1003	F6P	C4-C5-C6-O6
2	E	1006	F6P	C4-C5-C6-O6
2	G	1008	F6P	C4-C5-C6-O6
2	G	1008	F6P	O5-C5-C6-O6
2	H	1007	F6P	O5-C5-C6-O6
2	H	1007	F6P	C4-C5-C6-O6
2	G	1008	F6P	C5-C6-O6-P

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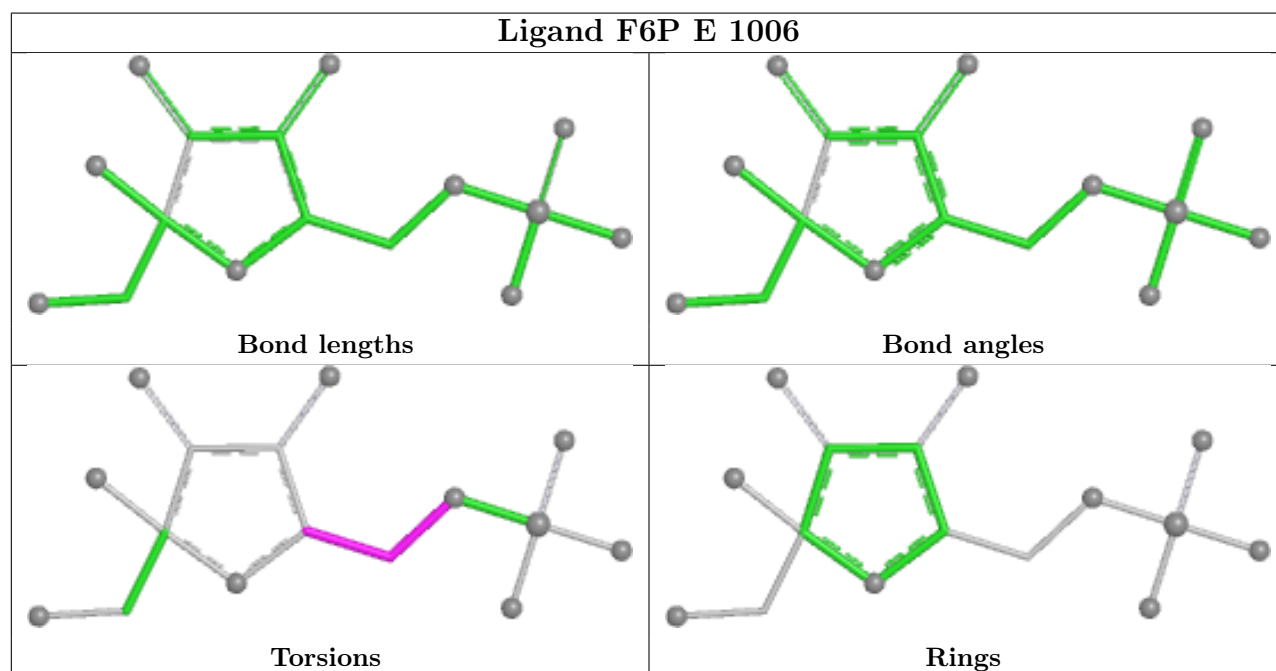
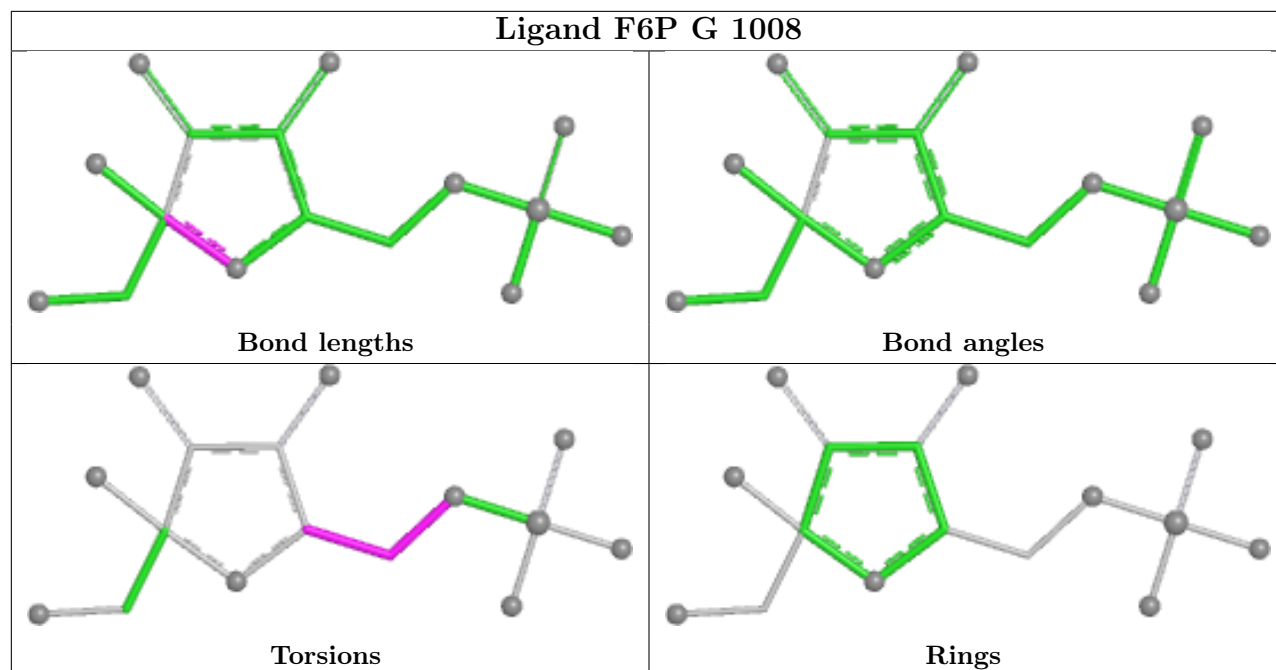
Mol	Chain	Res	Type	Atoms
2	E	1006	F6P	C5-C6-O6-P
2	H	1007	F6P	C5-C6-O6-P
2	A	1002	F6P	C5-C6-O6-P

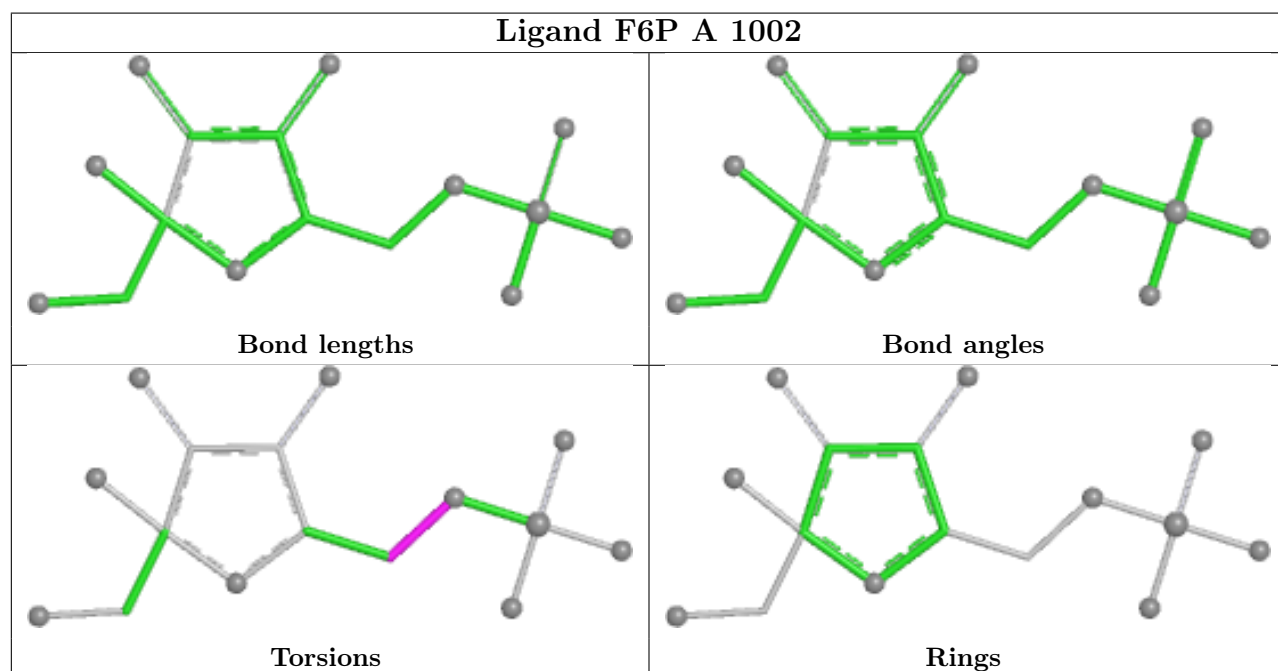
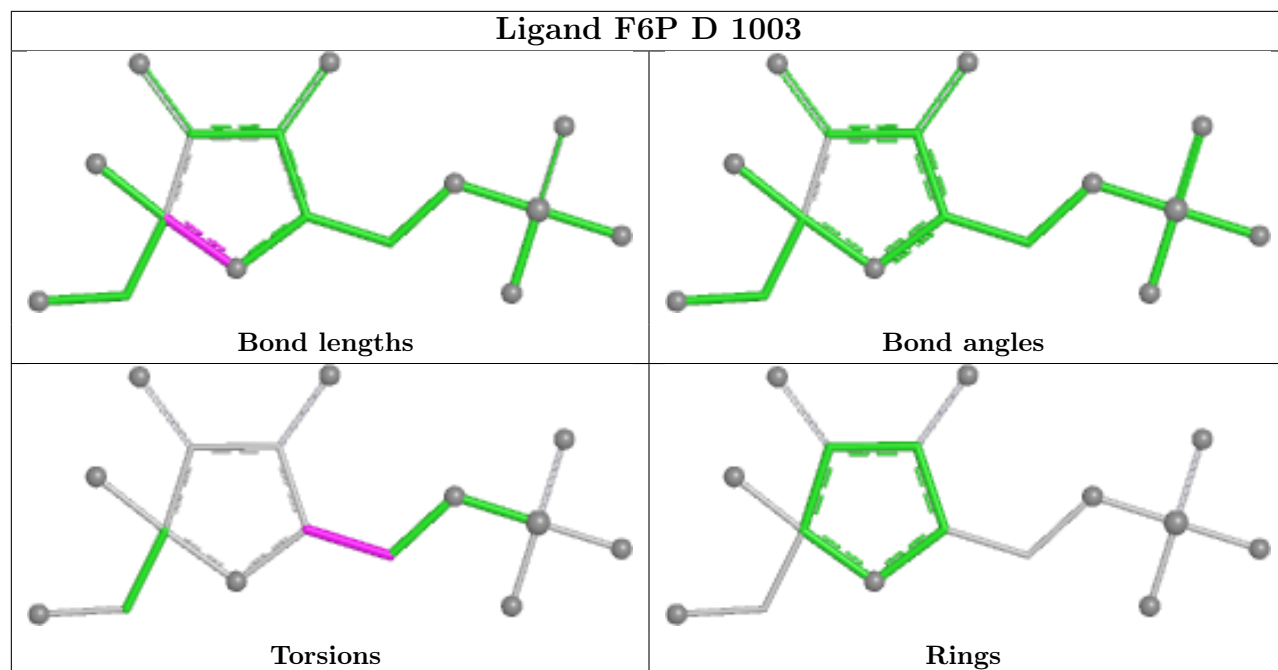
There are no ring outliers.

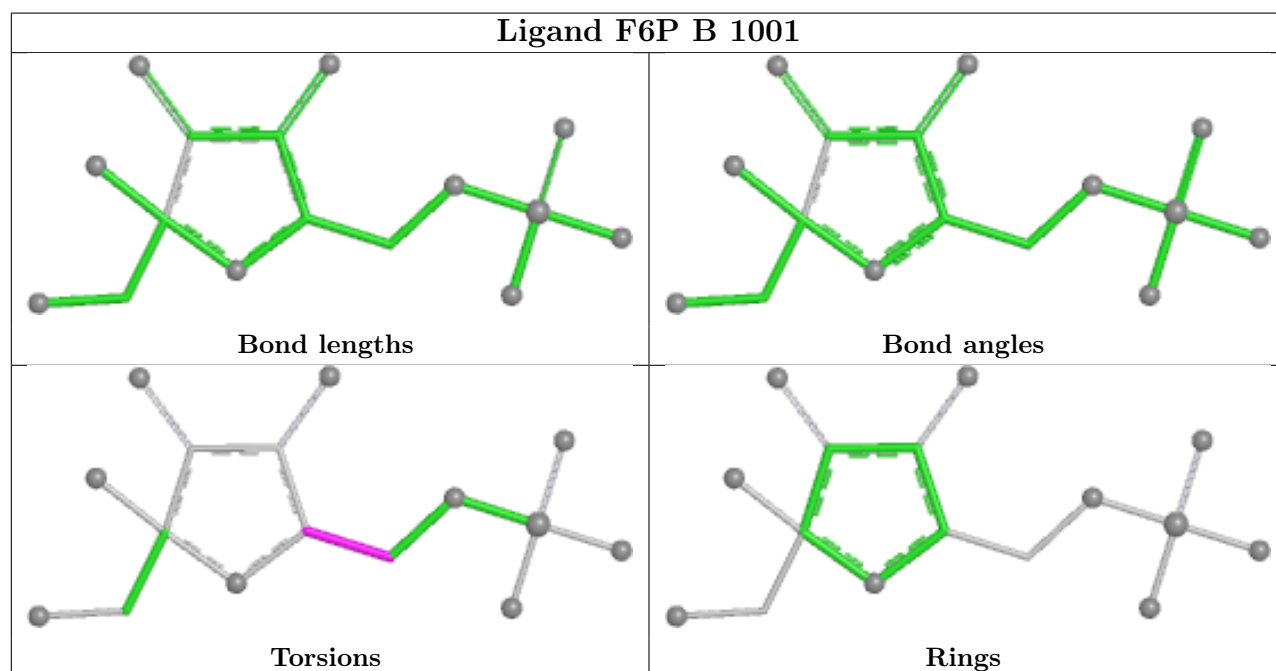
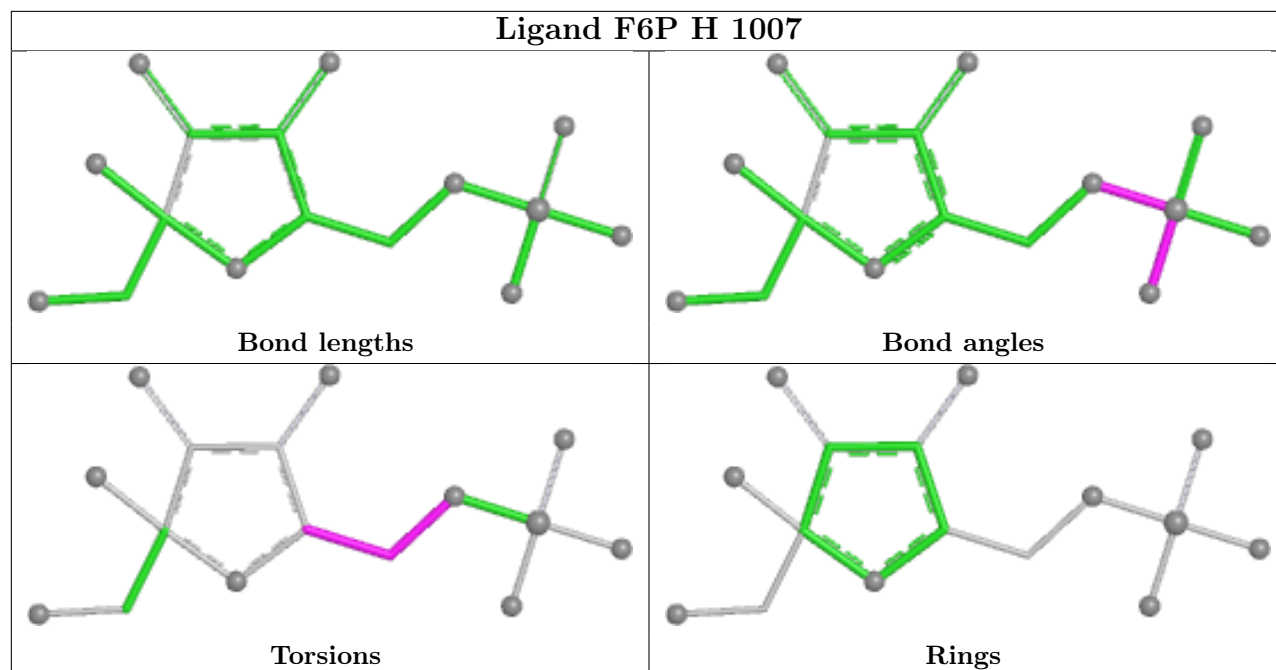
5 monomers are involved in 9 short contacts:

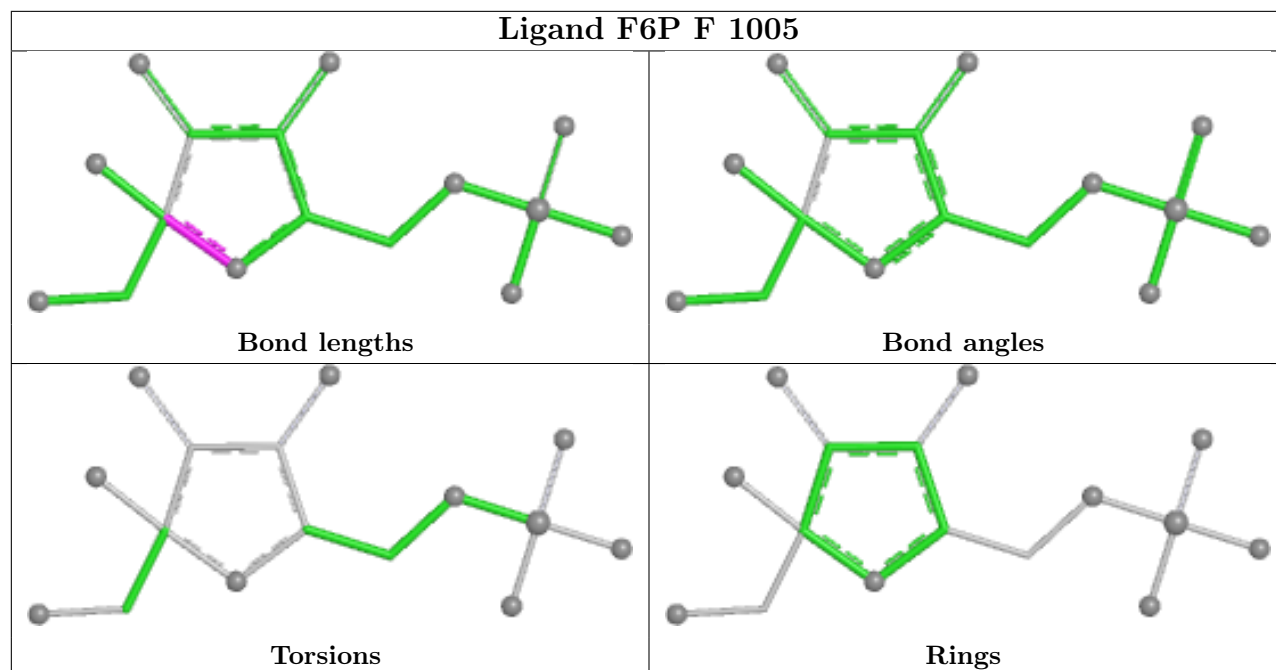
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1008	F6P	1	0
2	A	1002	F6P	1	0
2	C	1004	F6P	1	0
2	H	1007	F6P	4	0
2	F	1005	F6P	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.