Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 11:15 AM EDT

PDB ID	:	1RDX
Title	:	R-STATE STRUCTURE OF THE ARG 243 TO ALA MUTANT OF PIG KIDNEY FRUCTOSE 1,6-BISPHOSPHATASE EXPRESSED IN E. COLI
Authors	:	Stec, B.; Abraham, R.; Giroux, E.; Kantrowitz, E.R.
Deposited on	:	1996-05-17
Resolution	:	2.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

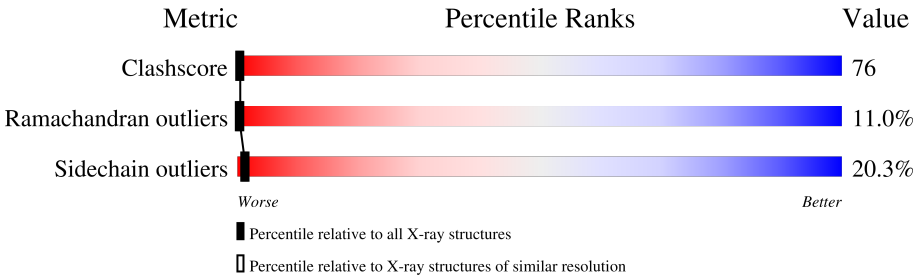
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	337	23% 54% 21% .
1	B	337	20% 60% 18% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5223 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.

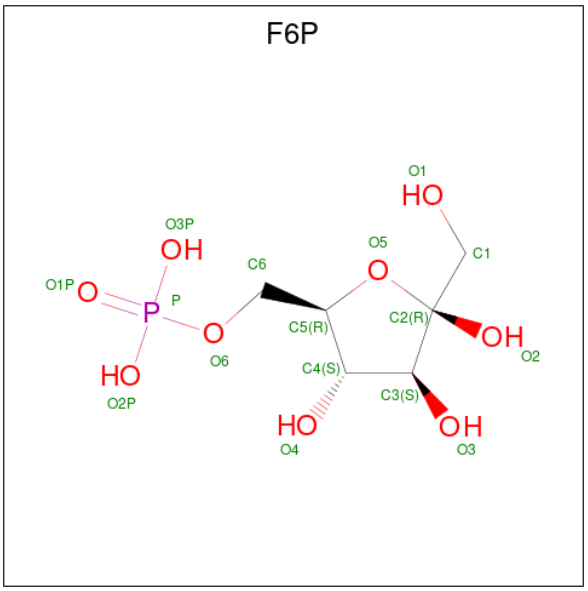
- Molecule 1 is a protein called FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2566	1630	431	490	15			
1	B	337	Total	C	N	O	S	0	0	0
			2566	1630	431	490	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P00636
A	96	THR	SER	conflict	UNP P00636
A	199	ASN	ASP	conflict	UNP P00636
A	243	ALA	ARG	engineered mutation	UNP P00636
B	20	GLN	GLU	conflict	UNP P00636
B	96	THR	SER	conflict	UNP P00636
B	199	ASN	ASP	conflict	UNP P00636
B	243	ALA	ARG	engineered mutation	UNP P00636

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 16 6 9 1	0	0
2	B	1	Total C O P 16 6 9 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	29	Total O 29 29	0	0
3	B	30	Total O 30 30	0	0

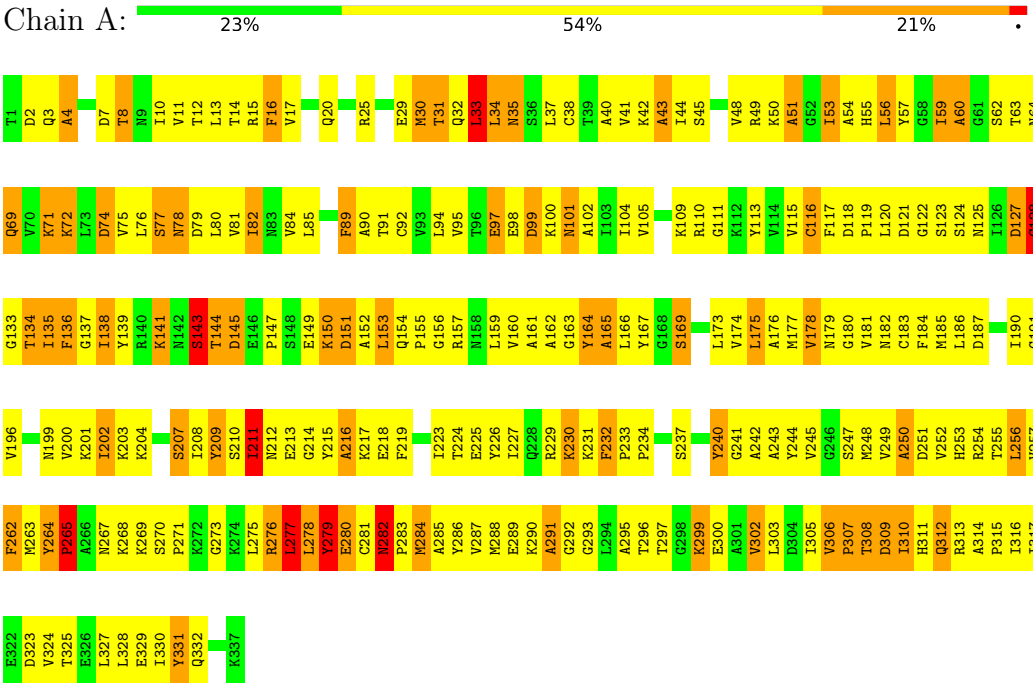
3 Residue-property plots (i)

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.

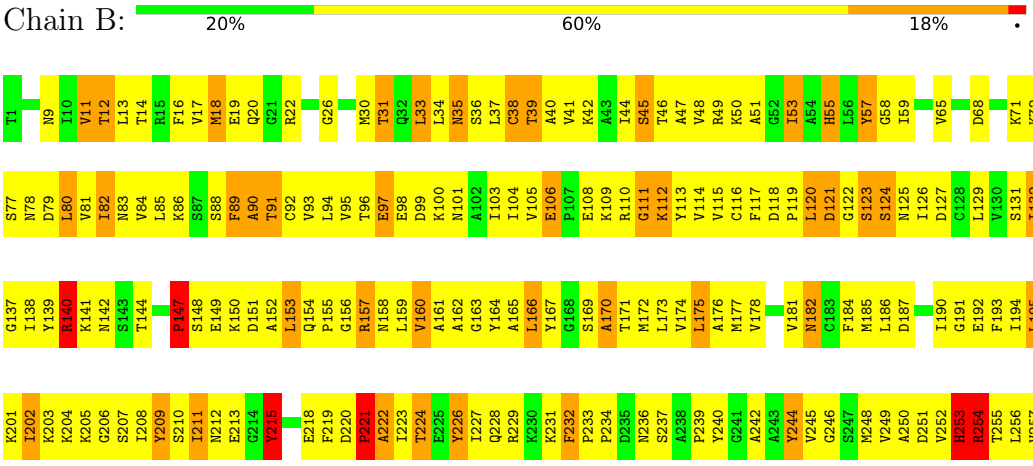
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

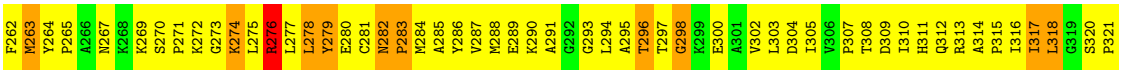
Chain A:



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B:




F262
M263
Y264
P265
A266
N267
K268
K269
S270
P271
K272
G273
K274
L275
R276
L277
L278
Y279
E280
C281
M282
P283
M284
A285
Y286
V287
M288
E289
K290
A291
G292
G293
L294
A295
T296
T297
G298
K299
E300
A301
V302
L303
D304
I305
V306
P307
T308
D309
I310
H311
Q312
R313
A314
P315
I316
I317
L318
G319
S320
P321


E322
D323
V324
T325
E326
L327
L328
E329
I330
Y331
Q332
K333
H334
A335
A336
K337

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.31Å 131.31Å 66.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.75	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.75)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.223 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5223	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.58	0/2609	0.92	5/3531 (0.1%)
1	B	0.56	0/2609	0.89	3/3531 (0.1%)
All	All	0.57	0/5218	0.91	8/7062 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	LEU	CA-CB-CG	7.19	131.84	115.30
1	A	169	SER	N-CA-C	-6.88	92.44	111.00
1	A	33	LEU	CA-CB-CG	6.72	130.76	115.30
1	B	298	GLY	N-CA-C	-6.58	96.66	113.10
1	A	306	VAL	N-CA-C	-5.77	95.42	111.00
1	B	118	ASP	N-CA-C	-5.16	97.08	111.00
1	A	211	ILE	N-CA-C	-5.11	97.19	111.00
1	B	140	ARG	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	TYR	Sidechain

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	2566	0	2620	396	0
1	B	2566	0	2620	427	0
2	A	16	0	11	1	0
2	B	16	0	11	1	0
3	A	29	0	0	2	0
3	B	30	0	0	2	0
All	All	5223	0	5262	791	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 76.

All (791) 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:297:THR:HB	1:A:315:PRO:HG2	1.21	1.15
1:A:97:GLU:HB3	1:A:279:TYR:HE2	1.08	1.13
1:A:224:THR:HA	1:A:227:ILE:HD12	1.34	1.09
1:A:174:VAL:HA	1:A:183:CYS:HA	1.33	1.09
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.33	1.07
1:B:90:ALA:HA	1:B:111:GLY:HA3	1.39	1.04
1:A:156:GLY:HA3	1:A:303:LEU:HD22	1.37	1.03
1:A:318:LEU:HA	1:A:324:VAL:HG21	1.36	1.03
1:A:175:LEU:HB3	1:A:184:PHE:HE2	1.22	1.03
1:B:281:CYS:SG	1:B:314:ALA:HB3	2.00	1.02
1:A:263:MET:HA	1:A:317:ILE:HG12	1.43	1.01
1:A:41:VAL:HG21	1:A:173:LEU:HD12	1.41	1.00
1:A:78:ASN:HA	1:A:81:VAL:HB	1.42	0.99
1:B:106:GLU:HB2	1:B:108:GLU:HG2	1.45	0.98
1:A:97:GLU:HB3	1:A:279:TYR:CE2	1.99	0.96
1:A:208:ILE:HG23	1:A:242:ALA:HA	1.45	0.96
1:B:167:TYR:HD1	1:B:171:THR:HG1	1.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HA	1:A:330:ILE:HD12	1.50	0.93
1:A:49:ARG:HA	1:B:170:ALA:HB2	1.49	0.93
1:A:13:LEU:HD11	1:A:175:LEU:HD22	1.48	0.93
1:A:95:VAL:HB	1:A:116:CYS:HA	1.49	0.93
1:A:45:SER:HA	1:A:167:TYR:CD2	2.03	0.92
1:B:185:MET:HE2	1:B:196:VAL:HG21	1.52	0.92
1:B:120:LEU:HA	1:B:134:THR:OG1	1.70	0.91
1:A:175:LEU:HB3	1:A:184:PHE:CE2	2.05	0.91
1:A:320:SER:HB2	1:A:323:ASP:HB2	1.52	0.91
1:B:263:MET:HB2	1:B:317:ILE:HG12	1.53	0.90
1:A:243:ALA:HB1	1:B:246:GLY:HA3	1.53	0.89
1:B:194:ILE:HG22	1:B:196:VAL:HG13	1.55	0.88
1:B:192:GLU:HG3	1:B:194:ILE:HG13	1.53	0.87
1:B:295:ALA:HA	1:B:318:LEU:HB3	1.56	0.87
1:B:209:TYR:HA	1:B:261:ILE:HG22	1.56	0.87
1:B:40:ALA:HB1	1:B:81:VAL:HG22	1.55	0.87
1:A:275:LEU:HB3	1:A:280:GLU:HB3	1.57	0.86
1:B:38:CYS:SG	1:B:42:LYS:HD2	2.15	0.86
1:B:277:LEU:HA	1:B:281:CYS:SG	2.16	0.86
1:B:281:CYS:O	1:B:285:ALA:HB3	1.74	0.86
1:B:162:ALA:HB1	1:B:283:PRO:HA	1.58	0.85
1:A:204:LYS:HA	1:A:321:PRO:HD2	1.58	0.85
1:B:113:TYR:HA	1:B:139:TYR:O	1.76	0.85
1:A:53:ILE:HG23	1:A:54:ALA:H	1.41	0.85
1:A:174:VAL:HG12	1:A:181:VAL:HG12	1.57	0.85
1:B:31:THR:HA	1:B:34:LEU:HB2	1.59	0.85
1:A:13:LEU:HD23	1:A:38:CYS:SG	2.17	0.84
1:B:273:GLY:HA3	1:B:315:PRO:HG3	1.58	0.84
1:A:11:VAL:HG13	1:A:15:ARG:HH12	1.42	0.83
1:A:156:GLY:HA2	1:A:159:LEU:HB3	1.61	0.83
1:B:248:MET:SD	1:B:275:LEU:HD13	2.19	0.83
1:A:277:LEU:HB2	1:A:281:CYS:SG	2.20	0.82
1:A:4:ALA:HB1	1:B:58:GLY:HA2	1.62	0.81
1:A:174:VAL:HG13	1:A:183:CYS:SG	2.19	0.81
1:B:108:GLU:HG3	1:B:109:LYS:HG3	1.63	0.81
1:B:165:ALA:HB2	1:B:173:LEU:HD12	1.62	0.81
1:B:92:CYS:O	1:B:104:ILE:HG23	1.81	0.81
1:B:281:CYS:HB3	1:B:302:VAL:HG22	1.62	0.81
1:B:274:LYS:HA	1:B:313:ARG:HB3	1.63	0.80
1:A:45:SER:HA	1:A:167:TYR:CE2	2.16	0.80
1:A:53:ILE:HG21	1:B:196:VAL:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HD11	1:B:324:VAL:HG13	1.62	0.80
1:B:46:THR:HG22	1:B:49:ARG:HD3	1.65	0.79
1:B:81:VAL:O	1:B:85:LEU:HG	1.83	0.79
1:A:295:ALA:HA	1:A:318:LEU:HB3	1.63	0.79
1:A:317:ILE:HG22	1:A:324:VAL:HG23	1.64	0.79
1:A:41:VAL:O	1:A:45:SER:HB2	1.83	0.79
1:A:265:PRO:HA	1:A:315:PRO:HB3	1.63	0.79
1:A:277:LEU:HD12	1:A:281:CYS:SG	2.23	0.79
1:A:120:LEU:HD11	1:A:123:SER:HB3	1.65	0.78
1:B:39:THR:HA	1:B:42:LYS:HD3	1.63	0.78
1:B:114:VAL:HB	1:B:139:TYR:CB	2.13	0.77
1:A:139:TYR:CE2	1:A:154:GLN:HB2	2.18	0.77
1:A:71:LYS:HG2	1:A:74:ASP:HB3	1.64	0.77
1:A:248:MET:HA	1:A:262:PHE:CE2	2.20	0.77
1:A:85:LEU:HD13	1:A:94:LEU:HD22	1.66	0.76
1:A:13:LEU:CD1	1:A:175:LEU:HD22	2.14	0.76
1:B:321:PRO:O	1:B:325:THR:HB	1.84	0.76
1:A:160:VAL:HG12	1:A:178:VAL:HB	1.68	0.76
1:A:211:ILE:HB	1:A:263:MET:HB2	1.67	0.76
1:B:244:TYR:CE2	1:B:246:GLY:HA2	2.21	0.75
1:B:275:LEU:HB3	1:B:280:GLU:HG2	1.69	0.75
1:A:275:LEU:HD12	1:A:281:CYS:HB3	1.68	0.75
1:B:12:THR:HA	1:B:194:ILE:HG12	1.70	0.74
1:B:55:HIS:HB2	1:B:57:TYR:CE1	2.22	0.74
1:A:49:ARG:CA	1:B:170:ALA:HB2	2.16	0.74
1:B:93:VAL:HB	1:B:114:VAL:HG13	1.70	0.74
1:A:139:TYR:HE1	1:A:159:LEU:HD12	1.53	0.74
1:A:202:ILE:HD11	1:A:288:MET:SD	2.28	0.74
1:A:248:MET:HA	1:A:262:PHE:HE2	1.52	0.73
1:B:11:VAL:O	1:B:194:ILE:HG23	1.88	0.73
1:B:46:THR:HA	1:B:49:ARG:HB3	1.70	0.73
1:A:184:PHE:HA	1:A:195:LEU:HA	1.70	0.73
1:A:277:LEU:CB	1:A:281:CYS:SG	2.76	0.73
1:A:134:THR:H	1:A:165:ALA:HB3	1.51	0.73
1:B:261:ILE:HD13	1:B:323:ASP:HB3	1.69	0.73
1:A:16:PHE:O	1:A:20:GLN:HG2	1.88	0.73
1:A:50:LYS:HB3	1:A:55:HIS:CB	2.19	0.73
1:B:112:LYS:HG3	1:B:113:TYR:CE1	2.23	0.73
1:A:76:LEU:HA	1:A:79:ASP:HB2	1.70	0.73
1:A:128:CYS:HB3	1:B:254:ARG:HA	1.68	0.73
1:A:11:VAL:HA	1:A:15:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:MET:O	1:B:290:LYS:HE2	1.89	0.72
1:B:133:GLY:HA3	1:B:249:VAL:HG11	1.70	0.72
1:B:277:LEU:HD13	1:B:305:ILE:HB	1.70	0.72
1:B:134:THR:O	1:B:164:TYR:HB2	1.89	0.72
1:A:183:CYS:O	1:A:195:LEU:HA	1.89	0.72
1:A:162:ALA:HB1	1:A:283:PRO:HA	1.72	0.72
1:A:211:ILE:HG13	1:A:264:TYR:HD1	1.54	0.72
1:A:231:LYS:O	1:A:233:PRO:HD3	1.90	0.72
1:B:86:LYS:NZ	1:B:103:ILE:HG22	2.05	0.72
1:B:296:THR:HB	1:B:317:ILE:HB	1.71	0.72
1:A:42:LYS:O	1:A:45:SER:HB3	1.88	0.71
1:A:181:VAL:HB	1:A:200:VAL:HB	1.71	0.71
1:B:84:VAL:HG23	1:B:85:LEU:HD23	1.71	0.71
1:B:104:ILE:HG22	1:B:105:VAL:H	1.56	0.71
1:A:12:THR:HG22	1:A:192:GLU:HG3	1.73	0.71
1:B:37:LEU:HA	1:B:85:LEU:CD2	2.21	0.71
1:B:161:ALA:HA	1:B:176:ALA:O	1.91	0.71
1:B:209:TYR:HE1	1:B:242:ALA:HB2	1.56	0.71
1:A:296:THR:O	1:A:316:ILE:HA	1.91	0.70
1:B:185:MET:HB3	1:B:196:VAL:HG22	1.72	0.70
1:A:41:VAL:HG13	1:A:165:ALA:HB1	1.73	0.70
1:A:139:TYR:CZ	1:A:154:GLN:HB2	2.26	0.70
1:B:155:PRO:HB3	1:B:305:ILE:H	1.56	0.70
1:B:122:GLY:HA3	1:B:132:ILE:HD13	1.73	0.70
1:B:294:LEU:HG	1:B:321:PRO:HA	1.74	0.70
1:A:118:ASP:HB2	1:A:279:TYR:O	1.91	0.70
1:A:164:TYR:HD1	1:A:164:TYR:H	1.37	0.70
1:B:95:VAL:HG22	1:B:310:ILE:HD12	1.73	0.70
1:A:16:PHE:CE1	1:A:20:GLN:HG3	2.26	0.70
1:A:135:ILE:HA	1:A:164:TYR:HA	1.72	0.70
1:A:277:LEU:HA	1:A:281:CYS:SG	2.32	0.70
1:B:90:ALA:HA	1:B:111:GLY:CA	2.19	0.70
1:B:263:MET:HA	1:B:317:ILE:HA	1.72	0.70
1:B:245:VAL:HG11	1:B:250:ALA:HB3	1.73	0.70
1:A:203:LYS:HE2	1:A:258:TYR:O	1.92	0.69
1:B:252:VAL:HG21	1:B:284:MET:HG2	1.74	0.69
1:A:80:LEU:O	1:A:84:VAL:HG13	1.91	0.69
1:B:115:VAL:HA	1:B:138:ILE:HA	1.74	0.69
1:A:117:PHE:CB	1:A:136:PHE:HA	2.22	0.69
1:B:86:LYS:HZ1	1:B:103:ILE:HG22	1.56	0.69
1:B:226:TYR:CD2	1:B:327:LEU:HD13	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:HB2	1:A:181:VAL:HA	1.75	0.68
1:A:41:VAL:HA	1:A:167:TYR:OH	1.92	0.68
1:A:50:LYS:HB3	1:A:55:HIS:HB3	1.74	0.68
1:A:201:LYS:HA	1:A:291:ALA:O	1.94	0.68
1:B:264:TYR:CE2	1:B:274:LYS:HG2	2.29	0.68
1:B:96:THR:HA	1:B:117:PHE:O	1.93	0.68
1:B:248:MET:O	1:B:251:ASP:HB2	1.92	0.68
1:B:209:TYR:CA	1:B:261:ILE:HG22	2.24	0.68
1:A:55:HIS:O	1:A:56:LEU:HB2	1.91	0.68
1:A:173:LEU:O	1:A:184:PHE:HD2	1.76	0.68
1:A:277:LEU:CA	1:A:281:CYS:SG	2.82	0.67
1:A:130:VAL:HG13	1:A:131:SER:N	2.09	0.67
1:B:294:LEU:HB2	1:B:324:VAL:CG2	2.24	0.67
1:A:217:LYS:HD3	1:B:232:PHE:HB3	1.77	0.67
1:A:285:ALA:O	1:A:289:GLU:HG3	1.94	0.67
1:A:11:VAL:O	1:A:194:ILE:HA	1.95	0.67
1:A:49:ARG:HA	1:B:169:SER:O	1.95	0.67
1:A:121:ASP:N	1:A:135:ILE:HD11	2.10	0.67
1:A:233:PRO:HB2	1:A:237:SER:HB3	1.76	0.67
1:B:115:VAL:HG13	1:B:138:ILE:HG13	1.77	0.67
1:A:275:LEU:CD1	1:A:281:CYS:HB3	2.25	0.67
1:B:185:MET:HE2	1:B:196:VAL:CG2	2.25	0.66
1:B:41:VAL:HG11	1:B:173:LEU:CD1	2.26	0.66
1:B:202:ILE:HB	1:B:258:TYR:O	1.95	0.66
1:B:294:LEU:HB2	1:B:324:VAL:HG21	1.77	0.66
1:B:327:LEU:HA	1:B:330:ILE:HD12	1.77	0.66
1:A:231:LYS:NZ	1:B:213:GLU:HG2	2.10	0.66
1:A:208:ILE:HA	1:A:241:GLY:O	1.96	0.66
1:B:223:ILE:O	1:B:227:ILE:HG13	1.96	0.66
1:A:162:ALA:CB	1:A:283:PRO:HA	2.26	0.65
1:B:307:PRO:HA	1:B:312:GLN:OE1	1.97	0.65
1:B:182:ASN:HA	1:B:198:ARG:O	1.96	0.65
1:B:281:CYS:HB3	1:B:302:VAL:CG2	2.26	0.65
1:B:283:PRO:O	1:B:287:VAL:HG23	1.97	0.65
1:A:327:LEU:HD12	1:A:330:ILE:HB	1.77	0.65
1:A:57:TYR:HA	1:A:62:SER:HB3	1.78	0.65
1:B:105:VAL:HG12	1:B:109:LYS:HD2	1.79	0.65
1:B:202:ILE:HD12	1:B:259:GLY:HA2	1.79	0.65
1:B:288:MET:SD	1:B:293:GLY:HA3	2.37	0.64
1:B:37:LEU:HA	1:B:85:LEU:HD21	1.79	0.64
1:B:254:ARG:HH11	1:B:255:THR:H	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HB2	1:B:103:ILE:O	1.97	0.64
1:A:109:LYS:H	1:A:109:LYS:HD2	1.62	0.64
1:A:136:PHE:CD1	1:A:137:GLY:N	2.67	0.63
1:B:222:ALA:O	1:B:226:TYR:HB3	1.99	0.63
1:B:228:GLN:HA	1:B:231:LYS:CG	2.29	0.63
1:B:273:GLY:CA	1:B:315:PRO:HG3	2.26	0.63
1:A:212:ASN:HB3	1:A:215:TYR:CD2	2.33	0.63
1:B:226:TYR:HD2	1:B:330:ILE:HD13	1.64	0.63
1:B:263:MET:HE3	1:B:317:ILE:HG23	1.80	0.63
1:B:139:TYR:HE2	1:B:154:GLN:HB2	1.63	0.63
1:B:210:SER:O	1:B:211:ILE:HB	1.98	0.63
1:A:174:VAL:HA	1:A:183:CYS:CA	2.21	0.62
1:B:98:GLU:HB2	1:B:119:PRO:HG3	1.80	0.62
1:B:209:TYR:CE1	1:B:242:ALA:HB2	2.34	0.62
1:B:114:VAL:HG21	1:B:141:LYS:HD3	1.81	0.62
1:A:217:LYS:HB3	1:B:232:PHE:CD1	2.34	0.62
1:A:327:LEU:HA	1:A:330:ILE:CD1	2.25	0.62
1:B:41:VAL:HA	1:B:167:TYR:OH	1.98	0.62
1:A:99:ASP:HB3	1:A:101:ASN:O	1.99	0.62
1:A:278:LEU:C	1:A:279:TYR:HD1	2.03	0.62
1:B:91:THR:CB	1:B:105:VAL:HG21	2.30	0.62
1:B:277:LEU:HD11	1:B:282:ASN:HD21	1.64	0.62
1:B:126:ILE:O	1:B:129:LEU:HA	2.00	0.62
1:B:261:ILE:HG23	1:B:261:ILE:O	2.00	0.62
1:A:159:LEU:HD23	1:A:161:ALA:H	1.65	0.62
1:A:251:ASP:HA	1:A:254:ARG:NH1	2.15	0.62
1:B:277:LEU:HD12	1:B:281:CYS:HB2	1.82	0.62
1:A:136:PHE:N	1:A:163:GLY:O	2.32	0.61
1:B:186:LEU:HB2	1:B:193:PHE:CD1	2.35	0.61
1:A:137:GLY:HA2	1:A:162:ALA:HA	1.81	0.61
1:A:262:PHE:O	1:A:317:ILE:HA	2.00	0.61
1:B:112:LYS:C	1:B:113:TYR:HD1	2.04	0.61
1:B:275:LEU:HA	1:B:276:ARG:NH1	2.14	0.61
1:A:54:ALA:O	1:A:59:ILE:HG21	2.00	0.61
1:A:211:ILE:HG13	1:A:264:TYR:CD1	2.35	0.61
1:B:162:ALA:O	1:B:175:LEU:HA	1.99	0.61
1:A:66:THR:HG21	1:A:75:VAL:HG11	1.81	0.61
1:A:253:HIS:ND1	1:A:256:LEU:HD13	2.14	0.61
1:A:299:LYS:HD2	1:A:331:TYR:HE2	1.66	0.61
1:B:105:VAL:O	1:B:110:ARG:HG3	2.00	0.61
1:A:187:ASP:HB3	1:A:190:ILE:CG1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:HG22	1:A:315:PRO:O	2.01	0.61
1:B:99:ASP:O	1:B:100:LYS:HD2	2.01	0.61
1:B:114:VAL:CB	1:B:139:TYR:HB2	2.20	0.61
1:A:128:CYS:HB3	1:B:254:ARG:CA	2.30	0.61
1:A:173:LEU:O	1:A:184:PHE:CD2	2.54	0.61
1:B:14:THR:O	1:B:18:MET:HB2	2.00	0.61
1:B:93:VAL:HB	1:B:114:VAL:CG1	2.31	0.60
1:B:218:GLU:HB3	1:B:267:ASN:HB2	1.83	0.60
1:B:289:GLU:HG2	1:B:295:ALA:HB3	1.82	0.60
1:A:55:HIS:HA	1:A:59:ILE:HG23	1.83	0.60
1:A:176:ALA:HB2	1:A:181:VAL:HG13	1.83	0.60
1:B:275:LEU:O	1:B:280:GLU:HB2	2.00	0.60
1:A:257:VAL:HG12	1:A:258:TYR:H	1.67	0.60
1:B:33:LEU:O	1:B:37:LEU:HB2	2.01	0.60
1:A:244:TYR:HE1	1:A:262:PHE:CZ	2.18	0.60
1:A:169:SER:HB3	1:B:48:VAL:HG23	1.82	0.60
1:B:296:THR:HG22	1:B:297:THR:H	1.67	0.60
1:A:115:VAL:HA	1:A:138:ILE:HG23	1.82	0.60
1:B:33:LEU:HD21	1:B:85:LEU:HB3	1.83	0.60
1:A:12:THR:HA	1:A:193:PHE:O	2.02	0.60
1:A:37:LEU:O	1:A:41:VAL:HG23	2.02	0.60
1:B:104:ILE:HG22	1:B:105:VAL:N	2.16	0.60
1:A:156:GLY:CA	1:A:303:LEU:HD22	2.23	0.59
1:B:13:LEU:O	1:B:17:VAL:HG23	2.02	0.59
1:A:134:THR:CB	1:A:165:ALA:HB3	2.33	0.59
1:B:274:LYS:CA	1:B:313:ARG:HB3	2.32	0.59
1:A:89:PHE:HD1	1:A:109:LYS:HA	1.67	0.59
1:A:297:THR:CB	1:A:315:PRO:HG2	2.14	0.59
1:B:112:LYS:HG3	1:B:113:TYR:CD1	2.38	0.59
1:B:120:LEU:HD12	1:B:167:TYR:HE2	1.68	0.59
1:A:231:LYS:HZ2	1:B:213:GLU:HG2	1.67	0.59
1:B:132:ILE:O	1:B:166:LEU:HG	2.02	0.59
1:B:297:THR:HG23	1:B:315:PRO:HD2	1.85	0.59
1:A:204:LYS:O	1:A:320:SER:HB3	2.02	0.59
1:B:93:VAL:HA	1:B:104:ILE:HD12	1.84	0.59
1:A:41:VAL:CG1	1:A:167:TYR:HE1	2.16	0.58
1:A:318:LEU:CA	1:A:324:VAL:HG21	2.23	0.58
1:A:286:TYR:CE2	1:A:290:LYS:HD3	2.39	0.58
1:B:223:ILE:O	1:B:226:TYR:HD1	1.86	0.58
1:B:40:ALA:O	1:B:44:ILE:HG13	2.03	0.58
1:B:96:THR:HG22	1:B:97:GLU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:N	1:A:165:ALA:HB3	2.17	0.58
1:A:223:ILE:C	1:A:225:GLU:H	2.06	0.58
1:A:48:VAL:HA	1:A:51:ALA:CB	2.33	0.58
1:B:120:LEU:HD12	1:B:167:TYR:CE2	2.39	0.58
1:A:233:PRO:CB	1:A:237:SER:HB3	2.34	0.58
1:B:121:ASP:CG	1:B:134:THR:HA	2.24	0.58
1:B:141:LYS:HE2	1:B:151:ASP:HB3	1.86	0.58
1:B:196:VAL:O	1:B:196:VAL:HG23	2.03	0.58
1:B:218:GLU:HB3	1:B:267:ASN:CB	2.33	0.58
1:B:252:VAL:HB	1:B:284:MET:SD	2.43	0.58
1:A:131:SER:HB2	1:A:250:ALA:HB2	1.85	0.57
1:A:153:LEU:HD23	1:A:307:PRO:HB2	1.85	0.57
1:A:174:VAL:CG1	1:A:181:VAL:HG12	2.33	0.57
1:A:296:THR:CA	1:A:302:VAL:HG22	2.34	0.57
1:A:174:VAL:HG22	1:A:183:CYS:HB3	1.85	0.57
1:A:131:SER:HB2	1:A:250:ALA:CB	2.34	0.57
1:A:33:LEU:HD22	1:A:34:LEU:HD23	1.87	0.57
1:A:160:VAL:CG1	1:A:178:VAL:HB	2.33	0.57
1:A:166:LEU:HD22	1:A:253:HIS:CD2	2.40	0.57
1:B:223:ILE:HA	1:B:226:TYR:CD1	2.39	0.57
1:B:224:THR:C	1:B:226:TYR:H	2.06	0.57
1:B:327:LEU:O	1:B:330:ILE:HB	2.05	0.57
1:A:156:GLY:HA3	1:A:303:LEU:CD2	2.25	0.57
1:A:279:TYR:N	1:A:279:TYR:CD1	2.72	0.57
1:B:121:ASP:OD1	1:B:134:THR:HA	2.04	0.57
1:B:93:VAL:HA	1:B:104:ILE:CD1	2.35	0.57
1:A:296:THR:HA	1:A:302:VAL:H	1.70	0.57
1:A:120:LEU:HD11	1:A:123:SER:CB	2.34	0.56
1:A:217:LYS:HB3	1:B:232:PHE:CE1	2.40	0.56
1:A:139:TYR:CE1	1:A:159:LEU:HD12	2.35	0.56
1:A:150:LYS:O	1:A:152:ALA:N	2.38	0.56
1:B:263:MET:CB	1:B:317:ILE:HG12	2.28	0.56
1:B:228:GLN:HA	1:B:231:LYS:HB2	1.88	0.56
1:A:184:PHE:CD1	1:A:195:LEU:HB2	2.41	0.56
1:A:85:LEU:HB3	1:A:91:THR:HG21	1.86	0.56
1:A:226:TYR:HE2	1:A:261:ILE:HD12	1.71	0.56
1:A:141:LYS:HE3	1:A:143:SER:C	2.26	0.56
1:B:101:ASN:O	1:B:103:ILE:HD12	2.06	0.56
1:B:105:VAL:CG1	1:B:109:LYS:HD2	2.35	0.56
1:B:115:VAL:HG22	1:B:138:ILE:HG13	1.88	0.56
1:B:282:ASN:O	1:B:286:TYR:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PHE:CE1	1:A:195:LEU:HB2	2.39	0.56
1:A:244:TYR:HE1	1:A:262:PHE:HZ	1.52	0.56
1:A:245:VAL:HG11	1:A:250:ALA:HB3	1.86	0.56
1:B:30:MET:SD	1:B:113:TYR:HE2	2.28	0.56
1:B:207:SER:O	1:B:240:TYR:HA	2.06	0.56
1:A:59:ILE:HG23	1:A:59:ILE:O	2.05	0.56
1:A:121:ASP:H	1:A:135:ILE:HD11	1.71	0.56
1:B:33:LEU:HD21	1:B:85:LEU:CB	2.36	0.56
1:A:299:LYS:HE3	1:A:299:LYS:HA	1.88	0.55
1:B:187:ASP:O	1:B:191:GLY:N	2.39	0.55
1:A:186:LEU:HG	1:A:187:ASP:N	2.21	0.55
1:B:162:ALA:HB1	1:B:283:PRO:CA	2.33	0.55
1:B:302:VAL:C	1:B:304:ASP:H	2.10	0.55
1:A:248:MET:O	1:A:252:VAL:HG12	2.06	0.55
1:A:297:THR:HG23	1:A:300:GLU:O	2.07	0.55
1:B:269:LYS:O	1:B:269:LYS:HG2	2.06	0.55
1:A:41:VAL:HB	1:A:193:PHE:CE1	2.42	0.55
1:A:202:ILE:HG21	1:A:293:GLY:HA2	1.89	0.55
1:B:115:VAL:HG22	1:B:138:ILE:HG23	1.88	0.55
1:B:207:SER:HA	1:B:240:TYR:CE1	2.42	0.55
1:A:289:GLU:OE1	1:A:303:LEU:HD12	2.06	0.55
1:B:19:GLU:HA	1:B:22:ARG:HD3	1.89	0.55
1:B:47:ALA:HB1	1:B:73:LEU:HD11	1.89	0.55
1:B:263:MET:CE	1:B:317:ILE:HG23	2.36	0.55
1:B:282:ASN:HD22	1:B:282:ASN:N	2.03	0.55
1:A:133:GLY:HA3	1:A:165:ALA:O	2.06	0.55
1:B:328:LEU:O	1:B:332:GLN:HG3	2.07	0.55
1:A:33:LEU:HD11	1:A:138:ILE:HD13	1.88	0.54
1:A:278:LEU:C	1:A:279:TYR:CD1	2.81	0.54
1:B:89:PHE:CB	1:B:109:LYS:HB3	2.36	0.54
1:B:209:TYR:CB	1:B:261:ILE:HG22	2.38	0.54
1:B:275:LEU:HB3	1:B:280:GLU:CG	2.37	0.54
1:A:117:PHE:HB2	1:A:135:ILE:O	2.07	0.54
1:B:38:CYS:O	1:B:42:LYS:HG3	2.06	0.54
1:B:106:GLU:C	1:B:108:GLU:H	2.09	0.54
1:B:274:LYS:HA	1:B:313:ARG:CB	2.37	0.54
1:A:183:CYS:O	1:A:195:LEU:HD12	2.08	0.54
1:A:101:ASN:HA	1:A:310:ILE:HD13	1.89	0.54
1:A:156:GLY:C	1:A:303:LEU:HD13	2.28	0.54
1:B:327:LEU:HA	1:B:330:ILE:HB	1.90	0.54
1:A:217:LYS:HG3	1:A:218:GLU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HD22	1:A:273:GLY:HA2	1.73	0.54
1:A:285:ALA:HB2	1:A:316:ILE:HD11	1.90	0.54
1:B:204:LYS:HB3	1:B:322:GLU:OE1	2.08	0.54
1:A:41:VAL:O	1:A:167:TYR:CE1	2.61	0.54
1:A:185:MET:N	1:A:194:ILE:O	2.41	0.54
1:B:264:TYR:N	1:B:316:ILE:O	2.41	0.54
1:A:33:LEU:O	1:A:35:ASN:N	2.41	0.54
1:A:48:VAL:HA	1:A:51:ALA:HB3	1.90	0.54
1:B:226:TYR:HD2	1:B:330:ILE:CD1	2.21	0.54
1:A:16:PHE:CD2	1:A:184:PHE:HZ	2.26	0.53
1:A:49:ARG:HB3	1:B:170:ALA:HB2	1.89	0.53
1:B:135:ILE:HG22	1:B:283:PRO:HB2	1.90	0.53
1:A:49:ARG:HA	1:B:170:ALA:CB	2.31	0.53
1:A:174:VAL:HG22	1:A:183:CYS:CB	2.38	0.53
1:B:86:LYS:HE2	1:B:105:VAL:HG22	1.89	0.53
1:A:156:GLY:HA2	1:A:159:LEU:CB	2.37	0.53
1:A:218:GLU:O	1:A:268:LYS:HG3	2.07	0.53
1:A:328:LEU:O	1:A:332:GLN:HB2	2.07	0.53
1:A:99:ASP:O	1:A:311:HIS:CE1	2.61	0.53
1:A:305:ILE:O	1:A:307:PRO:HD3	2.08	0.53
1:A:285:ALA:HB2	1:A:316:ILE:CD1	2.38	0.53
1:B:279:TYR:CD1	1:B:279:TYR:N	2.77	0.53
1:A:202:ILE:HD11	1:A:255:THR:HG22	1.91	0.53
1:B:203:LYS:HE3	1:B:206:GLY:HA2	1.91	0.53
1:B:289:GLU:CG	1:B:295:ALA:HB3	2.39	0.53
1:A:178:VAL:HA	1:A:290:LYS:NZ	2.24	0.53
1:B:121:ASP:OD2	1:B:134:THR:HA	2.09	0.53
1:B:176:ALA:HB2	1:B:287:VAL:HA	1.91	0.53
1:A:186:LEU:HD12	1:A:192:GLU:O	2.09	0.53
1:B:245:VAL:HG21	1:B:250:ALA:CB	2.39	0.52
1:A:64:ASN:O	1:A:72:LYS:HE2	2.09	0.52
1:A:214:GLY:HA2	1:B:209:TYR:CZ	2.44	0.52
1:B:46:THR:HB	1:B:50:LYS:HB2	1.91	0.52
1:B:209:TYR:HB2	1:B:261:ILE:HG22	1.92	0.52
1:B:210:SER:N	1:B:261:ILE:O	2.43	0.52
1:A:49:ARG:CB	1:B:170:ALA:HB2	2.39	0.52
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.50	0.52
1:A:277:LEU:HD23	1:A:278:LEU:HD23	1.92	0.52
1:B:16:PHE:O	1:B:20:GLN:HB2	2.09	0.52
1:B:276:ARG:HA	1:B:312:GLN:O	2.08	0.52
1:A:295:ALA:O	1:A:296:THR:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HA	1:A:313:ARG:HA	1.91	0.52
1:A:127:ASP:HB3	1:B:257:VAL:HG11	1.92	0.52
1:A:151:ASP:C	1:A:153:LEU:H	2.13	0.52
1:B:207:SER:HA	1:B:240:TYR:CZ	2.44	0.52
1:B:309:ASP:C	1:B:311:HIS:H	2.13	0.52
1:A:202:ILE:HG13	1:A:293:GLY:HA3	1.91	0.52
1:B:226:TYR:O	1:B:229:ARG:HB3	2.10	0.52
1:A:53:ILE:HG12	1:A:54:ALA:N	2.25	0.52
1:A:122:GLY:HA3	2:A:338:F6P:O1	2.10	0.52
1:A:174:VAL:CG1	1:A:183:CYS:SG	2.95	0.52
1:A:308:THR:O	1:A:309:ASP:HB2	2.10	0.52
1:B:41:VAL:HG12	1:B:167:TYR:HE1	1.75	0.52
1:B:261:ILE:HG13	1:B:263:MET:SD	2.50	0.52
1:A:91:THR:O	1:A:110:ARG:HA	2.10	0.52
1:A:117:PHE:HB3	1:A:136:PHE:HA	1.92	0.52
1:A:176:ALA:HB1	1:A:180:GLY:O	2.09	0.52
1:A:230:LYS:HG3	1:A:240:TYR:CB	2.40	0.52
1:A:275:LEU:HA	1:A:280:GLU:OE2	2.10	0.52
1:A:169:SER:CB	1:B:48:VAL:HG23	2.39	0.51
1:A:253:HIS:HA	1:A:256:LEU:HD12	1.91	0.51
1:A:13:LEU:HD13	1:A:184:PHE:CE2	2.45	0.51
1:A:277:LEU:HA	1:A:281:CYS:H	1.75	0.51
1:A:310:ILE:HB	1:A:311:HIS:HD2	1.75	0.51
1:A:329:GLU:HA	1:A:332:GLN:HB2	1.91	0.51
1:A:12:THR:CG2	1:A:192:GLU:HG3	2.37	0.51
1:A:209:TYR:CD1	1:A:240:TYR:HD2	2.29	0.51
1:A:210:SER:O	1:A:263:MET:N	2.40	0.51
1:B:78:ASN:OD1	1:B:96:THR:HG21	2.11	0.51
1:B:89:PHE:CG	1:B:109:LYS:HB3	2.45	0.51
1:B:245:VAL:HG21	1:B:250:ALA:HB1	1.92	0.51
1:B:17:VAL:HG11	1:B:34:LEU:HD12	1.92	0.51
1:B:91:THR:OG1	1:B:105:VAL:HG21	2.10	0.51
1:A:230:LYS:HG3	1:A:240:TYR:HB2	1.93	0.51
1:A:30:MET:SD	1:A:113:TYR:CE1	3.04	0.51
1:A:104:ILE:HD11	1:A:149:GLU:N	2.26	0.51
1:B:81:VAL:HA	1:B:84:VAL:HG22	1.92	0.51
1:B:288:MET:HG3	1:B:293:GLY:O	2.11	0.51
1:A:214:GLY:HA2	1:B:209:TYR:OH	2.10	0.51
1:B:226:TYR:CD2	1:B:330:ILE:HD13	2.45	0.51
1:B:277:LEU:HD13	1:B:305:ILE:HD12	1.92	0.51
1:A:30:MET:HA	1:A:113:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PHE:O	1:A:194:ILE:HD13	2.10	0.51
1:A:248:MET:SD	1:A:280:GLU:O	2.69	0.51
1:A:11:VAL:H	1:A:194:ILE:HG23	1.77	0.50
1:A:178:VAL:HG22	1:A:178:VAL:O	2.11	0.50
1:B:297:THR:HG22	1:B:298:GLY:N	2.26	0.50
1:A:130:VAL:CG1	1:A:131:SER:N	2.74	0.50
1:A:217:LYS:HG3	1:A:218:GLU:H	1.76	0.50
1:B:33:LEU:HG	1:B:88:SER:OG	2.11	0.50
1:B:263:MET:CA	1:B:317:ILE:HA	2.41	0.50
1:A:245:VAL:HG11	1:A:250:ALA:CB	2.41	0.50
1:A:8:THR:HG22	1:A:8:THR:O	2.11	0.50
1:A:213:GLU:O	1:B:231:LYS:NZ	2.39	0.50
1:A:207:SER:HA	1:A:240:TYR:CE1	2.47	0.50
1:B:30:MET:HG3	1:B:34:LEU:CD1	2.42	0.50
1:A:41:VAL:HG12	1:A:167:TYR:HE1	1.76	0.50
1:A:230:LYS:HG3	1:A:240:TYR:CG	2.47	0.50
1:A:131:SER:O	1:A:250:ALA:HB2	2.11	0.50
1:B:77:SER:O	1:B:81:VAL:HG23	2.12	0.50
1:B:163:GLY:HA2	1:B:174:VAL:O	2.12	0.50
1:B:185:MET:HB3	1:B:196:VAL:CG2	2.39	0.50
1:B:223:ILE:HG13	1:B:265:PRO:CG	2.42	0.50
1:B:277:LEU:HA	1:B:281:CYS:CB	2.42	0.50
1:A:267:ASN:OD1	1:A:269:LYS:HB3	2.12	0.49
1:A:277:LEU:O	1:A:282:ASN:HB2	2.12	0.49
1:A:296:THR:N	1:A:302:VAL:HG22	2.26	0.49
1:A:310:ILE:HD12	1:A:311:HIS:CD2	2.47	0.49
1:B:86:LYS:CD	1:B:105:VAL:HG22	2.41	0.49
1:B:135:ILE:HA	1:B:164:TYR:HB2	1.93	0.49
1:A:16:PHE:HD2	1:A:184:PHE:HZ	1.61	0.49
1:A:184:PHE:HA	1:A:195:LEU:CA	2.42	0.49
1:A:243:ALA:CB	1:B:246:GLY:HA3	2.34	0.49
1:B:55:HIS:HB2	1:B:57:TYR:HE1	1.72	0.49
1:B:90:ALA:CA	1:B:111:GLY:HA3	2.27	0.49
1:A:247:SER:HB3	1:A:250:ALA:HB3	1.94	0.49
1:B:270:SER:N	1:B:271:PRO:HD3	2.27	0.49
1:B:289:GLU:HG2	1:B:295:ALA:CB	2.43	0.49
1:A:45:SER:CA	1:A:167:TYR:CE2	2.93	0.49
1:B:104:ILE:CG2	1:B:105:VAL:H	2.24	0.49
1:B:122:GLY:CA	1:B:132:ILE:HD13	2.41	0.49
1:B:330:ILE:O	1:B:334:HIS:ND1	2.46	0.49
1:A:134:THR:HG22	1:A:135:ILE:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:PRO:HG2	3:A:339:HOH:O	2.12	0.49
1:B:220:ASP:HB2	1:B:221:PRO:HD2	1.95	0.49
1:B:226:TYR:OH	1:B:263:MET:HE1	2.13	0.49
1:B:248:MET:CE	1:B:275:LEU:HD13	2.43	0.49
1:A:174:VAL:CA	1:A:183:CYS:HA	2.24	0.49
1:B:161:ALA:HB1	1:B:175:LEU:HG	1.95	0.49
1:B:181:VAL:HG21	1:B:291:ALA:CB	2.42	0.49
1:B:186:LEU:HB2	1:B:193:PHE:HD1	1.75	0.49
1:B:215:TYR:HD2	1:B:219:PHE:CE1	2.31	0.49
1:A:38:CYS:O	1:A:193:PHE:CZ	2.66	0.49
1:B:76:LEU:O	1:B:80:LEU:HB2	2.13	0.49
1:B:149:GLU:O	1:B:153:LEU:HG	2.13	0.49
1:A:110:ARG:NH1	1:A:147:PRO:HD2	2.28	0.49
1:A:245:VAL:HG12	1:A:247:SER:H	1.77	0.49
1:B:89:PHE:N	1:B:89:PHE:HD1	2.11	0.49
1:B:95:VAL:HB	1:B:116:CYS:SG	2.52	0.49
1:B:186:LEU:HA	1:B:192:GLU:O	2.13	0.49
1:A:30:MET:SD	1:A:113:TYR:CD1	3.06	0.48
1:B:201:LYS:HD3	1:B:291:ALA:O	2.13	0.48
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.95	0.48
1:A:186:LEU:HA	1:A:193:PHE:HA	1.96	0.48
1:A:248:MET:SD	1:A:284:MET:SD	3.10	0.48
1:A:134:THR:HB	1:A:165:ALA:CB	2.43	0.48
1:A:245:VAL:HG21	1:A:250:ALA:HB1	1.95	0.48
1:A:275:LEU:O	1:A:277:LEU:N	2.41	0.48
1:A:277:LEU:HD13	1:A:314:ALA:HB3	1.94	0.48
1:A:231:LYS:HB2	1:A:232:PHE:CD1	2.49	0.48
1:A:277:LEU:CD1	1:A:281:CYS:SG	2.98	0.48
1:B:137:GLY:C	1:B:138:ILE:HD12	2.34	0.48
1:A:91:THR:CG2	1:A:94:LEU:HD21	2.44	0.48
1:A:100:LYS:O	1:A:311:HIS:NE2	2.46	0.48
1:A:105:VAL:HG11	1:A:109:LYS:O	2.13	0.48
1:A:213:GLU:HB3	1:B:213:GLU:OE1	2.14	0.48
1:A:229:ARG:O	1:A:233:PRO:HA	2.12	0.48
1:B:122:GLY:O	1:B:124:SER:N	2.46	0.48
1:B:252:VAL:CB	1:B:284:MET:SD	3.01	0.48
1:A:17:VAL:HB	1:A:31:THR:HG23	1.96	0.48
1:A:44:ILE:O	1:A:45:SER:C	2.52	0.48
1:B:33:LEU:CD2	1:B:85:LEU:HD22	2.43	0.48
1:B:134:THR:HG22	1:B:136:PHE:HD2	1.78	0.48
1:B:229:ARG:HG2	1:B:326:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ALA:HA	1:B:253:HIS:HB2	1.94	0.48
1:B:89:PHE:N	1:B:89:PHE:CD1	2.81	0.48
1:B:254:ARG:HB3	1:B:254:ARG:NH1	2.29	0.48
1:B:98:GLU:CB	1:B:119:PRO:HG3	2.43	0.48
1:B:208:ILE:O	1:B:260:GLY:CA	2.62	0.48
1:A:297:THR:HB	1:A:315:PRO:CG	2.15	0.48
1:B:215:TYR:HB3	1:B:219:PHE:CZ	2.49	0.48
1:B:223:ILE:O	1:B:227:ILE:N	2.47	0.48
1:A:117:PHE:HE1	1:A:119:PRO:HB3	1.79	0.47
1:B:326:GLU:O	1:B:329:GLU:HB2	2.14	0.47
1:B:176:ALA:CB	1:B:287:VAL:HA	2.44	0.47
1:B:204:LYS:O	1:B:320:SER:HB3	2.14	0.47
1:B:254:ARG:HH11	1:B:255:THR:N	2.12	0.47
1:B:282:ASN:O	1:B:286:TYR:CB	2.62	0.47
1:B:45:SER:OG	1:B:167:TYR:HB3	2.14	0.47
1:B:95:VAL:HG22	1:B:310:ILE:CD1	2.43	0.47
1:B:228:GLN:HA	1:B:231:LYS:HG3	1.95	0.47
1:A:33:LEU:HD11	1:A:138:ILE:CD1	2.44	0.47
1:A:223:ILE:O	1:A:227:ILE:HG13	2.15	0.47
1:B:181:VAL:CG2	1:B:291:ALA:HA	2.44	0.47
1:A:55:HIS:HA	1:A:59:ILE:CG2	2.45	0.47
1:B:120:LEU:HD23	1:B:120:LEU:O	2.14	0.47
1:B:196:VAL:O	1:B:197:ASP:HB2	2.15	0.47
1:B:33:LEU:HD21	1:B:85:LEU:HA	1.96	0.47
1:B:42:LYS:HA	1:B:193:PHE:CZ	2.50	0.47
1:B:103:ILE:O	1:B:104:ILE:HD13	2.15	0.47
1:B:104:ILE:HG13	1:B:147:PRO:HB2	1.95	0.47
1:A:33:LEU:HD22	1:A:34:LEU:CD2	2.45	0.47
1:A:42:LYS:HG2	1:A:186:LEU:HD22	1.97	0.47
1:A:164:TYR:CG	1:A:165:ALA:N	2.83	0.47
1:A:187:ASP:HB3	1:A:190:ILE:HG12	1.96	0.47
1:A:241:GLY:HA2	1:B:212:ASN:HD21	1.80	0.47
1:A:284:MET:SD	1:A:284:MET:N	2.87	0.47
1:B:106:GLU:HB2	1:B:108:GLU:CG	2.31	0.47
1:B:187:ASP:O	1:B:192:GLU:N	2.47	0.47
1:B:261:ILE:O	1:B:261:ILE:CG2	2.62	0.47
1:A:40:ALA:HA	1:A:43:ALA:HB3	1.97	0.47
1:A:243:ALA:HB1	1:B:246:GLY:CA	2.34	0.47
1:A:68:ASP:O	1:A:69:GLN:HB3	2.15	0.47
1:B:53:ILE:HD13	1:B:53:ILE:HA	1.84	0.47
1:B:86:LYS:HG2	1:B:105:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG11	1:B:284:MET:CG	2.44	0.47
1:B:252:VAL:HG11	1:B:284:MET:HG3	1.96	0.46
1:B:253:HIS:O	1:B:254:ARG:C	2.53	0.46
1:B:33:LEU:HA	1:B:36:SER:HB2	1.96	0.46
1:B:121:ASP:O	1:B:132:ILE:HD12	2.15	0.46
1:B:178:VAL:HA	1:B:290:LYS:HZ3	1.81	0.46
1:B:12:THR:HG22	1:B:192:GLU:CD	2.35	0.46
1:A:81:VAL:HA	1:A:84:VAL:HG21	1.97	0.46
1:B:98:GLU:HG3	1:B:119:PRO:HG3	1.97	0.46
1:B:139:TYR:CE2	1:B:154:GLN:HB2	2.47	0.46
1:B:229:ARG:HD3	1:B:234:PRO:CD	2.45	0.46
1:B:317:ILE:O	1:B:317:ILE:HG22	2.15	0.46
1:B:252:VAL:HG11	1:B:284:MET:SD	2.55	0.46
1:A:11:VAL:HG13	1:A:15:ARG:NH1	2.19	0.46
1:B:182:ASN:N	1:B:182:ASN:HD22	2.13	0.46
1:B:329:GLU:HG2	1:B:332:GLN:NE2	2.30	0.46
1:A:141:LYS:HZ2	1:A:143:SER:HB2	1.81	0.46
1:A:186:LEU:HD12	1:A:187:ASP:H	1.81	0.46
1:B:42:LYS:HG2	1:B:193:PHE:CZ	2.50	0.46
1:B:228:GLN:HA	1:B:231:LYS:CB	2.46	0.46
1:B:263:MET:HB3	1:B:317:ILE:HG23	1.96	0.46
1:B:276:ARG:HD3	1:B:276:ARG:H	1.80	0.46
1:A:16:PHE:CD1	1:A:20:GLN:HG3	2.50	0.46
1:B:93:VAL:O	1:B:94:LEU:HD22	2.15	0.46
1:B:126:ILE:HD12	1:B:126:ILE:HA	1.85	0.46
1:B:288:MET:SD	1:B:291:ALA:HB3	2.55	0.46
1:B:127:ASP:C	1:B:129:LEU:H	2.20	0.46
1:A:41:VAL:HB	1:A:193:PHE:CZ	2.51	0.45
1:A:97:GLU:HG2	1:A:118:ASP:OD1	2.15	0.45
1:A:181:VAL:O	1:A:199:ASN:HA	2.16	0.45
1:A:230:LYS:O	1:A:233:PRO:HG3	2.15	0.45
1:A:243:ALA:HB3	1:A:254:ARG:NH2	2.30	0.45
1:A:41:VAL:HG21	1:A:173:LEU:CD1	2.30	0.45
1:B:156:GLY:C	1:B:158:ASN:H	2.19	0.45
1:B:215:TYR:HE2	1:B:267:ASN:ND2	2.15	0.45
1:A:120:LEU:HD21	1:A:123:SER:OG	2.16	0.45
1:A:110:ARG:CZ	1:A:147:PRO:HD2	2.47	0.45
1:A:244:TYR:CE1	1:A:262:PHE:CZ	3.02	0.45
1:A:174:VAL:HG12	1:A:181:VAL:CG1	2.39	0.45
1:A:185:MET:O	1:A:194:ILE:N	2.48	0.45
1:A:217:LYS:HD3	1:B:232:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:MET:HB3	1:A:196:VAL:CG1	2.47	0.45
1:B:33:LEU:HD21	1:B:85:LEU:CA	2.46	0.45
1:B:88:SER:O	1:B:89:PHE:HB2	2.16	0.45
1:B:178:VAL:HA	1:B:290:LYS:NZ	2.32	0.45
1:B:234:PRO:C	1:B:236:ASN:H	2.20	0.45
1:B:290:LYS:O	1:B:290:LYS:HG3	2.17	0.45
1:A:261:ILE:HA	1:A:318:LEU:O	2.17	0.45
1:A:277:LEU:HB2	1:A:314:ALA:HB3	1.99	0.45
1:A:288:MET:O	1:A:293:GLY:N	2.49	0.45
1:B:33:LEU:O	1:B:33:LEU:HD22	2.16	0.45
1:B:169:SER:O	1:B:170:ALA:CB	2.65	0.45
1:B:194:ILE:CG2	1:B:196:VAL:HG13	2.38	0.45
1:A:62:SER:OG	1:A:76:LEU:HD11	2.17	0.45
1:A:285:ALA:HA	1:A:318:LEU:CD2	2.47	0.45
1:B:140:ARG:HB2	1:B:160:VAL:HG21	1.98	0.45
1:B:215:TYR:CD2	1:B:219:PHE:CE1	3.05	0.45
1:A:34:LEU:O	1:A:38:CYS:N	2.46	0.45
1:B:208:ILE:O	1:B:260:GLY:HA2	2.17	0.45
1:A:53:ILE:HG23	1:A:54:ALA:N	2.21	0.45
1:B:18:MET:O	1:B:18:MET:SD	2.75	0.45
1:B:278:LEU:HD12	1:B:310:ILE:HA	1.99	0.45
1:A:29:GLU:HA	1:A:32:GLN:HG2	1.99	0.44
1:A:37:LEU:O	1:A:40:ALA:HB3	2.18	0.44
1:A:202:ILE:N	1:A:291:ALA:O	2.50	0.44
1:A:248:MET:CA	1:A:262:PHE:HE2	2.26	0.44
1:B:167:TYR:HA	1:B:171:THR:OG1	2.17	0.44
1:A:95:VAL:HG21	1:A:152:ALA:CB	2.47	0.44
1:A:139:TYR:C	1:A:141:LYS:H	2.20	0.44
1:A:177:MET:O	1:A:290:LYS:HE2	2.17	0.44
1:B:30:MET:O	1:B:34:LEU:HG	2.16	0.44
1:B:162:ALA:CB	1:B:283:PRO:HA	2.38	0.44
1:B:172:MET:HA	1:B:184:PHE:O	2.17	0.44
1:B:253:HIS:O	1:B:256:LEU:N	2.51	0.44
1:B:35:ASN:O	1:B:38:CYS:HB3	2.17	0.44
1:B:93:VAL:C	1:B:94:LEU:HD22	2.38	0.44
1:B:210:SER:HB3	1:B:261:ILE:C	2.38	0.44
1:B:279:TYR:N	1:B:279:TYR:HD1	2.14	0.44
1:A:105:VAL:O	1:A:110:ARG:NH2	2.50	0.44
1:A:16:PHE:HD2	1:A:184:PHE:CZ	2.36	0.44
1:B:302:VAL:O	1:B:304:ASP:N	2.50	0.44
1:B:41:VAL:HG11	1:B:173:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG22	1:B:65:VAL:O	2.18	0.44
1:B:133:GLY:CA	1:B:166:LEU:HA	2.48	0.44
1:B:152:ALA:O	1:B:154:GLN:N	2.51	0.44
1:B:185:MET:O	1:B:194:ILE:N	2.50	0.44
1:B:258:TYR:HB3	1:B:259:GLY:H	1.47	0.44
1:B:270:SER:HB3	1:B:273:GLY:O	2.18	0.44
1:A:95:VAL:HG21	1:A:152:ALA:HB1	2.00	0.44
1:A:327:LEU:CA	1:A:330:ILE:HD12	2.36	0.44
1:B:48:VAL:HB	1:B:126:ILE:HG12	2.00	0.44
1:B:223:ILE:HG13	1:B:265:PRO:HG2	2.00	0.44
1:A:253:HIS:O	1:A:256:LEU:HB2	2.18	0.44
1:A:297:THR:HG22	1:A:302:VAL:HG13	2.00	0.44
1:B:82:ILE:HD12	1:B:99:ASP:OD2	2.18	0.44
1:B:233:PRO:HD3	1:B:239:PRO:HA	1.99	0.44
1:A:123:SER:O	1:A:125:ASN:N	2.51	0.44
1:B:294:LEU:CG	1:B:321:PRO:HA	2.44	0.44
1:A:134:THR:CB	1:A:165:ALA:CB	2.96	0.43
1:A:134:THR:CA	1:A:165:ALA:HB3	2.48	0.43
1:A:143:SER:HB3	1:A:144:THR:H	1.59	0.43
1:B:98:GLU:HB2	1:B:119:PRO:CG	2.48	0.43
1:B:138:ILE:HD12	1:B:138:ILE:N	2.33	0.43
1:A:11:VAL:CG1	1:A:195:LEU:HB3	2.49	0.43
1:A:317:ILE:O	1:A:324:VAL:HG21	2.18	0.43
1:B:159:LEU:HD11	1:B:282:ASN:O	2.18	0.43
1:B:252:VAL:HG21	1:B:284:MET:CG	2.47	0.43
1:B:296:THR:HG21	1:B:328:LEU:HD23	2.00	0.43
1:A:80:LEU:C	1:A:82:ILE:H	2.21	0.43
1:B:202:ILE:HD11	1:B:320:SER:OG	2.19	0.43
1:A:17:VAL:HB	1:A:31:THR:CG2	2.48	0.43
1:A:217:LYS:HZ1	1:B:239:PRO:HG3	1.83	0.43
1:A:118:ASP:HB3	1:A:135:ILE:HB	2.00	0.43
1:A:305:ILE:HG22	1:A:306:VAL:N	2.34	0.43
1:B:30:MET:HG3	1:B:34:LEU:HD11	2.00	0.43
1:B:276:ARG:HG2	1:B:311:HIS:HA	1.99	0.43
1:A:59:ILE:O	1:A:60:ALA:HB2	2.19	0.43
1:A:181:VAL:HG11	1:A:287:VAL:HG13	2.00	0.43
1:A:268:LYS:HA	1:A:268:LYS:HD3	1.85	0.43
1:A:290:LYS:C	1:A:292:GLY:H	2.22	0.43
1:B:71:LYS:HD2	1:B:71:LYS:N	2.33	0.43
1:B:176:ALA:O	1:B:286:TYR:HE1	2.02	0.43
1:B:104:ILE:CG2	1:B:105:VAL:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:O	1:B:33:LEU:CD2	2.67	0.42
1:B:123:SER:O	1:B:126:ILE:N	2.51	0.42
1:B:229:ARG:HD3	1:B:234:PRO:CG	2.49	0.42
1:A:231:LYS:HZ1	1:B:213:GLU:HG2	1.82	0.42
1:B:86:LYS:CE	1:B:105:VAL:HG22	2.49	0.42
1:B:86:LYS:HZ1	1:B:103:ILE:CG2	2.27	0.42
1:B:89:PHE:O	1:B:91:THR:N	2.52	0.42
1:B:202:ILE:HG22	1:B:256:LEU:O	2.19	0.42
1:A:33:LEU:HD22	1:A:34:LEU:H	1.84	0.42
1:A:42:LYS:HD3	1:A:186:LEU:CD1	2.49	0.42
1:A:81:VAL:HG12	1:A:81:VAL:O	2.18	0.42
1:B:277:LEU:HD11	1:B:282:ASN:ND2	2.33	0.42
1:B:316:ILE:O	1:B:317:ILE:HG13	2.19	0.42
1:A:15:ARG:NH2	3:A:354:HOH:O	2.52	0.42
1:A:50:LYS:O	1:A:55:HIS:HB2	2.19	0.42
1:B:40:ALA:HB2	1:B:84:VAL:HG21	2.00	0.42
1:B:41:VAL:HG12	1:B:167:TYR:CE1	2.53	0.42
1:B:44:ILE:HB	1:B:167:TYR:CZ	2.55	0.42
1:B:275:LEU:HA	1:B:276:ARG:HH11	1.83	0.42
1:B:310:ILE:HG13	1:B:311:HIS:CE1	2.55	0.42
1:A:128:CYS:CB	1:B:254:ARG:HB2	2.50	0.42
1:B:271:PRO:O	1:B:272:LYS:HG2	2.19	0.42
1:B:330:ILE:O	1:B:334:HIS:N	2.49	0.42
1:A:286:TYR:O	1:A:290:LYS:HG2	2.20	0.42
1:B:31:THR:HA	1:B:34:LEU:CB	2.39	0.42
1:B:40:ALA:CB	1:B:81:VAL:HG22	2.38	0.42
1:B:93:VAL:HG12	1:B:94:LEU:N	2.35	0.42
1:B:186:LEU:HD13	1:B:193:PHE:CE1	2.55	0.42
1:A:231:LYS:C	1:A:233:PRO:HD3	2.40	0.42
1:B:92:CYS:SG	1:B:113:TYR:N	2.93	0.42
1:B:210:SER:CB	1:B:262:PHE:HA	2.50	0.42
1:B:288:MET:SD	1:B:288:MET:O	2.78	0.42
1:B:302:VAL:C	1:B:304:ASP:N	2.73	0.42
1:A:154:GLN:HA	1:A:155:PRO:HD3	1.87	0.42
1:A:215:TYR:HB2	1:A:219:PHE:CZ	2.54	0.42
1:A:267:ASN:HD21	1:A:270:SER:HB2	1.84	0.42
1:B:256:LEU:C	1:B:258:TYR:H	2.22	0.42
1:B:274:LYS:HA	1:B:313:ARG:CG	2.50	0.42
1:A:10:ILE:HD12	1:A:12:THR:HG23	2.02	0.42
1:B:33:LEU:HD23	1:B:36:SER:HB2	2.01	0.42
1:B:72:LYS:C	1:B:74:ASP:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HG12	1:B:117:PHE:HZ	1.84	0.42
1:A:164:TYR:CD1	1:A:164:TYR:N	2.85	0.41
1:B:95:VAL:HG11	1:B:310:ILE:HB	2.01	0.41
1:B:205:LYS:HB3	1:B:322:GLU:HB2	2.02	0.41
1:B:277:LEU:CD1	1:B:305:ILE:HB	2.42	0.41
1:B:309:ASP:C	1:B:311:HIS:N	2.73	0.41
1:A:56:LEU:O	1:A:60:ALA:HB3	2.20	0.41
1:A:90:ALA:O	1:A:111:GLY:HA3	2.21	0.41
1:B:136:PHE:HD1	1:B:136:PHE:O	2.04	0.41
1:A:7:ASP:HB3	1:A:8:THR:H	1.73	0.41
1:A:149:GLU:HG3	1:A:150:LYS:N	2.35	0.41
1:A:151:ASP:O	1:A:154:GLN:HG3	2.20	0.41
1:A:216:ALA:CB	1:B:231:LYS:HD2	2.50	0.41
1:A:249:VAL:HA	1:A:252:VAL:HG12	2.01	0.41
1:B:123:SER:O	1:B:126:ILE:HG22	2.21	0.41
1:B:133:GLY:HA3	1:B:166:LEU:HA	2.03	0.41
1:A:262:PHE:O	1:A:317:ILE:HG23	2.20	0.41
1:A:134:THR:HB	1:A:165:ALA:HB3	2.03	0.41
1:A:279:TYR:OH	1:A:311:HIS:HA	2.21	0.41
1:B:74:ASP:N	1:B:74:ASP:OD1	2.53	0.41
1:B:113:TYR:CD1	1:B:113:TYR:N	2.89	0.41
1:B:264:TYR:CE2	1:B:273:GLY:HA2	2.56	0.41
1:A:95:VAL:CG2	1:A:152:ALA:HB2	2.51	0.41
1:A:216:ALA:HB2	1:B:231:LYS:HZ2	1.84	0.41
1:A:253:HIS:HA	1:A:256:LEU:CD1	2.50	0.41
1:A:296:THR:HA	1:A:302:VAL:HG22	2.03	0.41
1:B:125:ASN:HB2	1:B:132:ILE:HG21	2.01	0.41
1:A:85:LEU:O	1:A:91:THR:CG2	2.69	0.41
1:A:186:LEU:CG	1:A:187:ASP:N	2.82	0.41
1:A:318:LEU:HA	1:A:324:VAL:CG2	2.27	0.41
1:B:252:VAL:HG22	1:B:262:PHE:CE2	2.56	0.41
1:B:330:ILE:HG23	1:B:334:HIS:CE1	2.55	0.41
1:A:13:LEU:HD22	1:A:173:LEU:HD22	2.03	0.41
1:A:77:SER:O	1:A:81:VAL:HG23	2.20	0.41
1:A:118:ASP:O	1:A:135:ILE:HD13	2.21	0.41
1:B:194:ILE:CG2	1:B:195:LEU:N	2.84	0.41
1:B:210:SER:HB3	1:B:262:PHE:CA	2.51	0.41
1:A:16:PHE:HE1	1:A:20:GLN:HG3	1.78	0.41
1:A:33:LEU:HD11	1:A:138:ILE:HG21	2.02	0.41
1:A:42:LYS:HE3	1:A:193:PHE:CE2	2.56	0.41
1:A:48:VAL:HA	1:A:51:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG23	1:A:85:LEU:N	2.36	0.41
1:A:92:CYS:SG	1:A:111:GLY:C	2.99	0.41
1:A:203:LYS:O	1:A:321:PRO:HD2	2.21	0.41
1:B:51:ALA:HA	1:B:55:HIS:CD2	2.56	0.41
1:B:51:ALA:O	1:B:53:ILE:N	2.54	0.41
1:B:136:PHE:CE2	1:B:164:TYR:HA	2.55	0.41
1:B:150:LYS:HA	1:B:153:LEU:HG	2.02	0.41
1:B:224:THR:C	1:B:226:TYR:N	2.72	0.41
1:B:262:PHE:CD1	1:B:263:MET:N	2.89	0.41
1:B:277:LEU:HD22	1:B:307:PRO:HD3	2.02	0.41
1:A:80:LEU:O	1:A:84:VAL:HG22	2.21	0.41
1:B:79:ASP:O	1:B:83:ASN:N	2.54	0.41
1:B:297:THR:CG2	1:B:315:PRO:HD2	2.51	0.41
1:B:181:VAL:HG23	1:B:291:ALA:HA	2.04	0.40
1:B:223:ILE:O	1:B:226:TYR:CD1	2.70	0.40
1:B:276:ARG:H	1:B:276:ARG:HH11	1.67	0.40
1:A:30:MET:HB2	1:A:113:TYR:CZ	2.56	0.40
1:A:139:TYR:CD2	1:A:154:GLN:HB2	2.56	0.40
1:B:34:LEU:O	1:B:38:CYS:HB2	2.22	0.40
1:B:328:LEU:HD22	1:B:328:LEU:HA	1.88	0.40
1:A:54:ALA:C	1:A:59:ILE:HG21	2.42	0.40
1:A:286:TYR:CD1	1:A:286:TYR:C	2.94	0.40
1:B:115:VAL:HG13	1:B:137:GLY:O	2.21	0.40
1:B:187:ASP:OD2	1:B:190:ILE:HG12	2.22	0.40
1:B:246:GLY:O	2:B:338:F6P:H4	2.21	0.40
1:B:322:GLU:HB3	3:B:349:HOH:O	2.21	0.40
1:B:327:LEU:HA	1:B:330:ILE:CD1	2.48	0.40
1:A:117:PHE:HB2	1:A:136:PHE:HA	2.02	0.40
1:A:190:ILE:O	1:A:191:GLY:C	2.60	0.40
1:A:227:ILE:O	1:A:231:LYS:HG3	2.22	0.40
1:A:312:GLN:HE21	1:A:312:GLN:HB3	1.68	0.40
1:B:205:LYS:HB2	3:B:357:HOH:O	2.21	0.40
1:A:35:ASN:HA	1:A:38:CYS:SG	2.62	0.40
1:A:42:LYS:HD3	1:A:186:LEU:HD13	2.04	0.40
1:A:78:ASN:HB2	1:A:119:PRO:CB	2.52	0.40
1:A:210:SER:O	1:A:262:PHE:HD1	2.05	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	335/337 (99%)	209 (62%)	84 (25%)	42 (12%)	0 0
1	B	335/337 (99%)	206 (62%)	97 (29%)	32 (10%)	0 0
All	All	670/674 (99%)	415 (62%)	181 (27%)	74 (11%)	0 0

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	8	THR
1	A	33	LEU
1	A	34	LEU
1	A	56	LEU
1	A	60	ALA
1	A	65	VAL
1	A	69	GLN
1	A	124	SER
1	A	128	CYS
1	A	141	LYS
1	A	145	ASP
1	A	150	LYS
1	A	151	ASP
1	A	258	TYR
1	A	277	LEU
1	A	309	ASP
1	B	9	ASN
1	B	59	ILE
1	B	106	GLU
1	B	112	LYS
1	B	123	SER
1	B	147	PRO
1	B	153	LEU
1	B	170	ALA

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Mol	Chain	Res	Type
1	B	197	ASP
1	B	198	ARG
1	B	211	ILE
1	B	276	ARG
1	B	283	PRO
1	B	336	ALA
1	A	4	ALA
1	A	51	ALA
1	A	53	ILE
1	A	102	ALA
1	A	143	SER
1	A	178	VAL
1	A	211	ILE
1	A	234	PRO
1	A	250	ALA
1	A	265	PRO
1	B	26	GLY
1	B	90	ALA
1	B	221	PRO
1	B	237	SER
1	B	244	TYR
1	B	253	HIS
1	B	303	LEU
1	A	72	LYS
1	A	207	SER
1	A	278	LEU
1	A	279	TYR
1	B	38	CYS
1	B	111	GLY
1	B	157	ARG
1	A	25	ARG
1	A	77	SER
1	A	165	ALA
1	A	282	ASN
1	B	39	THR
1	B	222	ALA
1	B	274	LYS
1	A	43	ALA
1	A	216	ALA
1	A	259	GLY
1	A	291	ALA
1	A	307	PRO

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Mol	Chain	Res	Type
1	B	254	ARG
1	B	278	LEU
1	B	317	ILE
1	A	232	PHE
1	B	53	ILE
1	A	59	ILE
1	B	132	ILE

5.3.2 Protein sidechains (i)

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	278/278 (100%)	220 (79%)	58 (21%)	1	1
1	B	278/278 (100%)	223 (80%)	55 (20%)	1	1
All	All	556/556 (100%)	443 (80%)	113 (20%)	1	1

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	14	THR
1	A	16	PHE
1	A	30	MET
1	A	31	THR
1	A	33	LEU
1	A	35	ASN
1	A	63	THR
1	A	66	THR
1	A	71	LYS
1	A	74	ASP
1	A	78	ASN
1	A	82	ILE
1	A	89	PHE
1	A	97	GLU
1	A	98	GLU

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Mol	Chain	Res	Type
1	A	99	ASP
1	A	101	ASN
1	A	116	CYS
1	A	127	ASP
1	A	128	CYS
1	A	130	VAL
1	A	132	ILE
1	A	134	THR
1	A	135	ILE
1	A	136	PHE
1	A	138	ILE
1	A	143	SER
1	A	144	THR
1	A	145	ASP
1	A	157	ARG
1	A	164	TYR
1	A	175	LEU
1	A	179	ASN
1	A	182	ASN
1	A	194	ILE
1	A	202	ILE
1	A	209	TYR
1	A	230	LYS
1	A	240	TYR
1	A	256	LEU
1	A	261	ILE
1	A	262	PHE
1	A	264	TYR
1	A	265	PRO
1	A	276	ARG
1	A	277	LEU
1	A	279	TYR
1	A	280	GLU
1	A	282	ASN
1	A	284	MET
1	A	299	LYS
1	A	302	VAL
1	A	308	THR
1	A	310	ILE
1	A	312	GLN
1	A	325	THR
1	A	331	TYR

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Mol	Chain	Res	Type
1	B	11	VAL
1	B	12	THR
1	B	18	MET
1	B	31	THR
1	B	33	LEU
1	B	35	ASN
1	B	45	SER
1	B	55	HIS
1	B	57	TYR
1	B	68	ASP
1	B	74	ASP
1	B	75	VAL
1	B	76	LEU
1	B	80	LEU
1	B	82	ILE
1	B	89	PHE
1	B	91	THR
1	B	97	GLU
1	B	120	LEU
1	B	121	ASP
1	B	124	SER
1	B	131	SER
1	B	140	ARG
1	B	142	ASN
1	B	144	THR
1	B	147	PRO
1	B	148	SER
1	B	157	ARG
1	B	160	VAL
1	B	166	LEU
1	B	175	LEU
1	B	182	ASN
1	B	195	LEU
1	B	202	ILE
1	B	209	TYR
1	B	215	TYR
1	B	221	PRO
1	B	224	THR
1	B	226	TYR
1	B	232	PHE
1	B	253	HIS
1	B	254	ARG

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Mol	Chain	Res	Type
1	B	258	TYR
1	B	263	MET
1	B	276	ARG
1	B	279	TYR
1	B	282	ASN
1	B	296	THR
1	B	300	GLU
1	B	308	THR
1	B	318	LEU
1	B	324	VAL
1	B	325	THR
1	B	328	LEU
1	B	330	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	35	ASN
1	A	311	HIS
1	B	158	ASN
1	B	236	ASN
1	B	267	ASN
1	B	282	ASN
1	B	332	GLN
1	B	334	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	338	-	15,16,16	1.07	1 (6%)	17,25,25	0.97	1 (5%)
2	F6P	B	338	-	15,16,16	1.36	1 (6%)	17,25,25	1.45	2 (11%)

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	338	-	-	4/9/28/28	0/1/1/1
2	F6P	B	338	-	-	1/9/28/28	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	338	F6P	O5-C2	-4.15	1.36	1.43
2	A	338	F6P	O2-C2	2.45	1.44	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	338	F6P	O2-C2-O5	-3.50	102.74	109.50
2	B	338	F6P	P-O6-C6	2.32	124.69	118.30
2	A	338	F6P	O6-P-O1P	2.12	112.41	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

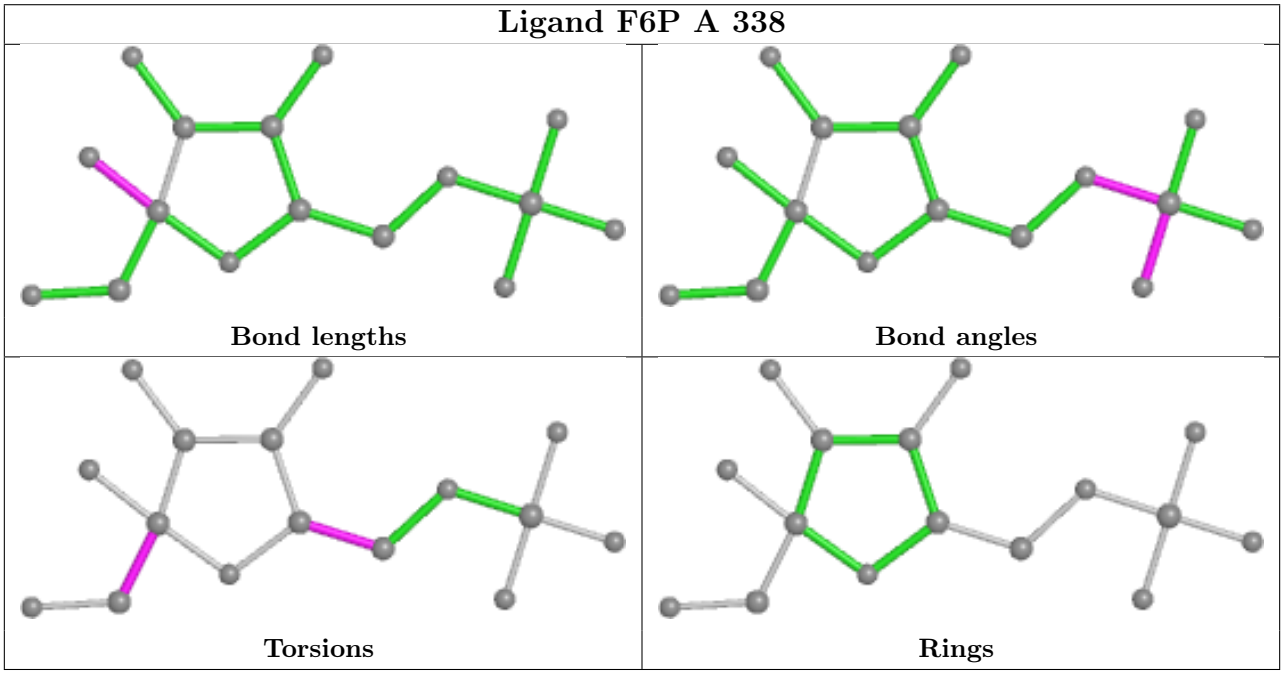
Mol	Chain	Res	Type	Atoms
2	A	338	F6P	O1-C1-C2-O2
2	A	338	F6P	O1-C1-C2-C3
2	A	338	F6P	O1-C1-C2-O5
2	B	338	F6P	C5-C6-O6-P
2	A	338	F6P	O5-C5-C6-O6

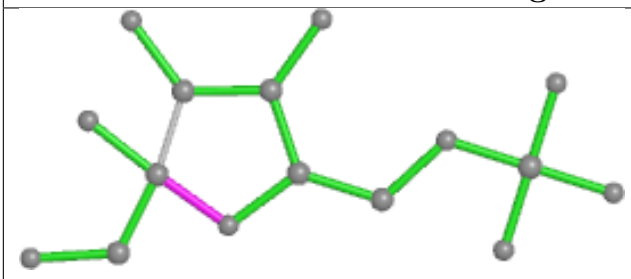
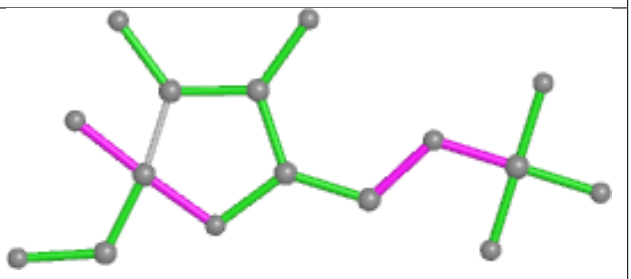
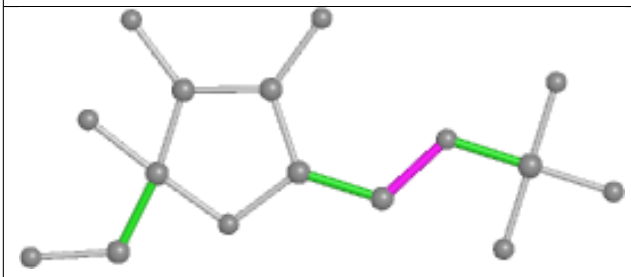
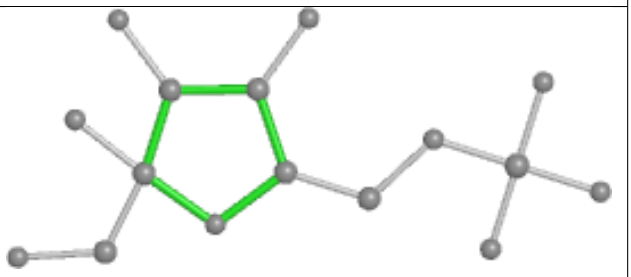
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	F6P	1	0
2	B	338	F6P	1	0

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



Ligand F6P B 338	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.