



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 08:45 AM EDT

PDB ID : 2I5J  
Title : Crystal structure of HIV-1 reverse transcriptase (RT) in complex with DHBNH, an RNASE H inhibitor  
Authors : Himmel, D.M.; Sarafianos, S.G.; Knight, J.L.; Levy, R.M.; Arnold, E.  
Deposited on : 2006-08-24  
Resolution : 3.15 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

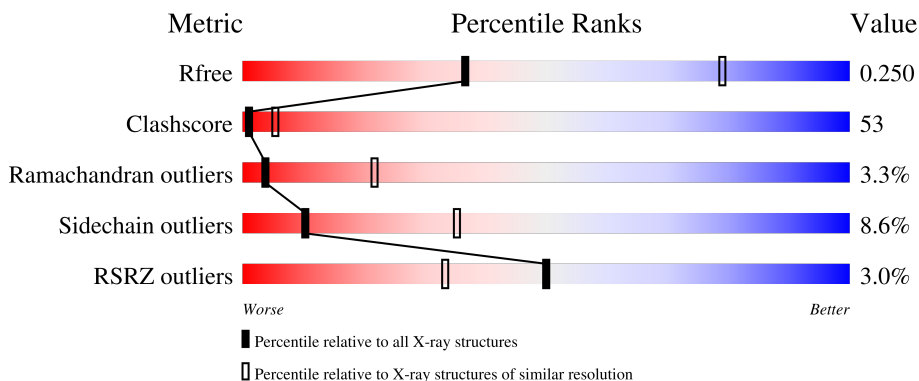
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	 3% 31% 60% 9%
2	B	429	 3% 37% 52% 8% ..
3	C	2	 50% 50%
3	D	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FRU	C	2	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8108 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 Reverse transcriptase/ribonuclease H P66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4499	2913	748	831	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

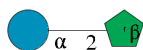
- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H P51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	420	3465	2254	575	630	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

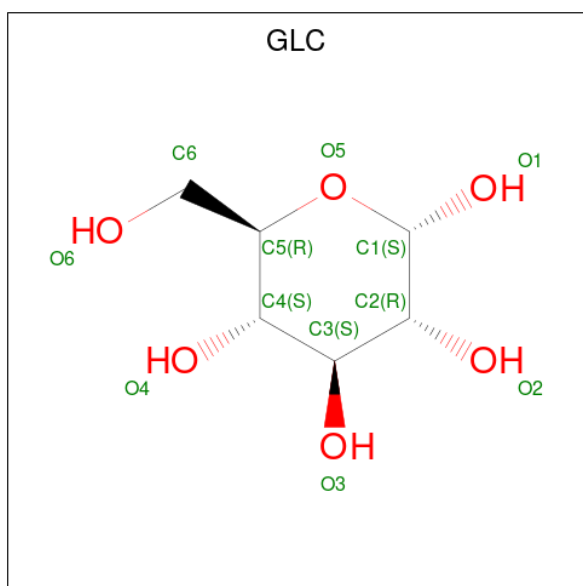
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



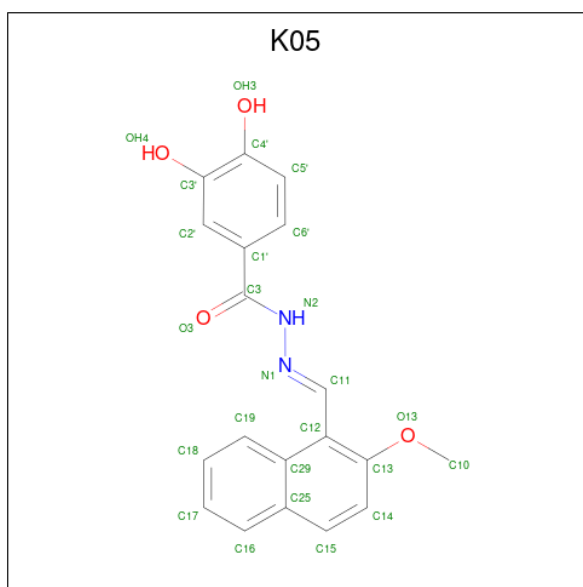
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	C	2	23	12	11	0	0	0
3	D	2	23	12	11	0	0	0

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0
4	A	1	Total C O 12 6 6	0	0
4	B	1	Total C O 12 6 6	0	0

- Molecule 5 is (E)-3,4-DIHYDROXY-N'-[(2-METHOXYNAPHTHALEN-1-YL)METHYLENE]BENZOHYDRAZIDE (three-letter code: K05) (formula: C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	19	2	4		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

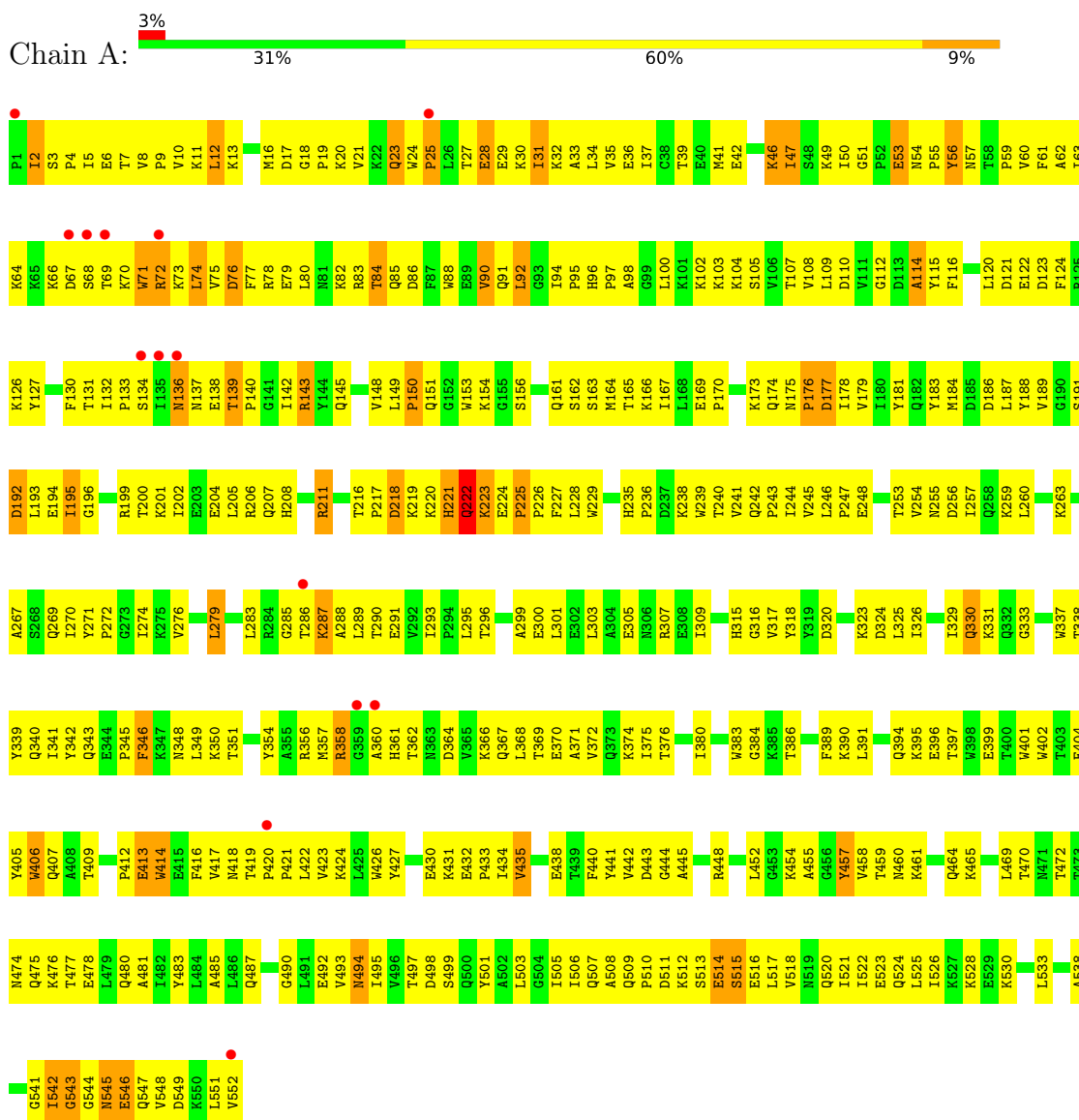
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total	O	0	0
			19	19		
7	B	17	Total	O	0	0
			17	17		

### 3 Residue-property plots i

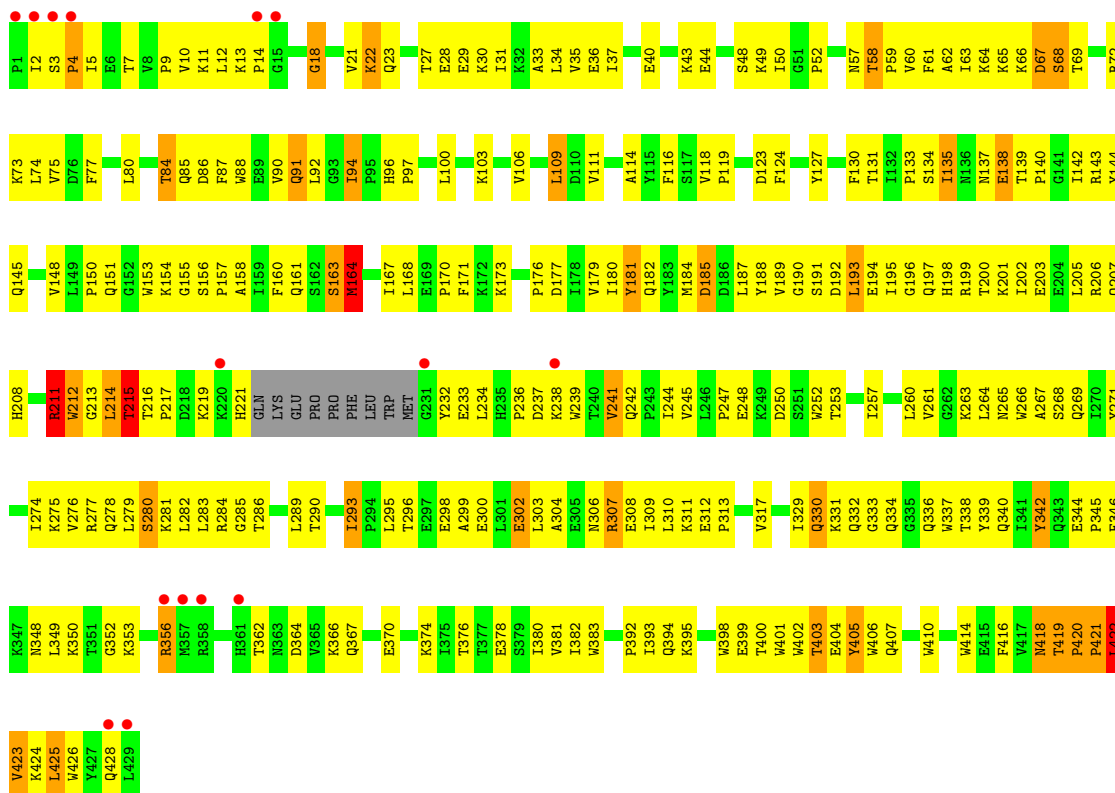
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Reverse transcriptase/ribonuclease H P66 subunit



- Molecule 2: Reverse transcriptase/ribonuclease H P51 subunit





- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain C: 50% 50%

GLC1  
FRU2

- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain D: 100%

GLC1  
FRU2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.81Å 68.90Å 104.66Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	25.71 – 3.15 25.71 – 3.15	Depositor EDS
% Data completeness (in resolution range)	87.7 (25.71-3.15) 87.7 (25.71-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.17Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.234 , 0.269 0.214 , 0.250	Depositor DCC
$R_{free}$ test set	676 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.4	Xtrriage
Anisotropy	0.108	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 90.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: GLC, FRU, K05, MG

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	0.52	0/4617	0.87	10/6271 (0.2%)
2	B	0.53	0/3564	0.83	8/4841 (0.2%)
All	All	0.52	0/8181	0.85	18/11112 (0.2%)

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	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	68	SER	N-CA-C	10.25	138.69	111.00
1	A	222	GLN	N-CA-C	10.06	138.16	111.00
1	A	219	LYS	N-CA-C	-9.79	84.57	111.00
2	B	422	LEU	N-CA-C	-8.46	88.16	111.00
1	A	285	GLY	N-CA-C	-8.42	92.06	113.10
1	A	67	ASP	N-CA-C	-7.94	89.57	111.00
2	B	211	ARG	O-C-N	-6.61	112.12	122.70
2	B	221	HIS	N-CA-C	-6.42	93.67	111.00
1	A	412	PRO	N-CA-C	6.37	128.65	112.10
2	B	419	THR	N-CA-C	6.31	128.03	111.00
2	B	420	PRO	N-CA-C	-6.03	96.43	112.10
1	A	150	PRO	CB-CA-C	5.98	126.96	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	N-CA-C	5.97	127.12	111.00
1	A	221	HIS	N-CA-C	-5.97	94.88	111.00
2	B	242	GLN	N-CA-C	5.82	126.72	111.00
1	A	288	ALA	CB-CA-C	5.80	118.79	110.10
2	B	66	LYS	N-CA-C	-5.76	95.43	111.00
2	B	215	THR	N-CA-C	-5.26	96.78	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	PRO	Peptide
2	B	211	ARG	Mainchain

## 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	4499	0	4560	553	0
2	B	3465	0	3506	339	0
3	C	23	0	21	4	0
3	D	23	0	21	1	0
4	A	24	0	24	3	0
4	B	12	0	12	1	0
5	A	25	0	15	7	0
6	A	1	0	0	0	0
7	A	19	0	0	0	0
7	B	17	0	0	1	0
All	All	8108	0	8159	866	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 53.

All (866) 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:27:THR:HG22	1:A:28:GLU:N	1.58	1.14
1:A:27:THR:HG22	1:A:28:GLU:H	1.01	1.12
1:A:543:GLY:CA	2:B:284:ARG:HA	1.78	1.12
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.25	1.11
1:A:23:GLN:O	1:A:25:PRO:HD3	1.51	1.10
1:A:295:LEU:HD13	1:A:300:GLU:HG2	1.32	1.08
2:B:13:LYS:HG3	2:B:14:PRO:HD2	1.11	1.08
2:B:206:ARG:HH12	2:B:219:LYS:HD3	0.95	1.08
1:A:59:PRO:HB2	1:A:61:PHE:CE1	1.88	1.08
1:A:228:LEU:HD22	1:A:242:GLN:HE21	1.18	1.07
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.11	1.07
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.35	1.06
2:B:263:LYS:HG3	2:B:425:LEU:HD22	1.33	1.05
1:A:497:THR:HG22	1:A:499:SER:H	1.21	1.05
2:B:241:VAL:HG12	2:B:241:VAL:O	1.46	1.05
1:A:27:THR:CG2	1:A:28:GLU:H	1.69	1.04
2:B:13:LYS:CG	2:B:14:PRO:HD2	1.87	1.04
2:B:307:ARG:HB3	2:B:307:ARG:HH11	1.17	1.04
1:A:242:GLN:HG2	1:A:243:PRO:HD2	1.39	1.04
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.40	1.04
2:B:296:THR:OG1	2:B:299:ALA:HB2	1.57	1.04
1:A:543:GLY:HA3	2:B:284:ARG:CA	1.88	1.03
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.15	1.02
2:B:114:ALA:HB2	2:B:215:THR:HG23	1.38	1.01
1:A:414:TRP:HE3	1:A:414:TRP:H	1.01	1.01
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.41	1.00
2:B:307:ARG:HB3	2:B:307:ARG:NH1	1.75	1.00
1:A:104:LYS:HB2	1:A:192:ASP:CA	1.91	0.99
1:A:104:LYS:H	1:A:192:ASP:HB3	1.29	0.98
1:A:90:VAL:HG23	1:A:161:GLN:OE1	1.65	0.96
2:B:13:LYS:HG3	2:B:14:PRO:CD	1.94	0.96
2:B:206:ARG:NH1	2:B:219:LYS:HD3	1.80	0.96
2:B:422:LEU:C	2:B:424:LYS:H	1.69	0.95
2:B:64:LYS:HD2	2:B:68:SER:HA	1.47	0.95
1:A:53:GLU:HB3	1:A:55:PRO:HD3	1.45	0.94
1:A:41:MET:HB2	1:A:47:ILE:HD11	1.50	0.94
1:A:59:PRO:HB2	1:A:61:PHE:HE1	1.28	0.93
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.04	0.92
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.04	0.92
2:B:207:GLN:O	2:B:211:ARG:HG3	1.71	0.91
1:A:452:LEU:HD21	1:A:470:THR:HG23	1.52	0.90
1:A:56:TYR:CD1	1:A:56:TYR:N	2.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PHE:HE2	1:A:418:ASN:HB2	1.37	0.90
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.53	0.90
1:A:543:GLY:HA3	2:B:284:ARG:HA	0.94	0.90
2:B:206:ARG:HH12	2:B:219:LYS:CD	1.85	0.89
1:A:50:ILE:HG21	1:A:145:GLN:HB3	1.53	0.89
1:A:74:LEU:O	1:A:74:LEU:HG	1.71	0.88
2:B:241:VAL:O	2:B:241:VAL:CG1	2.21	0.88
1:A:211:ARG:HG3	1:A:211:ARG:NH1	1.78	0.88
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.54	0.88
1:A:90:VAL:HG22	1:A:91:GLN:H	1.39	0.88
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.09	0.87
1:A:46:LYS:H	1:A:46:LYS:HD2	1.40	0.87
2:B:307:ARG:O	2:B:311:LYS:HG3	1.75	0.87
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.54	0.87
2:B:340:GLN:HG2	2:B:426:TRP:CH2	2.10	0.87
2:B:111:VAL:HG22	2:B:185:ASP:O	1.76	0.86
1:A:30:LYS:O	1:A:34:LEU:HG	1.75	0.86
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.07	0.85
1:A:452:LEU:CD2	1:A:470:THR:HG23	2.08	0.84
2:B:213:GLY:O	2:B:214:LEU:HG	1.78	0.84
2:B:244:ILE:HD11	2:B:310:LEU:HD22	1.59	0.83
2:B:263:LYS:HA	2:B:425:LEU:HD13	1.61	0.83
1:A:107:THR:HG22	1:A:108:VAL:H	1.44	0.83
1:A:238:LYS:HD3	1:A:315:HIS:HB3	1.58	0.83
1:A:211:ARG:HH11	1:A:211:ARG:CG	1.92	0.82
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.60	0.82
1:A:440:PHE:HA	1:A:459:THR:HG22	1.61	0.82
1:A:253:THR:H	1:A:256:ASP:HB2	1.42	0.81
2:B:65:LYS:HE2	2:B:72:ARG:HD3	1.61	0.81
1:A:427:TYR:CZ	1:A:509:GLN:HA	2.14	0.81
2:B:86:ASP:O	2:B:90:VAL:HB	1.81	0.81
1:A:108:VAL:HB	5:A:4001:K05:H6 <sup>7</sup>	1.60	0.81
1:A:27:THR:HG22	1:A:29:GLU:H	1.43	0.81
2:B:263:LYS:HA	2:B:425:LEU:CD1	2.10	0.81
1:A:69:THR:HG23	1:A:70:LYS:HG2	1.63	0.80
2:B:3:SER:HB2	2:B:4:PRO:HD2	1.62	0.80
2:B:206:ARG:CZ	2:B:219:LYS:HB3	2.11	0.80
2:B:31:ILE:O	2:B:35:VAL:HG23	1.81	0.80
1:A:90:VAL:HG22	1:A:91:GLN:N	1.96	0.80
2:B:193:LEU:HD12	2:B:198:HIS:N	1.97	0.80
1:A:542:ILE:HB	1:A:545:ASN:HB3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:THR:OG1	1:A:476:LYS:HB3	1.81	0.79
1:A:228:LEU:HD22	1:A:242:GLN:NE2	1.96	0.79
1:A:224:GLU:HB2	1:A:225:PRO:HD2	1.65	0.79
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.65	0.79
1:A:324:ASP:O	1:A:343:GLN:HG2	1.83	0.79
1:A:424:LYS:HD3	1:A:426:TRP:CH2	2.18	0.79
1:A:498:ASP:CB	1:A:538:ALA:HB2	2.12	0.79
1:A:62:ALA:O	1:A:63:ILE:HD13	1.83	0.78
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.47	0.78
2:B:3:SER:HB2	2:B:4:PRO:CD	2.13	0.78
2:B:63:ILE:HG22	2:B:403:THR:O	1.83	0.78
1:A:32:LYS:CG	1:A:33:ALA:N	2.47	0.78
1:A:104:LYS:N	1:A:192:ASP:HB3	1.98	0.78
1:A:143:ARG:HG2	1:A:143:ARG:NH1	1.87	0.78
1:A:195:ILE:N	1:A:195:ILE:HD12	1.97	0.78
1:A:107:THR:HG21	1:A:202:ILE:HG21	1.64	0.78
1:A:53:GLU:HG3	1:A:54:ASN:H	1.49	0.77
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.67	0.77
1:A:31:ILE:HD13	1:A:133:PRO:HB2	1.65	0.76
2:B:282:LEU:HB3	2:B:293:ILE:HD12	1.67	0.76
1:A:53:GLU:HB3	1:A:55:PRO:CD	2.16	0.76
2:B:307:ARG:HH11	2:B:307:ARG:CB	1.97	0.76
2:B:398:TRP:O	2:B:402:TRP:HD1	1.68	0.76
1:A:542:ILE:HD12	1:A:542:ILE:H	1.49	0.76
2:B:91:GLN:HG2	2:B:92:LEU:CD2	2.17	0.75
1:A:74:LEU:O	1:A:74:LEU:CG	2.33	0.75
2:B:263:LYS:CG	2:B:425:LEU:HD22	2.16	0.75
1:A:131:THR:CG2	1:A:143:ARG:HH11	1.99	0.74
1:A:201:LYS:O	1:A:204:GLU:HB2	1.87	0.74
1:A:469:LEU:CD1	1:A:480:GLN:HG2	2.17	0.74
1:A:46:LYS:HD2	1:A:46:LYS:N	1.98	0.74
1:A:200:THR:O	1:A:204:GLU:HG3	1.87	0.74
2:B:215:THR:O	2:B:217:PRO:HD3	1.86	0.74
1:A:427:TYR:OH	1:A:509:GLN:HA	1.88	0.74
1:A:131:THR:HG23	1:A:143:ARG:NH1	2.03	0.73
1:A:36:GLU:O	1:A:39:THR:HG22	1.87	0.73
1:A:406:TRP:CE3	2:B:419:THR:HG22	2.23	0.73
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.19	0.72
1:A:27:THR:HG22	1:A:29:GLU:N	2.02	0.72
2:B:193:LEU:HD12	2:B:198:HIS:CA	2.19	0.72
2:B:333:GLY:O	2:B:336:GLN:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.72	0.72
1:A:107:THR:HG22	1:A:108:VAL:N	2.04	0.72
1:A:151:GLN:HE21	4:A:2001:GLC:H1	1.54	0.72
2:B:208:HIS:HE1	2:B:212:TRP:HD1	1.37	0.72
1:A:317:VAL:HG12	1:A:348:ASN:O	1.89	0.72
1:A:545:ASN:C	1:A:547:GLN:H	1.92	0.72
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.70	0.72
1:A:523:GLU:HA	1:A:526:ILE:HD12	1.72	0.71
2:B:13:LYS:CG	2:B:14:PRO:CD	2.61	0.71
1:A:356:ARG:O	1:A:356:ARG:HG2	1.88	0.71
1:A:376:THR:O	1:A:380:ILE:HG13	1.90	0.71
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.70	0.71
1:A:16:MET:HE1	1:A:83:ARG:HA	1.71	0.71
1:A:30:LYS:C	1:A:32:LYS:H	1.93	0.71
1:A:543:GLY:O	2:B:285:GLY:N	2.22	0.70
1:A:443:ASP:HB3	1:A:548:VAL:HG12	1.71	0.70
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.26	0.70
2:B:214:LEU:O	2:B:216:THR:N	2.25	0.70
1:A:201:LYS:HD3	1:A:204:GLU:OE1	1.91	0.70
1:A:296:THR:HG23	1:A:299:ALA:H	1.56	0.70
2:B:12:LEU:HD21	2:B:124:PHE:HE1	1.56	0.70
1:A:189:VAL:CG1	1:A:202:ILE:HD12	2.22	0.70
2:B:94:ILE:HD13	2:B:161:GLN:NE2	2.06	0.70
1:A:270:ILE:O	1:A:272:PRO:HD3	1.91	0.70
2:B:206:ARG:NH1	2:B:219:LYS:HB3	2.07	0.70
2:B:424:LYS:C	2:B:426:TRP:H	1.95	0.70
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.27	0.69
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.73	0.69
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.55	0.69
2:B:296:THR:OG1	2:B:299:ALA:CB	2.37	0.69
1:A:317:VAL:HG13	1:A:349:LEU:HD13	1.74	0.69
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.57	0.69
2:B:206:ARG:HG3	2:B:206:ARG:HH11	1.58	0.69
2:B:264:LEU:HD23	2:B:276:VAL:HG12	1.73	0.69
1:A:177:ASP:O	1:A:178:ILE:HD13	1.92	0.69
2:B:418:ASN:O	2:B:418:ASN:ND2	2.22	0.68
1:A:206:ARG:HG3	1:A:216:THR:OG1	1.93	0.68
1:A:189:VAL:HG11	1:A:202:ILE:HD12	1.76	0.68
2:B:303:LEU:O	2:B:307:ARG:HG3	1.93	0.68
1:A:460:ASN:ND2	1:A:461:LYS:HG3	2.09	0.68
2:B:67:ASP:O	2:B:69:THR:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:OE2	1:A:433:PRO:HD2	1.93	0.68
1:A:138:GLU:HG3	1:A:140:PRO:HD2	1.76	0.68
2:B:33:ALA:O	2:B:36:GLU:HG2	1.94	0.68
1:A:339:TYR:O	1:A:351:THR:HB	1.95	0.67
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.29	0.67
1:A:239:TRP:HB3	1:A:318:TYR:HE2	1.59	0.67
1:A:3:SER:OG	1:A:5:ILE:HG13	1.94	0.67
2:B:65:LYS:O	2:B:407:GLN:NE2	2.27	0.67
2:B:282:LEU:HD23	2:B:293:ILE:HB	1.75	0.67
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.29	0.67
2:B:422:LEU:O	2:B:424:LYS:N	2.27	0.67
1:A:50:ILE:CG2	1:A:145:GLN:HB3	2.24	0.67
2:B:91:GLN:HG2	2:B:92:LEU:HD23	1.75	0.67
2:B:422:LEU:C	2:B:424:LYS:N	2.39	0.67
1:A:16:MET:CE	1:A:83:ARG:HA	2.25	0.67
2:B:423:VAL:HG12	2:B:423:VAL:O	1.93	0.67
1:A:195:ILE:N	1:A:195:ILE:CD1	2.58	0.67
2:B:103:LYS:HA	2:B:192:ASP:OD1	1.95	0.66
1:A:240:THR:HG22	1:A:241:VAL:N	2.09	0.66
1:A:295:LEU:HD13	1:A:300:GLU:CG	2.19	0.66
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.75	0.66
2:B:40:GLU:O	2:B:44:GLU:HG2	1.96	0.66
2:B:2:ILE:HD13	2:B:5:ILE:HD11	1.78	0.66
1:A:28:GLU:O	1:A:28:GLU:HG2	1.96	0.66
1:A:435:VAL:HG13	2:B:290:THR:CG2	2.21	0.66
1:A:23:GLN:OE1	1:A:60:VAL:N	2.28	0.66
2:B:60:VAL:HG12	2:B:75:VAL:HG12	1.78	0.66
2:B:281:LYS:HA	2:B:284:ARG:NH1	2.10	0.66
1:A:107:THR:HB	1:A:189:VAL:HG13	1.78	0.65
2:B:139:THR:HB	2:B:140:PRO:HD2	1.79	0.65
2:B:213:GLY:C	2:B:214:LEU:HG	2.16	0.65
1:A:542:ILE:O	1:A:546:GLU:HG2	1.96	0.65
2:B:307:ARG:HH12	2:B:311:LYS:HE2	1.61	0.65
1:A:84:THR:HG22	1:A:154:LYS:HD3	1.78	0.65
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.26	0.65
1:A:441:TYR:O	1:A:548:VAL:HG21	1.96	0.65
1:A:514:GLU:HG3	1:A:515:SER:H	1.60	0.65
1:A:23:GLN:O	1:A:25:PRO:CD	2.37	0.65
2:B:57:ASN:OD1	2:B:130:PHE:HA	1.97	0.65
1:A:495:ILE:HB	1:A:533:LEU:HD12	1.78	0.65
1:A:279:LEU:CD1	1:A:299:ALA:HB1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:HG2	2:B:72:ARG:HD3	1.79	0.64
2:B:206:ARG:NH1	2:B:219:LYS:CB	2.60	0.64
1:A:469:LEU:HD11	1:A:480:GLN:CG	2.24	0.64
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.79	0.64
1:A:71:TRP:CD1	1:A:71:TRP:N	2.65	0.64
1:A:71:TRP:HD1	1:A:71:TRP:H	1.44	0.64
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.31	0.64
1:A:317:VAL:HG22	1:A:318:TYR:N	2.11	0.64
2:B:208:HIS:CE1	2:B:212:TRP:HD1	2.15	0.64
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.27	0.64
2:B:264:LEU:CD2	2:B:276:VAL:HG12	2.27	0.64
1:A:27:THR:CG2	1:A:29:GLU:H	2.11	0.64
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.33	0.64
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.96	0.64
1:A:28:GLU:O	1:A:32:LYS:HB3	1.98	0.64
1:A:413:GLU:HG3	1:A:413:GLU:O	1.98	0.64
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.32	0.64
1:A:546:GLU:OE1	1:A:546:GLU:HA	1.98	0.63
1:A:32:LYS:HG3	1:A:33:ALA:N	2.14	0.63
1:A:452:LEU:HD23	1:A:470:THR:HA	1.79	0.63
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.27	0.63
1:A:90:VAL:CG2	1:A:91:GLN:H	2.11	0.63
1:A:188:TYR:CD2	1:A:188:TYR:O	2.52	0.63
2:B:330:GLN:HB2	2:B:424:LYS:HE2	1.81	0.63
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.80	0.63
1:A:238:LYS:HD3	1:A:315:HIS:CB	2.29	0.63
2:B:27:THR:HG22	2:B:29:GLU:H	1.64	0.63
2:B:156:SER:N	2:B:157:PRO:HD2	2.13	0.63
2:B:208:HIS:HE1	2:B:212:TRP:CD1	2.17	0.63
1:A:222:GLN:O	1:A:222:GLN:HG3	1.99	0.62
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.29	0.62
1:A:366:LYS:O	1:A:370:GLU:HG3	1.98	0.62
1:A:478:GLU:HG3	1:A:499:SER:HB2	1.81	0.62
2:B:23:GLN:HB2	7:B:1018:HOH:O	1.99	0.62
2:B:50:ILE:HG13	2:B:143:ARG:HB3	1.81	0.62
2:B:96:HIS:HD1	2:B:181:TYR:HE2	1.43	0.62
1:A:104:LYS:HB2	1:A:192:ASP:CB	2.28	0.62
1:A:183:TYR:CD2	1:A:184:MET:HG2	2.34	0.62
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.82	0.62
2:B:131:THR:HA	2:B:142:ILE:O	1.99	0.62
1:A:167:ILE:O	1:A:170:PRO:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:HA	2:B:31:ILE:HD12	1.80	0.62
1:A:224:GLU:HB2	1:A:225:PRO:CD	2.29	0.62
1:A:181:TYR:CD1	1:A:188:TYR:HD2	2.18	0.62
1:A:460:ASN:HD21	1:A:461:LYS:HG3	1.65	0.62
2:B:257:ILE:HD12	2:B:293:ILE:HD11	1.82	0.62
2:B:80:LEU:HG	2:B:80:LEU:O	2.00	0.61
1:A:115:TYR:HE2	1:A:156:SER:HB3	1.62	0.61
1:A:192:ASP:O	1:A:193:LEU:HD23	1.99	0.61
1:A:427:TYR:CD1	1:A:525:LEU:HD13	2.36	0.61
1:A:544:GLY:O	1:A:547:GLN:HG2	2.01	0.61
2:B:247:PRO:O	2:B:252:TRP:HH2	1.84	0.61
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.35	0.61
1:A:131:THR:HG23	1:A:143:ARG:HH11	1.64	0.61
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.47	0.61
2:B:276:VAL:O	2:B:276:VAL:HG23	2.01	0.61
1:A:138:GLU:HG3	1:A:140:PRO:CD	2.31	0.61
1:A:454:LYS:O	1:A:552:VAL:HG11	2.01	0.61
2:B:84:THR:O	2:B:87:PHE:HB3	2.01	0.61
1:A:73:LYS:HZ3	1:A:75:VAL:HG22	1.63	0.60
1:A:151:GLN:NE2	4:A:2001:GLC:H1	2.14	0.60
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.29	0.60
1:A:508:ALA:HB3	1:A:510:PRO:HD3	1.83	0.60
2:B:142:ILE:N	2:B:142:ILE:HD12	2.16	0.60
2:B:171:PHE:HB2	2:B:208:HIS:HD2	1.65	0.60
2:B:275:LYS:O	2:B:302:GLU:CG	2.48	0.60
2:B:275:LYS:O	2:B:302:GLU:HG3	2.01	0.60
2:B:300:GLU:HA	2:B:303:LEU:HB2	1.83	0.60
1:A:346:PHE:H	3:C:1:GLC:H62	1.65	0.60
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.66	0.60
1:A:552:VAL:OXT	1:A:552:VAL:HG12	2.00	0.60
2:B:23:GLN:HG2	2:B:133:PRO:HD3	1.83	0.60
2:B:106:VAL:HG23	2:B:236:PRO:HD3	1.83	0.60
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.83	0.60
2:B:193:LEU:CD1	2:B:198:HIS:HA	2.32	0.60
2:B:257:ILE:O	2:B:261:VAL:HG23	2.01	0.60
1:A:241:VAL:HG11	1:A:244:ILE:HD11	1.83	0.60
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.37	0.60
2:B:261:VAL:O	2:B:265:ASN:N	2.35	0.60
1:A:41:MET:CB	1:A:47:ILE:HD11	2.26	0.59
1:A:53:GLU:CG	1:A:54:ASN:H	2.10	0.59
1:A:546:GLU:OE1	1:A:546:GLU:CA	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TYR:CD1	1:A:188:TYR:CD2	2.90	0.59
1:A:76:ASP:CG	1:A:76:ASP:O	2.41	0.59
1:A:401:TRP:CH2	1:A:409:THR:HG21	2.37	0.59
2:B:260:LEU:O	2:B:264:LEU:HB2	2.02	0.59
2:B:422:LEU:HD12	2:B:426:TRP:HE1	1.66	0.59
1:A:73:LYS:NZ	1:A:75:VAL:HG22	2.18	0.59
1:A:254:VAL:HG23	1:A:291:GLU:HB3	1.85	0.59
1:A:443:ASP:HB3	1:A:548:VAL:CG1	2.33	0.59
1:A:497:THR:CG2	1:A:499:SER:HB3	2.32	0.59
1:A:218:ASP:C	1:A:220:LYS:N	2.44	0.59
2:B:245:VAL:HG12	2:B:428:GLN:HG2	1.84	0.59
2:B:266:TRP:CE3	2:B:425:LEU:HD12	2.37	0.59
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.32	0.59
2:B:282:LEU:HD11	2:B:296:THR:HG23	1.85	0.59
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.84	0.59
1:A:511:ASP:OD1	1:A:512:LYS:N	2.36	0.59
1:A:542:ILE:HD12	1:A:542:ILE:N	2.17	0.59
2:B:18:GLY:HA3	2:B:127:TYR:HD1	1.67	0.59
1:A:73:LYS:NZ	1:A:75:VAL:CG2	2.66	0.59
1:A:329:ILE:HG22	1:A:330:GLN:N	2.16	0.59
2:B:257:ILE:HD12	2:B:293:ILE:CD1	2.32	0.59
1:A:195:ILE:HG22	1:A:199:ARG:HH21	1.67	0.58
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.38	0.58
1:A:27:THR:CG2	1:A:28:GLU:N	2.31	0.58
1:A:102:LYS:O	1:A:103:LYS:HD2	2.03	0.58
1:A:509:GLN:N	1:A:510:PRO:CD	2.66	0.58
1:A:506:ILE:C	1:A:508:ALA:H	2.07	0.58
1:A:542:ILE:C	1:A:544:GLY:H	2.07	0.58
1:A:545:ASN:ND2	1:A:546:GLU:OE1	2.36	0.58
1:A:341:ILE:HD13	1:A:383:TRP:HZ3	1.68	0.58
1:A:509:GLN:N	1:A:510:PRO:HD3	2.18	0.58
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.69	0.58
1:A:13:LYS:HD2	1:A:16:MET:HE2	1.86	0.58
1:A:32:LYS:HG2	1:A:33:ALA:H	1.68	0.58
1:A:54:ASN:N	1:A:55:PRO:CD	2.67	0.58
1:A:108:VAL:CB	5:A:4001:K05:H6'	2.32	0.58
1:A:541:GLY:N	1:A:546:GLU:OE2	2.37	0.58
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.84	0.58
2:B:13:LYS:CB	2:B:14:PRO:HD2	2.33	0.58
2:B:264:LEU:O	2:B:267:ALA:HB3	2.04	0.58
2:B:163:SER:O	2:B:167:ILE:HG13	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:HG12	2:B:428:GLN:CG	2.33	0.57
2:B:248:GLU:O	2:B:248:GLU:HG3	2.02	0.57
2:B:271:TYR:HB2	2:B:274:ILE:HD11	1.86	0.57
1:A:104:LYS:H	1:A:192:ASP:CB	2.09	0.57
1:A:218:ASP:HB2	1:A:220:LYS:C	2.25	0.57
1:A:290:THR:HG23	1:A:290:THR:O	2.04	0.57
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.40	0.57
2:B:193:LEU:HD12	2:B:197:GLN:C	2.24	0.57
1:A:170:PRO:O	1:A:174:GLN:HG3	2.05	0.57
2:B:349:LEU:HB3	2:B:383:TRP:CZ2	2.39	0.57
1:A:193:LEU:O	1:A:194:GLU:C	2.41	0.57
1:A:20:LYS:HG2	1:A:56:TYR:HB3	1.87	0.57
1:A:317:VAL:CG2	1:A:318:TYR:N	2.67	0.57
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.87	0.57
1:A:181:TYR:CE2	2:B:138:GLU:HG2	2.40	0.57
1:A:195:ILE:CD1	1:A:195:ILE:H	2.18	0.57
2:B:199:ARG:HH21	2:B:233:GLU:HG3	1.70	0.57
2:B:362:THR:HA	2:B:366:LYS:HD3	1.86	0.57
1:A:376:THR:HG23	1:A:386:THR:HG22	1.87	0.56
1:A:31:ILE:O	1:A:31:ILE:HG22	2.05	0.56
1:A:346:PHE:N	3:C:1:GLC:H62	2.20	0.56
2:B:252:TRP:NE1	2:B:295:LEU:HD11	2.20	0.56
2:B:96:HIS:HE1	2:B:381:VAL:O	1.88	0.56
1:A:103:LYS:HG2	1:A:191:SER:HA	1.86	0.56
1:A:414:TRP:CE3	1:A:414:TRP:N	2.66	0.56
2:B:63:ILE:CD1	2:B:74:LEU:HD22	2.36	0.56
2:B:65:LYS:CE	2:B:72:ARG:HD3	2.34	0.56
2:B:237:ASP:OD1	2:B:238:LYS:N	2.38	0.56
2:B:349:LEU:HB3	2:B:383:TRP:HZ2	1.71	0.56
1:A:12:LEU:HB3	1:A:83:ARG:O	2.05	0.56
1:A:360:ALA:O	1:A:361:HIS:ND1	2.39	0.56
2:B:422:LEU:CD1	2:B:426:TRP:HE1	2.19	0.56
2:B:236:PRO:HG2	2:B:237:ASP:H	1.70	0.56
1:A:200:THR:O	1:A:204:GLU:CG	2.54	0.56
2:B:75:VAL:HG21	2:B:77:PHE:CE2	2.41	0.56
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.87	0.55
1:A:542:ILE:HG22	1:A:545:ASN:H	1.71	0.55
2:B:376:THR:O	2:B:380:ILE:HG13	2.05	0.55
1:A:404:GLU:OE2	1:A:431:LYS:HE2	2.07	0.55
1:A:445:ALA:H	1:A:552:VAL:HG12	1.71	0.55
1:A:545:ASN:O	1:A:549:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG22	1:A:544:GLY:H	1.71	0.55
2:B:195:ILE:O	2:B:195:ILE:HG22	2.06	0.55
1:A:259:LYS:HG2	1:A:263:LYS:HE2	1.88	0.55
1:A:208:HIS:O	1:A:211:ARG:HB2	2.06	0.55
1:A:325:LEU:C	1:A:326:ILE:HD12	2.27	0.55
1:A:368:LEU:O	1:A:372:VAL:HG23	2.07	0.55
1:A:476:LYS:O	1:A:480:GLN:HB2	2.07	0.55
1:A:483:TYR:O	1:A:487:GLN:HG3	2.07	0.55
2:B:194:GLU:C	2:B:196:GLY:H	2.10	0.55
2:B:148:VAL:O	2:B:150:PRO:HD3	2.06	0.55
1:A:131:THR:CG2	1:A:143:ARG:NH1	2.63	0.55
1:A:518:VAL:HG12	1:A:522:ILE:CD1	2.36	0.55
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.06	0.55
1:A:60:VAL:HG13	1:A:73:LYS:HZ3	1.72	0.54
2:B:362:THR:HG22	2:B:367:GLN:NE2	2.21	0.54
1:A:329:ILE:HG22	1:A:330:GLN:H	1.70	0.54
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.43	0.54
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.42	0.54
1:A:188:TYR:HB2	5:A:4001:K05:OH3	2.06	0.54
1:A:497:THR:HG21	1:A:499:SER:HB3	1.89	0.54
2:B:181:TYR:HD1	2:B:182:GLN:N	2.05	0.54
2:B:263:LYS:HA	2:B:425:LEU:HD11	1.87	0.54
1:A:8:VAL:O	1:A:10:VAL:HG23	2.07	0.54
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.89	0.54
2:B:402:TRP:CE2	2:B:403:THR:HG22	2.42	0.54
1:A:399:GLU:HA	1:A:402:TRP:HE1	1.72	0.54
1:A:457:TYR:C	1:A:457:TYR:CD2	2.81	0.54
1:A:497:THR:HG22	1:A:499:SER:N	2.05	0.54
1:A:542:ILE:O	1:A:544:GLY:N	2.41	0.54
1:A:543:GLY:C	2:B:285:GLY:H	2.07	0.54
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.43	0.54
1:A:457:TYR:C	1:A:457:TYR:HD2	2.10	0.54
2:B:424:LYS:C	2:B:426:TRP:N	2.61	0.54
2:B:60:VAL:HG11	2:B:130:PHE:HB2	1.90	0.54
2:B:422:LEU:HD23	2:B:422:LEU:H	1.72	0.54
1:A:72:ARG:HB3	1:A:72:ARG:CZ	2.37	0.54
2:B:11:LYS:HG3	2:B:12:LEU:O	2.08	0.54
1:A:253:THR:HA	1:A:291:GLU:O	2.08	0.53
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.42	0.53
2:B:393:ILE:HG12	2:B:394:GLN:N	2.24	0.53
1:A:53:GLU:C	1:A:55:PRO:CD	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:O	1:A:211:ARG:HG2	2.08	0.53
1:A:405:TYR:HE2	1:A:407:GLN:HE21	1.53	0.53
2:B:198:HIS:O	2:B:202:ILE:HG12	2.07	0.53
1:A:107:THR:CG2	1:A:108:VAL:H	2.19	0.53
1:A:330:GLN:HE22	1:A:340:GLN:CD	2.12	0.53
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.43	0.53
1:A:13:LYS:HB2	1:A:16:MET:HE2	1.89	0.53
1:A:136:ASN:HD22	1:A:137:ASN:H	1.56	0.53
1:A:30:LYS:C	1:A:32:LYS:N	2.58	0.53
1:A:366:LYS:O	1:A:369:THR:HB	2.08	0.53
1:A:88:TRP:NE1	2:B:143:ARG:HD3	2.24	0.53
2:B:103:LYS:O	2:B:236:PRO:CG	2.57	0.53
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.39	0.53
1:A:517:LEU:HA	1:A:520:GLN:OE1	2.09	0.53
1:A:542:ILE:H	1:A:542:ILE:CD1	2.21	0.53
1:A:53:GLU:C	1:A:55:PRO:HD2	2.30	0.52
1:A:120:LEU:HD12	1:A:121:ASP:H	1.73	0.52
1:A:103:LYS:CG	1:A:191:SER:HA	2.39	0.52
2:B:11:LYS:HE2	2:B:13:LYS:HZ2	1.73	0.52
1:A:56:TYR:H	1:A:56:TYR:HD1	1.39	0.52
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.91	0.52
1:A:337:TRP:CH2	1:A:368:LEU:HB2	2.44	0.52
1:A:498:ASP:HB2	1:A:538:ALA:CB	2.25	0.52
2:B:422:LEU:HD23	2:B:422:LEU:N	2.25	0.52
1:A:240:THR:CG2	1:A:241:VAL:N	2.72	0.52
2:B:11:LYS:HE3	2:B:13:LYS:HD2	1.91	0.52
2:B:103:LYS:O	2:B:236:PRO:HG2	2.09	0.52
1:A:74:LEU:C	1:A:74:LEU:HD12	2.30	0.52
2:B:263:LYS:CA	2:B:425:LEU:HD13	2.35	0.52
1:A:545:ASN:C	1:A:547:GLN:N	2.62	0.52
1:A:112:GLY:O	1:A:114:ALA:N	2.38	0.52
1:A:196:GLY:HA2	1:A:199:ARG:CZ	2.40	0.52
1:A:90:VAL:O	1:A:92:LEU:HD23	2.10	0.52
1:A:181:TYR:HE2	2:B:138:GLU:HG2	1.75	0.52
1:A:324:ASP:OD1	1:A:326:ILE:HD11	2.10	0.52
1:A:345:PRO:HA	3:C:1:GLC:H61	1.92	0.52
1:A:544:GLY:N	2:B:283:LEU:O	2.43	0.52
2:B:7:THR:O	2:B:9:PRO:HD3	2.10	0.52
2:B:304:ALA:HA	2:B:307:ARG:HB2	1.91	0.51
2:B:420:PRO:O	2:B:422:LEU:HD23	2.10	0.51
1:A:360:ALA:O	1:A:361:HIS:CG	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:CE1	1:A:98:ALA:H	2.28	0.51
1:A:110:ASP:HB3	1:A:217:PRO:HG3	1.93	0.51
1:A:149:LEU:HD23	1:A:149:LEU:N	2.25	0.51
1:A:478:GLU:CG	1:A:499:SER:HB2	2.39	0.51
1:A:542:ILE:C	1:A:544:GLY:N	2.63	0.51
1:A:340:GLN:HA	1:A:351:THR:HA	1.93	0.51
1:A:418:ASN:O	1:A:419:THR:HG23	2.10	0.51
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.46	0.51
1:A:61:PHE:CD1	1:A:61:PHE:N	2.78	0.51
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.76	0.51
1:A:376:THR:HG23	1:A:386:THR:CG2	2.41	0.51
1:A:493:VAL:HG22	1:A:494:ASN:N	2.25	0.51
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.93	0.51
2:B:103:LYS:HB3	2:B:191:SER:O	2.10	0.51
1:A:246:LEU:HD23	1:A:307:ARG:HG2	1.93	0.51
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.93	0.51
2:B:50:ILE:HG23	2:B:145:GLN:HG2	1.92	0.51
1:A:223:LYS:HB3	1:A:227:PHE:CE2	2.45	0.51
1:A:248:GLU:HG2	1:A:307:ARG:CZ	2.40	0.51
1:A:394:GLN:NE2	1:A:396:GLU:OE1	2.43	0.51
2:B:405:TYR:CD1	2:B:405:TYR:N	2.79	0.51
1:A:228:LEU:H	5:A:4001:K05:H19	1.75	0.50
1:A:31:ILE:HG21	1:A:134:SER:O	2.11	0.50
1:A:109:LEU:HB2	1:A:187:LEU:HB2	1.92	0.50
1:A:132:ILE:HG12	1:A:142:ILE:HB	1.93	0.50
1:A:223:LYS:HB3	1:A:227:PHE:HE2	1.75	0.50
1:A:508:ALA:C	1:A:510:PRO:HD3	2.31	0.50
2:B:199:ARG:NH2	2:B:233:GLU:HG3	2.27	0.50
1:A:131:THR:HG22	1:A:143:ARG:CG	2.41	0.50
2:B:345:PRO:O	2:B:346:PHE:HB2	2.11	0.50
1:A:181:TYR:HB2	1:A:188:TYR:CB	2.41	0.50
1:A:389:PHE:HD1	1:A:391:LEU:HD21	1.77	0.50
2:B:23:GLN:CG	2:B:133:PRO:HD3	2.41	0.50
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.41	0.50
1:A:207:GLN:O	1:A:211:ARG:CG	2.59	0.50
1:A:458:VAL:CG1	2:B:286:THR:HG21	2.41	0.50
1:A:305:GLU:O	1:A:309:ILE:HG13	2.12	0.50
1:A:460:ASN:ND2	1:A:461:LYS:N	2.60	0.50
2:B:13:LYS:HD2	2:B:14:PRO:HD3	1.93	0.50
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.42	0.50
1:A:457:TYR:O	1:A:458:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:GLN:HG2	2:B:426:TRP:CZ3	2.47	0.50
2:B:96:HIS:CE1	2:B:381:VAL:O	2.65	0.49
1:A:32:LYS:CG	1:A:33:ALA:H	2.19	0.49
2:B:40:GLU:O	2:B:43:LYS:HB3	2.12	0.49
2:B:401:TRP:O	2:B:404:GLU:HB2	2.12	0.49
1:A:420:PRO:HA	1:A:421:PRO:C	2.32	0.49
2:B:49:LYS:HA	2:B:143:ARG:O	2.13	0.49
2:B:253:THR:O	2:B:257:ILE:HG13	2.12	0.49
2:B:424:LYS:O	2:B:426:TRP:N	2.38	0.49
1:A:195:ILE:CG2	1:A:199:ARG:HH21	2.25	0.49
1:A:242:GLN:CG	1:A:243:PRO:HD2	2.26	0.49
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.27	0.49
2:B:164:MET:O	2:B:167:ILE:N	2.43	0.49
2:B:234:LEU:HD22	2:B:239:TRP:HZ2	1.77	0.49
1:A:17:ASP:O	1:A:83:ARG:HD3	2.12	0.49
1:A:189:VAL:HG13	1:A:202:ILE:HD12	1.92	0.49
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.93	0.49
2:B:203:GLU:HA	2:B:206:ARG:HB2	1.94	0.49
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.28	0.49
1:A:108:VAL:O	1:A:109:LEU:HD23	2.13	0.49
2:B:342:TYR:N	2:B:342:TYR:CD2	2.81	0.49
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.78	0.49
1:A:279:LEU:HD21	1:A:303:LEU:HD13	1.94	0.49
1:A:296:THR:O	1:A:300:GLU:OE1	2.31	0.49
1:A:317:VAL:HG12	1:A:348:ASN:C	2.33	0.49
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.09	0.49
1:A:389:PHE:HB3	1:A:391:LEU:CD2	2.41	0.49
1:A:492:GLU:HA	1:A:530:LYS:O	2.13	0.49
1:A:542:ILE:CB	1:A:545:ASN:HB3	2.37	0.49
2:B:206:ARG:HH11	2:B:206:ARG:CG	2.22	0.49
1:A:110:ASP:O	1:A:217:PRO:HD3	2.13	0.48
1:A:218:ASP:HB2	1:A:220:LYS:O	2.13	0.48
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.41	0.48
2:B:106:VAL:O	2:B:234:LEU:HB2	2.13	0.48
1:A:188:TYR:HD1	5:A:4001:K05:C5'	2.26	0.48
1:A:248:GLU:HG2	1:A:307:ARG:NH1	2.28	0.48
1:A:259:LYS:HG2	1:A:263:LYS:CE	2.43	0.48
1:A:271:TYR:HB3	1:A:274:ILE:HD11	1.94	0.48
1:A:271:TYR:O	1:A:274:ILE:HG12	2.13	0.48
1:A:331:LYS:NZ	1:A:333:GLY:HA2	2.28	0.48
2:B:94:ILE:HD11	2:B:158:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:N	1:A:55:PRO:HD3	2.27	0.48
1:A:427:TYR:OH	1:A:510:PRO:HD2	2.14	0.48
2:B:109:LEU:N	2:B:109:LEU:HD23	2.28	0.48
2:B:156:SER:N	2:B:157:PRO:CD	2.76	0.48
2:B:257:ILE:HD11	2:B:293:ILE:HG13	1.94	0.48
2:B:277:ARG:C	2:B:279:LEU:H	2.17	0.48
1:A:195:ILE:O	1:A:199:ARG:NE	2.46	0.48
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.49	0.48
2:B:50:ILE:CG1	2:B:143:ARG:HB3	2.43	0.48
2:B:269:GLN:HB3	2:B:346:PHE:CE1	2.49	0.48
1:A:84:THR:HG21	1:A:154:LYS:HB3	1.95	0.48
1:A:241:VAL:HG12	1:A:242:GLN:O	2.13	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.95	0.48
2:B:302:GLU:O	2:B:306:ASN:HB2	2.14	0.48
2:B:381:VAL:HG12	2:B:382:ILE:N	2.27	0.48
2:B:422:LEU:HD12	2:B:426:TRP:NE1	2.29	0.48
2:B:332:GLN:HB3	2:B:336:GLN:HB3	1.95	0.48
1:A:108:VAL:CG1	5:A:4001:K05:H6 <sup>+</sup>	2.44	0.48
1:A:341:ILE:HD13	1:A:383:TRP:CZ3	2.47	0.48
1:A:362:THR:CG2	1:A:367:GLN:HG3	2.44	0.48
1:A:148:VAL:HG23	1:A:149:LEU:O	2.14	0.48
2:B:261:VAL:HG21	2:B:283:LEU:HD11	1.96	0.48
1:A:192:ASP:OD1	1:A:192:ASP:N	2.41	0.47
1:A:413:GLU:O	1:A:413:GLU:CG	2.62	0.47
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.49	0.47
1:A:342:TYR:HA	1:A:349:LEU:CD2	2.43	0.47
1:A:424:LYS:HD3	1:A:426:TRP:CZ3	2.47	0.47
2:B:167:ILE:HG23	2:B:212:TRP:HB3	1.95	0.47
2:B:173:LYS:O	2:B:176:PRO:HD3	2.13	0.47
2:B:268:SER:HB3	2:B:274:ILE:HB	1.95	0.47
1:A:5:ILE:HG22	1:A:6:GLU:N	2.28	0.47
1:A:12:LEU:HG	1:A:124:PHE:HE1	1.79	0.47
1:A:269:GLN:O	1:A:351:THR:O	2.32	0.47
1:A:345:PRO:HA	3:C:1:GLC:C6	2.45	0.47
2:B:67:ASP:C	2:B:69:THR:H	2.15	0.47
2:B:114:ALA:HB2	2:B:215:THR:CG2	2.28	0.47
1:A:5:ILE:HD13	1:A:163:SER:HB3	1.97	0.47
1:A:523:GLU:OE1	1:A:526:ILE:HD12	2.14	0.47
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.48	0.47
1:A:432:GLU:OE2	1:A:432:GLU:HA	2.15	0.47
1:A:245:VAL:HG12	1:A:245:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:HG23	1:A:276:VAL:O	2.15	0.47
1:A:330:GLN:HG2	1:A:338:THR:HG23	1.97	0.47
2:B:404:GLU:HB3	2:B:405:TYR:CD1	2.49	0.47
1:A:90:VAL:HG23	1:A:161:GLN:CD	2.34	0.47
1:A:139:THR:HG22	1:A:139:THR:O	2.14	0.47
1:A:189:VAL:CG1	1:A:202:ILE:CD1	2.91	0.47
2:B:194:GLU:C	2:B:196:GLY:N	2.67	0.47
2:B:298:GLU:O	2:B:298:GLU:HG2	2.13	0.47
2:B:370:GLU:OE2	4:B:2003:GLC:H61	2.14	0.47
1:A:260:LEU:HD11	1:A:303:LEU:HD11	1.97	0.47
1:A:521:ILE:O	1:A:525:LEU:HG	2.14	0.47
2:B:271:TYR:HD2	2:B:309:ILE:HG22	1.80	0.47
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.97	0.47
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.97	0.47
2:B:85:GLN:C	2:B:87:PHE:N	2.68	0.47
2:B:206:ARG:NH1	2:B:206:ARG:CG	2.78	0.47
2:B:268:SER:HA	2:B:274:ILE:HD12	1.96	0.47
1:A:143:ARG:HH11	1:A:143:ARG:CG	2.01	0.47
1:A:238:LYS:HG2	1:A:316:GLY:O	2.15	0.47
1:A:455:ALA:HB2	1:A:480:GLN:HB3	1.97	0.47
1:A:222:GLN:O	1:A:222:GLN:CG	2.62	0.46
1:A:269:GLN:O	1:A:350:LYS:HG3	2.15	0.46
2:B:244:ILE:HG13	2:B:244:ILE:O	2.16	0.46
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.15	0.46
1:A:61:PHE:HD1	1:A:61:PHE:H	1.61	0.46
1:A:406:TRP:CD2	2:B:419:THR:HG22	2.50	0.46
1:A:21:VAL:O	1:A:57:ASN:HB3	2.15	0.46
1:A:253:THR:HB	1:A:291:GLU:H	1.81	0.46
1:A:541:GLY:O	1:A:543:GLY:N	2.48	0.46
2:B:94:ILE:HD13	2:B:161:GLN:CD	2.36	0.46
2:B:137:ASN:O	2:B:138:GLU:C	2.53	0.46
1:A:235:HIS:N	1:A:238:LYS:O	2.46	0.46
2:B:106:VAL:HA	2:B:189:VAL:O	2.16	0.46
2:B:197:GLN:O	2:B:200:THR:N	2.36	0.46
1:A:326:ILE:HD12	1:A:326:ILE:N	2.30	0.46
1:A:406:TRP:CH2	2:B:418:ASN:CA	2.90	0.46
1:A:516:GLU:HG2	1:A:517:LEU:N	2.31	0.46
2:B:181:TYR:C	2:B:181:TYR:CD1	2.86	0.46
1:A:189:VAL:HG13	1:A:189:VAL:O	2.15	0.46
1:A:164:MET:O	1:A:167:ILE:HB	2.15	0.46
1:A:207:GLN:O	1:A:211:ARG:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:O	1:A:247:PRO:HD3	2.16	0.46
2:B:13:LYS:HD3	2:B:86:ASP:OD2	2.15	0.46
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.46	0.46
1:A:193:LEU:C	1:A:194:GLU:O	2.49	0.46
1:A:217:PRO:O	1:A:218:ASP:HB3	2.15	0.46
1:A:259:LYS:HG2	1:A:263:LYS:NZ	2.30	0.46
2:B:67:ASP:C	2:B:69:THR:N	2.69	0.46
2:B:278:GLN:OE1	2:B:278:GLN:CA	2.63	0.46
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.96	0.46
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.81	0.46
2:B:91:GLN:HG2	2:B:92:LEU:HD21	1.95	0.46
2:B:402:TRP:C	2:B:404:GLU:H	2.18	0.46
1:A:17:ASP:O	1:A:83:ARG:NE	2.50	0.45
2:B:203:GLU:O	2:B:207:GLN:HG2	2.16	0.45
2:B:332:GLN:HE21	2:B:338:THR:HG23	1.81	0.45
1:A:77:PHE:O	1:A:80:LEU:N	2.35	0.45
1:A:136:ASN:ND2	1:A:137:ASN:H	2.13	0.45
2:B:12:LEU:HD21	2:B:124:PHE:CE1	2.45	0.45
2:B:48:SER:O	2:B:144:TYR:HA	2.15	0.45
2:B:73:LYS:HB3	2:B:73:LYS:HZ2	1.80	0.45
1:A:30:LYS:HE2	1:A:71:TRP:HZ3	1.81	0.45
1:A:88:TRP:HB3	2:B:52:PRO:HA	1.97	0.45
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.31	0.45
1:A:544:GLY:C	1:A:547:GLN:HG2	2.37	0.45
1:A:165:THR:O	1:A:167:ILE:N	2.50	0.45
2:B:266:TRP:CD2	2:B:425:LEU:HD12	2.50	0.45
2:B:266:TRP:HB3	2:B:425:LEU:HD12	1.98	0.45
2:B:398:TRP:C	2:B:400:THR:H	2.20	0.45
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.51	0.45
1:A:73:LYS:HZ3	1:A:75:VAL:CG2	2.27	0.45
1:A:175:ASN:N	1:A:176:PRO:HD3	2.29	0.45
1:A:372:VAL:HG13	1:A:389:PHE:CE1	2.52	0.45
1:A:518:VAL:HG12	1:A:522:ILE:HD11	1.99	0.45
2:B:65:LYS:HG2	2:B:72:ARG:CD	2.45	0.45
1:A:62:ALA:O	1:A:63:ILE:CD1	2.60	0.45
1:A:179:VAL:HG23	1:A:179:VAL:O	2.17	0.45
1:A:419:THR:H	1:A:422:LEU:HD11	1.81	0.45
1:A:544:GLY:O	1:A:547:GLN:CG	2.64	0.45
1:A:547:GLN:HB2	1:A:548:VAL:H	1.67	0.45
2:B:213:GLY:C	2:B:214:LEU:CG	2.84	0.45
1:A:32:LYS:HG2	1:A:33:ALA:N	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:CD1	4:A:2001:GLC:H3	2.52	0.45
1:A:181:TYR:HD1	1:A:188:TYR:HD2	1.60	0.45
1:A:206:ARG:HG3	1:A:216:THR:HG1	1.81	0.45
1:A:301:LEU:O	1:A:305:GLU:HG3	2.16	0.45
1:A:371:ALA:O	1:A:375:ILE:HG13	2.17	0.45
1:A:178:ILE:HG21	1:A:189:VAL:HG23	1.98	0.45
1:A:418:ASN:O	1:A:419:THR:CG2	2.65	0.45
1:A:441:TYR:HB2	1:A:458:VAL:O	2.15	0.45
1:A:239:TRP:HB3	1:A:318:TYR:CE2	2.44	0.45
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.52	0.45
1:A:514:GLU:HG3	1:A:515:SER:N	2.30	0.45
2:B:30:LYS:HB3	2:B:62:ALA:HB3	1.98	0.45
2:B:135:ILE:H	2:B:135:ILE:HG13	1.55	0.45
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.46	0.45
1:A:175:ASN:C	1:A:177:ASP:H	2.20	0.44
1:A:257:ILE:CB	1:A:283:LEU:HD21	2.39	0.44
1:A:291:GLU:O	1:A:293:ILE:HG13	2.16	0.44
1:A:523:GLU:O	1:A:526:ILE:HB	2.16	0.44
2:B:248:GLU:O	2:B:248:GLU:CG	2.65	0.44
2:B:290:THR:HG22	2:B:290:THR:O	2.17	0.44
2:B:332:GLN:HB3	2:B:336:GLN:CB	2.47	0.44
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.49	0.44
2:B:100:LEU:O	2:B:100:LEU:HD12	2.17	0.44
2:B:195:ILE:O	2:B:199:ARG:HG3	2.17	0.44
2:B:271:TYR:N	2:B:271:TYR:CD1	2.85	0.44
1:A:37:ILE:HG12	1:A:70:LYS:NZ	2.32	0.44
1:A:246:LEU:HD12	1:A:260:LEU:HD12	1.98	0.44
1:A:394:GLN:HG2	1:A:416:PHE:CD1	2.52	0.44
1:A:405:TYR:CE2	1:A:407:GLN:NE2	2.81	0.44
2:B:421:PRO:O	2:B:422:LEU:C	2.55	0.44
1:A:84:THR:O	1:A:154:LYS:NZ	2.51	0.44
1:A:104:LYS:CB	1:A:192:ASP:CB	2.96	0.44
1:A:196:GLY:HA2	1:A:199:ARG:NH1	2.32	0.44
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.31	0.44
1:A:490:GLY:O	1:A:528:LYS:NZ	2.28	0.44
1:A:107:THR:O	1:A:108:VAL:CG1	2.66	0.44
1:A:131:THR:CG2	1:A:143:ARG:CG	2.93	0.44
1:A:317:VAL:CG2	1:A:318:TYR:H	2.30	0.44
1:A:362:THR:HG22	1:A:367:GLN:HE21	1.82	0.44
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.17	0.44
2:B:353:LYS:HB2	2:B:353:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:HG21	1:A:383:TRP:CZ3	2.53	0.44
2:B:84:THR:O	2:B:87:PHE:N	2.41	0.44
2:B:206:ARG:NH1	2:B:206:ARG:HG3	2.28	0.44
2:B:308:GLU:C	2:B:310:LEU:N	2.70	0.44
1:A:163:SER:O	1:A:167:ILE:HG13	2.18	0.43
1:A:330:GLN:CG	1:A:338:THR:HG23	2.48	0.43
1:A:405:TYR:HE2	1:A:407:GLN:NE2	2.16	0.43
2:B:280:SER:O	2:B:284:ARG:NH1	2.49	0.43
2:B:312:GLU:HA	2:B:313:PRO:HD3	1.70	0.43
2:B:366:LYS:HB2	2:B:405:TYR:CE2	2.52	0.43
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.83	0.43
1:A:201:LYS:O	1:A:204:GLU:N	2.46	0.43
1:A:506:ILE:C	1:A:508:ALA:N	2.72	0.43
2:B:13:LYS:CB	2:B:14:PRO:CD	2.96	0.43
2:B:50:ILE:HG21	2:B:145:GLN:HG2	1.99	0.43
1:A:73:LYS:HZ2	1:A:75:VAL:CG2	2.30	0.43
1:A:516:GLU:H	1:A:516:GLU:CD	2.21	0.43
2:B:13:LYS:CD	2:B:14:PRO:HD3	2.48	0.43
1:A:20:LYS:CG	1:A:56:TYR:HB3	2.47	0.43
1:A:95:PRO:HG2	1:A:229:TRP:HH2	1.83	0.43
1:A:131:THR:HG22	1:A:143:ARG:HA	2.00	0.43
2:B:195:ILE:O	2:B:195:ILE:CG2	2.66	0.43
2:B:350:LYS:CE	2:B:378:GLU:OE1	2.66	0.43
2:B:374:LYS:HA	2:B:374:LYS:HD2	1.89	0.43
1:A:173:LYS:O	1:A:176:PRO:HD3	2.18	0.43
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.99	0.43
1:A:291:GLU:OE1	1:A:293:ILE:HG12	2.19	0.43
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.99	0.43
1:A:542:ILE:HG23	2:B:283:LEU:HB3	2.01	0.43
1:A:543:GLY:N	2:B:283:LEU:O	2.51	0.43
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.76	0.43
2:B:281:LYS:HA	2:B:284:ARG:HH11	1.84	0.43
1:A:54:ASN:OD1	1:A:55:PRO:N	2.51	0.43
1:A:76:ASP:O	1:A:76:ASP:OD1	2.37	0.43
1:A:121:ASP:O	1:A:123:ASP:N	2.51	0.43
1:A:542:ILE:C	1:A:546:GLU:HG2	2.39	0.43
2:B:58:THR:HG22	2:B:59:PRO:HD2	2.01	0.43
2:B:244:ILE:CD1	2:B:310:LEU:HD22	2.39	0.43
1:A:7:THR:O	1:A:9:PRO:HD3	2.18	0.43
1:A:18:GLY:CA	1:A:56:TYR:CD2	3.02	0.43
1:A:27:THR:O	1:A:31:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:C	1:A:167:ILE:H	2.21	0.43
2:B:317:VAL:HG11	2:B:348:ASN:O	2.19	0.43
1:A:55:PRO:O	1:A:143:ARG:NH2	2.52	0.42
1:A:240:THR:HG22	1:A:241:VAL:H	1.82	0.42
2:B:329:ILE:O	2:B:392:PRO:HG3	2.19	0.42
1:A:13:LYS:HB2	1:A:16:MET:CE	2.49	0.42
1:A:253:THR:OG1	1:A:256:ASP:OD1	2.37	0.42
1:A:295:LEU:HB3	1:A:300:GLU:CD	2.39	0.42
1:A:402:TRP:CE3	2:B:364:ASP:OD2	2.72	0.42
2:B:263:LYS:HG3	2:B:425:LEU:CD2	2.24	0.42
2:B:339:TYR:C	2:B:340:GLN:NE2	2.72	0.42
2:B:342:TYR:N	2:B:342:TYR:HD2	2.17	0.42
1:A:150:PRO:HB2	1:A:153:TRP:HB2	2.00	0.42
1:A:226:PRO:O	5:A:4001:K05:H18	2.20	0.42
1:A:320:ASP:O	1:A:343:GLN:NE2	2.40	0.42
1:A:218:ASP:HB2	1:A:220:LYS:CA	2.49	0.42
1:A:384:GLY:O	2:B:27:THR:HA	2.18	0.42
2:B:3:SER:CB	2:B:4:PRO:CD	2.86	0.42
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.55	0.42
1:A:33:ALA:HA	1:A:36:GLU:OE1	2.20	0.42
1:A:115:TYR:HD1	1:A:115:TYR:H	1.67	0.42
1:A:290:THR:O	1:A:290:THR:CG2	2.66	0.42
1:A:416:PHE:CE2	1:A:418:ASN:CB	2.93	0.42
2:B:103:LYS:HD2	2:B:192:ASP:OD2	2.19	0.42
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.16	0.42
2:B:401:TRP:O	2:B:404:GLU:CB	2.67	0.42
2:B:407:GLN:O	2:B:407:GLN:HG3	2.18	0.42
2:B:421:PRO:C	2:B:422:LEU:O	2.44	0.42
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.55	0.42
1:A:541:GLY:HA2	1:A:546:GLU:HG3	2.01	0.42
1:A:545:ASN:O	1:A:545:ASN:CG	2.57	0.42
2:B:208:HIS:CE1	2:B:212:TRP:CD1	2.99	0.42
1:A:79:GLU:OE2	1:A:82:LYS:HD3	2.20	0.42
1:A:246:LEU:O	1:A:307:ARG:NH1	2.53	0.42
1:A:362:THR:HG21	1:A:367:GLN:HG3	2.02	0.42
2:B:180:ILE:HG23	2:B:187:LEU:HD11	2.02	0.42
2:B:295:LEU:HD13	2:B:300:GLU:HG2	2.02	0.42
2:B:406:TRP:HZ2	2:B:410:TRP:O	2.03	0.42
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.49	0.42
1:A:240:THR:CG2	1:A:241:VAL:H	2.33	0.42
1:A:253:THR:C	1:A:293:ILE:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:HZ1	1:A:333:GLY:HA2	1.85	0.42
2:B:2:ILE:HD13	2:B:5:ILE:CD1	2.48	0.42
2:B:33:ALA:O	2:B:37:ILE:HG13	2.19	0.42
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.48	0.42
2:B:356:ARG:HD3	2:B:356:ARG:C	2.40	0.42
1:A:77:PHE:HB3	1:A:80:LEU:HB3	2.00	0.42
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.76	0.42
1:A:286:THR:CG2	1:A:287:LYS:N	2.83	0.42
1:A:360:ALA:C	1:A:361:HIS:CG	2.93	0.42
1:A:380:ILE:O	1:A:380:ILE:HG22	2.19	0.42
1:A:394:GLN:O	1:A:396:GLU:N	2.53	0.42
1:A:472:THR:HG1	1:A:476:LYS:HB3	1.83	0.42
1:A:516:GLU:CD	1:A:516:GLU:N	2.73	0.42
1:A:524:GLN:O	1:A:528:LYS:HG2	2.19	0.42
1:A:547:GLN:HG3	2:B:286:THR:CG2	2.50	0.42
2:B:85:GLN:C	2:B:87:PHE:H	2.22	0.42
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.90	0.42
2:B:179:VAL:HG22	2:B:190:GLY:CA	2.50	0.42
2:B:184:MET:HB3	2:B:185:ASP:OD1	2.19	0.42
1:A:239:TRP:HZ2	1:A:349:LEU:O	2.02	0.42
1:A:543:GLY:C	2:B:284:ARG:HA	2.37	0.42
2:B:22:LYS:HD2	2:B:22:LYS:O	2.20	0.42
1:A:254:VAL:CA	1:A:293:ILE:HD11	2.50	0.41
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.49	0.41
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.02	0.41
2:B:333:GLY:O	2:B:334:GLN:HB2	2.19	0.41
2:B:344:GLU:O	2:B:345:PRO:C	2.58	0.41
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.55	0.41
1:A:107:THR:C	1:A:108:VAL:HG13	2.40	0.41
2:B:60:VAL:CG1	2:B:75:VAL:HG12	2.49	0.41
2:B:402:TRP:C	2:B:404:GLU:N	2.72	0.41
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.56	0.41
1:A:11:LYS:N	1:A:85:GLN:OE1	2.54	0.41
1:A:357:MET:C	1:A:358:ARG:HG3	2.41	0.41
1:A:394:GLN:C	1:A:396:GLU:N	2.74	0.41
1:A:483:TYR:CE2	1:A:487:GLN:OE1	2.73	0.41
1:A:63:ILE:HG22	1:A:64:LYS:H	1.86	0.41
1:A:402:TRP:HE3	2:B:364:ASP:OD2	2.03	0.41
2:B:13:LYS:HD2	2:B:13:LYS:HA	1.78	0.41
2:B:60:VAL:HG11	2:B:130:PHE:CB	2.50	0.41
2:B:266:TRP:CZ3	2:B:425:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:HG1	1:A:124:PHE:HZ	1.69	0.41
1:A:255:ASN:HB2	1:A:289:LEU:O	2.20	0.41
1:A:391:LEU:N	1:A:391:LEU:HD23	2.36	0.41
1:A:354:TYR:OH	1:A:370:GLU:HB2	2.21	0.41
1:A:389:PHE:CD1	1:A:391:LEU:HD21	2.54	0.41
1:A:457:TYR:CE2	1:A:465:LYS:N	2.89	0.41
1:A:458:VAL:HG11	2:B:286:THR:HG21	2.02	0.41
2:B:118:VAL:HA	2:B:119:PRO:HD2	1.94	0.41
1:A:74:LEU:O	1:A:74:LEU:CD1	2.68	0.41
1:A:460:ASN:ND2	1:A:461:LYS:H	2.19	0.41
1:A:497:THR:HG22	1:A:498:ASP:N	2.35	0.41
2:B:188:TYR:CD1	2:B:188:TYR:N	2.89	0.41
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.21	0.41
1:A:329:ILE:CG2	1:A:330:GLN:N	2.84	0.41
1:A:330:GLN:HG2	1:A:338:THR:O	2.20	0.41
1:A:493:VAL:HG22	1:A:494:ASN:H	1.85	0.41
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.36	0.41
2:B:114:ALA:HB1	2:B:160:PHE:CE2	2.56	0.41
2:B:153:TRP:C	2:B:155:GLY:H	2.25	0.41
2:B:213:GLY:C	2:B:215:THR:N	2.74	0.41
2:B:171:PHE:CD1	2:B:171:PHE:C	2.93	0.41
1:A:66:LYS:HD3	1:A:66:LYS:HA	1.84	0.40
1:A:116:PHE:HA	1:A:148:VAL:HG21	2.03	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.76	0.40
1:A:239:TRP:CZ2	1:A:349:LEU:O	2.74	0.40
1:A:356:ARG:HH22	1:A:513:SER:HA	1.86	0.40
2:B:339:TYR:OH	2:B:350:LYS:HE3	2.22	0.40
1:A:2:ILE:H	1:A:2:ILE:HG12	1.54	0.40
1:A:109:LEU:CD1	1:A:205:LEU:HD23	2.50	0.40
1:A:238:LYS:CD	1:A:315:HIS:HB3	2.41	0.40
2:B:58:THR:HA	2:B:59:PRO:HD3	1.89	0.40
1:A:3:SER:HA	1:A:4:PRO:HD3	1.90	0.40
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.37	0.40
1:A:126:LYS:HG3	1:A:127:TYR:CE1	2.56	0.40
1:A:254:VAL:N	1:A:293:ILE:HD11	2.36	0.40
1:A:394:GLN:HG2	1:A:416:PHE:CE1	2.56	0.40
2:B:139:THR:CB	2:B:140:PRO:HD2	2.48	0.40
1:A:10:VAL:HG12	1:A:11:LYS:N	2.37	0.40
1:A:23:GLN:NE2	1:A:131:THR:O	2.54	0.40
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.80	0.40
2:B:34:LEU:HD21	2:B:61:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:TYR:CE2	2:B:352:GLY:HA3	2.57	0.40
3:D:1:GLC:H61	3:D:2:FRU:H61	2.03	0.40
1:A:96:HIS:ND1	1:A:96:HIS:C	2.74	0.40
2:B:237:ASP:CG	2:B:238:LYS:N	2.75	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	550/552 (100%)	433 (79%)	101 (18%)	16 (3%)	4	25
2	B	416/429 (97%)	324 (78%)	76 (18%)	16 (4%)	3	19
All	All	966/981 (98%)	757 (78%)	177 (18%)	32 (3%)	4	22

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	406	TRP
2	B	423	VAL
1	A	78	ARG
1	A	90	VAL
1	A	122	GLU
1	A	515	SER
2	B	68	SER
2	B	91	GLN
2	B	154	LYS
2	B	241	VAL
1	A	114	ALA
1	A	162	SER
1	A	166	LYS

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Mol	Chain	Res	Type
1	A	507	GLN
2	B	123	ASP
2	B	215	THR
2	B	232	TYR
2	B	425	LEU
1	A	31	ILE
1	A	542	ILE
2	B	399	GLU
1	A	51	GLY
1	A	218	ASP
1	A	543	GLY
2	B	138	GLU
2	B	164	MET
2	B	18	GLY
1	A	176	PRO
2	B	4	PRO
2	B	421	PRO
2	B	170	PRO

### 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	494/494 (100%)	449 (91%)	45 (9%)	9 32
2	B	382/391 (98%)	352 (92%)	30 (8%)	12 40
All	All	876/885 (99%)	801 (91%)	75 (9%)	10 35

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	12	LEU
1	A	23	GLN
1	A	24	TRP
1	A	28	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	35	VAL
1	A	46	LYS
1	A	47	ILE
1	A	53	GLU
1	A	56	TYR
1	A	71	TRP
1	A	72	ARG
1	A	74	LEU
1	A	76	ASP
1	A	84	THR
1	A	92	LEU
1	A	100	LEU
1	A	105	SER
1	A	136	ASN
1	A	143	ARG
1	A	177	ASP
1	A	186	ASP
1	A	192	ASP
1	A	195	ILE
1	A	211	ARG
1	A	221	HIS
1	A	223	LYS
1	A	225	PRO
1	A	279	LEU
1	A	287	LYS
1	A	330	GLN
1	A	346	PHE
1	A	358	ARG
1	A	397	THR
1	A	413	GLU
1	A	414	TRP
1	A	435	VAL
1	A	448	ARG
1	A	457	TYR
1	A	474	ASN
1	A	494	ASN
1	A	514	GLU
1	A	545	ASN
1	A	546	GLU
1	A	551	LEU
2	B	22	LYS
2	B	58	THR

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Mol	Chain	Res	Type
2	B	67	ASP
2	B	84	THR
2	B	94	ILE
2	B	109	LEU
2	B	134	SER
2	B	135	ILE
2	B	163	SER
2	B	164	MET
2	B	177	ASP
2	B	181	TYR
2	B	185	ASP
2	B	193	LEU
2	B	211	ARG
2	B	212	TRP
2	B	214	LEU
2	B	250	ASP
2	B	280	SER
2	B	293	ILE
2	B	302	GLU
2	B	307	ARG
2	B	330	GLN
2	B	342	TYR
2	B	356	ARG
2	B	403	THR
2	B	405	TYR
2	B	414	TRP
2	B	418	ASN
2	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	ASN
1	A	151	GLN
1	A	161	GLN
1	A	197	GLN
1	A	242	GLN
1	A	330	GLN
1	A	340	GLN
1	A	407	GLN
1	A	545	ASN

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Mol	Chain	Res	Type
1	A	547	GLN
2	B	161	GLN
2	B	208	HIS
2	B	330	GLN
2	B	332	GLN
2	B	340	GLN
2	B	407	GLN

### 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](#)

4 monosaccharides 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
3	GLC	C	1	3	11,11,12	1.08	1 (9%)	15,15,17	1.06	2 (13%)
3	FRU	C	2	3	11,12,12	1.38	2 (18%)	10,18,18	0.89	0
3	GLC	D	1	3	11,11,12	1.25	1 (9%)	15,15,17	1.56	3 (20%)
3	FRU	D	2	3	11,12,12	1.39	2 (18%)	10,18,18	1.07	1 (10%)

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
3	GLC	C	1	3	-	1/2/19/22	0/1/1/1
3	FRU	C	2	3	-	3/5/24/24	0/1/1/1
3	GLC	D	1	3	-	1/2/19/22	0/1/1/1
3	FRU	D	2	3	-	0/5/24/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	FRU	C1-C2	3.47	1.57	1.52
3	C	2	FRU	C1-C2	3.07	1.57	1.52
3	C	2	FRU	O2-C2	3.06	1.46	1.40
3	D	1	GLC	C4-C5	2.70	1.58	1.53
3	D	2	FRU	O2-C2	2.67	1.45	1.40
3	C	1	GLC	C1-C2	2.14	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	GLC	C2-C3-C4	-3.25	105.27	110.89
3	D	1	GLC	O5-C5-C6	2.74	111.50	107.20
3	D	1	GLC	O5-C1-C2	-2.61	106.74	110.77
3	C	1	GLC	C1-O5-C5	2.55	115.64	112.19
3	C	1	GLC	C2-C3-C4	-2.33	106.86	110.89
3	D	2	FRU	O2-C2-O5	2.17	113.69	109.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	FRU	O1-C1-C2-C3
3	C	2	FRU	O1-C1-C2-O2
3	C	2	FRU	O1-C1-C2-O5
3	C	1	GLC	O5-C5-C6-O6
3	D	1	GLC	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

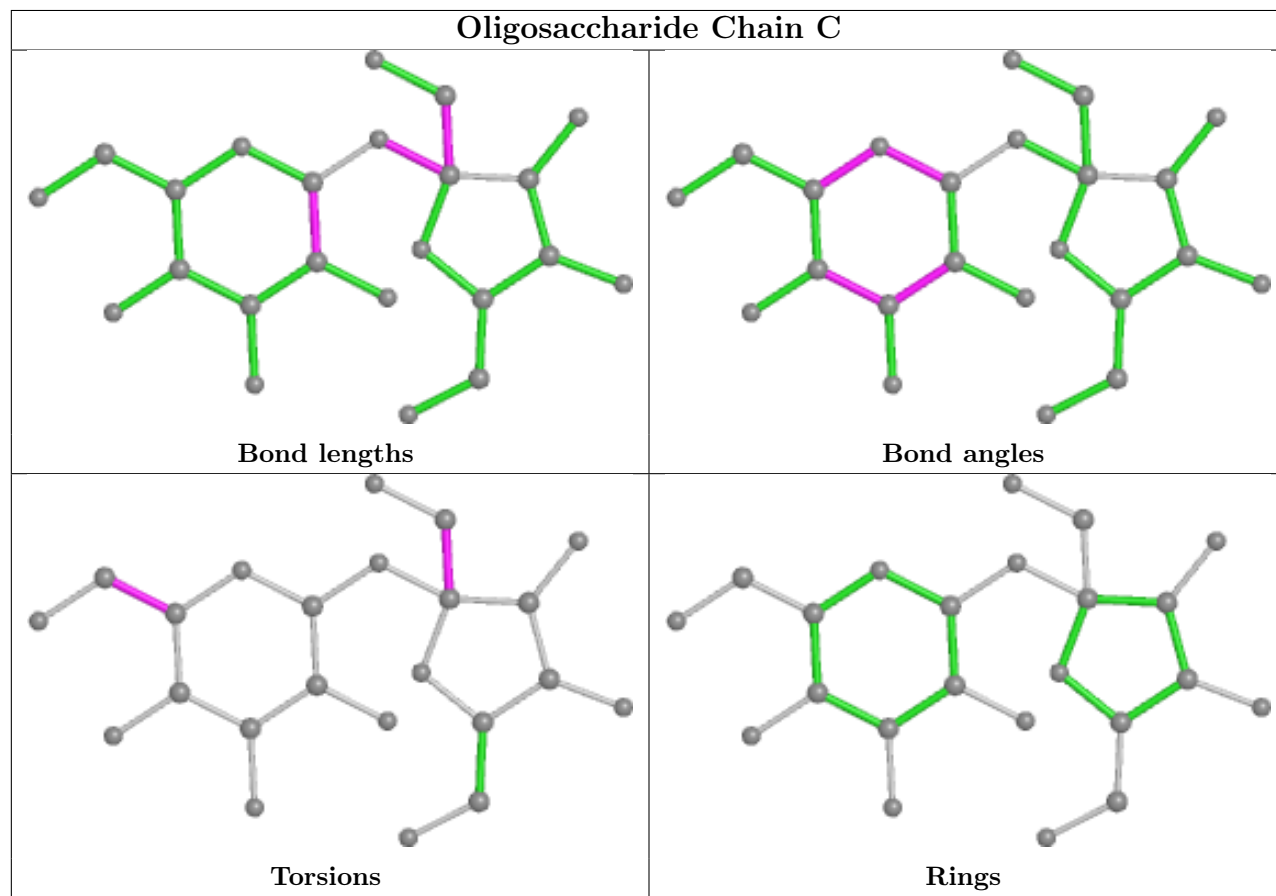
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	GLC	4	0
3	D	2	FRU	1	0

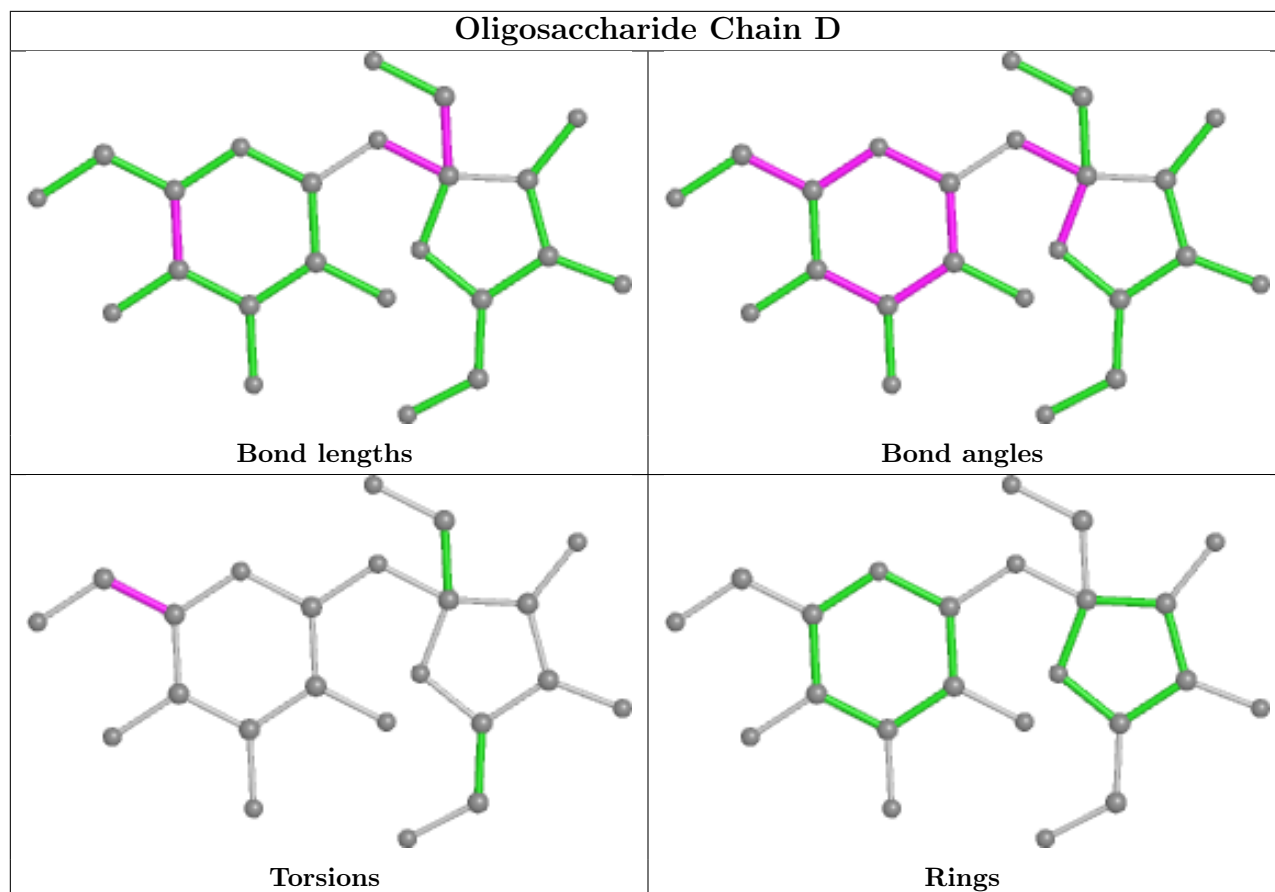
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GLC	B	2003	-	12,12,12	0.76	0	17,17,17	0.81	1 (5%)
4	GLC	A	2002	-	12,12,12	0.59	0	17,17,17	0.85	1 (5%)
4	GLC	A	2001	-	12,12,12	0.56	0	17,17,17	1.20	2 (11%)
5	K05	A	4001	-	27,27,27	5.43	18 (66%)	37,37,37	1.53	5 (13%)

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
4	GLC	B	2003	-	-	0/2/22/22	0/1/1/1
4	GLC	A	2002	-	-	0/2/22/22	0/1/1/1
4	GLC	A	2001	-	-	1/2/22/22	0/1/1/1
5	K05	A	4001	-	-	2/12/12/12	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4001	K05	O3-C3	13.62	1.51	1.23
5	A	4001	K05	C3-N2	10.90	1.49	1.35
5	A	4001	K05	C29-C25	8.19	1.57	1.43
5	A	4001	K05	C11-N1	7.76	1.37	1.28
5	A	4001	K05	C2'-C3'	7.54	1.49	1.38
5	A	4001	K05	N2-N1	-7.14	1.29	1.38
5	A	4001	K05	C2'-C1'	6.50	1.49	1.39
5	A	4001	K05	C14-C13	6.07	1.52	1.39
5	A	4001	K05	C6'-C1'	5.54	1.48	1.39
5	A	4001	K05	C12-C13	5.32	1.52	1.41
5	A	4001	K05	C5'-C4'	4.36	1.47	1.39
5	A	4001	K05	C17-C16	4.36	1.46	1.36
5	A	4001	K05	C18-C19	4.28	1.46	1.36
5	A	4001	K05	C18-C17	3.52	1.47	1.38
5	A	4001	K05	C15-C14	3.48	1.43	1.36
5	A	4001	K05	C6'-C5'	3.24	1.44	1.38
5	A	4001	K05	C4'-C3'	2.86	1.44	1.40
5	A	4001	K05	C16-C25	2.59	1.48	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4001	K05	C10-O13-C13	4.40	124.17	117.53
5	A	4001	K05	C29-C12-C11	3.57	125.96	121.09
4	A	2001	GLC	C4-C3-C2	3.19	116.39	110.82
4	A	2001	GLC	C3-C4-C5	2.77	115.17	110.24
5	A	4001	K05	C17-C18-C19	2.59	124.08	120.44
4	B	2003	GLC	C3-C4-C5	2.34	114.41	110.24
5	A	4001	K05	C1'-C3-N2	2.22	119.10	115.97
4	A	2002	GLC	C3-C4-C5	2.16	114.10	110.24
5	A	4001	K05	C5'-C6'-C1'	2.04	123.16	120.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

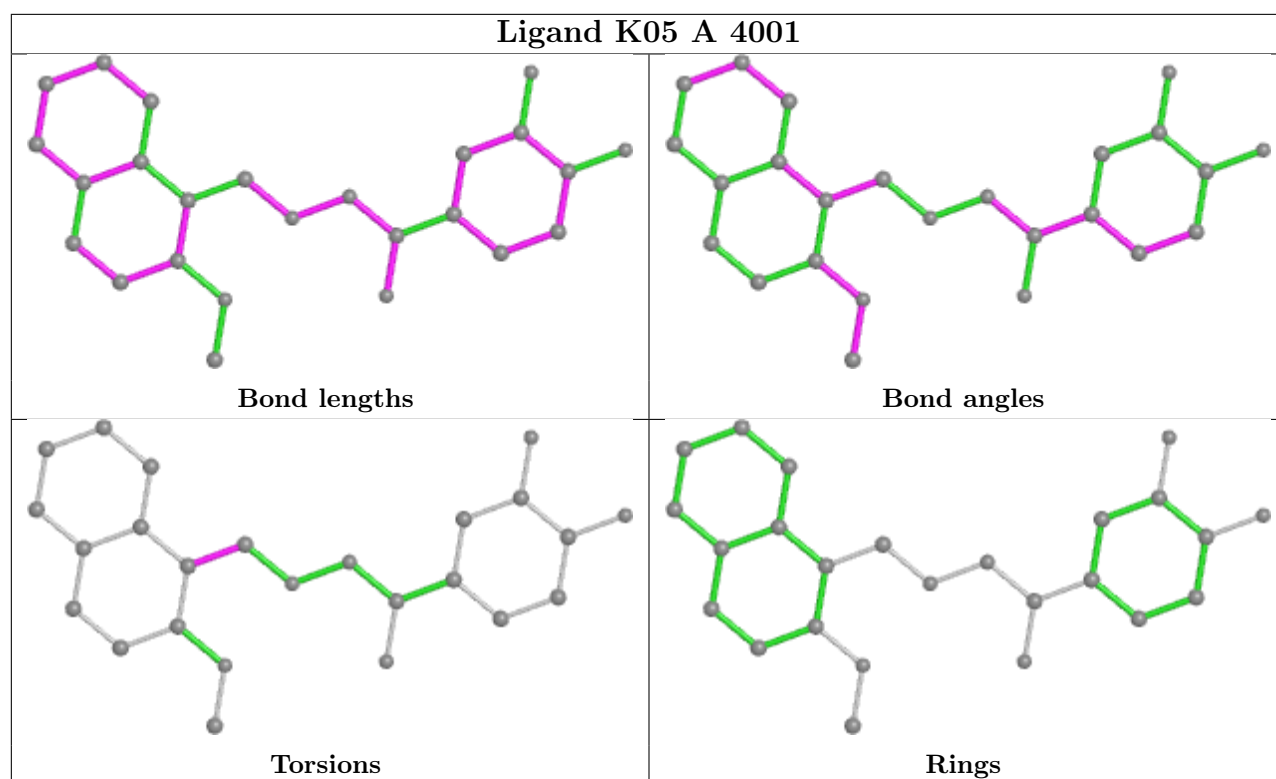
Mol	Chain	Res	Type	Atoms
5	A	4001	K05	N1-C11-C12-C29
5	A	4001	K05	N1-C11-C12-C13
4	A	2001	GLC	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2003	GLC	1	0
4	A	2001	GLC	3	0
5	A	4001	K05	7	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	552/552 (100%)	-0.18	14 (2%) 57 42	38, 93, 143, 150	0
2	B	420/429 (97%)	-0.24	15 (3%) 42 26	35, 77, 145, 150	0
All	All	972/981 (99%)	-0.20	29 (2%) 50 33	35, 88, 144, 150	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	9.3
2	B	428	GLN	6.1
2	B	3	SER	5.9
1	A	67	ASP	4.6
2	B	1	PRO	4.6
1	A	134	SER	4.1
2	B	231	GLY	4.0
2	B	2	ILE	3.5
2	B	4	PRO	3.4
1	A	1	PRO	3.1
1	A	136	ASN	3.1
1	A	552	VAL	3.1
1	A	69	THR	3.0
1	A	359	GLY	3.0
2	B	15	GLY	2.9
1	A	360	ALA	2.9
2	B	361	HIS	2.9
2	B	238	LYS	2.9
1	A	68	SER	2.7
2	B	429	LEU	2.6
2	B	358	ARG	2.5
2	B	357	MET	2.4
2	B	14	PRO	2.4
2	B	356	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	25	PRO	2.3
1	A	72	ARG	2.3
1	A	286	THR	2.1
1	A	420	PRO	2.0
2	B	220	LYS	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

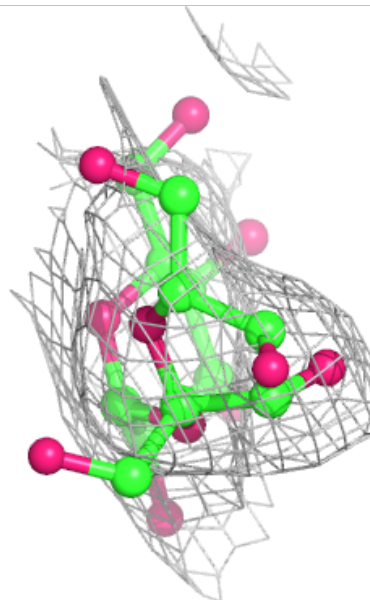
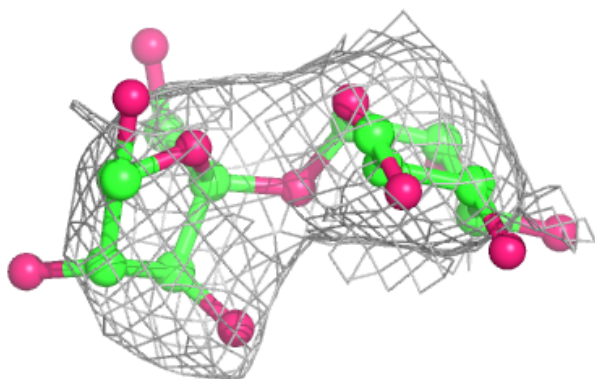
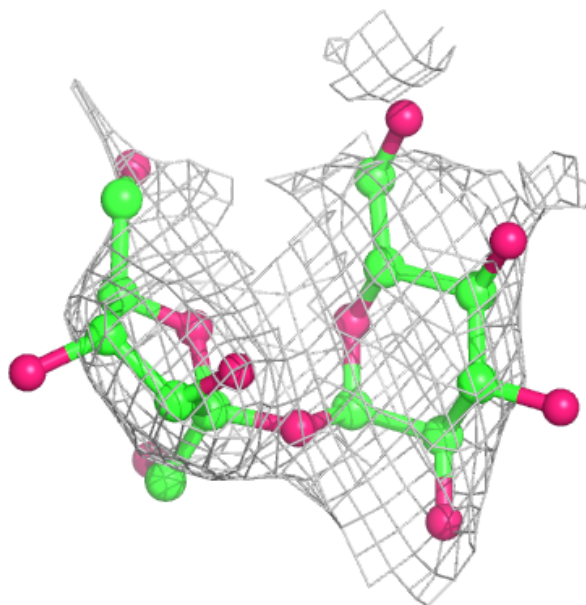
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

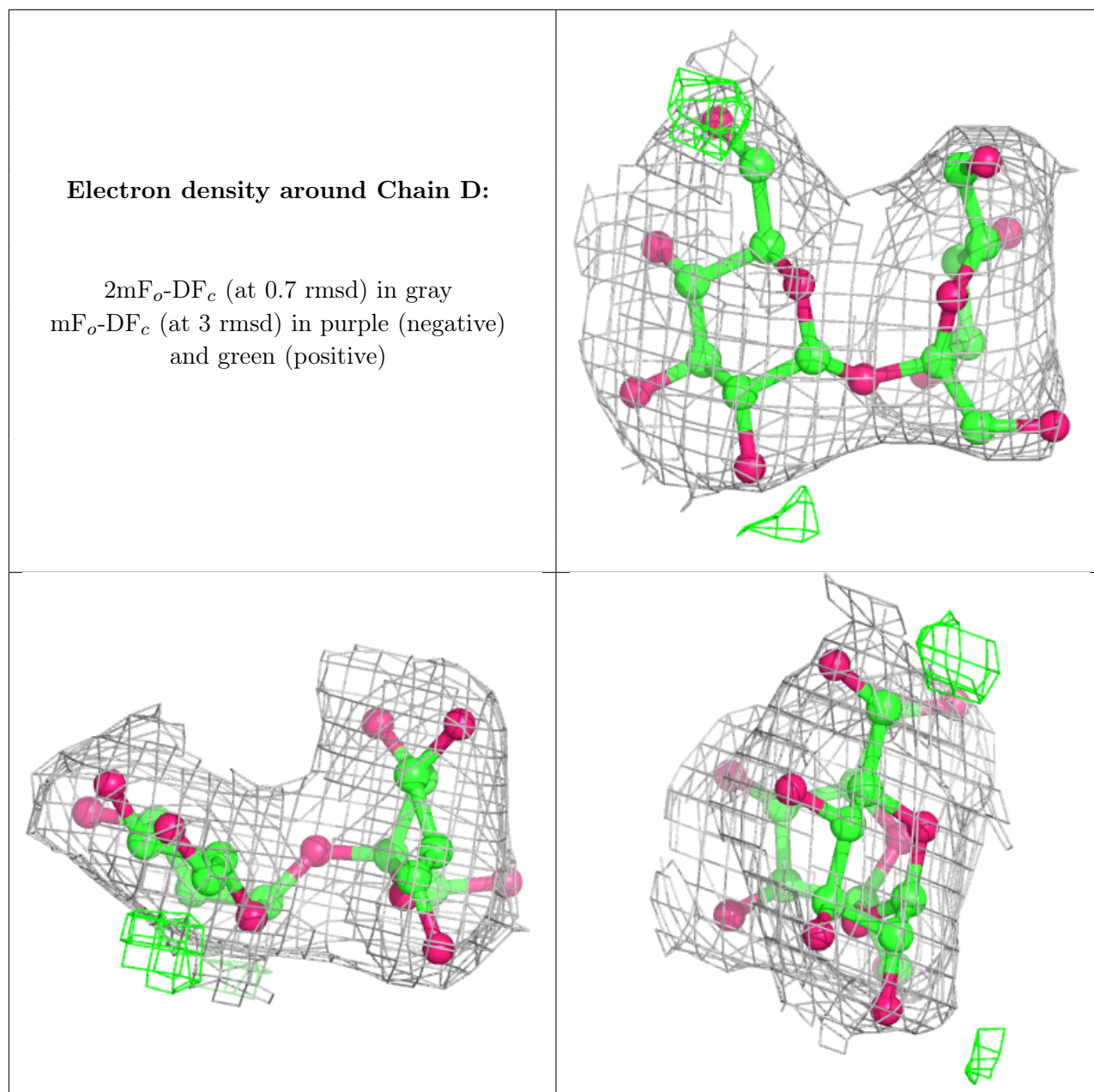
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FRU	C	2	12/12	0.78	0.43	110,137,143,146	0
3	GLC	C	1	11/12	0.88	0.28	105,124,134,134	0
3	GLC	D	1	11/12	0.95	0.17	47,60,70,99	0
3	FRU	D	2	12/12	0.96	0.14	54,69,83,84	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

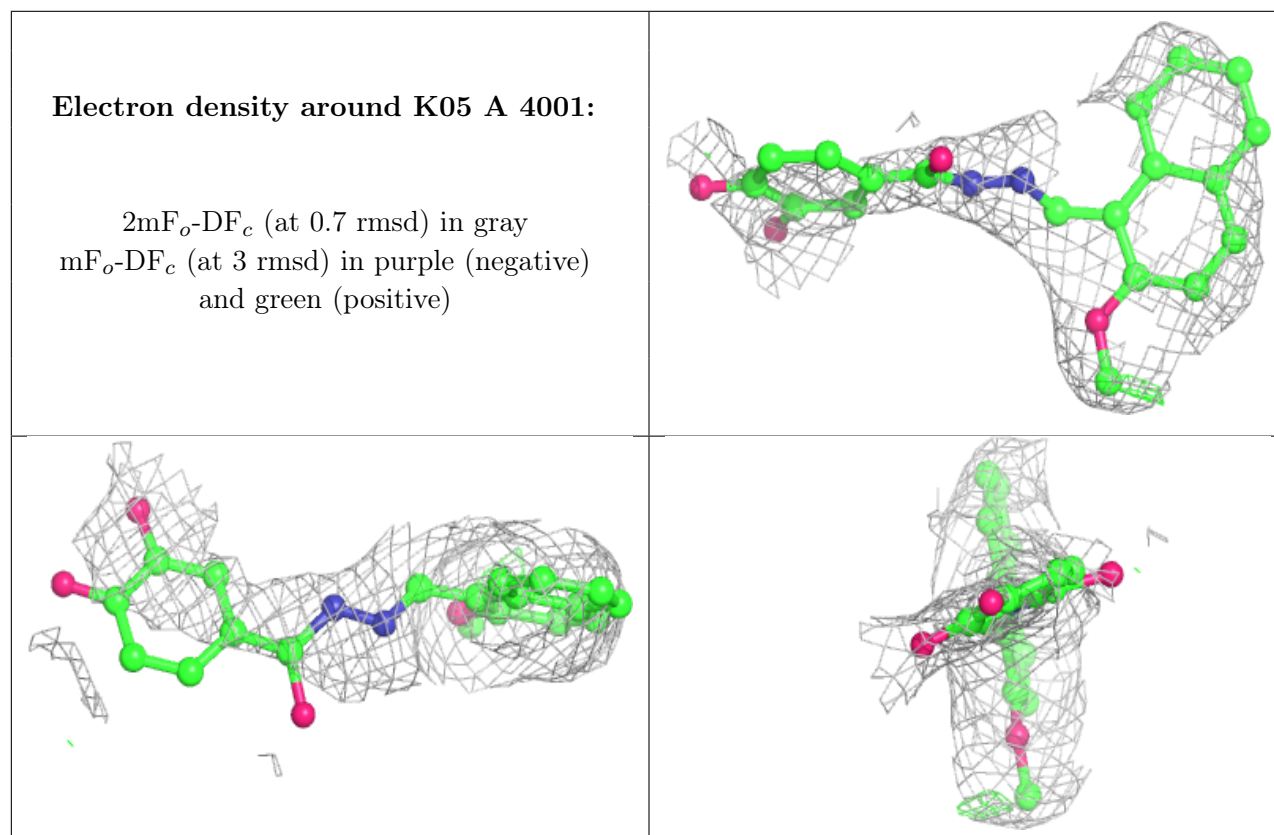
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GLC	B	2003	12/12	0.78	0.38	101,134,142,150	0
4	GLC	A	2002	12/12	0.85	0.24	92,123,130,139	0
4	GLC	A	2001	12/12	0.87	0.36	113,138,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	K05	A	4001	25/25	0.88	0.23	86,105,111,113	0
6	MG	A	5001	1/1	0.94	0.19	75,75,75,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.