Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 10:52 PM EDT

PDB ID	:	2WRF
Title	:	structure of H2 avian jena hemagglutinin with human receptor
Authors	:	Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on	:	2009-09-01
Resolution	:	3.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

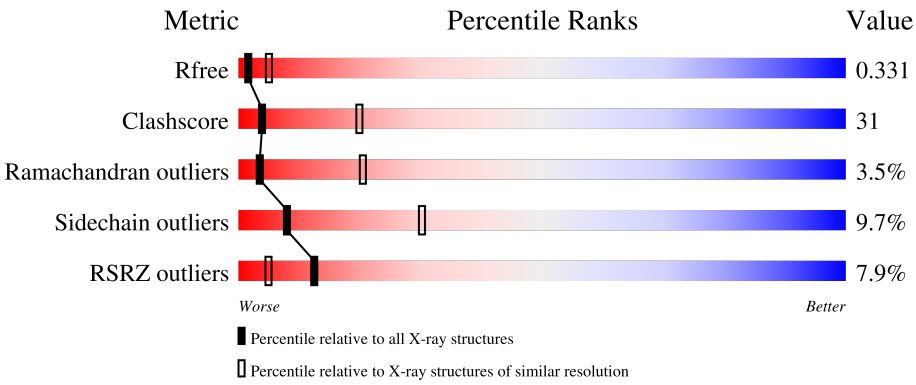
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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% 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	507	4% 32% 48% 15% • •
1	B	507	5% 54% 37% • •
1	C	507	6% 55% 37% • •
1	D	507	8% 37% 49% 9% • •
1	E	507	12% 53% 39% • •

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Mol	Chain	Length	Quality of chain
1	F	507	8% 53% 39%
1	G	507	9% 49% 36% 9%
1	H	507	10% 54% 36% 5%
1	I	507	7% 56% 35% 5%
2	J	2	50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34577 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	486	3837	2409	656	748	24	0	0	0
1	B	486	3837	2409	656	748	24	0	0	0
1	C	486	3834	2408	655	747	24	0	0	0
1	D	486	3837	2409	656	748	24	0	0	0
1	E	486	3837	2409	656	748	24	0	0	0
1	F	486	3834	2408	655	747	24	0	0	0
1	G	486	3837	2409	656	748	24	0	0	0
1	H	486	3837	2409	656	748	24	0	0	0
1	I	486	3834	2408	655	747	24	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ILE	LEU	conflict	UNP Q67326
A	142	ASP	GLY	conflict	UNP Q67326
A	374	PHE	ILE	conflict	UNP Q67326
A	459	VAL	ALA	conflict	UNP Q67326
B	109	ILE	LEU	conflict	UNP Q67326
B	142	ASP	GLY	conflict	UNP Q67326
B	374	PHE	ILE	conflict	UNP Q67326
B	459	VAL	ALA	conflict	UNP Q67326
C	109	ILE	LEU	conflict	UNP Q67326
C	142	ASP	GLY	conflict	UNP Q67326
C	374	PHE	ILE	conflict	UNP Q67326

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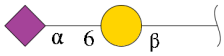
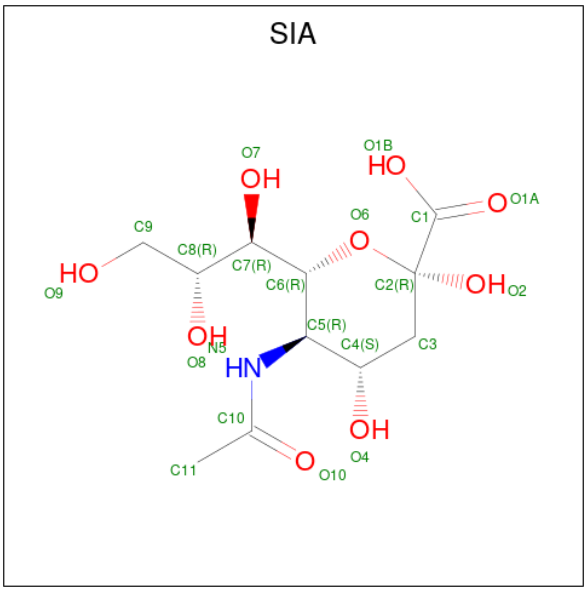
Chain	Residue	Modelled	Actual	Comment	Reference
C	459	VAL	ALA	conflict	UNP Q67326
D	109	ILE	LEU	conflict	UNP Q67326
D	142	ASP	GLY	conflict	UNP Q67326
D	374	PHE	ILE	conflict	UNP Q67326
D	459	VAL	ALA	conflict	UNP Q67326
E	109	ILE	LEU	conflict	UNP Q67326
E	142	ASP	GLY	conflict	UNP Q67326
E	374	PHE	ILE	conflict	UNP Q67326
E	459	VAL	ALA	conflict	UNP Q67326
F	109	ILE	LEU	conflict	UNP Q67326
F	142	ASP	GLY	conflict	UNP Q67326
F	374	PHE	ILE	conflict	UNP Q67326
F	459	VAL	ALA	conflict	UNP Q67326
G	109	ILE	LEU	conflict	UNP Q67326
G	142	ASP	GLY	conflict	UNP Q67326
G	374	PHE	ILE	conflict	UNP Q67326
G	459	VAL	ALA	conflict	UNP Q67326
H	109	ILE	LEU	conflict	UNP Q67326
H	142	ASP	GLY	conflict	UNP Q67326
H	374	PHE	ILE	conflict	UNP Q67326
H	459	VAL	ALA	conflict	UNP Q67326
I	109	ILE	LEU	conflict	UNP Q67326
I	142	ASP	GLY	conflict	UNP Q67326
I	374	PHE	ILE	conflict	UNP Q67326
I	459	VAL	ALA	conflict	UNP Q67326

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	J	2	32	17	1	14	0	0	0

- Molecule 3 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



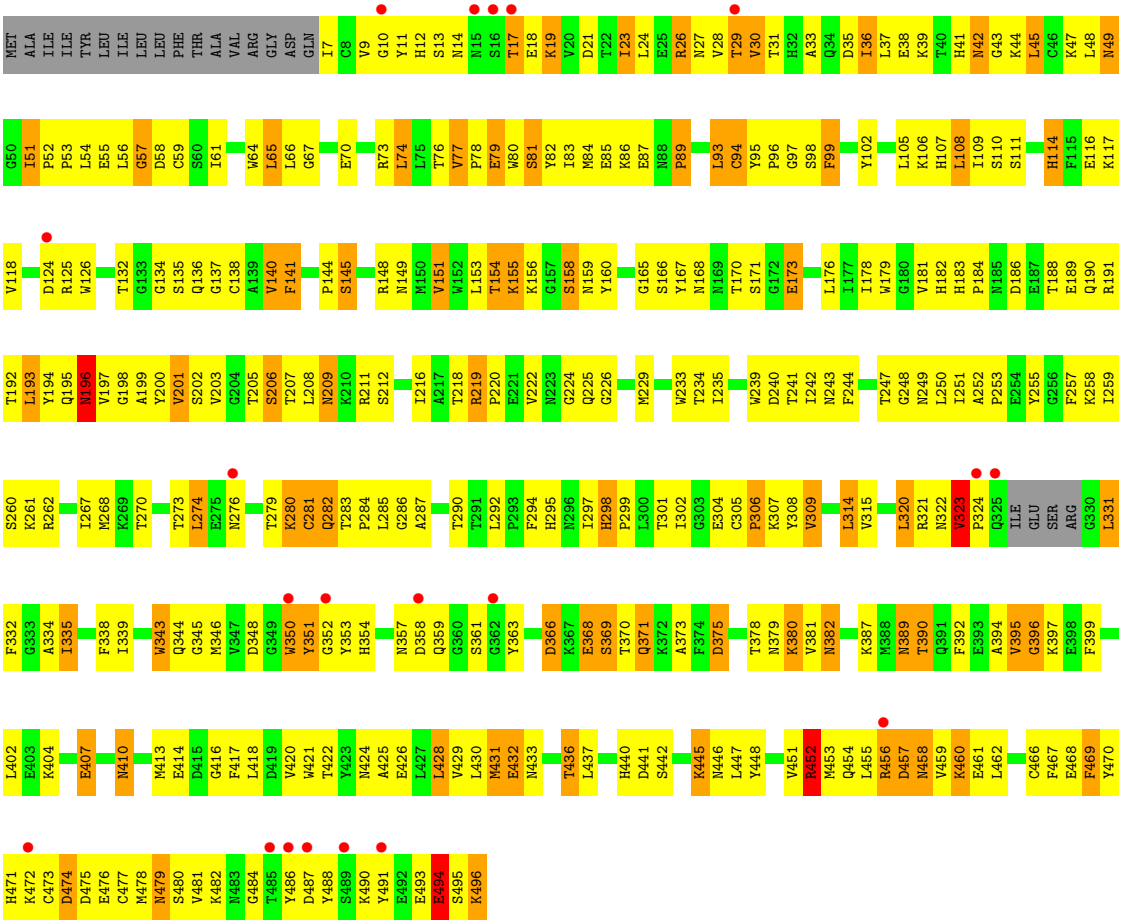
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	D	1	21	11	1	9	0	0

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 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.

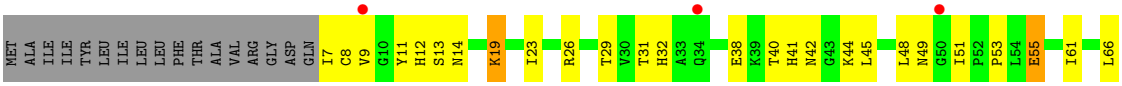
• Molecule 1: HEMAGGLUTININ

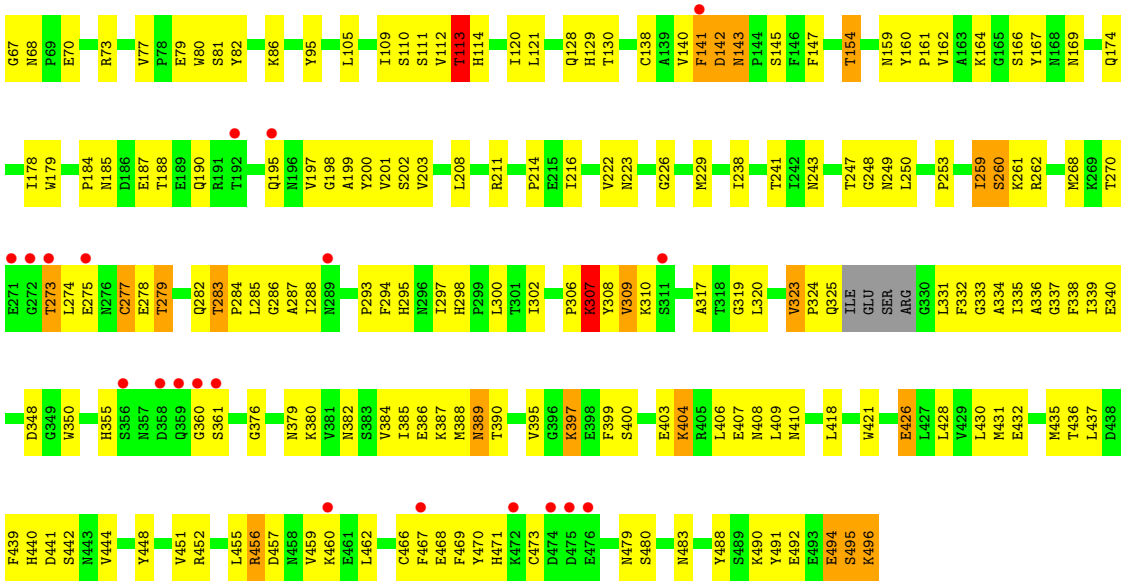
Chain A:



• Molecule 1: HEMAGGLUTININ

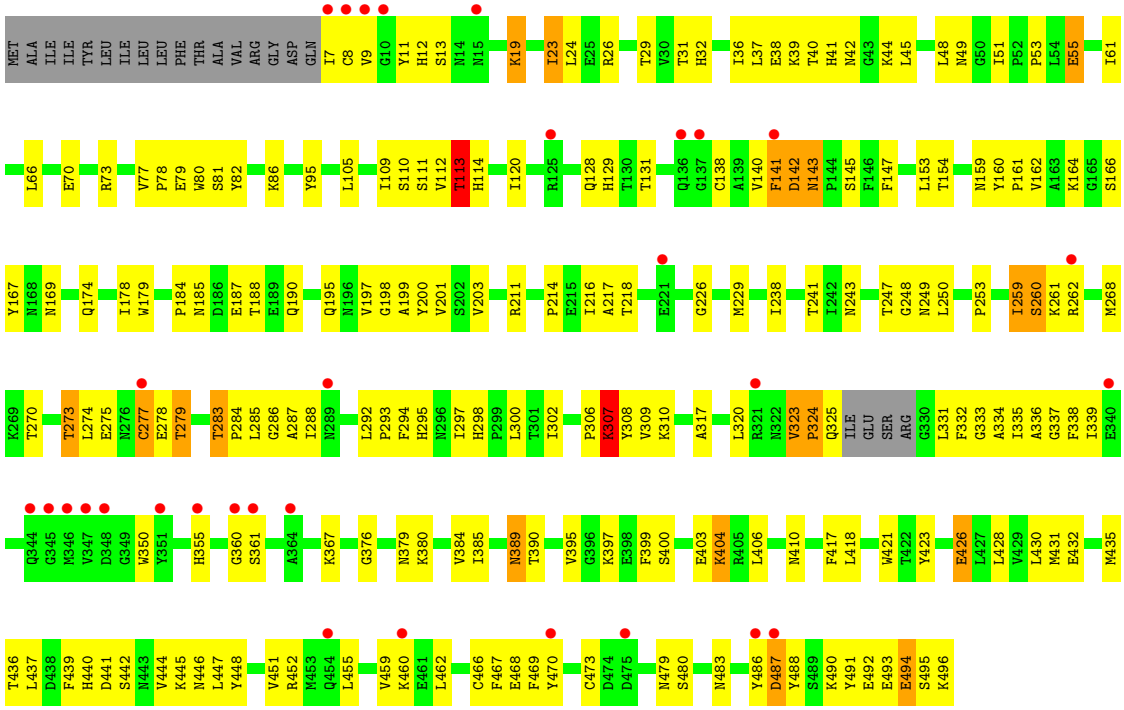
Chain B:





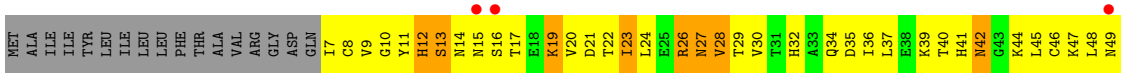
- Molecule 1: HEMAGGLUTININ

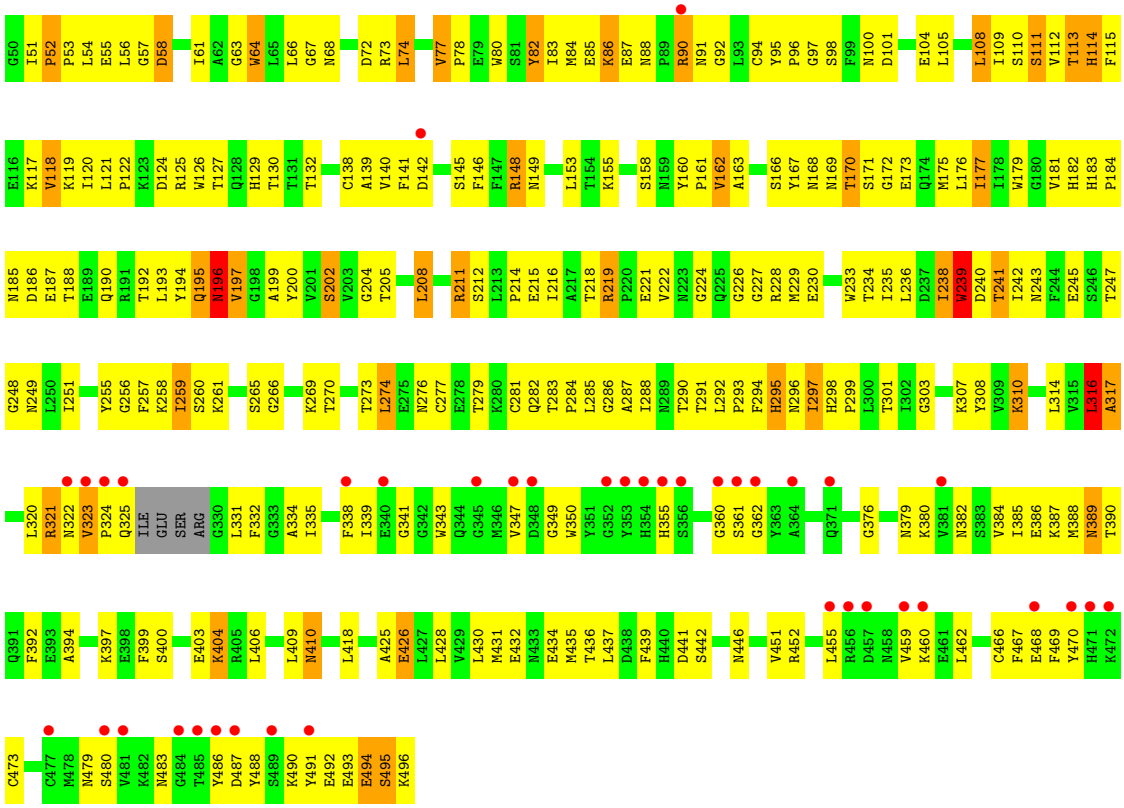
Chain C:



- Molecule 1: HEMAGGLUTININ

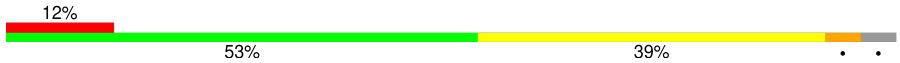
Chain D:

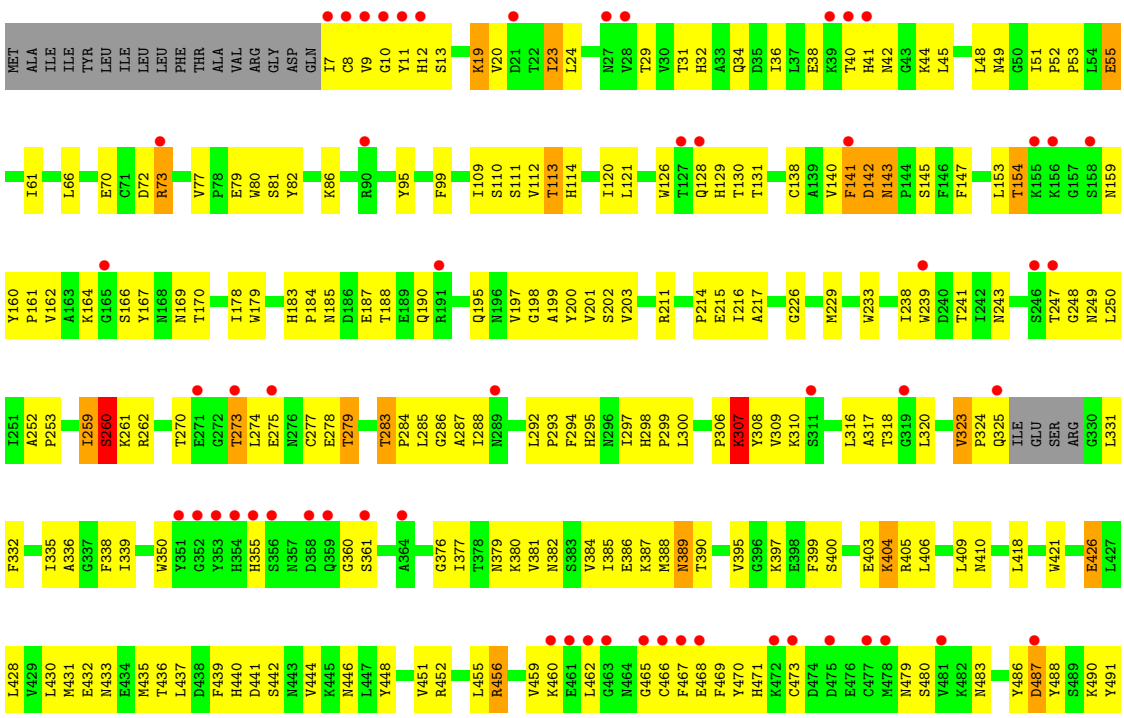




- Molecule 1: HEMAGGLUTININ

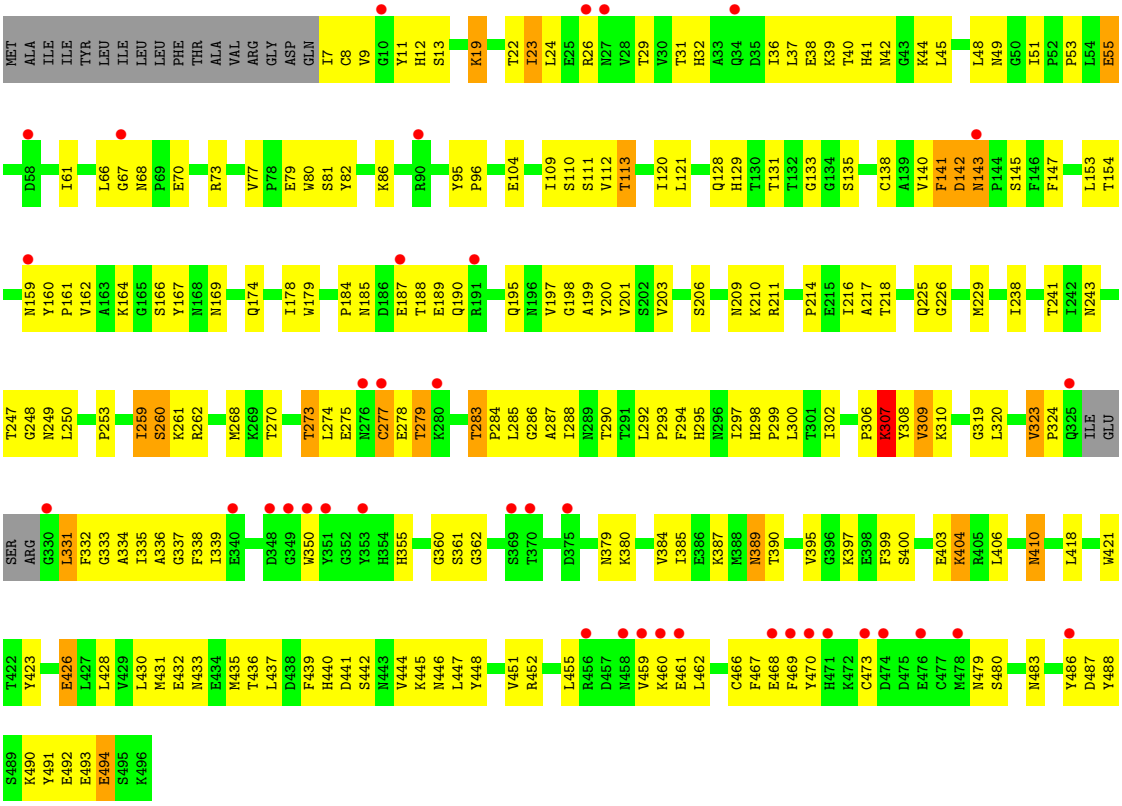
Chain E:





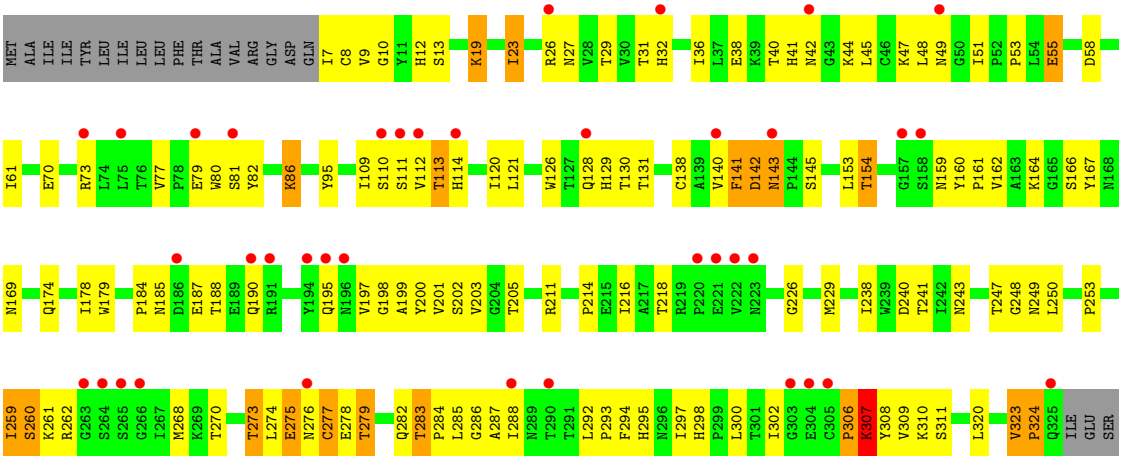
• Molecule 1: HEMAGGLUTININ

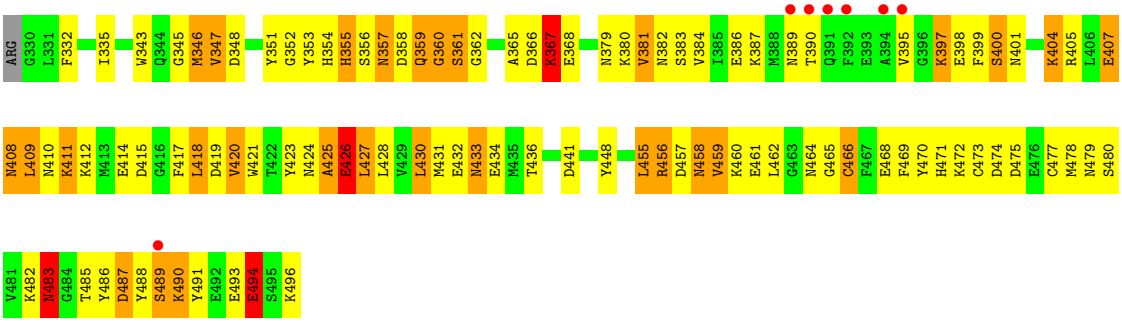
Chain F:



• Molecule 1: HEMAGGLUTININ

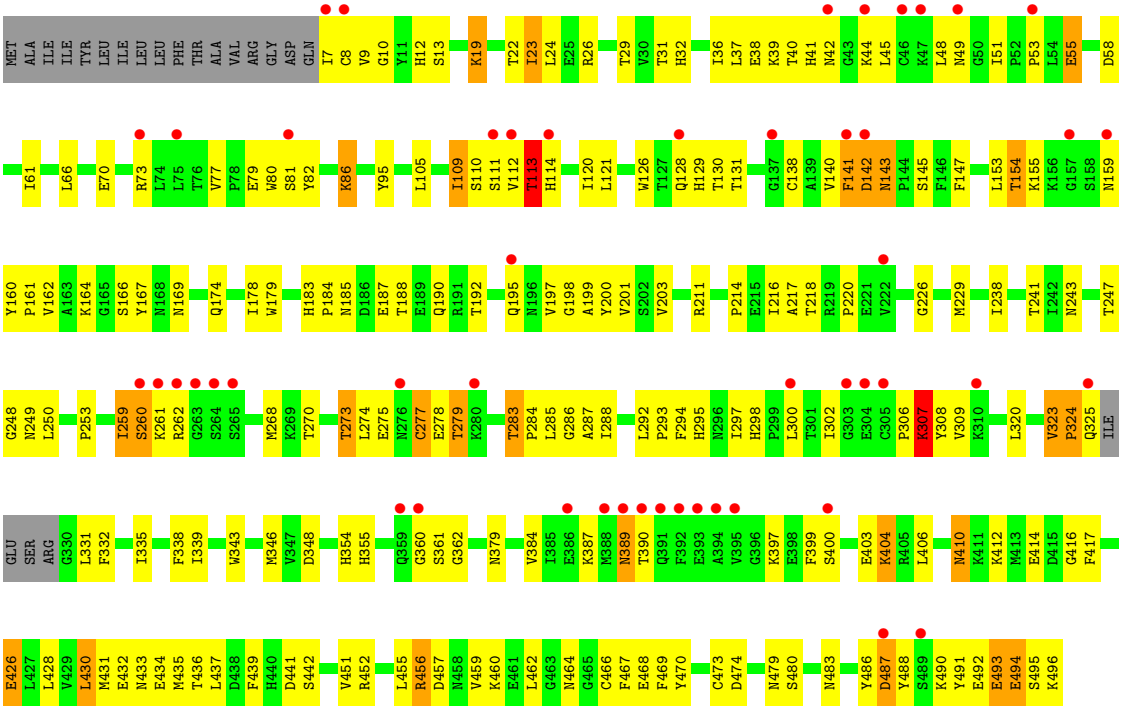
Chain G:





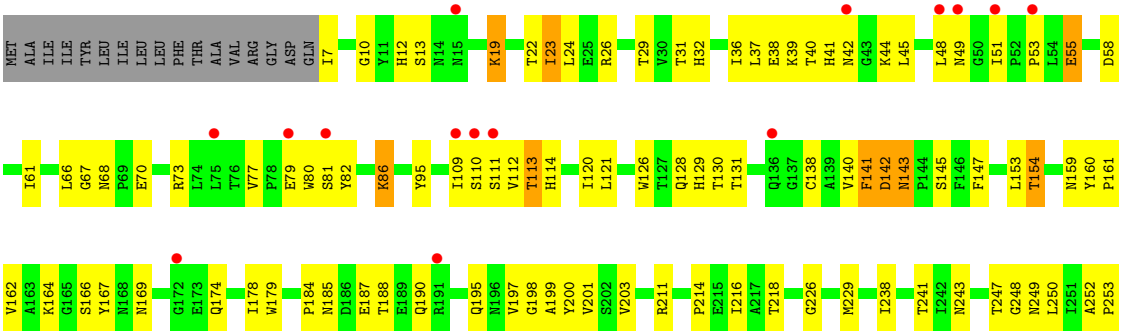
- Molecule 1: HEMAGGLUTININ

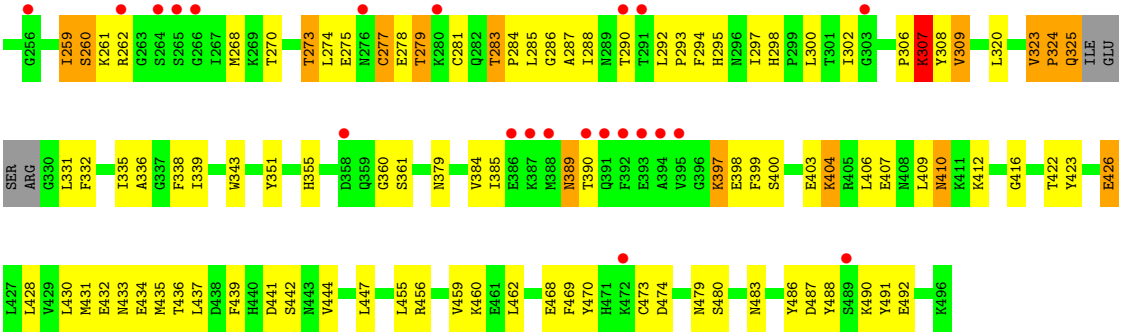
Chain H:



- Molecule 1: HEMAGGLUTININ

Chain I:





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.17Å 113.28Å 184.67Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	29.92 – 3.10 29.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.8 (29.92-3.10) 99.6 (29.92-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.11Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.273 , 0.337 0.270 , 0.331	Depositor DCC
R_{free} test set	4993 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	34577	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GAL, SIA

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	0.47	0/3923	0.68	1/5309 (0.0%)
1	B	0.40	0/3923	0.53	0/5309
1	C	0.38	0/3920	0.51	0/5305
1	D	0.44	0/3923	0.63	1/5309 (0.0%)
1	E	0.35	0/3923	0.50	0/5309
1	F	0.34	0/3920	0.49	0/5305
1	G	0.47	0/3923	0.63	0/5309
1	H	0.41	0/3923	0.53	0/5309
1	I	0.40	0/3920	0.52	0/5305
All	All	0.41	0/35298	0.56	2/47769 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	314	LEU	CA-CB-CG	5.74	128.51	115.30
1	D	251	ILE	N-CA-C	-5.12	97.19	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3837	0	3674	344	0
1	B	3837	0	3672	205	0
1	C	3834	0	3666	211	0
1	D	3837	0	3672	308	0
1	E	3837	0	3672	264	0
1	F	3834	0	3666	234	0
1	G	3837	0	3672	289	0
1	H	3837	0	3672	216	0
1	I	3834	0	3666	185	0
2	J	32	0	28	7	0
3	D	21	0	18	1	0
All	All	34577	0	33078	2079	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 31.

All (2079) 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:B:471:HIS:HB3	1:B:494:GLU:HG2	1.19	1.18
1:E:11:TYR:CE2	1:E:335:ILE:HA	1.83	1.14
1:G:7:ILE:HD11	1:G:482:LYS:HE3	1.15	1.12
1:C:9:VAL:HG21	1:C:448:TYR:HA	1.31	1.11
1:G:459:VAL:HG12	1:G:469:PHE:HA	1.22	1.11
1:H:7:ILE:HA	1:H:355:HIS:HA	1.28	1.11
1:F:9:VAL:HG21	1:F:448:TYR:HA	1.31	1.10
1:E:72:ASP:HB3	1:G:275:GLU:HB2	1.35	1.09
1:D:293:PRO:HG3	1:D:385:ILE:HA	1.34	1.09
1:E:9:VAL:HG21	1:E:448:TYR:HA	1.22	1.09
1:E:387:LYS:HD3	1:F:426:GLU:HG2	1.34	1.09
1:E:7:ILE:HG22	1:E:467:PHE:HB2	1.29	1.06
1:D:236:LEU:HD22	1:D:242:ILE:HG22	1.37	1.06
1:A:459:VAL:HG12	1:A:469:PHE:HA	1.32	1.05
1:E:283:THR:HG22	1:E:285:LEU:H	1.21	1.05
1:H:283:THR:HG22	1:H:285:LEU:H	1.21	1.05
1:B:9:VAL:HG21	1:B:448:TYR:HA	1.35	1.04
1:D:168:ASN:HA	1:D:241:THR:HB	1.38	1.03
1:I:283:THR:HG22	1:I:285:LEU:H	1.21	1.02
1:G:409:LEU:HD11	1:I:410:ASN:HB2	1.42	1.02
1:C:283:THR:HG22	1:C:285:LEU:H	1.21	1.01
1:A:181:VAL:HG22	1:A:201:VAL:HG21	1.41	1.00
1:B:283:THR:HG22	1:B:285:LEU:H	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:TYR:HD2	1:D:229:MET:HG3	1.26	1.00
1:F:283:THR:HG22	1:F:285:LEU:H	1.23	0.99
1:G:283:THR:HG22	1:G:285:LEU:H	1.26	0.99
1:E:73:ARG:HB2	1:G:44:LYS:HZ1	1.26	0.98
1:E:259:ILE:HG23	1:E:260:SER:H	1.30	0.97
1:H:190:GLN:HE22	1:H:249:ASN:HD21	1.11	0.97
1:C:259:ILE:HG23	1:C:260:SER:H	1.29	0.96
1:G:7:ILE:HA	1:G:355:HIS:HA	1.48	0.96
1:E:9:VAL:O	1:E:339:ILE:HD13	1.65	0.95
1:H:384:VAL:HG22	1:H:428:LEU:HD21	1.48	0.95
1:B:190:GLN:HE22	1:B:249:ASN:HD21	1.06	0.95
1:B:259:ILE:HG23	1:B:260:SER:H	1.31	0.95
1:E:141:PHE:CE1	1:G:47:LYS:HE2	2.02	0.95
1:C:190:GLN:HE22	1:C:249:ASN:HD21	1.11	0.95
1:D:95:TYR:CD2	1:D:229:MET:HG3	2.03	0.94
1:B:459:VAL:HG12	1:B:469:PHE:HA	1.49	0.93
1:D:23:ILE:HG13	1:F:380:LYS:HA	1.48	0.93
1:G:190:GLN:HE22	1:G:249:ASN:HD21	1.11	0.93
1:A:410:ASN:HB2	1:B:409:LEU:HD11	1.50	0.93
1:E:9:VAL:HG11	1:E:448:TYR:HB2	1.49	0.93
1:G:408:ASN:HD21	1:I:397:LYS:NZ	1.67	0.93
1:I:459:VAL:HG12	1:I:469:PHE:HA	1.50	0.92
1:B:7:ILE:HG22	1:B:467:PHE:HB2	1.52	0.92
1:D:283:THR:HG22	1:D:285:LEU:H	1.33	0.92
1:D:23:ILE:HD11	1:F:380:LYS:HE2	1.51	0.92
1:H:8:CYS:N	1:H:354:HIS:O	2.02	0.92
1:H:23:ILE:HG22	1:H:434:GLU:HG2	1.49	0.92
1:A:282:GLN:HE21	1:A:283:THR:H	1.17	0.92
1:E:190:GLN:HE22	1:E:249:ASN:HD21	1.10	0.92
1:F:190:GLN:HE22	1:F:249:ASN:HD21	1.08	0.92
1:H:455:LEU:HD23	1:H:459:VAL:HG21	1.52	0.91
1:A:197:VAL:HG12	1:A:198:GLY:H	1.32	0.91
1:F:259:ILE:HG23	1:F:260:SER:H	1.35	0.91
1:E:459:VAL:HG12	1:E:469:PHE:HA	1.51	0.91
1:G:8:CYS:O	1:G:353:TYR:HA	1.70	0.91
1:I:190:GLN:HE22	1:I:249:ASN:HD21	1.11	0.90
1:I:259:ILE:HG23	1:I:260:SER:H	1.36	0.90
1:B:259:ILE:HG23	1:B:260:SER:N	1.86	0.90
1:I:384:VAL:HG22	1:I:428:LEU:HD21	1.54	0.90
1:B:387:LYS:HD3	1:C:426:GLU:HG2	1.51	0.90
1:D:459:VAL:HG12	1:D:469:PHE:HA	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:ILE:HG23	1:F:260:SER:N	1.87	0.89
1:A:282:GLN:HE21	1:A:283:THR:N	1.71	0.89
1:H:459:VAL:HG12	1:H:469:PHE:HA	1.51	0.89
1:E:259:ILE:HG23	1:E:260:SER:N	1.86	0.89
1:A:190:GLN:HE22	1:A:249:ASN:HD21	1.21	0.89
1:H:259:ILE:HG23	1:H:260:SER:H	1.35	0.89
1:E:9:VAL:HB	1:E:448:TYR:HD1	1.37	0.89
1:E:11:TYR:HB3	1:E:444:VAL:HG21	1.55	0.89
1:E:72:ASP:HB3	1:G:275:GLU:CB	2.02	0.88
1:F:459:VAL:HG12	1:F:469:PHE:HA	1.53	0.88
1:C:459:VAL:HG12	1:C:469:PHE:HA	1.55	0.88
1:D:279:THR:HB	1:D:287:ALA:HB1	1.56	0.88
1:G:259:ILE:HG23	1:G:260:SER:H	1.36	0.88
1:D:227:GLY:O	1:D:228:ARG:HD3	1.73	0.88
1:C:7:ILE:HG22	1:C:467:PHE:HB2	1.53	0.88
1:D:384:VAL:HG22	1:D:428:LEU:HD21	1.56	0.87
1:G:243:ASN:HB2	1:H:218:THR:O	1.74	0.87
1:C:259:ILE:HG23	1:C:260:SER:N	1.87	0.87
1:E:169:ASN:HD22	1:E:238:ILE:HA	1.39	0.87
1:D:141:PHE:N	1:D:142:ASP:HA	1.89	0.87
1:A:53:PRO:HD2	1:A:274:LEU:HD22	1.57	0.86
1:I:23:ILE:HG22	1:I:434:GLU:HG2	1.58	0.86
1:B:384:VAL:HG22	1:B:428:LEU:HD21	1.57	0.86
1:D:53:PRO:HD2	1:D:274:LEU:HD13	1.58	0.86
1:D:108:LEU:HD21	1:D:235:ILE:HD11	1.57	0.86
1:E:7:ILE:O	1:E:467:PHE:N	2.09	0.86
1:I:259:ILE:HG23	1:I:260:SER:N	1.90	0.86
1:E:471:HIS:HB3	1:E:494:GLU:HG2	1.57	0.86
1:G:395:VAL:HG22	1:H:412:LYS:HE2	1.57	0.86
1:A:184:PRO:HB3	1:A:189:GLU:HG2	1.58	0.86
1:E:72:ASP:CB	1:G:275:GLU:HB2	2.06	0.86
1:G:459:VAL:CG1	1:G:469:PHE:HA	2.06	0.85
1:A:431:MET:O	1:A:433:ASN:N	2.09	0.85
1:A:94:CYS:HB2	1:A:138:CYS:SG	2.17	0.85
1:G:7:ILE:CD1	1:G:482:LYS:HE3	2.03	0.85
1:G:259:ILE:HG23	1:G:260:SER:N	1.91	0.85
1:G:283:THR:HB	1:G:286:GLY:O	1.77	0.85
1:C:141:PHE:N	1:C:142:ASP:HA	1.90	0.85
1:H:259:ILE:HG23	1:H:260:SER:N	1.91	0.85
1:C:455:LEU:HD23	1:C:459:VAL:HG21	1.59	0.84
1:E:384:VAL:HG22	1:E:428:LEU:HD21	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:THR:HB	1:E:286:GLY:O	1.76	0.84
1:A:335:ILE:HG13	1:A:441:ASP:HA	1.59	0.84
1:A:262:ARG:HH11	1:A:262:ARG:HG3	1.42	0.84
1:G:432:GLU:OE1	1:G:432:GLU:HA	1.76	0.84
1:D:120:ILE:O	1:D:121:LEU:HD23	1.78	0.84
1:E:73:ARG:CB	1:G:44:LYS:HZ1	1.89	0.84
1:A:166:SER:HB2	1:A:243:ASN:ND2	1.93	0.83
1:B:471:HIS:CB	1:B:494:GLU:HG2	2.04	0.83
1:I:462:LEU:HD11	1:I:468:GLU:HB2	1.60	0.83
1:H:283:THR:HB	1:H:286:GLY:O	1.78	0.83
1:I:141:PHE:N	1:I:142:ASP:HA	1.93	0.83
1:D:205:THR:HG22	1:D:242:ILE:HA	1.59	0.83
1:C:384:VAL:HG22	1:C:428:LEU:HD21	1.59	0.83
1:F:384:VAL:HG22	1:F:428:LEU:HD21	1.58	0.83
1:F:462:LEU:HD11	1:F:468:GLU:HB2	1.61	0.83
1:H:169:ASN:HD22	1:H:238:ILE:HA	1.43	0.83
1:E:141:PHE:HE1	1:G:47:LYS:HE2	1.43	0.83
1:I:143:ASN:HD22	1:I:143:ASN:N	1.77	0.83
1:G:259:ILE:O	1:G:260:SER:HB2	1.78	0.83
1:F:141:PHE:N	1:F:142:ASP:HA	1.93	0.83
1:A:399:PHE:CG	1:A:407:GLU:HB2	2.15	0.82
1:G:41:HIS:HB3	1:G:297:ILE:HD13	1.60	0.82
1:G:141:PHE:N	1:G:142:ASP:HA	1.93	0.82
1:E:141:PHE:N	1:E:142:ASP:HA	1.94	0.82
1:C:143:ASN:HD22	1:C:143:ASN:N	1.74	0.82
1:D:455:LEU:HD23	1:D:459:VAL:HG21	1.60	0.82
1:E:455:LEU:HD23	1:E:459:VAL:HG21	1.59	0.82
1:F:169:ASN:HD22	1:F:238:ILE:HA	1.43	0.82
1:H:41:HIS:HB3	1:H:297:ILE:HD13	1.60	0.82
1:F:41:HIS:HB3	1:F:297:ILE:HD13	1.60	0.82
1:H:143:ASN:HD22	1:H:143:ASN:N	1.76	0.82
1:B:455:LEU:HD23	1:B:459:VAL:HG21	1.62	0.82
1:E:9:VAL:HG21	1:E:448:TYR:CA	2.09	0.82
1:E:320:LEU:HD12	1:E:335:ILE:HD13	1.61	0.82
1:F:185:ASN:HD21	1:F:226:GLY:HA3	1.45	0.82
1:F:283:THR:HB	1:F:286:GLY:O	1.80	0.82
1:C:185:ASN:HD21	1:C:226:GLY:HA3	1.43	0.81
1:E:143:ASN:HD22	1:E:143:ASN:N	1.75	0.81
1:E:300:LEU:HA	1:E:395:VAL:HB	1.60	0.81
1:G:143:ASN:HD22	1:G:143:ASN:N	1.76	0.81
1:I:185:ASN:HD21	1:I:226:GLY:HA3	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:ILE:O	1:E:260:SER:HB2	1.78	0.81
1:F:7:ILE:HG22	1:F:467:PHE:HB2	1.61	0.81
1:B:143:ASN:N	1:B:143:ASN:HD22	1.75	0.81
1:B:169:ASN:HD22	1:B:238:ILE:HA	1.45	0.81
1:B:185:ASN:HD21	1:B:226:GLY:HA3	1.43	0.81
1:G:185:ASN:HD21	1:G:226:GLY:HA3	1.45	0.81
1:I:169:ASN:HD22	1:I:238:ILE:HA	1.46	0.81
1:F:455:LEU:HD23	1:F:459:VAL:HG21	1.63	0.81
1:A:44:LYS:O	1:A:286:GLY:HA2	1.81	0.81
1:A:334:ALA:HB2	1:A:445:LYS:HB2	1.61	0.81
1:B:141:PHE:N	1:B:142:ASP:HA	1.93	0.81
1:B:462:LEU:HD11	1:B:468:GLU:HB2	1.62	0.81
1:C:169:ASN:HD22	1:C:238:ILE:HA	1.44	0.81
1:H:141:PHE:N	1:H:142:ASP:HA	1.93	0.81
1:C:143:ASN:HD21	1:G:19:LYS:HD3	1.46	0.81
1:I:455:LEU:HD23	1:I:459:VAL:HG21	1.61	0.81
1:H:8:CYS:O	1:H:343:TRP:HH2	1.65	0.81
1:B:320:LEU:HD12	1:B:335:ILE:HD13	1.61	0.80
1:D:175:MET:HA	1:D:257:PHE:O	1.81	0.80
1:D:283:THR:HB	1:D:286:GLY:O	1.82	0.80
1:I:283:THR:HB	1:I:286:GLY:O	1.79	0.80
1:C:283:THR:HB	1:C:286:GLY:O	1.81	0.80
1:D:12:HIS:CD2	1:D:13:SER:H	1.99	0.80
1:D:462:LEU:HD11	1:D:468:GLU:HB2	1.64	0.80
1:G:387:LYS:NZ	1:H:426:GLU:HG2	1.97	0.80
1:I:295:HIS:HD2	1:I:297:ILE:H	1.27	0.80
1:D:28:VAL:O	1:D:30:VAL:HG13	1.80	0.80
1:B:9:VAL:HB	1:B:448:TYR:HD1	1.46	0.80
1:E:380:LYS:HA	1:F:23:ILE:HG12	1.63	0.80
1:B:283:THR:HB	1:B:286:GLY:O	1.81	0.80
1:H:462:LEU:HD11	1:H:468:GLU:HB2	1.63	0.79
1:C:41:HIS:HB3	1:C:297:ILE:HD13	1.64	0.79
1:D:168:ASN:CA	1:D:241:THR:HB	2.12	0.79
1:E:41:HIS:HB3	1:E:297:ILE:HD13	1.63	0.79
1:E:471:HIS:CB	1:E:494:GLU:HG2	2.12	0.79
1:G:8:CYS:O	1:G:354:HIS:N	2.14	0.79
1:A:346:MET:HE3	1:A:352:GLY:HA3	1.64	0.79
1:A:56:LEU:HD12	1:A:85:GLU:HB2	1.64	0.79
1:B:259:ILE:O	1:B:260:SER:HB2	1.80	0.79
1:E:293:PRO:HG3	1:E:385:ILE:HA	1.64	0.79
1:F:143:ASN:HD22	1:F:143:ASN:N	1.77	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:LEU:HD11	1:C:468:GLU:HB2	1.62	0.79
1:D:80:TRP:CE2	1:D:112:VAL:HG22	2.17	0.79
1:E:185:ASN:HD21	1:E:226:GLY:HA3	1.46	0.79
1:G:169:ASN:HD22	1:G:238:ILE:HA	1.46	0.79
1:E:320:LEU:CD1	1:E:335:ILE:HD13	2.12	0.79
1:A:321:ARG:HH21	1:A:437:LEU:HD23	1.48	0.79
1:E:295:HIS:HD2	1:E:297:ILE:H	1.30	0.79
1:C:295:HIS:HD2	1:C:297:ILE:H	1.31	0.78
1:D:218:THR:O	1:F:243:ASN:HB2	1.82	0.78
1:E:11:TYR:CD2	1:E:335:ILE:HG12	2.17	0.78
1:F:11:TYR:CE2	1:F:335:ILE:HA	2.19	0.78
1:H:185:ASN:HD21	1:H:226:GLY:HA3	1.46	0.78
1:D:41:HIS:CD2	1:D:297:ILE:HD13	2.18	0.78
1:E:379:ASN:HD22	1:F:26:ARG:NH1	1.81	0.78
1:D:36:ILE:HA	1:D:292:LEU:HD22	1.63	0.78
1:E:462:LEU:HD11	1:E:468:GLU:HB2	1.63	0.78
1:F:295:HIS:HD2	1:F:297:ILE:H	1.30	0.78
1:B:41:HIS:HB3	1:B:297:ILE:HD13	1.66	0.78
1:G:493:GLU:O	1:G:494:GLU:HB2	1.81	0.78
1:B:11:TYR:CE2	1:B:335:ILE:HA	2.19	0.78
1:H:7:ILE:HG13	1:H:355:HIS:HB3	1.64	0.77
1:A:451:VAL:O	1:A:467:PHE:HE2	1.67	0.77
1:E:7:ILE:HG22	1:E:467:PHE:CB	2.11	0.77
1:G:458:ASN:O	1:G:459:VAL:HG13	1.84	0.77
1:D:202:SER:OG	1:E:217:ALA:HB2	1.84	0.77
1:C:9:VAL:O	1:C:339:ILE:HD13	1.85	0.77
1:C:324:PRO:O	1:C:325:GLN:HB2	1.85	0.77
1:D:187:GLU:O	1:D:190:GLN:HB3	1.84	0.77
1:A:47:LYS:HB3	1:A:51:ILE:O	1.84	0.76
1:A:282:GLN:HE21	1:A:282:GLN:HA	1.50	0.76
1:F:9:VAL:O	1:F:339:ILE:HD13	1.85	0.76
1:C:259:ILE:O	1:C:260:SER:HB2	1.86	0.76
1:F:320:LEU:HB3	1:F:440:HIS:CG	2.20	0.76
1:F:259:ILE:O	1:F:260:SER:HB2	1.82	0.76
1:I:259:ILE:O	1:I:260:SER:HB2	1.82	0.76
1:A:332:PHE:CE2	1:A:442:SER:HB2	2.21	0.76
1:H:7:ILE:HA	1:H:355:HIS:CA	2.12	0.75
1:C:11:TYR:CE2	1:C:335:ILE:HA	2.22	0.75
1:I:41:HIS:HB3	1:I:297:ILE:HD13	1.66	0.75
1:C:143:ASN:HD21	1:G:19:LYS:CD	1.99	0.75
1:A:12:HIS:HB2	1:A:350:TRP:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:HB	1:C:448:TYR:HD1	1.51	0.75
1:A:323:VAL:N	1:A:324:PRO:HD3	2.02	0.75
1:D:26:ARG:HH11	1:F:379:ASN:HD22	1.35	0.75
1:E:320:LEU:HB3	1:E:440:HIS:CG	2.22	0.75
1:A:302:ILE:HG23	1:A:394:ALA:HB2	1.69	0.75
1:A:307:LYS:HE2	1:A:421:TRP:CE2	2.22	0.75
1:E:202:SER:HB2	1:F:217:ALA:HB2	1.68	0.75
1:A:282:GLN:NE2	1:A:283:THR:H	1.84	0.75
1:I:283:THR:CG2	1:I:285:LEU:H	2.00	0.75
1:A:66:LEU:O	1:A:149:ASN:HB2	1.86	0.74
1:C:320:LEU:HB3	1:C:440:HIS:CG	2.22	0.74
1:G:211:ARG:NH1	1:H:216:ILE:HB	2.00	0.74
1:I:283:THR:HG22	1:I:285:LEU:N	2.00	0.74
1:B:320:LEU:HB3	1:B:440:HIS:CG	2.22	0.74
1:E:376:GLY:C	1:F:24:LEU:HD22	2.07	0.74
1:A:38:GLU:OE1	1:A:290:THR:HB	1.88	0.73
1:B:190:GLN:HE22	1:B:249:ASN:ND2	1.83	0.73
1:H:8:CYS:O	1:H:354:HIS:N	2.20	0.73
1:F:189:GLU:OE2	2:J:2:SIA:H92	1.87	0.73
1:G:7:ILE:HD11	1:G:482:LYS:CE	2.08	0.73
1:G:409:LEU:HD11	1:I:410:ASN:CB	2.16	0.73
1:A:58:ASP:HB3	1:A:86:LYS:HD3	1.70	0.73
1:D:22:THR:HB	1:D:434:GLU:OE2	1.89	0.73
1:H:283:THR:HG22	1:H:285:LEU:N	2.00	0.73
1:A:19:LYS:HZ3	1:A:27:ASN:HB3	1.53	0.73
1:D:45:LEU:HD11	1:D:270:THR:HG21	1.71	0.73
1:H:259:ILE:O	1:H:260:SER:HB2	1.88	0.73
1:E:283:THR:HG22	1:E:285:LEU:N	2.02	0.73
1:F:320:LEU:HD12	1:F:335:ILE:HD13	1.71	0.73
1:B:278:GLU:HG3	1:B:279:THR:N	2.04	0.72
1:G:308:TYR:CD2	1:G:418:LEU:HD11	2.24	0.72
1:B:7:ILE:O	1:B:467:PHE:N	2.22	0.72
1:B:283:THR:HG22	1:B:285:LEU:N	2.02	0.72
1:E:278:GLU:HG3	1:E:279:THR:N	2.03	0.72
1:H:295:HIS:HD2	1:H:297:ILE:H	1.36	0.72
1:C:283:THR:HG22	1:C:285:LEU:N	2.01	0.72
1:G:8:CYS:HB2	1:G:354:HIS:HB3	1.69	0.72
1:B:190:GLN:NE2	1:B:249:ASN:HD21	1.85	0.72
1:B:283:THR:CG2	1:B:285:LEU:H	2.02	0.72
1:F:190:GLN:HE22	1:F:249:ASN:ND2	1.86	0.72
1:D:26:ARG:HD3	1:F:379:ASN:HD22	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:THR:HG22	1:F:285:LEU:N	2.03	0.72
1:A:493:GLU:O	1:A:494:GLU:HB2	1.90	0.72
1:E:320:LEU:HB3	1:E:440:HIS:CB	2.20	0.71
1:B:323:VAL:HG11	1:B:336:ALA:HB2	1.72	0.71
1:C:9:VAL:HG11	1:C:448:TYR:HB2	1.72	0.71
1:E:11:TYR:CE1	1:E:335:ILE:HG23	2.25	0.71
1:A:158:SER:O	1:A:195:GLN:HG2	1.89	0.71
1:B:295:HIS:HD2	1:B:297:ILE:H	1.37	0.71
1:E:141:PHE:CZ	1:G:47:LYS:HE2	2.25	0.71
1:E:379:ASN:HD22	1:F:26:ARG:CZ	2.03	0.71
1:A:380:LYS:HG3	1:A:380:LYS:O	1.87	0.71
1:C:143:ASN:ND2	1:G:19:LYS:HE3	2.05	0.71
1:C:199:ALA:HB3	1:C:249:ASN:HD22	1.56	0.71
1:C:283:THR:CG2	1:C:285:LEU:H	2.00	0.71
1:F:320:LEU:HD23	1:F:320:LEU:H	1.55	0.71
1:D:282:GLN:HG3	1:D:283:THR:H	1.56	0.70
1:G:8:CYS:O	1:G:353:TYR:CA	2.39	0.70
1:G:295:HIS:HD2	1:G:297:ILE:H	1.36	0.70
1:I:190:GLN:HE22	1:I:249:ASN:ND2	1.88	0.70
1:I:324:PRO:O	1:I:325:GLN:HB2	1.90	0.70
1:C:320:LEU:HD12	1:C:335:ILE:HD13	1.73	0.70
1:G:382:ASN:O	1:G:386:GLU:HG3	1.91	0.70
1:H:7:ILE:CA	1:H:355:HIS:HA	2.16	0.70
1:A:99:PHE:HZ	1:A:178:ILE:HD13	1.57	0.70
1:A:282:GLN:HE21	1:A:282:GLN:CA	2.03	0.70
1:B:9:VAL:HG11	1:B:448:TYR:HB2	1.73	0.70
1:H:283:THR:CG2	1:H:285:LEU:H	2.01	0.70
1:D:41:HIS:HD2	1:D:297:ILE:HD13	1.56	0.70
1:F:9:VAL:HB	1:F:448:TYR:HD1	1.56	0.70
1:E:320:LEU:HD23	1:E:320:LEU:H	1.56	0.70
1:A:208:LEU:HD12	1:A:209:ASN:H	1.57	0.70
1:B:379:ASN:HD22	1:C:26:ARG:CZ	2.05	0.69
1:D:139:ALA:HB1	1:D:142:ASP:HB2	1.73	0.69
1:H:496:LYS:HD2	1:H:496:LYS:N	2.07	0.69
1:A:201:VAL:HG13	1:A:250:LEU:HB2	1.74	0.69
1:G:480:SER:HB2	1:G:485:THR:O	1.91	0.69
1:C:293:PRO:HG3	1:C:385:ILE:HA	1.75	0.69
1:E:387:LYS:CD	1:F:426:GLU:HG2	2.19	0.69
1:A:197:VAL:HG12	1:A:198:GLY:N	2.08	0.69
1:F:283:THR:CG2	1:F:285:LEU:H	2.01	0.69
1:E:8:CYS:HA	1:E:466:CYS:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:VAL:CB	1:E:448:TYR:HD1	2.04	0.69
1:E:190:GLN:HE22	1:E:249:ASN:ND2	1.88	0.69
1:G:408:ASN:HD21	1:I:397:LYS:HZ3	1.41	0.69
1:H:24:LEU:HD12	1:H:434:GLU:OE1	1.93	0.69
1:G:283:THR:HG22	1:G:285:LEU:N	2.05	0.69
1:B:379:ASN:HD22	1:C:26:ARG:NH1	1.90	0.69
1:E:9:VAL:CG2	1:E:448:TYR:HA	2.12	0.69
1:E:11:TYR:CZ	1:E:335:ILE:HA	2.27	0.69
1:F:300:LEU:HA	1:F:395:VAL:HB	1.74	0.68
1:A:97:GLY:HA3	1:A:229:MET:O	1.93	0.68
1:E:190:GLN:NE2	1:E:249:ASN:HD21	1.89	0.68
1:H:199:ALA:HB3	1:H:249:ASN:HD22	1.58	0.68
1:D:426:GLU:HG2	1:F:387:LYS:HD3	1.74	0.68
1:I:19:LYS:HE2	1:I:29:THR:OG1	1.93	0.68
1:A:203:VAL:HG22	1:A:244:PHE:CD1	2.29	0.68
1:A:95:TYR:CE1	1:A:225:GLN:HG3	2.29	0.68
1:E:9:VAL:HB	1:E:448:TYR:CD1	2.26	0.68
1:G:346:MET:SD	1:G:352:GLY:HA3	2.34	0.68
1:G:479:ASN:O	1:G:483:ASN:HB2	1.92	0.68
1:I:199:ALA:HB3	1:I:249:ASN:HD22	1.58	0.68
1:A:14:ASN:H	1:A:322:ASN:HD21	1.40	0.68
1:A:281:CYS:HB2	1:A:304:GLU:O	1.94	0.68
1:D:387:LYS:HD3	1:E:426:GLU:HG2	1.76	0.68
1:G:448:TYR:CE1	1:G:465:GLY:HA2	2.29	0.68
1:A:410:ASN:HB2	1:B:409:LEU:CD1	2.23	0.67
1:F:190:GLN:NE2	1:F:249:ASN:HD21	1.88	0.67
1:I:190:GLN:NE2	1:I:249:ASN:HD21	1.90	0.67
1:A:154:THR:O	1:A:155:LYS:HB3	1.94	0.67
1:B:293:PRO:CG	1:B:385:ILE:HG12	2.24	0.67
1:G:190:GLN:HE22	1:G:249:ASN:ND2	1.89	0.67
1:A:282:GLN:HA	1:A:282:GLN:NE2	2.09	0.67
1:C:143:ASN:ND2	1:G:19:LYS:HD3	2.08	0.67
1:C:190:GLN:HE22	1:C:249:ASN:ND2	1.88	0.67
1:A:205:THR:HG22	1:A:242:ILE:HA	1.75	0.67
1:D:26:ARG:HD3	1:F:379:ASN:ND2	2.09	0.67
1:E:283:THR:CG2	1:E:285:LEU:H	2.03	0.67
1:G:199:ALA:HB3	1:G:249:ASN:HD22	1.59	0.67
1:F:199:ALA:HB3	1:F:249:ASN:HD22	1.60	0.67
1:H:459:VAL:CG1	1:H:469:PHE:HA	2.25	0.67
1:A:379:ASN:HD22	1:B:26:ARG:NH1	1.91	0.67
1:G:332:PHE:HB2	1:G:441:ASP:OD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:TYR:CD2	1:H:229:MET:HG3	2.30	0.67
1:I:320:LEU:HD23	1:I:320:LEU:H	1.60	0.67
1:G:259:ILE:O	1:G:260:SER:CB	2.43	0.67
1:H:355:HIS:H	1:H:355:HIS:CD2	2.12	0.67
1:I:278:GLU:HG3	1:I:279:THR:N	2.09	0.67
1:A:455:LEU:HB3	1:A:459:VAL:CG2	2.25	0.67
1:F:293:PRO:HG3	1:F:385:ILE:HA	1.77	0.67
1:A:302:ILE:HG23	1:A:394:ALA:CB	2.24	0.67
1:B:320:LEU:CD1	1:B:335:ILE:HD13	2.24	0.67
1:F:133:GLY:HA3	2:J:2:SIA:H113	1.75	0.67
1:B:199:ALA:HB3	1:B:249:ASN:HD22	1.59	0.66
1:D:53:PRO:CD	1:D:274:LEU:HD13	2.25	0.66
1:E:199:ALA:HB3	1:E:249:ASN:HD22	1.58	0.66
1:G:425:ALA:O	1:G:427:LEU:N	2.27	0.66
1:A:486:TYR:CG	1:A:487:ASP:N	2.64	0.66
1:F:9:VAL:HG11	1:F:448:TYR:HB2	1.76	0.66
1:H:8:CYS:O	1:H:343:TRP:CH2	2.48	0.66
1:D:12:HIS:CG	1:D:13:SER:H	2.14	0.66
1:I:459:VAL:CG1	1:I:469:PHE:HA	2.26	0.66
1:A:9:VAL:HG21	1:A:448:TYR:HA	1.77	0.66
1:C:278:GLU:HG3	1:C:279:THR:N	2.11	0.66
1:A:399:PHE:CD2	1:A:407:GLU:HB2	2.30	0.66
1:A:457:ASP:C	1:A:459:VAL:H	1.99	0.66
1:B:320:LEU:HD23	1:B:320:LEU:H	1.61	0.66
1:C:190:GLN:NE2	1:C:249:ASN:HD21	1.89	0.66
1:D:248:GLY:O	1:D:249:ASN:HB2	1.94	0.66
1:A:12:HIS:CD2	1:A:13:SER:N	2.64	0.66
1:A:248:GLY:C	1:A:249:ASN:HD22	1.99	0.66
1:A:476:GLU:O	1:A:480:SER:HB3	1.95	0.66
1:G:320:LEU:HD23	1:G:320:LEU:H	1.60	0.66
1:H:190:GLN:HE22	1:H:249:ASN:ND2	1.89	0.66
1:E:95:TYR:CD2	1:E:229:MET:HG3	2.31	0.66
1:G:283:THR:CG2	1:G:285:LEU:H	2.05	0.66
1:A:320:LEU:HD23	1:A:320:LEU:H	1.61	0.66
1:E:323:VAL:HG11	1:E:336:ALA:HB2	1.78	0.66
1:A:166:SER:HB2	1:A:243:ASN:HD22	1.56	0.66
1:G:346:MET:HE1	1:G:365:ALA:CA	2.25	0.66
1:D:45:LEU:HA	1:D:282:GLN:NE2	2.11	0.65
1:F:479:ASN:O	1:F:483:ASN:HB2	1.96	0.65
1:G:211:ARG:HH11	1:H:216:ILE:HB	1.61	0.65
1:G:345:GLY:O	1:G:347:VAL:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:408:ASN:HD21	1:I:397:LYS:HZ1	1.44	0.65
1:I:95:TYR:CD2	1:I:229:MET:HG3	2.31	0.65
1:B:431:MET:O	1:B:432:GLU:HB2	1.96	0.65
1:D:109:ILE:HG22	1:D:259:ILE:HD11	1.77	0.65
1:D:182:HIS:O	1:D:184:PRO:HD3	1.96	0.65
1:E:11:TYR:HB3	1:E:444:VAL:CG2	2.25	0.65
1:H:8:CYS:H	1:H:354:HIS:C	2.00	0.65
1:H:190:GLN:NE2	1:H:249:ASN:HD21	1.91	0.65
1:E:259:ILE:O	1:E:260:SER:CB	2.44	0.65
1:G:95:TYR:CD2	1:G:229:MET:HG3	2.32	0.65
1:D:186:ASP:HA	1:D:216:ILE:HG21	1.77	0.65
1:E:73:ARG:HD2	1:G:276:ASN:O	1.96	0.65
1:E:211:ARG:HD2	1:F:216:ILE:O	1.96	0.65
1:F:278:GLU:HG3	1:F:279:THR:N	2.12	0.65
1:G:379:ASN:HB3	1:H:26:ARG:CZ	2.26	0.65
1:A:38:GLU:HG2	1:A:290:THR:HG21	1.78	0.65
1:C:11:TYR:HB3	1:C:444:VAL:HG21	1.77	0.65
1:A:343:TRP:CZ3	1:A:354:HIS:HB2	2.32	0.65
1:B:459:VAL:CG1	1:B:469:PHE:HA	2.24	0.65
1:C:7:ILE:O	1:C:467:PHE:N	2.28	0.65
1:D:32:HIS:CE1	1:D:350:TRP:HE1	2.15	0.65
1:D:479:ASN:O	1:D:483:ASN:HB2	1.97	0.65
1:F:133:GLY:CA	2:J:2:SIA:H113	2.27	0.65
1:F:320:LEU:HB3	1:F:440:HIS:CB	2.27	0.65
1:G:166:SER:HB2	1:G:243:ASN:HD22	1.62	0.65
1:A:23:ILE:HD11	1:C:380:LYS:HG3	1.79	0.65
1:A:41:HIS:HB3	1:A:297:ILE:HD13	1.78	0.65
1:A:105:LEU:HB2	1:A:233:TRP:CE2	2.32	0.65
1:C:320:LEU:HD23	1:C:320:LEU:H	1.61	0.65
1:D:24:LEU:HD12	1:D:434:GLU:CD	2.16	0.65
1:D:182:HIS:CD2	1:D:194:TYR:OH	2.50	0.65
1:D:238:ILE:HG23	1:D:239:TRP:CD2	2.33	0.64
1:F:11:TYR:HB3	1:F:444:VAL:HG21	1.78	0.64
1:G:367:LYS:HA	1:G:367:LYS:HE2	1.79	0.64
1:H:278:GLU:HG3	1:H:279:THR:N	2.12	0.64
1:H:293:PRO:HB2	1:H:294:PHE:CE2	2.32	0.64
1:A:455:LEU:HB3	1:A:459:VAL:HG22	1.79	0.64
1:B:202:SER:HB2	1:C:217:ALA:HB2	1.80	0.64
1:H:455:LEU:HB3	1:H:459:VAL:HG22	1.78	0.64
1:C:78:PRO:HG2	1:E:114:HIS:CE1	2.32	0.64
1:G:379:ASN:HB3	1:H:26:ARG:NH2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LYS:HD2	1:B:426:GLU:HG2	1.78	0.64
1:D:111:SER:O	1:D:261:LYS:HE3	1.98	0.64
1:D:431:MET:O	1:D:432:GLU:HB2	1.97	0.64
1:E:159:ASN:O	1:E:161:PRO:HD3	1.98	0.64
1:H:479:ASN:O	1:H:483:ASN:HB2	1.98	0.64
1:E:11:TYR:CZ	1:E:335:ILE:HG23	2.32	0.64
1:H:293:PRO:HB2	1:H:294:PHE:CD2	2.32	0.64
1:D:120:ILE:HG12	1:D:256:GLY:H	1.63	0.64
1:D:282:GLN:HG3	1:D:283:THR:N	2.13	0.64
1:E:7:ILE:HG23	1:E:467:PHE:CD2	2.33	0.64
1:I:431:MET:O	1:I:432:GLU:HB2	1.98	0.64
1:A:26:ARG:HD3	1:C:379:ASN:ND2	2.13	0.64
1:A:451:VAL:O	1:A:467:PHE:CE2	2.51	0.64
1:H:10:GLY:N	1:H:343:TRP:CH2	2.65	0.64
1:I:159:ASN:O	1:I:161:PRO:HD3	1.98	0.64
1:C:199:ALA:HB3	1:C:249:ASN:ND2	2.13	0.64
1:E:459:VAL:CG1	1:E:469:PHE:HA	2.26	0.64
1:E:479:ASN:O	1:E:483:ASN:HB2	1.98	0.63
1:F:259:ILE:O	1:F:260:SER:CB	2.46	0.63
1:A:108:LEU:HD12	1:A:261:LYS:HD2	1.80	0.63
1:B:293:PRO:HG3	1:B:385:ILE:HA	1.80	0.63
1:D:37:LEU:HB2	1:D:314:LEU:HB2	1.80	0.63
1:D:294:PHE:CE1	1:D:425:ALA:HB2	2.33	0.63
1:G:19:LYS:HE2	1:G:29:THR:OG1	1.97	0.63
1:B:320:LEU:HB3	1:B:440:HIS:CB	2.27	0.63
1:B:479:ASN:O	1:B:483:ASN:HB2	1.98	0.63
1:C:455:LEU:HB3	1:C:459:VAL:HG22	1.80	0.63
1:E:143:ASN:N	1:E:143:ASN:ND2	2.45	0.63
1:G:293:PRO:HB2	1:G:294:PHE:CE2	2.33	0.63
1:A:413:MET:HG2	1:A:414:GLU:N	2.13	0.63
1:E:73:ARG:CB	1:G:44:LYS:NZ	2.61	0.63
1:I:259:ILE:O	1:I:260:SER:CB	2.46	0.63
1:A:334:ALA:HB3	1:A:441:ASP:OD1	1.98	0.63
1:D:108:LEU:HD12	1:D:261:LYS:HD2	1.80	0.63
1:E:7:ILE:N	1:E:467:PHE:O	2.31	0.63
1:E:11:TYR:OH	1:E:336:ALA:N	2.24	0.63
1:E:307:LYS:HE2	1:E:421:TRP:CE2	2.34	0.63
1:G:159:ASN:O	1:G:161:PRO:HD3	1.98	0.63
1:A:42:ASN:HB2	1:A:287:ALA:HB3	1.79	0.63
1:A:478:MET:C	1:A:480:SER:H	2.00	0.63
1:C:335:ILE:HG13	1:C:441:ASP:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:LEU:HB3	1:E:459:VAL:HG22	1.80	0.63
1:I:479:ASN:O	1:I:483:ASN:HB2	1.98	0.63
1:D:109:ILE:CG2	1:D:259:ILE:HD11	2.29	0.63
1:B:259:ILE:O	1:B:260:SER:CB	2.46	0.63
1:C:141:PHE:O	1:G:19:LYS:HB2	1.99	0.63
1:A:10:GLY:HA3	1:A:343:TRP:CZ2	2.34	0.62
1:B:293:PRO:HB2	1:B:294:PHE:CD2	2.34	0.62
1:C:143:ASN:N	1:C:143:ASN:ND2	2.46	0.62
1:D:288:ILE:HG12	1:D:297:ILE:HD12	1.81	0.62
1:C:389:ASN:HD22	1:C:390:THR:H	1.47	0.62
1:C:479:ASN:O	1:C:483:ASN:HB2	1.98	0.62
1:D:182:HIS:HD2	1:D:194:TYR:OH	1.82	0.62
1:F:389:ASN:HD22	1:F:390:THR:H	1.47	0.62
1:A:379:ASN:HD22	1:B:26:ARG:CZ	2.12	0.62
1:A:431:MET:C	1:A:433:ASN:H	2.01	0.62
1:D:205:THR:CG2	1:D:242:ILE:HA	2.29	0.62
1:D:120:ILE:HD13	1:D:177:ILE:HD13	1.80	0.62
1:D:298:HIS:ND1	1:D:299:PRO:HD2	2.13	0.62
1:F:455:LEU:HB3	1:F:459:VAL:HG22	1.82	0.62
1:G:53:PRO:HD2	1:G:274:LEU:HD13	1.81	0.62
1:A:335:ILE:CG1	1:A:441:ASP:HA	2.28	0.62
1:A:462:LEU:HD13	1:A:466:CYS:O	1.99	0.62
1:H:23:ILE:HG22	1:H:434:GLU:CG	2.27	0.62
1:I:55:GLU:OE2	1:I:273:THR:HG22	1.99	0.62
1:A:183:HIS:HB3	1:A:219:ARG:NH2	2.15	0.62
1:G:293:PRO:HB2	1:G:294:PHE:CD2	2.35	0.62
1:H:431:MET:O	1:H:432:GLU:HB2	1.99	0.62
1:A:51:ILE:HG22	1:A:52:PRO:CD	2.30	0.62
1:B:295:HIS:CE1	1:B:308:TYR:HB2	2.35	0.62
1:C:320:LEU:HB3	1:C:440:HIS:CB	2.29	0.62
1:D:459:VAL:CG1	1:D:469:PHE:HA	2.30	0.62
1:F:159:ASN:O	1:F:161:PRO:HD3	2.00	0.62
1:F:199:ALA:HB3	1:F:249:ASN:ND2	2.15	0.62
1:G:455:LEU:HB3	1:G:459:VAL:CG2	2.30	0.62
1:A:168:ASN:CA	1:A:241:THR:HG22	2.30	0.62
1:C:159:ASN:O	1:C:161:PRO:HD3	1.99	0.62
1:E:166:SER:HB2	1:E:243:ASN:HD22	1.65	0.62
1:H:22:THR:HG22	1:H:433:ASN:HB3	1.82	0.62
1:F:178:ILE:O	1:F:253:PRO:HG3	1.99	0.62
1:F:389:ASN:HD22	1:F:390:THR:N	1.97	0.62
1:G:190:GLN:NE2	1:G:249:ASN:HD21	1.91	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:CYS:HB3	1:A:306:PRO:HD2	1.81	0.61
1:C:338:PHE:CE1	1:C:339:ILE:HG13	2.35	0.61
1:D:310:LYS:NZ	1:D:418:LEU:HD23	2.15	0.61
1:E:166:SER:CB	1:E:243:ASN:HD22	2.13	0.61
1:D:108:LEU:CD1	1:D:261:LYS:HD2	2.31	0.61
1:F:143:ASN:N	1:F:143:ASN:ND2	2.48	0.61
1:H:332:PHE:CZ	1:I:331:LEU:HD12	2.35	0.61
1:A:118:VAL:HG11	1:A:258:LYS:HD2	1.82	0.61
1:B:95:TYR:CD2	1:B:229:MET:HG3	2.35	0.61
1:D:7:ILE:HG22	1:D:467:PHE:HB2	1.82	0.61
1:A:282:GLN:NE2	1:A:283:THR:N	2.43	0.61
1:B:389:ASN:HD22	1:B:390:THR:H	1.48	0.61
1:C:143:ASN:ND2	1:G:19:LYS:CE	2.63	0.61
1:H:19:LYS:HE2	1:H:29:THR:OG1	2.00	0.61
1:A:168:ASN:HA	1:A:241:THR:HG22	1.81	0.61
1:C:259:ILE:O	1:C:260:SER:CB	2.47	0.61
1:H:178:ILE:O	1:H:253:PRO:HG3	1.99	0.61
1:B:278:GLU:HG3	1:B:279:THR:H	1.66	0.61
1:G:346:MET:HE1	1:G:365:ALA:HA	1.82	0.61
1:H:159:ASN:O	1:H:161:PRO:HD3	2.00	0.61
1:H:199:ALA:HB3	1:H:249:ASN:ND2	2.15	0.61
1:A:183:HIS:HB3	1:A:219:ARG:HH22	1.66	0.61
1:G:455:LEU:HB3	1:G:459:VAL:HG21	1.83	0.61
1:I:142:ASP:C	1:I:143:ASN:HD22	2.04	0.61
1:I:248:GLY:O	1:I:249:ASN:HB2	2.00	0.61
1:B:9:VAL:O	1:B:339:ILE:HD13	2.01	0.61
1:C:495:SER:C	1:C:496:LYS:HD2	2.21	0.61
1:E:389:ASN:HD22	1:E:390:THR:H	1.48	0.61
1:F:225:GLN:NE2	2:J:2:SIA:O1A	2.34	0.61
1:G:248:GLY:O	1:G:249:ASN:HB2	2.01	0.61
1:G:357:ASN:HB3	1:G:359:GLN:H	1.66	0.61
1:H:389:ASN:HD22	1:H:390:THR:H	1.48	0.61
1:B:159:ASN:O	1:B:161:PRO:HD3	2.00	0.61
1:C:12:HIS:N	1:C:350:TRP:O	2.24	0.61
1:E:389:ASN:HD22	1:E:390:THR:N	1.99	0.61
1:G:278:GLU:HG3	1:G:279:THR:N	2.15	0.61
1:C:140:VAL:C	1:C:142:ASP:HA	2.22	0.61
1:D:389:ASN:HD22	1:D:390:THR:N	1.98	0.61
1:D:455:LEU:HB3	1:D:459:VAL:HG22	1.81	0.61
1:F:323:VAL:HG11	1:F:336:ALA:HB2	1.82	0.61
1:D:11:TYR:CE2	1:D:335:ILE:HA	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLN:HE21	1:D:195:GLN:HA	1.66	0.60
1:E:19:LYS:HE2	1:E:29:THR:OG1	2.01	0.60
1:E:248:GLY:O	1:E:249:ASN:HB2	2.01	0.60
1:B:355:HIS:H	1:B:355:HIS:CD2	2.19	0.60
1:E:199:ALA:HB3	1:E:249:ASN:ND2	2.15	0.60
1:E:431:MET:O	1:E:432:GLU:HB2	2.00	0.60
1:G:7:ILE:HA	1:G:355:HIS:CA	2.28	0.60
1:G:111:SER:O	1:G:261:LYS:HE3	2.01	0.60
1:H:248:GLY:O	1:H:249:ASN:HB2	2.00	0.60
1:H:389:ASN:HD22	1:H:390:THR:N	2.00	0.60
1:A:283:THR:HG23	1:A:298:HIS:HB3	1.82	0.60
1:A:382:ASN:HD22	1:A:382:ASN:N	1.99	0.60
1:B:338:PHE:CE1	1:B:339:ILE:HG13	2.36	0.60
1:C:53:PRO:HD2	1:C:274:LEU:HD13	1.84	0.60
1:C:166:SER:HB2	1:C:243:ASN:HD22	1.65	0.60
1:D:310:LYS:HZ2	1:D:418:LEU:HD23	1.66	0.60
1:B:55:GLU:OE2	1:B:273:THR:HG22	2.01	0.60
1:B:143:ASN:N	1:B:143:ASN:ND2	2.46	0.60
1:C:300:LEU:HA	1:C:395:VAL:HB	1.83	0.60
1:D:130:THR:HG22	1:D:132:THR:H	1.67	0.60
1:D:171:SER:HB2	1:D:258:LYS:NZ	2.16	0.60
1:D:322:ASN:O	1:D:323:VAL:HG13	2.01	0.60
1:A:37:LEU:HB2	1:A:314:LEU:HB2	1.83	0.60
1:A:452:ARG:HG3	1:A:467:PHE:CZ	2.36	0.60
1:D:20:VAL:HG13	1:D:30:VAL:HG21	1.83	0.60
1:F:95:TYR:CD2	1:F:229:MET:HG3	2.37	0.60
1:I:389:ASN:HD22	1:I:390:THR:H	1.48	0.60
1:A:338:PHE:CE1	1:A:339:ILE:HG13	2.35	0.60
1:B:455:LEU:HB3	1:B:459:VAL:HG22	1.83	0.60
1:C:459:VAL:CG1	1:C:469:PHE:HA	2.30	0.60
1:F:355:HIS:H	1:F:355:HIS:CD2	2.18	0.60
1:G:346:MET:HE1	1:G:365:ALA:N	2.16	0.60
1:A:30:VAL:HA	1:A:321:ARG:HA	1.82	0.60
1:E:355:HIS:H	1:E:355:HIS:CD2	2.19	0.60
1:E:471:HIS:HB3	1:E:494:GLU:CG	2.31	0.60
1:H:259:ILE:O	1:H:260:SER:CB	2.49	0.60
1:B:111:SER:O	1:B:261:LYS:HE3	2.01	0.60
1:D:279:THR:CB	1:D:287:ALA:HB1	2.31	0.60
1:E:338:PHE:CE1	1:E:339:ILE:HG13	2.36	0.60
1:I:355:HIS:H	1:I:355:HIS:CD2	2.20	0.60
1:D:66:LEU:O	1:D:149:ASN:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ARG:NH1	1:E:216:ILE:O	2.35	0.60
1:F:431:MET:O	1:F:432:GLU:HB2	2.00	0.60
1:G:199:ALA:HB3	1:G:249:ASN:ND2	2.15	0.60
1:H:53:PRO:HD2	1:H:274:LEU:HD13	1.83	0.60
1:E:111:SER:O	1:E:261:LYS:HE3	2.01	0.60
1:I:323:VAL:HG11	1:I:336:ALA:HB2	1.83	0.60
1:I:455:LEU:HB3	1:I:459:VAL:HG22	1.82	0.60
1:B:389:ASN:HD22	1:B:390:THR:N	1.99	0.59
1:F:166:SER:HB2	1:F:243:ASN:HD22	1.67	0.59
1:G:178:ILE:O	1:G:253:PRO:HG3	2.02	0.59
1:E:32:HIS:CE1	1:E:350:TRP:HE1	2.21	0.59
1:H:143:ASN:N	1:H:143:ASN:ND2	2.47	0.59
1:I:259:ILE:CG2	1:I:260:SER:N	2.63	0.59
1:A:424:ASN:O	1:A:426:GLU:N	2.33	0.59
1:G:420:VAL:HG12	1:G:421:TRP:N	2.17	0.59
1:H:142:ASP:C	1:H:143:ASN:HD22	2.06	0.59
1:D:24:LEU:HA	1:F:379:ASN:HB2	1.85	0.59
1:D:162:VAL:CG2	1:D:247:THR:HG22	2.31	0.59
1:A:471:HIS:CE1	1:A:491:TYR:CD1	2.90	0.59
1:C:295:HIS:CE1	1:C:308:TYR:HB2	2.37	0.59
1:E:278:GLU:HG3	1:E:279:THR:H	1.67	0.59
1:F:185:ASN:HD21	1:F:226:GLY:CA	2.15	0.59
1:B:11:TYR:HB3	1:B:444:VAL:HG21	1.85	0.59
1:H:111:SER:O	1:H:261:LYS:HE3	2.02	0.59
1:H:166:SER:CB	1:H:243:ASN:HD22	2.16	0.59
1:I:199:ALA:HB3	1:I:249:ASN:ND2	2.16	0.59
1:A:47:LYS:O	1:A:279:THR:HG22	2.02	0.59
1:A:282:GLN:NE2	1:A:282:GLN:CA	2.66	0.59
1:A:455:LEU:HD12	1:A:486:TYR:CE2	2.38	0.59
1:F:53:PRO:HD2	1:F:274:LEU:HD13	1.84	0.59
1:D:238:ILE:O	1:D:240:ASP:N	2.36	0.59
1:F:338:PHE:CE1	1:F:339:ILE:HG13	2.38	0.59
1:A:140:VAL:HG12	1:A:141:PHE:N	2.18	0.59
1:E:142:ASP:C	1:E:143:ASN:HD22	2.05	0.59
1:G:409:LEU:CD1	1:I:410:ASN:HB2	2.25	0.59
1:I:389:ASN:HD22	1:I:390:THR:N	2.00	0.59
1:B:293:PRO:HB2	1:B:294:PHE:CE2	2.38	0.58
1:C:293:PRO:CG	1:C:385:ILE:HG12	2.33	0.58
1:D:389:ASN:HD22	1:D:390:THR:H	1.48	0.58
1:F:295:HIS:CE1	1:F:308:TYR:HB2	2.38	0.58
1:G:166:SER:CB	1:G:243:ASN:HD22	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:382:ASN:HB3	1:G:386:GLU:OE2	2.03	0.58
1:B:248:GLY:O	1:B:249:ASN:HB2	2.01	0.58
1:D:23:ILE:CD1	1:F:380:LYS:HE2	2.30	0.58
1:D:118:VAL:HG23	1:D:120:ILE:HG23	1.84	0.58
1:D:183:HIS:HB3	1:D:219:ARG:HH22	1.68	0.58
1:D:214:PRO:HG3	1:D:249:ASN:OD1	2.02	0.58
1:G:458:ASN:ND2	1:G:491:TYR:HB2	2.18	0.58
1:A:93:LEU:H	1:A:93:LEU:HD12	1.68	0.58
1:D:108:LEU:CD2	1:D:235:ILE:HD11	2.31	0.58
1:H:335:ILE:HG13	1:H:441:ASP:HA	1.84	0.58
1:A:382:ASN:N	1:A:382:ASN:ND2	2.51	0.58
1:C:389:ASN:HD22	1:C:390:THR:N	1.99	0.58
1:F:11:TYR:HB3	1:F:444:VAL:CG2	2.33	0.58
1:G:142:ASP:C	1:G:143:ASN:HD22	2.06	0.58
1:A:282:GLN:HE22	1:A:286:GLY:C	2.07	0.58
1:A:351:TYR:CD2	1:A:351:TYR:N	2.65	0.58
1:A:418:LEU:O	1:A:422:THR:HB	2.04	0.58
1:D:53:PRO:HG3	1:D:82:TYR:CE2	2.38	0.58
1:D:355:HIS:CD2	1:D:355:HIS:H	2.20	0.58
1:E:7:ILE:CG2	1:E:467:PHE:CD2	2.86	0.58
1:H:320:LEU:HD23	1:H:320:LEU:H	1.67	0.58
1:I:185:ASN:HD21	1:I:226:GLY:CA	2.16	0.58
1:I:293:PRO:HB2	1:I:294:PHE:CE2	2.38	0.58
1:A:219:ARG:HG3	1:A:226:GLY:O	2.04	0.58
1:A:413:MET:O	1:A:416:GLY:N	2.35	0.58
1:C:355:HIS:H	1:C:355:HIS:CD2	2.20	0.58
1:D:265:SER:OG	1:D:266:GLY:N	2.37	0.58
1:E:259:ILE:CG2	1:E:260:SER:H	2.06	0.58
1:F:480:SER:HA	1:F:483:ASN:HB2	1.85	0.58
1:A:176:LEU:HA	1:A:235:ILE:HD13	1.84	0.58
1:A:396:GLY:O	1:A:397:LYS:HG2	2.03	0.58
1:B:142:ASP:C	1:B:143:ASN:HD22	2.05	0.58
1:C:95:TYR:CD2	1:C:229:MET:HG3	2.38	0.58
1:D:19:LYS:HE2	1:D:29:THR:OG1	2.04	0.58
1:E:9:VAL:C	1:E:339:ILE:HD13	2.23	0.58
1:E:295:HIS:CE1	1:E:308:TYR:HB2	2.38	0.58
1:E:310:LYS:HD2	1:E:418:LEU:CD2	2.33	0.58
1:C:111:SER:O	1:C:261:LYS:HE3	2.04	0.58
1:C:185:ASN:HD21	1:C:226:GLY:CA	2.15	0.58
1:D:295:HIS:HD2	1:D:296:ASN:N	2.02	0.58
1:A:490:LYS:HE3	1:A:491:TYR:CE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:CYS:HA	1:B:466:CYS:HA	1.86	0.58
1:B:166:SER:CB	1:B:243:ASN:HD22	2.17	0.58
1:F:19:LYS:HE2	1:F:29:THR:OG1	2.03	0.58
1:H:259:ILE:CG2	1:H:260:SER:N	2.63	0.58
1:A:56:LEU:O	1:A:57:GLY:C	2.42	0.58
1:B:243:ASN:HB2	1:C:218:THR:O	2.04	0.58
1:G:489:SER:O	1:G:490:LYS:HB2	2.04	0.58
1:I:288:ILE:CD1	1:I:297:ILE:HD12	2.34	0.58
1:I:480:SER:HA	1:I:483:ASN:HB2	1.85	0.58
1:A:155:LYS:HE2	1:A:192:THR:O	2.04	0.57
1:D:310:LYS:NZ	1:D:418:LEU:CD2	2.67	0.57
1:G:357:ASN:ND2	1:G:473:CYS:O	2.34	0.57
1:I:53:PRO:HD2	1:I:274:LEU:HD13	1.86	0.57
1:A:279:THR:C	1:A:280:LYS:HD2	2.24	0.57
1:A:451:VAL:O	1:A:451:VAL:HG12	2.04	0.57
1:B:199:ALA:HB3	1:B:249:ASN:ND2	2.19	0.57
1:E:480:SER:HA	1:E:483:ASN:HB2	1.85	0.57
1:F:459:VAL:CG1	1:F:469:PHE:HA	2.29	0.57
1:G:259:ILE:CG2	1:G:260:SER:N	2.63	0.57
1:G:308:TYR:HD2	1:G:418:LEU:HD11	1.68	0.57
1:D:193:LEU:HB2	1:D:194:TYR:CD2	2.40	0.57
1:G:143:ASN:N	1:G:143:ASN:ND2	2.46	0.57
1:A:283:THR:HG22	1:A:285:LEU:H	1.69	0.57
1:A:350:TRP:H	1:A:370:THR:CG2	2.17	0.57
1:C:431:MET:O	1:C:432:GLU:HB2	2.03	0.57
1:F:335:ILE:HG13	1:F:441:ASP:HA	1.86	0.57
1:B:179:TRP:CE2	1:B:203:VAL:HG21	2.40	0.57
1:C:11:TYR:HB3	1:C:444:VAL:CG2	2.34	0.57
1:D:13:SER:CB	1:D:324:PRO:HG3	2.34	0.57
1:D:42:ASN:HD22	1:D:44:LYS:HB2	1.70	0.57
1:F:142:ASP:C	1:F:143:ASN:HD22	2.06	0.57
1:H:480:SER:HA	1:H:483:ASN:HB2	1.86	0.57
1:B:211:ARG:NH1	1:C:216:ILE:HB	2.19	0.57
1:D:376:GLY:C	1:E:24:LEU:HD22	2.24	0.57
1:F:12:HIS:HB2	1:F:350:TRP:HA	1.85	0.57
1:I:111:SER:O	1:I:261:LYS:HE3	2.04	0.57
1:A:19:LYS:HD2	1:A:29:THR:HG23	1.87	0.57
1:D:308:TYR:O	1:D:418:LEU:HD12	2.05	0.57
1:A:45:LEU:HD11	1:A:270:THR:HG21	1.87	0.57
1:A:203:VAL:HG22	1:A:244:PHE:HD1	1.69	0.57
1:D:295:HIS:C	1:D:295:HIS:CD2	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PRO:HD2	1:E:274:LEU:HD13	1.85	0.57
1:F:248:GLY:O	1:F:249:ASN:HB2	2.05	0.57
1:F:293:PRO:HB2	1:F:294:PHE:CE2	2.40	0.57
1:G:381:VAL:HG12	1:G:382:ASN:N	2.18	0.57
1:A:10:GLY:HA3	1:A:343:TRP:CH2	2.39	0.57
1:A:23:ILE:HB	1:A:430:LEU:HB3	1.86	0.57
1:B:480:SER:HA	1:B:483:ASN:HB2	1.87	0.57
1:C:248:GLY:O	1:C:249:ASN:HB2	2.04	0.57
1:C:294:PHE:HB3	1:C:309:VAL:HG22	1.87	0.57
1:C:320:LEU:CD1	1:C:335:ILE:HD13	2.34	0.57
1:D:228:ARG:NH2	1:F:206:SER:HA	2.20	0.57
1:D:493:GLU:O	1:D:494:GLU:HB2	2.05	0.57
1:A:51:ILE:HD13	1:A:51:ILE:N	2.20	0.57
1:A:54:LEU:HD13	1:A:80:TRP:CE3	2.40	0.57
1:A:284:PRO:HD2	1:A:298:HIS:ND1	2.20	0.57
1:E:335:ILE:HG13	1:E:441:ASP:HA	1.86	0.57
1:G:379:ASN:HB3	1:H:26:ARG:NH1	2.20	0.57
1:G:473:CYS:SG	1:G:478:MET:HE2	2.45	0.57
1:D:168:ASN:HA	1:D:241:THR:CB	2.25	0.56
1:F:12:HIS:CB	1:F:350:TRP:HA	2.35	0.56
1:G:387:LYS:HZ2	1:H:426:GLU:HG2	1.69	0.56
1:H:387:LYS:HD3	1:I:426:GLU:HG2	1.86	0.56
1:A:165:GLY:O	1:A:244:PHE:N	2.34	0.56
1:D:338:PHE:CE1	1:D:339:ILE:HG13	2.40	0.56
1:A:189:GLU:HG3	1:A:193:LEU:HD12	1.86	0.56
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.40	0.56
1:C:480:SER:HA	1:C:483:ASN:HB2	1.87	0.56
1:E:456:ARG:HD2	1:F:461:GLU:O	2.05	0.56
1:F:293:PRO:HB2	1:F:294:PHE:CD2	2.40	0.56
1:G:140:VAL:C	1:G:142:ASP:HA	2.25	0.56
1:H:379:ASN:HB3	1:I:26:ARG:CZ	2.36	0.56
1:H:379:ASN:HD22	1:I:26:ARG:CZ	2.18	0.56
1:I:166:SER:HB2	1:I:243:ASN:HD22	1.70	0.56
1:I:178:ILE:O	1:I:253:PRO:HG3	2.05	0.56
1:I:306:PRO:O	1:I:308:TYR:N	2.38	0.56
1:A:81:SER:HB2	1:A:82:TYR:HD2	1.70	0.56
1:A:332:PHE:CD2	1:A:442:SER:HB2	2.41	0.56
1:C:32:HIS:CE1	1:C:350:TRP:HE1	2.24	0.56
1:C:166:SER:CB	1:C:243:ASN:HD22	2.17	0.56
1:D:63:GLY:HA2	1:D:92:GLY:O	2.05	0.56
1:I:166:SER:CB	1:I:243:ASN:HD22	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:197:VAL:HG12	1:I:198:GLY:N	2.21	0.56
1:A:23:ILE:CD1	1:C:380:LYS:HE2	2.35	0.56
1:C:12:HIS:HB2	1:C:350:TRP:HA	1.88	0.56
1:H:114:HIS:O	1:H:259:ILE:O	2.24	0.56
1:A:366:ASP:HB3	1:A:369:SER:HB3	1.87	0.56
1:B:140:VAL:C	1:B:142:ASP:HA	2.25	0.56
1:F:197:VAL:HG12	1:F:198:GLY:N	2.21	0.56
1:H:460:LYS:HD2	1:H:470:TYR:CE1	2.40	0.56
1:I:293:PRO:HB2	1:I:294:PHE:CD2	2.39	0.56
1:E:141:PHE:CE2	1:G:274:LEU:HD11	2.41	0.56
1:H:140:VAL:C	1:H:142:ASP:HA	2.25	0.56
1:H:410:ASN:HB2	1:I:409:LEU:CD1	2.35	0.56
1:B:332:PHE:CE2	1:B:442:SER:HB2	2.41	0.56
1:C:19:LYS:HE2	1:C:29:THR:OG1	2.06	0.56
1:D:195:GLN:O	1:D:195:GLN:HG3	2.05	0.56
1:F:140:VAL:C	1:F:142:ASP:HA	2.26	0.56
1:G:214:PRO:HG2	1:G:249:ASN:ND2	2.21	0.56
1:G:470:TYR:O	1:G:471:HIS:HB3	2.06	0.56
1:A:160:TYR:CE2	1:A:248:GLY:N	2.74	0.56
1:G:384:VAL:O	1:G:384:VAL:HG12	2.06	0.56
1:I:160:TYR:CZ	1:I:248:GLY:HA2	2.41	0.56
1:A:45:LEU:HD22	1:A:84:MET:CE	2.36	0.56
1:B:284:PRO:HG2	1:B:298:HIS:CE1	2.40	0.56
1:C:12:HIS:CB	1:C:350:TRP:HA	2.36	0.56
1:D:124:ASP:O	1:D:126:TRP:N	2.39	0.56
1:D:295:HIS:CD2	1:D:296:ASN:N	2.74	0.56
1:G:55:GLU:OE2	1:G:273:THR:HG22	2.06	0.56
1:H:379:ASN:HB3	1:I:26:ARG:NH1	2.21	0.56
1:I:278:GLU:HG3	1:I:279:THR:H	1.69	0.56
1:C:142:ASP:C	1:C:143:ASN:HD22	2.09	0.55
1:D:113:THR:HG23	1:D:113:THR:O	2.06	0.55
1:D:238:ILE:HG23	1:D:239:TRP:CE2	2.40	0.55
1:F:111:SER:O	1:F:261:LYS:HE3	2.06	0.55
1:G:428:LEU:O	1:G:432:GLU:HB2	2.05	0.55
1:A:211:ARG:HD2	1:B:216:ILE:O	2.05	0.55
1:D:120:ILE:CD1	1:D:177:ILE:HD13	2.36	0.55
1:E:140:VAL:C	1:E:142:ASP:HA	2.26	0.55
1:E:460:LYS:HD2	1:E:470:TYR:CE1	2.41	0.55
1:H:197:VAL:HG12	1:H:198:GLY:N	2.22	0.55
1:I:187:GLU:O	1:I:190:GLN:HB3	2.07	0.55
1:B:376:GLY:C	1:C:24:LEU:HD22	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:HIS:HE1	1:D:347:VAL:HA	1.71	0.55
1:D:124:ASP:C	1:D:126:TRP:H	2.09	0.55
1:G:420:VAL:O	1:G:423:TYR:HB3	2.07	0.55
1:H:399:PHE:CE1	1:H:406:LEU:HG	2.41	0.55
1:A:55:GLU:O	1:A:74:LEU:HD21	2.07	0.55
1:D:288:ILE:CG1	1:D:297:ILE:HD12	2.37	0.55
1:F:293:PRO:CG	1:F:385:ILE:HG12	2.36	0.55
1:G:387:LYS:HZ1	1:H:426:GLU:HG2	1.71	0.55
1:C:55:GLU:HG3	1:C:274:LEU:HD22	1.88	0.55
1:C:143:ASN:ND2	1:G:19:LYS:CD	2.69	0.55
1:D:129:HIS:NE2	1:D:161:PRO:O	2.39	0.55
1:F:460:LYS:HD2	1:F:470:TYR:CE1	2.41	0.55
1:G:42:ASN:OD1	1:G:44:LYS:HE2	2.07	0.55
1:I:214:PRO:HG2	1:I:249:ASN:ND2	2.21	0.55
1:I:460:LYS:HD2	1:I:470:TYR:CE1	2.42	0.55
1:I:42:ASN:HB3	1:I:287:ALA:H	1.71	0.55
1:B:185:ASN:HD21	1:B:226:GLY:CA	2.17	0.55
1:C:197:VAL:HG12	1:C:198:GLY:N	2.22	0.55
1:F:11:TYR:CD2	1:F:335:ILE:HG12	2.42	0.55
1:F:259:ILE:CG2	1:F:260:SER:N	2.59	0.55
1:G:185:ASN:HD21	1:G:226:GLY:CA	2.17	0.55
1:E:55:GLU:OE2	1:E:273:THR:HG22	2.07	0.55
1:E:310:LYS:HD2	1:E:418:LEU:HD21	1.89	0.55
1:H:55:GLU:OE2	1:H:273:THR:HG22	2.07	0.55
1:A:382:ASN:ND2	1:A:382:ASN:H	2.05	0.55
1:B:211:ARG:NH1	1:C:216:ILE:O	2.40	0.55
1:D:53:PRO:HG3	1:D:82:TYR:CZ	2.42	0.55
1:E:288:ILE:CD1	1:E:297:ILE:HD12	2.37	0.55
1:E:317:ALA:N	1:E:433:ASN:OD1	2.26	0.55
1:F:12:HIS:N	1:F:350:TRP:O	2.26	0.55
1:F:166:SER:CB	1:F:243:ASN:HD22	2.19	0.55
1:F:320:LEU:CD1	1:F:335:ILE:HD13	2.35	0.55
1:B:293:PRO:HG3	1:B:385:ILE:HG23	1.88	0.55
1:C:259:ILE:CG2	1:C:260:SER:H	2.06	0.55
1:I:143:ASN:N	1:I:143:ASN:ND2	2.47	0.55
1:B:55:GLU:HG3	1:B:274:LEU:HD22	1.89	0.54
1:B:310:LYS:HD2	1:B:418:LEU:HD21	1.89	0.54
1:D:108:LEU:HD12	1:D:108:LEU:C	2.28	0.54
1:D:480:SER:HA	1:D:483:ASN:HB2	1.88	0.54
1:E:169:ASN:ND2	1:E:238:ILE:HA	2.17	0.54
1:E:197:VAL:HG12	1:E:198:GLY:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ILE:CD1	1:G:297:ILE:HD12	2.37	0.54
1:G:343:TRP:HE3	1:G:346:MET:CG	2.20	0.54
1:I:293:PRO:HG3	1:I:385:ILE:HG12	1.88	0.54
1:A:51:ILE:HG21	1:A:79:GLU:HG2	1.87	0.54
1:A:77:VAL:HG22	1:A:79:GLU:H	1.70	0.54
1:F:179:TRP:CE2	1:F:203:VAL:HG21	2.43	0.54
1:H:42:ASN:HB3	1:H:287:ALA:H	1.72	0.54
1:H:166:SER:HB2	1:H:243:ASN:HD22	1.71	0.54
1:H:185:ASN:HD21	1:H:226:GLY:CA	2.16	0.54
1:I:140:VAL:C	1:I:142:ASP:HA	2.27	0.54
1:A:36:ILE:O	1:A:292:LEU:HD22	2.07	0.54
1:A:445:LYS:HG3	1:A:445:LYS:O	2.07	0.54
1:B:166:SER:HB2	1:B:243:ASN:HD22	1.73	0.54
1:B:197:VAL:HG12	1:B:198:GLY:N	2.21	0.54
1:A:160:TYR:CZ	1:A:248:GLY:HA2	2.42	0.54
1:G:26:ARG:CZ	1:I:379:ASN:HD22	2.21	0.54
1:G:197:VAL:HG12	1:G:198:GLY:N	2.22	0.54
1:H:278:GLU:HG3	1:H:279:THR:H	1.71	0.54
1:A:460:LYS:HG3	1:A:468:GLU:CG	2.37	0.54
1:C:460:LYS:HD2	1:C:470:TYR:CE1	2.43	0.54
1:A:351:TYR:HE2	1:A:370:THR:HA	1.73	0.54
1:E:376:GLY:HA2	1:F:24:LEU:HB3	1.89	0.54
1:F:399:PHE:CE1	1:F:406:LEU:HG	2.43	0.54
1:A:64:TRP:HE1	1:A:76:THR:HG22	1.73	0.54
1:A:117:LYS:HG3	1:A:257:PHE:CE1	2.43	0.54
1:D:158:SER:O	1:D:195:GLN:HG2	2.08	0.54
1:D:239:TRP:CD2	1:D:239:TRP:N	2.76	0.54
1:E:320:LEU:HD13	1:E:335:ILE:HD13	1.90	0.54
1:E:376:GLY:CA	1:F:24:LEU:HB3	2.37	0.54
1:G:179:TRP:CE2	1:G:203:VAL:HG21	2.43	0.54
1:G:455:LEU:CG	1:G:459:VAL:HG21	2.38	0.54
1:H:160:TYR:CZ	1:H:248:GLY:HA2	2.43	0.54
1:A:78:PRO:O	1:A:114:HIS:HB2	2.07	0.54
1:E:488:TYR:O	1:E:492:GLU:HB2	2.07	0.54
1:G:379:ASN:HD22	1:H:26:ARG:CZ	2.20	0.54
1:B:53:PRO:HD2	1:B:274:LEU:HD13	1.89	0.54
1:B:436:THR:O	1:B:439:PHE:HB3	2.07	0.54
1:D:160:TYR:CZ	1:D:248:GLY:HA2	2.42	0.54
1:H:432:GLU:H	1:H:435:MET:HG3	1.71	0.54
1:C:323:VAL:HG11	1:C:336:ALA:HB2	1.90	0.54
1:F:187:GLU:O	1:F:190:GLN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:CYS:O	1:G:353:TYR:C	2.47	0.54
1:D:55:GLU:OE1	1:D:274:LEU:HD23	2.08	0.53
1:D:108:LEU:HD21	1:D:235:ILE:CD1	2.34	0.53
1:D:140:VAL:HG12	1:D:141:PHE:CD2	2.43	0.53
1:D:290:THR:OG1	1:D:291:THR:N	2.41	0.53
1:G:23:ILE:HG22	1:G:434:GLU:HG2	1.90	0.53
1:D:303:GLY:HA2	1:D:392:PHE:CD1	2.43	0.53
1:G:42:ASN:HB3	1:G:287:ALA:H	1.74	0.53
1:G:360:GLY:O	1:G:361:SER:HB2	2.08	0.53
1:A:417:PHE:CD1	1:C:417:PHE:HE1	2.26	0.53
1:C:288:ILE:CD1	1:C:297:ILE:HD12	2.38	0.53
1:F:284:PRO:HG2	1:F:298:HIS:CE1	2.44	0.53
1:G:160:TYR:CZ	1:G:248:GLY:HA2	2.43	0.53
1:G:448:TYR:HE1	1:G:465:GLY:HA2	1.72	0.53
1:A:202:SER:HB3	1:A:211:ARG:HG3	1.91	0.53
1:B:288:ILE:CD1	1:B:297:ILE:HD12	2.38	0.53
1:B:380:LYS:HA	1:C:23:ILE:HG12	1.90	0.53
1:D:80:TRP:CE2	1:D:112:VAL:CG2	2.90	0.53
1:D:460:LYS:HD2	1:D:470:TYR:CE1	2.43	0.53
1:E:293:PRO:HB2	1:E:294:PHE:CD2	2.44	0.53
1:G:427:LEU:HD12	1:G:431:MET:HE2	1.91	0.53
1:I:268:MET:HE3	1:I:302:ILE:HD12	1.90	0.53
1:I:462:LEU:HD11	1:I:468:GLU:CB	2.37	0.53
1:C:214:PRO:HG2	1:C:249:ASN:ND2	2.24	0.53
1:F:214:PRO:HG2	1:F:249:ASN:ND2	2.22	0.53
1:G:184:PRO:O	1:G:216:ILE:HG23	2.09	0.53
1:I:24:LEU:HD12	1:I:434:GLU:OE1	2.08	0.53
1:I:490:LYS:HE3	1:I:491:TYR:CE2	2.44	0.53
1:A:51:ILE:HG22	1:A:52:PRO:HD2	1.90	0.53
1:D:36:ILE:HG13	1:D:314:LEU:HB3	1.91	0.53
1:D:288:ILE:HG12	1:D:297:ILE:CD1	2.38	0.53
1:G:166:SER:HB2	1:G:243:ASN:ND2	2.24	0.53
1:G:408:ASN:ND2	1:I:397:LYS:NZ	2.48	0.53
1:G:455:LEU:O	1:G:456:ARG:HB2	2.08	0.53
1:I:306:PRO:O	1:I:307:LYS:C	2.47	0.53
1:B:494:GLU:O	1:B:495:SER:C	2.47	0.53
1:E:379:ASN:HB2	1:F:24:LEU:HA	1.91	0.53
1:G:9:VAL:HA	1:G:352:GLY:O	2.09	0.53
1:G:284:PRO:HG2	1:G:298:HIS:CE1	2.44	0.53
1:G:404:LYS:HA	1:G:404:LYS:HE3	1.90	0.53
1:I:128:GLN:HB3	1:I:161:PRO:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:TYR:O	1:B:492:GLU:HB2	2.08	0.53
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.43	0.53
1:D:26:ARG:O	1:D:27:ASN:HB2	2.08	0.53
1:D:42:ASN:HB2	1:D:44:LYS:H	1.74	0.53
1:F:55:GLU:OE2	1:F:273:THR:HG22	2.08	0.53
1:G:26:ARG:CZ	1:I:379:ASN:HB3	2.39	0.53
1:G:408:ASN:ND2	1:G:408:ASN:C	2.62	0.53
1:A:461:GLU:HG3	1:A:467:PHE:HE1	1.72	0.53
1:C:178:ILE:O	1:C:253:PRO:HG3	2.09	0.53
1:D:215:GLU:OE1	1:F:210:LYS:HA	2.09	0.53
1:E:284:PRO:HG2	1:E:298:HIS:CE1	2.44	0.53
1:F:462:LEU:HD11	1:F:468:GLU:CB	2.36	0.53
1:A:218:THR:HG22	1:A:218:THR:O	2.09	0.53
1:A:451:VAL:O	1:A:452:ARG:HB2	2.08	0.53
1:B:294:PHE:HB3	1:B:309:VAL:HG22	1.90	0.53
1:C:114:HIS:O	1:C:259:ILE:O	2.26	0.53
1:D:310:LYS:HZ2	1:D:418:LEU:CD2	2.22	0.53
1:E:376:GLY:C	1:F:24:LEU:CD2	2.77	0.53
1:F:55:GLU:HG3	1:F:274:LEU:HD22	1.91	0.53
1:G:460:LYS:HD3	1:G:470:TYR:OH	2.09	0.53
1:H:338:PHE:CE1	1:H:339:ILE:HG13	2.44	0.53
1:H:436:THR:O	1:H:439:PHE:HB3	2.09	0.53
1:A:199:ALA:HA	1:A:247:THR:OG1	2.09	0.52
1:C:55:GLU:OE2	1:C:273:THR:HG22	2.08	0.52
1:D:57:GLY:O	1:D:86:LYS:HD3	2.10	0.52
1:D:72:ASP:O	1:D:74:LEU:N	2.41	0.52
1:E:293:PRO:HB2	1:E:294:PHE:CE2	2.43	0.52
1:H:214:PRO:HG2	1:H:249:ASN:ND2	2.23	0.52
1:A:23:ILE:O	1:A:23:ILE:HG12	2.08	0.52
1:A:38:GLU:N	1:A:294:PHE:O	2.39	0.52
1:B:200:TYR:CE1	1:B:247:THR:HG23	2.44	0.52
1:B:460:LYS:HD2	1:B:470:TYR:CE1	2.44	0.52
1:E:214:PRO:HG2	1:E:249:ASN:ND2	2.23	0.52
1:F:307:LYS:HE2	1:F:421:TRP:CE2	2.44	0.52
1:A:392:PHE:C	1:A:392:PHE:CD2	2.83	0.52
1:B:160:TYR:CZ	1:B:248:GLY:HA2	2.44	0.52
1:C:8:CYS:HA	1:C:466:CYS:HA	1.92	0.52
1:D:12:HIS:CD2	1:D:13:SER:N	2.74	0.52
1:E:8:CYS:HA	1:E:465:GLY:O	2.09	0.52
1:E:55:GLU:HG3	1:E:274:LEU:HD22	1.90	0.52
1:H:9:VAL:C	1:H:343:TRP:CH2	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HD3	1:C:379:ASN:HD22	1.75	0.52
1:A:82:TYR:CE1	1:A:268:MET:HE2	2.44	0.52
1:A:190:GLN:HG2	1:A:197:VAL:HG22	1.90	0.52
1:A:495:SER:O	1:A:496:LYS:HB2	2.09	0.52
1:B:11:TYR:CD2	1:B:335:ILE:HG12	2.44	0.52
1:B:201:VAL:HG22	1:B:250:LEU:HB2	1.91	0.52
1:D:30:VAL:HG12	1:D:321:ARG:HA	1.92	0.52
1:D:45:LEU:CD1	1:D:270:THR:HG21	2.37	0.52
1:D:80:TRP:CZ2	1:D:112:VAL:HG21	2.45	0.52
1:F:278:GLU:HG3	1:F:279:THR:H	1.74	0.52
1:H:488:TYR:O	1:H:492:GLU:HB2	2.08	0.52
1:A:53:PRO:HG3	1:A:82:TYR:CZ	2.44	0.52
1:A:94:CYS:CB	1:A:138:CYS:SG	2.95	0.52
1:A:460:LYS:HG2	1:A:470:TYR:CE1	2.44	0.52
1:D:105:LEU:HB2	1:D:233:TRP:CE2	2.45	0.52
1:D:162:VAL:HG22	1:D:247:THR:HG22	1.91	0.52
1:E:42:ASN:HB3	1:E:287:ALA:H	1.75	0.52
1:E:294:PHE:HB3	1:E:309:VAL:HG22	1.92	0.52
1:F:288:ILE:CD1	1:F:297:ILE:HD12	2.40	0.52
1:G:55:GLU:HG3	1:G:274:LEU:HD22	1.92	0.52
1:G:167:TYR:CE2	1:G:169:ASN:HA	2.45	0.52
1:G:311:SER:HB3	1:G:426:GLU:OE2	2.10	0.52
1:B:11:TYR:HB3	1:B:444:VAL:CG2	2.40	0.52
1:C:162:VAL:HG12	1:C:164:LYS:HG3	1.92	0.52
1:D:67:GLY:O	1:D:68:ASN:C	2.47	0.52
1:D:120:ILE:HG12	1:D:256:GLY:N	2.24	0.52
1:G:7:ILE:HG13	1:G:355:HIS:HB3	1.90	0.52
1:G:493:GLU:O	1:G:494:GLU:CB	2.57	0.52
1:G:243:ASN:CB	1:H:218:THR:HB	2.40	0.52
1:G:397:LYS:HG2	1:G:397:LYS:O	2.10	0.52
1:A:331:LEU:HD22	1:C:442:SER:OG	2.10	0.52
1:F:169:ASN:ND2	1:F:238:ILE:HA	2.20	0.52
1:G:367:LYS:HE2	1:G:367:LYS:CA	2.40	0.52
1:A:23:ILE:HD11	1:C:380:LYS:CG	2.40	0.52
1:A:420:VAL:HG12	1:A:421:TRP:N	2.25	0.52
1:B:259:ILE:CG2	1:B:260:SER:N	2.59	0.52
1:C:493:GLU:O	1:C:494:GLU:CB	2.58	0.52
1:D:67:GLY:O	1:D:148:ARG:HG2	2.09	0.52
1:E:160:TYR:CZ	1:E:248:GLY:HA2	2.45	0.52
1:E:307:LYS:HD2	1:E:421:TRP:CD1	2.45	0.52
1:G:162:VAL:HG12	1:G:164:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:PRO:O	1:G:307:LYS:C	2.47	0.52
1:G:343:TRP:HE3	1:G:346:MET:HG2	1.75	0.52
1:A:151:VAL:N	1:A:252:ALA:O	2.36	0.52
1:A:197:VAL:CG1	1:A:198:GLY:H	2.15	0.52
1:B:214:PRO:HG2	1:B:249:ASN:ND2	2.25	0.52
1:B:300:LEU:HA	1:B:395:VAL:HB	1.91	0.52
1:C:42:ASN:HB3	1:C:287:ALA:H	1.74	0.52
1:D:183:HIS:CE1	1:D:215:GLU:HB2	2.44	0.52
1:D:195:GLN:O	1:D:196:ASN:HB3	2.09	0.52
1:E:442:SER:OG	1:F:331:LEU:O	2.26	0.52
1:F:294:PHE:HB3	1:F:309:VAL:HG22	1.92	0.52
1:H:332:PHE:CE2	1:H:442:SER:HB2	2.45	0.52
1:I:332:PHE:CE2	1:I:442:SER:HB2	2.45	0.52
1:A:195:GLN:O	1:A:196:ASN:HB3	2.10	0.51
1:C:462:LEU:HD11	1:C:468:GLU:CB	2.37	0.51
1:D:219:ARG:HD3	1:D:226:GLY:O	2.09	0.51
1:D:221:GLU:OE1	1:D:224:GLY:HA2	2.10	0.51
1:G:379:ASN:O	1:G:380:LYS:C	2.46	0.51
1:A:116:GLU:OE1	1:A:258:LYS:HD3	2.10	0.51
1:A:417:PHE:CD1	1:C:417:PHE:CE1	2.97	0.51
1:C:187:GLU:O	1:C:190:GLN:HB3	2.10	0.51
1:F:310:LYS:HD2	1:F:418:LEU:HD21	1.91	0.51
1:I:53:PRO:HG3	1:I:82:TYR:CZ	2.45	0.51
1:A:478:MET:C	1:A:480:SER:N	2.64	0.51
1:B:48:LEU:O	1:B:49:ASN:HB2	2.10	0.51
1:C:259:ILE:CG2	1:C:260:SER:N	2.60	0.51
1:C:284:PRO:HG2	1:C:298:HIS:CE1	2.45	0.51
1:C:293:PRO:HB2	1:C:294:PHE:CE2	2.45	0.51
1:E:12:HIS:HB2	1:E:350:TRP:HA	1.91	0.51
1:G:128:GLN:HB3	1:G:161:PRO:HG2	1.92	0.51
1:G:457:ASP:C	1:G:459:VAL:H	2.13	0.51
1:A:59:CYS:O	1:A:89:PRO:HB3	2.10	0.51
1:A:305:CYS:O	1:A:306:PRO:O	2.29	0.51
1:D:10:GLY:HA2	1:D:339:ILE:HG21	1.92	0.51
1:F:162:VAL:HG12	1:F:164:LYS:HG3	1.92	0.51
1:F:332:PHE:CE2	1:F:442:SER:HB2	2.46	0.51
1:H:174:GLN:O	1:H:259:ILE:HG22	2.11	0.51
1:A:102:TYR:O	1:A:106:LYS:HB2	2.10	0.51
1:B:32:HIS:CE1	1:B:350:TRP:HE1	2.29	0.51
1:D:23:ILE:CG1	1:F:380:LYS:HA	2.30	0.51
1:D:96:PRO:HG3	1:D:222:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLN:O	1:D:196:ASN:CB	2.59	0.51
1:E:9:VAL:CG2	1:E:448:TYR:HD1	2.23	0.51
1:F:488:TYR:O	1:F:492:GLU:HB2	2.10	0.51
1:G:409:LEU:HD11	1:I:410:ASN:OD1	2.10	0.51
1:I:432:GLU:H	1:I:435:MET:HG3	1.76	0.51
1:A:323:VAL:N	1:A:324:PRO:CD	2.74	0.51
1:A:424:ASN:C	1:A:426:GLU:H	2.13	0.51
1:B:9:VAL:CB	1:B:448:TYR:HD1	2.22	0.51
1:C:293:PRO:HB2	1:C:294:PHE:CD2	2.45	0.51
1:D:404:LYS:HB2	1:F:104:GLU:OE1	2.10	0.51
1:F:7:ILE:O	1:F:467:PHE:N	2.38	0.51
1:F:160:TYR:CZ	1:F:248:GLY:HA2	2.45	0.51
1:H:10:GLY:HA3	1:H:343:TRP:CE2	2.46	0.51
1:A:13:SER:CB	1:A:324:PRO:HG3	2.40	0.51
1:E:243:ASN:HB2	1:F:218:THR:O	2.10	0.51
1:E:400:SER:OG	1:E:403:GLU:HG3	2.11	0.51
1:I:184:PRO:O	1:I:216:ILE:HG23	2.11	0.51
1:D:126:TRP:CZ3	1:D:153:LEU:HD11	2.46	0.51
1:E:48:LEU:O	1:E:49:ASN:HB2	2.11	0.51
1:E:185:ASN:HD21	1:E:226:GLY:CA	2.19	0.51
1:G:218:THR:O	1:I:243:ASN:HB2	2.11	0.51
1:A:7:ILE:O	1:A:467:PHE:HB2	2.11	0.51
1:D:216:ILE:HB	1:F:211:ARG:NH1	2.25	0.51
1:D:332:PHE:CE2	1:D:442:SER:HB2	2.46	0.51
1:I:399:PHE:CE1	1:I:406:LEU:HG	2.46	0.51
1:A:9:VAL:O	1:A:339:ILE:HD13	2.10	0.51
1:A:83:ILE:HB	1:A:267:ILE:HG13	1.93	0.51
1:C:48:LEU:O	1:C:49:ASN:HB2	2.10	0.51
1:C:166:SER:HB2	1:C:243:ASN:ND2	2.25	0.51
1:I:335:ILE:HG13	1:I:441:ASP:HA	1.92	0.51
1:A:178:ILE:O	1:A:253:PRO:HG3	2.11	0.50
1:A:457:ASP:C	1:A:459:VAL:N	2.65	0.50
1:A:475:ASP:O	1:A:479:ASN:HB3	2.11	0.50
1:D:52:PRO:O	1:D:80:TRP:HA	2.11	0.50
1:E:10:GLY:HA2	1:E:339:ILE:HG21	1.91	0.50
1:E:20:VAL:HB	1:E:433:ASN:ND2	2.26	0.50
1:I:22:THR:HG22	1:I:433:ASN:HB3	1.93	0.50
1:A:179:TRP:CE2	1:A:203:VAL:HG21	2.46	0.50
1:A:181:VAL:CG2	1:A:201:VAL:HG21	2.29	0.50
1:A:461:GLU:HG3	1:A:467:PHE:CE1	2.46	0.50
1:D:11:TYR:CZ	1:D:335:ILE:HG23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:SER:HB2	1:E:243:ASN:ND2	2.25	0.50
1:F:295:HIS:HD2	1:F:297:ILE:N	2.06	0.50
1:G:458:ASN:C	1:G:459:VAL:HG22	2.31	0.50
1:H:486:TYR:CG	1:H:487:ASP:N	2.79	0.50
1:I:294:PHE:HB3	1:I:309:VAL:HG22	1.93	0.50
1:A:166:SER:CB	1:A:243:ASN:ND2	2.71	0.50
1:A:395:VAL:O	1:A:396:GLY:O	2.29	0.50
1:D:83:ILE:HD11	1:D:109:ILE:O	2.12	0.50
1:E:332:PHE:CE2	1:E:442:SER:HB2	2.45	0.50
1:G:405:ARG:HD2	1:I:398:GLU:O	2.11	0.50
1:A:462:LEU:HD12	1:A:462:LEU:N	2.27	0.50
1:C:310:LYS:HD2	1:C:418:LEU:HD21	1.94	0.50
1:D:196:ASN:O	1:D:196:ASN:ND2	2.33	0.50
1:D:293:PRO:HD3	1:D:385:ILE:HG12	1.93	0.50
1:D:335:ILE:HG13	1:D:441:ASP:HA	1.93	0.50
1:I:284:PRO:HG2	1:I:298:HIS:CE1	2.46	0.50
1:A:351:TYR:H	1:A:351:TYR:HD2	1.56	0.50
1:B:169:ASN:ND2	1:B:238:ILE:HA	2.23	0.50
1:C:317:ALA:O	1:C:436:THR:HG21	2.12	0.50
1:H:7:ILE:CG1	1:H:355:HIS:HB3	2.38	0.50
1:H:167:TYR:CE2	1:H:169:ASN:HA	2.46	0.50
1:I:486:TYR:CG	1:I:487:ASP:N	2.79	0.50
1:D:488:TYR:O	1:D:492:GLU:HB2	2.12	0.50
1:E:7:ILE:O	1:E:467:PHE:HD2	1.94	0.50
1:F:129:HIS:NE2	1:F:161:PRO:HD2	2.27	0.50
1:G:458:ASN:HD21	1:G:491:TYR:HB2	1.74	0.50
1:H:490:LYS:HE3	1:H:491:TYR:CE2	2.46	0.50
1:I:293:PRO:CG	1:I:385:ILE:HG12	2.41	0.50
1:A:282:GLN:HE22	1:A:287:ALA:N	2.10	0.50
1:C:129:HIS:NE2	1:C:161:PRO:HD2	2.26	0.50
1:C:332:PHE:CE2	1:C:442:SER:HB2	2.46	0.50
1:E:141:PHE:HE2	1:G:274:LEU:HD11	1.76	0.50
1:E:278:GLU:CG	1:E:279:THR:N	2.73	0.50
1:E:388:MET:HE2	1:F:423:TYR:CE1	2.47	0.50
1:E:490:LYS:HE3	1:E:491:TYR:CE2	2.47	0.50
1:A:219:ARG:HG2	1:A:219:ARG:HH11	1.77	0.50
1:A:283:THR:HA	1:A:301:THR:HG22	1.94	0.50
1:A:452:ARG:C	1:A:454:GLN:H	2.14	0.50
1:E:73:ARG:CZ	1:G:276:ASN:O	2.59	0.50
1:E:436:THR:O	1:E:439:PHE:HB3	2.12	0.50
1:G:366:ASP:C	1:G:368:GLU:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451:VAL:HG12	1:H:452:ARG:N	2.26	0.50
1:C:42:ASN:OD1	1:C:44:LYS:HE2	2.12	0.50
1:C:294:PHE:HB3	1:C:309:VAL:CG2	2.41	0.50
1:C:432:GLU:H	1:C:435:MET:HG3	1.77	0.50
1:C:490:LYS:HE3	1:C:491:TYR:CE2	2.46	0.50
1:E:259:ILE:CG2	1:E:260:SER:N	2.59	0.50
1:H:128:GLN:HB3	1:H:161:PRO:HG2	1.94	0.50
1:I:120:ILE:O	1:I:121:LEU:HD23	2.12	0.50
1:A:389:ASN:HD22	1:A:390:THR:H	1.59	0.49
1:C:444:VAL:O	1:C:447:LEU:N	2.44	0.49
1:D:36:ILE:O	1:D:292:LEU:HB3	2.11	0.49
1:D:211:ARG:HB2	1:E:215:GLU:HB3	1.93	0.49
1:D:380:LYS:HA	1:E:23:ILE:HG12	1.93	0.49
1:D:409:LEU:CD1	1:F:410:ASN:HB2	2.42	0.49
1:E:178:ILE:O	1:E:253:PRO:HG3	2.11	0.49
1:E:184:PRO:O	1:E:216:ILE:HG23	2.12	0.49
1:G:53:PRO:CD	1:G:274:LEU:HD13	2.42	0.49
1:A:94:CYS:SG	1:A:138:CYS:SG	3.10	0.49
1:A:216:ILE:HB	1:C:211:ARG:NH1	2.27	0.49
1:B:332:PHE:CD2	1:B:442:SER:HB2	2.48	0.49
1:D:240:ASP:C	1:D:241:THR:HG22	2.32	0.49
1:E:138:CYS:O	1:E:145:SER:HB3	2.12	0.49
1:E:432:GLU:H	1:E:435:MET:HG3	1.76	0.49
1:C:128:GLN:HB3	1:C:161:PRO:HG2	1.94	0.49
1:D:8:CYS:HB3	1:D:343:TRP:HZ2	1.78	0.49
1:D:12:HIS:CG	1:D:13:SER:N	2.78	0.49
1:D:20:VAL:CG1	1:D:30:VAL:HG21	2.41	0.49
1:A:320:LEU:HD23	1:A:320:LEU:N	2.27	0.49
1:C:307:LYS:HE2	1:C:421:TRP:CE2	2.47	0.49
1:D:100:ASN:O	1:D:101:ASP:HB2	2.12	0.49
1:D:283:THR:HG22	1:D:285:LEU:N	2.14	0.49
1:D:432:GLU:H	1:D:435:MET:HG3	1.78	0.49
1:E:11:TYR:HE2	1:E:335:ILE:HA	1.62	0.49
1:E:162:VAL:HG12	1:E:164:LYS:HG3	1.94	0.49
1:F:120:ILE:O	1:F:121:LEU:HD23	2.12	0.49
1:G:26:ARG:NH1	1:I:379:ASN:HB3	2.27	0.49
1:G:45:LEU:H	1:G:45:LEU:HD12	1.77	0.49
1:G:306:PRO:O	1:G:308:TYR:N	2.45	0.49
1:G:430:LEU:C	1:G:431:MET:O	2.48	0.49
1:G:474:ASP:O	1:G:477:CYS:HB3	2.13	0.49
1:D:14:ASN:O	1:D:16:SER:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ILE:O	1:E:121:LEU:HD23	2.12	0.49
1:F:184:PRO:O	1:F:216:ILE:HG23	2.12	0.49
1:F:338:PHE:CE1	1:F:339:ILE:CG1	2.96	0.49
1:G:243:ASN:HB3	1:H:218:THR:HB	1.95	0.49
1:G:424:ASN:O	1:G:425:ALA:O	2.30	0.49
1:H:53:PRO:HG3	1:H:82:TYR:CZ	2.48	0.49
1:H:493:GLU:O	1:H:494:GLU:CB	2.60	0.49
1:H:493:GLU:O	1:H:494:GLU:HB3	2.12	0.49
1:A:28:VAL:HG12	1:A:30:VAL:HG12	1.93	0.49
1:A:282:GLN:HE21	1:A:282:GLN:C	2.16	0.49
1:A:460:LYS:O	1:A:468:GLU:HB3	2.12	0.49
1:C:142:ASP:OD2	1:G:27:ASN:OD1	2.31	0.49
1:D:23:ILE:CG1	1:D:23:ILE:O	2.61	0.49
1:I:174:GLN:O	1:I:259:ILE:HG22	2.13	0.49
1:I:201:VAL:HG22	1:I:250:LEU:HB2	1.95	0.49
1:A:107:HIS:ND1	1:A:107:HIS:C	2.65	0.49
1:B:162:VAL:HG12	1:B:164:LYS:HG3	1.94	0.49
1:C:167:TYR:CE2	1:C:169:ASN:HA	2.48	0.49
1:D:14:ASN:OD1	1:D:16:SER:HB2	2.11	0.49
1:D:42:ASN:CB	1:D:44:LYS:H	2.25	0.49
1:D:486:TYR:CG	1:D:487:ASP:N	2.79	0.49
1:F:189:GLU:OE2	2:J:2:SIA:C9	2.59	0.49
1:H:10:GLY:O	1:H:346:MET:HE1	2.12	0.49
1:C:143:ASN:HD21	1:G:19:LYS:CE	2.23	0.49
1:F:128:GLN:HB3	1:F:161:PRO:HG2	1.93	0.49
1:G:295:HIS:CE1	1:G:308:TYR:HB2	2.48	0.49
1:B:317:ALA:O	1:B:436:THR:HG21	2.12	0.49
1:D:204:GLY:HA2	1:D:208:LEU:O	2.13	0.49
1:E:9:VAL:HG11	1:E:448:TYR:CB	2.34	0.49
1:G:187:GLU:O	1:G:190:GLN:HB3	2.12	0.49
1:G:288:ILE:HD11	1:G:297:ILE:HD12	1.95	0.49
1:I:167:TYR:CE2	1:I:169:ASN:HA	2.47	0.49
1:B:128:GLN:HB3	1:B:161:PRO:HG2	1.94	0.49
1:B:432:GLU:H	1:B:435:MET:HG3	1.77	0.49
1:D:80:TRP:CZ2	1:D:112:VAL:CG2	2.96	0.49
1:E:167:TYR:CE2	1:E:169:ASN:HA	2.47	0.49
1:E:179:TRP:CE2	1:E:203:VAL:HG21	2.48	0.49
1:E:471:HIS:HB2	1:E:494:GLU:HG2	1.91	0.49
1:F:32:HIS:CE1	1:F:350:TRP:HE1	2.31	0.49
1:F:48:LEU:O	1:F:49:ASN:HB2	2.12	0.49
1:H:55:GLU:HG3	1:H:274:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:PRO:HG2	1:H:298:HIS:CE1	2.47	0.49
1:I:179:TRP:CE2	1:I:203:VAL:HG21	2.48	0.49
1:I:295:HIS:CE1	1:I:308:TYR:HB2	2.48	0.49
1:A:135:SER:N	1:A:144:PRO:HB3	2.28	0.48
1:B:293:PRO:HG3	1:B:385:ILE:HG12	1.93	0.48
1:E:7:ILE:HG23	1:E:467:PHE:HD2	1.78	0.48
1:E:295:HIS:HD2	1:E:297:ILE:N	2.06	0.48
1:F:42:ASN:OD1	1:F:44:LYS:HE2	2.13	0.48
1:G:205:THR:C	1:H:220:PRO:HD2	2.34	0.48
1:G:428:LEU:O	1:G:431:MET:O	2.31	0.48
1:H:410:ASN:HB2	1:I:409:LEU:HD11	1.95	0.48
1:I:169:ASN:ND2	1:I:238:ILE:HA	2.23	0.48
1:B:335:ILE:HG13	1:B:441:ASP:HA	1.95	0.48
1:D:462:LEU:HD11	1:D:468:GLU:CB	2.38	0.48
1:E:486:TYR:CG	1:E:487:ASP:N	2.79	0.48
1:H:53:PRO:CD	1:H:274:LEU:HD13	2.43	0.48
1:A:369:SER:H	1:A:371:GLN:H	1.61	0.48
1:A:460:LYS:HE2	1:A:468:GLU:HG2	1.95	0.48
1:B:167:TYR:CE2	1:B:169:ASN:HA	2.48	0.48
1:B:462:LEU:HD11	1:B:468:GLU:CB	2.39	0.48
1:D:12:HIS:CE1	1:D:347:VAL:HA	2.48	0.48
1:E:140:VAL:HG12	1:E:141:PHE:N	2.28	0.48
1:F:45:LEU:CD2	1:F:270:THR:HG21	2.43	0.48
1:F:133:GLY:HA3	2:J:2:SIA:C11	2.41	0.48
1:F:490:LYS:HE3	1:F:491:TYR:CE2	2.48	0.48
1:H:184:PRO:O	1:H:216:ILE:HG23	2.13	0.48
1:H:187:GLU:O	1:H:190:GLN:HB3	2.13	0.48
1:A:140:VAL:HG12	1:A:141:PHE:H	1.78	0.48
1:B:184:PRO:O	1:B:216:ILE:HG23	2.14	0.48
1:E:128:GLN:HB3	1:E:161:PRO:HG2	1.94	0.48
1:E:316:LEU:HD11	1:E:384:VAL:HG11	1.95	0.48
1:E:399:PHE:CE1	1:E:406:LEU:HG	2.49	0.48
1:H:31:THR:C	1:H:32:HIS:CG	2.86	0.48
1:H:294:PHE:HB3	1:H:309:VAL:CG2	2.43	0.48
1:A:17:THR:O	1:A:18:GLU:C	2.50	0.48
1:A:262:ARG:HG3	1:A:262:ARG:NH1	2.19	0.48
1:B:294:PHE:HB3	1:B:309:VAL:CG2	2.43	0.48
1:D:23:ILE:O	1:F:379:ASN:C	2.52	0.48
1:D:87:GLU:OE1	1:D:269:LYS:HD2	2.14	0.48
1:D:168:ASN:O	1:D:170:THR:HG22	2.13	0.48
1:E:9:VAL:CG2	1:E:448:TYR:CD1	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LYS:HB2	1:E:418:LEU:HD21	1.95	0.48
1:F:42:ASN:HB3	1:F:287:ALA:H	1.79	0.48
1:G:278:GLU:HG3	1:G:279:THR:H	1.79	0.48
1:G:355:HIS:CD2	1:G:361:SER:HB3	2.48	0.48
1:G:455:LEU:HD23	1:G:459:VAL:HG21	1.95	0.48
1:I:294:PHE:HB3	1:I:309:VAL:CG2	2.43	0.48
1:I:488:TYR:O	1:I:492:GLU:HB2	2.13	0.48
1:A:206:SER:HG	1:A:240:ASP:CG	2.17	0.48
1:B:19:LYS:HE2	1:B:29:THR:OG1	2.14	0.48
1:C:338:PHE:CE1	1:C:339:ILE:CG1	2.97	0.48
1:C:486:TYR:CG	1:C:487:ASP:N	2.79	0.48
1:D:108:LEU:HD12	1:D:108:LEU:O	2.14	0.48
1:D:494:GLU:O	1:D:494:GLU:HG3	2.12	0.48
1:E:114:HIS:O	1:E:259:ILE:O	2.32	0.48
1:F:53:PRO:HG3	1:F:82:TYR:CZ	2.49	0.48
1:I:66:LEU:O	1:I:147:PHE:HB3	2.13	0.48
1:I:278:GLU:O	1:I:279:THR:HB	2.13	0.48
1:B:42:ASN:HB3	1:B:287:ALA:H	1.79	0.48
1:C:293:PRO:HG3	1:C:385:ILE:HG23	1.95	0.48
1:E:42:ASN:OD1	1:E:44:LYS:HE2	2.13	0.48
1:H:45:LEU:H	1:H:45:LEU:HD12	1.79	0.48
1:H:48:LEU:O	1:H:49:ASN:HB2	2.14	0.48
1:H:306:PRO:O	1:H:308:TYR:N	2.47	0.48
1:C:488:TYR:O	1:C:492:GLU:HB2	2.13	0.48
1:D:83:ILE:HD12	1:D:110:SER:HA	1.96	0.48
1:D:183:HIS:ND1	1:F:209:ASN:ND2	2.59	0.48
1:D:294:PHE:O	1:D:295:HIS:HB3	2.13	0.48
1:H:77:VAL:HG22	1:H:79:GLU:O	2.14	0.48
1:H:278:GLU:O	1:H:279:THR:HB	2.14	0.48
1:I:42:ASN:OD1	1:I:44:LYS:HE2	2.13	0.48
1:I:436:THR:O	1:I:439:PHE:HB3	2.13	0.48
1:B:278:GLU:CG	1:B:279:THR:N	2.74	0.48
1:D:119:LYS:HA	1:D:255:TYR:CD1	2.48	0.48
1:D:294:PHE:CZ	1:D:425:ALA:HB2	2.49	0.48
1:D:490:LYS:HE3	1:D:491:TYR:CE2	2.48	0.48
1:G:38:GLU:OE2	1:G:40:THR:HG22	2.14	0.48
1:G:200:TYR:CE1	1:G:211:ARG:NH2	2.82	0.48
1:G:332:PHE:CZ	1:H:331:LEU:HD12	2.49	0.48
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.17	0.48
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.48	0.48
1:D:36:ILE:C	1:D:292:LEU:HD13	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLU:OE2	1:E:405:ARG:HB2	2.14	0.48
1:D:242:ILE:HG12	1:D:243:ASN:N	2.29	0.48
1:F:200:TYR:CE1	1:F:211:ARG:NH2	2.82	0.48
1:H:162:VAL:HG12	1:H:164:LYS:HG3	1.95	0.48
1:H:166:SER:HB2	1:H:243:ASN:ND2	2.29	0.48
1:A:61:ILE:O	1:A:65:LEU:HD12	2.14	0.47
1:A:124:ASP:OD2	1:A:125:ARG:HG3	2.14	0.47
1:B:490:LYS:HE3	1:B:491:TYR:CE2	2.49	0.47
1:C:200:TYR:CE1	1:C:247:THR:HG23	2.49	0.47
1:G:268:MET:HE3	1:G:302:ILE:HD12	1.95	0.47
1:H:179:TRP:CE2	1:H:203:VAL:HG21	2.49	0.47
1:H:200:TYR:CE1	1:H:211:ARG:NH2	2.82	0.47
1:A:36:ILE:HD11	1:A:429:VAL:CG2	2.44	0.47
1:A:375:ASP:OD1	1:A:375:ASP:N	2.35	0.47
1:A:417:PHE:CE1	1:C:417:PHE:CE1	3.02	0.47
1:B:399:PHE:CE1	1:B:406:LEU:HG	2.49	0.47
1:F:432:GLU:H	1:F:435:MET:HG3	1.78	0.47
1:G:417:PHE:CE1	1:H:416:GLY:C	2.87	0.47
1:G:490:LYS:O	1:G:493:GLU:HB2	2.15	0.47
1:H:200:TYR:CE1	1:H:247:THR:HG23	2.49	0.47
1:I:162:VAL:HG12	1:I:164:LYS:HG3	1.95	0.47
1:I:166:SER:HB2	1:I:243:ASN:ND2	2.29	0.47
1:A:378:THR:O	1:A:381:VAL:HB	2.15	0.47
1:E:490:LYS:C	1:E:492:GLU:H	2.17	0.47
1:F:277:CYS:HB2	1:F:278:GLU:H	1.59	0.47
1:H:120:ILE:O	1:H:121:LEU:HD23	2.15	0.47
1:I:55:GLU:HG3	1:I:274:LEU:HD22	1.96	0.47
1:I:114:HIS:O	1:I:259:ILE:O	2.32	0.47
1:A:171:SER:HB2	1:A:258:LYS:HE3	1.97	0.47
1:B:11:TYR:CZ	1:B:335:ILE:HA	2.50	0.47
1:D:186:ASP:HA	1:D:216:ILE:CG2	2.42	0.47
1:D:325:GLN:HG3	1:D:341:GLY:HA3	1.95	0.47
1:D:400:SER:OG	1:D:403:GLU:HG3	2.14	0.47
1:E:73:ARG:CA	1:G:44:LYS:NZ	2.78	0.47
1:E:293:PRO:CG	1:E:385:ILE:HG12	2.44	0.47
1:F:400:SER:OG	1:F:403:GLU:HG3	2.15	0.47
1:G:174:GLN:O	1:G:259:ILE:HG22	2.13	0.47
1:H:332:PHE:CD2	1:H:442:SER:HB2	2.48	0.47
1:B:130:THR:HB	1:B:154:THR:OG1	2.13	0.47
1:C:143:ASN:HD21	1:G:19:LYS:HE3	1.79	0.47
1:C:169:ASN:ND2	1:C:238:ILE:HA	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:HG3	1:C:279:THR:H	1.77	0.47
1:D:266:GLY:HA3	1:D:394:ALA:HB1	1.95	0.47
1:F:53:PRO:CD	1:F:274:LEU:HD13	2.45	0.47
1:H:306:PRO:O	1:H:307:LYS:C	2.51	0.47
1:I:404:LYS:HA	1:I:404:LYS:HD2	1.63	0.47
1:C:11:TYR:CD2	1:C:335:ILE:HG12	2.49	0.47
1:E:66:LEU:O	1:E:147:PHE:HB3	2.15	0.47
1:E:278:GLU:O	1:E:279:THR:HB	2.15	0.47
1:E:294:PHE:HB3	1:E:309:VAL:CG2	2.45	0.47
1:A:178:ILE:HG12	1:A:233:TRP:HB3	1.96	0.47
1:A:458:ASN:OD1	1:A:488:TYR:CE1	2.68	0.47
1:A:460:LYS:HG3	1:A:468:GLU:HG2	1.95	0.47
1:C:80:TRP:CE2	1:C:112:VAL:HG22	2.49	0.47
1:C:129:HIS:CD2	1:C:161:PRO:HD2	2.50	0.47
1:D:20:VAL:HG13	1:D:30:VAL:CG2	2.43	0.47
1:D:34:GLN:CG	1:D:35:ASP:N	2.78	0.47
1:D:163:ALA:O	1:D:245:GLU:HA	2.15	0.47
1:D:219:ARG:NH2	1:F:209:ASN:OD1	2.44	0.47
1:E:187:GLU:O	1:E:190:GLN:HB3	2.15	0.47
1:E:201:VAL:HG22	1:E:250:LEU:HB2	1.96	0.47
1:E:211:ARG:NH1	1:F:216:ILE:HB	2.29	0.47
1:E:324:PRO:O	1:E:325:GLN:HB2	2.15	0.47
1:F:66:LEU:O	1:F:147:PHE:HB3	2.14	0.47
1:F:310:LYS:HD2	1:F:418:LEU:CD2	2.44	0.47
1:G:240:ASP:OD1	1:H:220:PRO:HG2	2.15	0.47
1:G:462:LEU:CD1	1:G:462:LEU:H	2.27	0.47
1:H:42:ASN:OD1	1:H:44:LYS:HE2	2.15	0.47
1:H:201:VAL:HG22	1:H:250:LEU:HB2	1.96	0.47
1:I:295:HIS:HD2	1:I:297:ILE:N	2.05	0.47
1:I:490:LYS:C	1:I:492:GLU:H	2.17	0.47
1:A:248:GLY:O	1:A:249:ASN:HB2	2.14	0.47
1:B:277:CYS:HB2	1:B:278:GLU:H	1.60	0.47
1:B:307:LYS:HE2	1:B:421:TRP:CE2	2.50	0.47
1:D:436:THR:O	1:D:439:PHE:HB3	2.14	0.47
1:E:379:ASN:HB3	1:F:23:ILE:O	2.14	0.47
1:G:42:ASN:HB2	1:G:287:ALA:O	2.15	0.47
1:G:471:HIS:CE1	1:G:491:TYR:CD1	3.03	0.47
1:A:38:GLU:OE2	1:A:39:LYS:N	2.44	0.47
1:A:81:SER:HB2	1:A:82:TYR:CD2	2.50	0.47
1:A:117:LYS:HE3	1:A:255:TYR:CG	2.50	0.47
1:E:73:ARG:CD	1:G:276:ASN:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:ILE:HB	1:G:478:MET:SD	2.54	0.47
1:H:23:ILE:CG2	1:H:434:GLU:HG2	2.34	0.47
1:H:42:ASN:HB2	1:H:287:ALA:O	2.14	0.47
1:H:268:MET:HE3	1:H:302:ILE:HD12	1.95	0.47
1:H:288:ILE:CD1	1:H:297:ILE:HD12	2.44	0.47
1:H:417:PHE:CZ	1:I:416:GLY:HA3	2.49	0.47
1:A:95:TYR:HD2	1:A:229:MET:HG3	1.79	0.47
1:A:138:CYS:O	1:A:145:SER:HB3	2.15	0.47
1:A:455:LEU:HB3	1:A:459:VAL:HG21	1.97	0.47
1:B:120:ILE:O	1:B:121:LEU:HD23	2.15	0.47
1:B:178:ILE:O	1:B:253:PRO:HG3	2.15	0.47
1:D:155:LYS:HE2	1:D:192:THR:O	2.14	0.47
1:F:294:PHE:HB3	1:F:309:VAL:CG2	2.45	0.47
1:I:288:ILE:HD11	1:I:297:ILE:HD12	1.97	0.47
1:A:77:VAL:HG23	1:A:78:PRO:HD2	1.97	0.46
1:A:404:LYS:HA	1:A:404:LYS:HD3	1.54	0.46
1:B:166:SER:HB2	1:B:243:ASN:ND2	2.30	0.46
1:H:31:THR:O	1:H:32:HIS:CD2	2.69	0.46
1:H:462:LEU:HD11	1:H:468:GLU:CB	2.39	0.46
1:I:142:ASP:OD2	1:I:142:ASP:N	2.48	0.46
1:A:154:THR:O	1:A:193:LEU:O	2.34	0.46
1:A:168:ASN:CB	1:A:241:THR:HG22	2.45	0.46
1:A:459:VAL:HG12	1:A:469:PHE:CA	2.23	0.46
1:B:80:TRP:CE2	1:B:112:VAL:HG22	2.50	0.46
1:C:138:CYS:O	1:C:145:SER:HB3	2.14	0.46
1:D:185:ASN:O	1:D:186:ASP:HB3	2.15	0.46
1:D:248:GLY:C	1:D:249:ASN:HD22	2.18	0.46
1:E:9:VAL:O	1:E:339:ILE:CD1	2.50	0.46
1:E:200:TYR:CE1	1:E:211:ARG:NH2	2.82	0.46
1:H:169:ASN:ND2	1:H:238:ILE:HA	2.22	0.46
1:I:138:CYS:O	1:I:145:SER:HB3	2.14	0.46
1:A:12:HIS:CD2	1:A:13:SER:C	2.89	0.46
1:A:95:TYR:CD2	1:A:229:MET:HG3	2.50	0.46
1:B:42:ASN:OD1	1:B:44:LYS:HE2	2.16	0.46
1:B:382:ASN:O	1:B:386:GLU:N	2.47	0.46
1:D:193:LEU:HB2	1:D:194:TYR:CE2	2.50	0.46
1:E:462:LEU:HD11	1:E:468:GLU:CB	2.39	0.46
1:G:48:LEU:O	1:G:49:ASN:HB2	2.14	0.46
1:G:200:TYR:CE1	1:G:247:THR:HG23	2.51	0.46
1:G:448:TYR:OH	1:G:461:GLU:HG3	2.15	0.46
1:H:410:ASN:HB2	1:I:409:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:ILE:HA	1:I:355:HIS:HA	1.96	0.46
1:I:338:PHE:CE1	1:I:339:ILE:HG13	2.50	0.46
1:A:154:THR:O	1:A:155:LYS:CB	2.60	0.46
1:B:12:HIS:N	1:B:350:TRP:O	2.32	0.46
1:B:268:MET:HE3	1:B:302:ILE:HD12	1.98	0.46
1:B:310:LYS:HD2	1:B:418:LEU:CD2	2.45	0.46
1:B:323:VAL:HA	1:B:324:PRO:HD3	1.62	0.46
1:E:7:ILE:HG22	1:E:467:PHE:CG	2.51	0.46
1:E:456:ARG:CD	1:F:461:GLU:O	2.64	0.46
1:F:166:SER:HB2	1:F:243:ASN:ND2	2.29	0.46
1:G:357:ASN:OD1	1:G:475:ASP:OD1	2.33	0.46
1:A:117:LYS:HG3	1:A:257:PHE:CD1	2.51	0.46
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.67	0.46
1:A:428:LEU:C	1:A:428:LEU:HD23	2.35	0.46
1:B:187:GLU:O	1:B:190:GLN:HB3	2.15	0.46
1:D:155:LYS:HD3	1:D:195:GLN:HB2	1.98	0.46
1:F:278:GLU:O	1:F:279:THR:HB	2.15	0.46
1:F:490:LYS:C	1:F:492:GLU:H	2.19	0.46
1:G:383:SER:HB3	1:H:26:ARG:NH2	2.30	0.46
1:I:332:PHE:CD2	1:I:442:SER:HB2	2.50	0.46
1:A:94:CYS:HB3	1:A:137:GLY:O	2.15	0.46
1:B:12:HIS:CB	1:B:350:TRP:HA	2.46	0.46
1:C:141:PHE:N	1:C:142:ASP:CA	2.73	0.46
1:C:436:THR:O	1:C:439:PHE:HB3	2.15	0.46
1:D:118:VAL:CG2	1:D:120:ILE:HG23	2.46	0.46
1:D:183:HIS:HB3	1:D:219:ARG:NH2	2.30	0.46
1:E:53:PRO:HG3	1:E:82:TYR:CZ	2.51	0.46
1:G:488:TYR:O	1:G:490:LYS:N	2.49	0.46
1:H:36:ILE:O	1:H:292:LEU:HB3	2.16	0.46
1:A:61:ILE:CG2	1:A:109:ILE:HD11	2.45	0.46
1:A:182:HIS:HD2	1:A:194:TYR:HE2	1.63	0.46
1:B:338:PHE:CE1	1:B:339:ILE:CG1	2.98	0.46
1:C:295:HIS:HD2	1:C:297:ILE:N	2.07	0.46
1:D:399:PHE:CE1	1:D:406:LEU:HG	2.51	0.46
1:F:442:SER:O	1:F:446:ASN:HB2	2.16	0.46
1:G:201:VAL:HG22	1:G:250:LEU:HB2	1.97	0.46
1:H:12:HIS:CE1	1:H:13:SER:O	2.68	0.46
1:I:42:ASN:HB2	1:I:287:ALA:O	2.15	0.46
1:I:53:PRO:CD	1:I:274:LEU:HD13	2.45	0.46
1:C:77:VAL:HG22	1:C:79:GLU:O	2.16	0.46
1:C:490:LYS:C	1:C:492:GLU:H	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:TYR:HE2	1:D:335:ILE:HA	1.80	0.46
1:D:58:ASP:HB3	1:D:90:ARG:HB2	1.97	0.46
1:E:338:PHE:CE1	1:E:339:ILE:CG1	2.99	0.46
1:F:167:TYR:CE2	1:F:169:ASN:HA	2.50	0.46
1:G:310:LYS:HD3	1:I:389:ASN:OD1	2.15	0.46
1:I:200:TYR:CE1	1:I:247:THR:HG23	2.50	0.46
1:I:324:PRO:HB2	1:I:325:GLN:H	1.53	0.46
1:A:61:ILE:HD11	1:A:83:ILE:HD13	1.98	0.46
1:A:93:LEU:HD12	1:A:93:LEU:N	2.31	0.46
1:B:129:HIS:NE2	1:B:161:PRO:HD2	2.31	0.46
1:B:278:GLU:O	1:B:279:THR:HB	2.16	0.46
1:B:387:LYS:CD	1:C:426:GLU:HG2	2.34	0.46
1:C:38:GLU:OE2	1:C:40:THR:HG22	2.16	0.46
1:C:201:VAL:HG22	1:C:250:LEU:HB2	1.96	0.46
1:C:333:GLY:O	1:C:337:GLY:HA3	2.16	0.46
1:D:7:ILE:O	1:D:466:CYS:HA	2.16	0.46
1:D:51:ILE:HG23	1:D:52:PRO:HD2	1.97	0.46
1:D:54:LEU:HD21	1:D:64:TRP:CZ3	2.51	0.46
1:D:293:PRO:HG3	1:D:385:ILE:CA	2.25	0.46
1:E:288:ILE:HD11	1:E:297:ILE:HD12	1.97	0.46
1:G:399:PHE:HB2	1:G:407:GLU:HG2	1.98	0.46
1:H:140:VAL:HG12	1:H:141:PHE:N	2.30	0.46
1:H:400:SER:OG	1:H:403:GLU:HG3	2.16	0.46
1:I:38:GLU:OE2	1:I:40:THR:HG22	2.16	0.46
1:B:306:PRO:O	1:B:308:TYR:N	2.49	0.46
1:E:211:ARG:NH1	1:F:216:ILE:O	2.45	0.46
1:F:278:GLU:CG	1:F:279:THR:N	2.79	0.46
1:G:346:MET:HA	1:G:346:MET:HE3	1.98	0.46
1:H:10:GLY:HA3	1:H:343:TRP:CZ2	2.52	0.46
1:H:490:LYS:C	1:H:492:GLU:H	2.19	0.46
1:I:23:ILE:H	1:I:434:GLU:HB2	1.81	0.46
1:I:200:TYR:CE1	1:I:211:ARG:NH2	2.84	0.46
1:A:61:ILE:HG21	1:A:109:ILE:HD11	1.97	0.45
1:A:229:MET:SD	1:A:251:ILE:HG13	2.56	0.45
1:A:371:GLN:CA	1:A:371:GLN:HE21	2.29	0.45
1:C:53:PRO:HG3	1:C:82:TYR:CZ	2.51	0.45
1:C:278:GLU:O	1:C:279:THR:HB	2.15	0.45
1:C:404:LYS:HA	1:C:404:LYS:HD2	1.65	0.45
1:D:53:PRO:HG2	1:D:84:MET:SD	2.57	0.45
1:D:490:LYS:C	1:D:492:GLU:H	2.19	0.45
1:E:200:TYR:CE1	1:E:247:THR:HG23	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:TYR:CZ	1:F:335:ILE:HG23	2.51	0.45
1:F:36:ILE:O	1:F:292:LEU:HB3	2.16	0.45
1:F:38:GLU:OE2	1:F:40:THR:HG22	2.17	0.45
1:G:138:CYS:O	1:G:145:SER:HB3	2.16	0.45
1:G:480:SER:HA	1:G:483:ASN:HB2	1.97	0.45
1:H:460:LYS:CG	1:H:468:GLU:HB3	2.46	0.45
1:I:36:ILE:O	1:I:292:LEU:HB3	2.16	0.45
1:I:48:LEU:O	1:I:49:ASN:HB2	2.15	0.45
1:A:36:ILE:HG13	1:A:314:LEU:HB3	1.98	0.45
1:B:105:LEU:O	1:B:109:ILE:HG12	2.16	0.45
1:B:288:ILE:HD11	1:B:297:ILE:HD12	1.97	0.45
1:C:174:GLN:O	1:C:259:ILE:HG22	2.17	0.45
1:C:184:PRO:O	1:C:216:ILE:HG23	2.16	0.45
1:D:37:LEU:CB	1:D:314:LEU:HB2	2.46	0.45
1:D:181:VAL:O	1:D:181:VAL:HG12	2.16	0.45
1:A:477:CYS:O	1:A:481:VAL:HG23	2.16	0.45
1:C:278:GLU:CG	1:C:279:THR:N	2.78	0.45
1:D:288:ILE:HG22	1:D:290:THR:HG22	1.98	0.45
1:G:140:VAL:HG12	1:G:141:PHE:N	2.30	0.45
1:G:288:ILE:HG12	1:G:297:ILE:HD12	1.98	0.45
1:H:45:LEU:CD2	1:H:270:THR:HG21	2.46	0.45
1:A:353:TYR:CD2	1:A:482:LYS:HE3	2.52	0.45
1:A:380:LYS:HE3	1:A:380:LYS:HB2	1.55	0.45
1:A:397:LYS:NZ	1:B:408:ASN:HD22	2.15	0.45
1:B:496:LYS:N	1:B:496:LYS:HE3	2.32	0.45
1:D:216:ILE:O	1:F:211:ARG:HD2	2.17	0.45
1:E:53:PRO:CD	1:E:274:LEU:HD13	2.46	0.45
1:F:486:TYR:CG	1:F:487:ASP:N	2.80	0.45
1:G:366:ASP:O	1:G:368:GLU:N	2.49	0.45
1:G:459:VAL:HG12	1:G:468:GLU:O	2.17	0.45
1:H:295:HIS:CE1	1:H:308:TYR:HB2	2.51	0.45
1:I:10:GLY:HA3	1:I:343:TRP:CZ2	2.52	0.45
1:I:460:LYS:CG	1:I:468:GLU:HB3	2.46	0.45
1:A:173:GLU:CD	1:A:260:SER:HB2	2.37	0.45
1:B:31:THR:C	1:B:32:HIS:CG	2.89	0.45
1:C:45:LEU:CD2	1:C:270:THR:HG21	2.46	0.45
1:C:306:PRO:O	1:C:308:TYR:N	2.49	0.45
1:D:293:PRO:HB2	1:D:294:PHE:CE2	2.52	0.45
1:C:277:CYS:HB2	1:C:278:GLU:H	1.58	0.45
1:D:146:PHE:HE1	1:D:229:MET:HE3	1.80	0.45
1:G:77:VAL:HG22	1:G:79:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:408:ASN:O	1:G:412:LYS:HB2	2.16	0.45
1:G:430:LEU:O	1:G:433:ASN:HB2	2.16	0.45
1:H:38:GLU:OE2	1:H:40:THR:HG22	2.17	0.45
1:I:77:VAL:HG22	1:I:79:GLU:O	2.16	0.45
1:I:140:VAL:HG12	1:I:141:PHE:N	2.32	0.45
1:I:277:CYS:HB2	1:I:278:GLU:H	1.60	0.45
1:A:345:GLY:HA3	1:A:363:TYR:CE2	2.52	0.45
1:B:45:LEU:CD2	1:B:270:THR:HG21	2.47	0.45
1:C:51:ILE:HB	1:C:81:SER:HB3	1.98	0.45
1:C:332:PHE:CD2	1:C:442:SER:HB2	2.51	0.45
1:D:23:ILE:HD11	1:F:380:LYS:CG	2.47	0.45
1:D:190:GLN:HE21	1:D:197:VAL:HA	1.82	0.45
1:E:12:HIS:CE1	1:E:13:SER:O	2.70	0.45
1:F:140:VAL:HG12	1:F:141:PHE:N	2.32	0.45
1:G:45:LEU:HD12	1:G:45:LEU:N	2.32	0.45
1:G:53:PRO:HG3	1:G:82:TYR:CZ	2.52	0.45
1:G:464:ASN:OD1	1:G:466:CYS:HB2	2.17	0.45
1:H:31:THR:O	1:H:32:HIS:CG	2.70	0.45
1:H:58:ASP:HA	1:H:86:LYS:HD3	1.98	0.45
1:H:130:THR:HB	1:H:154:THR:OG1	2.16	0.45
1:H:277:CYS:HB2	1:H:278:GLU:H	1.58	0.45
1:A:11:TYR:HA	1:A:351:TYR:HA	1.98	0.45
1:A:13:SER:CB	1:A:344:GLN:NE2	2.79	0.45
1:A:283:THR:HG22	1:A:284:PRO:N	2.32	0.45
1:B:319:GLY:C	1:B:440:HIS:NE2	2.70	0.45
1:B:451:VAL:HG12	1:B:452:ARG:N	2.32	0.45
1:D:47:LYS:O	1:D:279:THR:HG22	2.17	0.45
1:D:361:SER:HA	1:D:362:GLY:HA3	1.73	0.45
1:E:332:PHE:CD2	1:E:442:SER:HB2	2.52	0.45
1:E:460:LYS:CG	1:E:468:GLU:HB3	2.47	0.45
1:F:80:TRP:CE2	1:F:112:VAL:HG22	2.52	0.45
1:A:31:THR:HG23	1:A:320:LEU:O	2.17	0.45
1:B:129:HIS:CD2	1:B:161:PRO:HD2	2.52	0.45
1:C:142:ASP:OD2	1:C:142:ASP:N	2.50	0.45
1:E:278:GLU:CG	1:E:279:THR:H	2.29	0.45
1:E:452:ARG:HB2	1:E:467:PHE:HZ	1.81	0.45
1:F:460:LYS:CG	1:F:468:GLU:HB3	2.47	0.45
1:G:120:ILE:O	1:G:121:LEU:HD23	2.17	0.45
1:A:170:THR:HG22	1:A:239:TRP:CE3	2.52	0.45
1:B:278:GLU:CG	1:B:279:THR:H	2.29	0.45
1:B:320:LEU:HB3	1:B:440:HIS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:TYR:CE1	1:D:247:THR:HG23	2.52	0.45
1:E:442:SER:O	1:E:446:ASN:HB2	2.17	0.45
1:G:455:LEU:O	1:G:456:ARG:CB	2.65	0.45
1:H:166:SER:HB3	1:H:243:ASN:HD22	1.82	0.45
1:A:195:GLN:O	1:A:196:ASN:CB	2.64	0.44
1:B:77:VAL:HG22	1:B:79:GLU:O	2.16	0.44
1:B:138:CYS:O	1:B:145:SER:HB3	2.17	0.44
1:C:53:PRO:CD	1:C:274:LEU:HD13	2.46	0.44
1:C:200:TYR:CE1	1:C:211:ARG:NH2	2.85	0.44
1:D:26:ARG:HG2	1:F:379:ASN:HD21	1.81	0.44
1:D:77:VAL:HA	1:D:78:PRO:HD3	1.81	0.44
1:G:414:GLU:OE2	1:H:412:LYS:NZ	2.49	0.44
1:H:452:ARG:HB2	1:H:467:PHE:HZ	1.82	0.44
1:B:179:TRP:CH2	1:B:208:LEU:HD21	2.52	0.44
1:C:268:MET:HE3	1:C:302:ILE:HD12	1.99	0.44
1:C:288:ILE:HD11	1:C:297:ILE:HD12	2.00	0.44
1:D:172:GLY:HA2	1:D:239:TRP:CH2	2.52	0.44
1:D:238:ILE:HG23	1:D:239:TRP:CG	2.52	0.44
1:D:248:GLY:O	1:D:249:ASN:CB	2.65	0.44
1:F:436:THR:O	1:F:439:PHE:HB3	2.16	0.44
1:G:455:LEU:CB	1:G:459:VAL:HG21	2.47	0.44
1:I:45:LEU:CD2	1:I:270:THR:HG21	2.47	0.44
1:I:129:HIS:CD2	1:I:161:PRO:HD2	2.52	0.44
1:A:126:TRP:CZ3	1:A:153:LEU:HD11	2.52	0.44
1:A:469:PHE:CE1	1:A:471:HIS:CE1	3.05	0.44
1:D:239:TRP:N	1:D:239:TRP:CE3	2.77	0.44
1:F:493:GLU:O	1:F:494:GLU:HB2	2.17	0.44
1:G:355:HIS:O	1:G:361:SER:HB2	2.18	0.44
1:H:278:GLU:CG	1:H:279:THR:N	2.80	0.44
1:A:67:GLY:O	1:A:148:ARG:HG2	2.18	0.44
1:A:343:TRP:CH2	1:A:354:HIS:HB2	2.52	0.44
1:A:436:THR:O	1:A:436:THR:HG22	2.17	0.44
1:B:38:GLU:OE2	1:B:40:THR:HG22	2.17	0.44
1:C:310:LYS:HD2	1:C:418:LEU:CD2	2.47	0.44
1:E:250:LEU:HD21	1:E:252:ALA:HB2	1.99	0.44
1:F:404:LYS:HA	1:F:404:LYS:HD2	1.60	0.44
1:G:202:SER:HB2	1:H:216:ILE:O	2.17	0.44
1:A:23:ILE:HD11	1:C:380:LYS:HE2	1.99	0.44
1:A:418:LEU:HD12	1:A:418:LEU:HA	1.63	0.44
1:B:360:GLY:O	1:B:361:SER:HB2	2.18	0.44
1:B:460:LYS:CG	1:B:468:GLU:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ILE:HG12	1:C:297:ILE:HD12	2.00	0.44
1:D:8:CYS:O	1:D:343:TRP:HH2	2.01	0.44
1:D:9:VAL:O	1:D:339:ILE:HD13	2.17	0.44
1:D:332:PHE:CD2	1:D:442:SER:HB2	2.53	0.44
1:G:462:LEU:HD12	1:G:462:LEU:N	2.32	0.44
1:A:219:ARG:CG	1:A:226:GLY:O	2.66	0.44
1:A:487:ASP:O	1:A:491:TYR:HD2	2.00	0.44
1:B:140:VAL:HG12	1:B:141:PHE:N	2.31	0.44
1:B:200:TYR:CE1	1:B:211:ARG:NH2	2.86	0.44
1:D:48:LEU:HD23	1:D:392:PHE:HE1	1.83	0.44
1:E:129:HIS:NE2	1:E:161:PRO:HD2	2.32	0.44
1:E:298:HIS:HE1	1:E:300:LEU:HD12	1.83	0.44
1:F:332:PHE:CD2	1:F:442:SER:HB2	2.52	0.44
1:G:417:PHE:CZ	1:H:416:GLY:HA3	2.52	0.44
1:I:460:LYS:HG2	1:I:468:GLU:HB3	2.00	0.44
1:A:460:LYS:HG3	1:A:468:GLU:HB3	1.99	0.44
1:B:388:MET:HE2	1:C:423:TYR:CE1	2.53	0.44
1:C:140:VAL:HG12	1:C:141:PHE:N	2.32	0.44
1:D:61:ILE:HG13	1:D:85:GLU:OE2	2.18	0.44
1:D:495:SER:O	1:D:496:LYS:C	2.56	0.44
1:E:376:GLY:O	1:F:24:LEU:HD23	2.17	0.44
1:E:452:ARG:HB2	1:E:467:PHE:CZ	2.53	0.44
1:H:288:ILE:HG12	1:H:297:ILE:HD12	2.00	0.44
1:H:332:PHE:HZ	1:I:331:LEU:HD12	1.80	0.44
1:A:280:LYS:HD2	1:A:280:LYS:N	2.33	0.44
1:A:351:TYR:CE2	1:A:370:THR:HA	2.50	0.44
1:B:7:ILE:N	1:B:467:PHE:O	2.51	0.44
1:B:53:PRO:CD	1:B:274:LEU:HD13	2.48	0.44
1:C:360:GLY:O	1:C:361:SER:HB2	2.18	0.44
1:D:409:LEU:HD11	1:F:410:ASN:HB2	2.00	0.44
1:D:410:ASN:HB2	1:E:409:LEU:HD11	2.00	0.44
1:E:306:PRO:O	1:E:308:TYR:N	2.50	0.44
1:E:404:LYS:HD2	1:E:404:LYS:HA	1.69	0.44
1:H:8:CYS:C	1:H:343:TRP:HH2	2.18	0.44
1:I:80:TRP:CE2	1:I:112:VAL:HG22	2.53	0.44
1:A:160:TYR:HE2	1:A:248:GLY:N	2.15	0.44
1:A:283:THR:HB	1:A:286:GLY:H	1.82	0.44
1:A:455:LEU:HD23	1:A:459:VAL:HG21	2.00	0.44
1:C:399:PHE:CE1	1:C:406:LEU:HG	2.53	0.44
1:E:31:THR:C	1:E:32:HIS:CG	2.91	0.44
1:E:80:TRP:CE2	1:E:112:VAL:HG22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:VAL:HG23	1:E:145:SER:CB	2.48	0.44
1:H:452:ARG:HB2	1:H:467:PHE:CZ	2.53	0.44
1:A:134:GLY:O	1:A:135:SER:HB2	2.18	0.43
1:A:358:ASP:HB2	1:A:472:LYS:NZ	2.33	0.43
1:A:476:GLU:OE1	1:A:476:GLU:HA	2.18	0.43
1:B:9:VAL:HG11	1:B:448:TYR:CB	2.45	0.43
1:B:66:LEU:O	1:B:147:PHE:HB3	2.18	0.43
1:C:12:HIS:CE1	1:C:13:SER:O	2.71	0.43
1:C:66:LEU:O	1:C:147:PHE:HB3	2.17	0.43
1:C:113:THR:HA	1:C:114:HIS:HA	1.89	0.43
1:D:12:HIS:HB2	1:D:350:TRP:HA	1.99	0.43
1:D:338:PHE:CE1	1:D:339:ILE:CG1	3.00	0.43
1:F:494:GLU:O	1:F:494:GLU:HG2	2.17	0.43
1:G:114:HIS:O	1:G:259:ILE:O	2.36	0.43
1:G:354:HIS:ND1	1:G:354:HIS:O	2.51	0.43
1:H:113:THR:HA	1:H:114:HIS:HA	1.88	0.43
1:H:460:LYS:HG2	1:H:468:GLU:HB3	2.00	0.43
1:I:129:HIS:NE2	1:I:161:PRO:HD2	2.32	0.43
1:A:170:THR:HG22	1:A:239:TRP:HE3	1.83	0.43
1:A:380:LYS:HZ3	1:A:432:GLU:HB3	1.84	0.43
1:B:166:SER:HB3	1:B:243:ASN:HD22	1.83	0.43
1:B:355:HIS:CD2	1:B:355:HIS:N	2.86	0.43
1:B:452:ARG:HB2	1:B:467:PHE:HZ	1.83	0.43
1:F:11:TYR:CZ	1:F:335:ILE:HA	2.53	0.43
1:F:12:HIS:CE1	1:F:13:SER:O	2.71	0.43
1:F:298:HIS:HA	1:F:299:PRO:HD3	1.88	0.43
1:G:414:GLU:HG3	1:H:412:LYS:HE3	1.99	0.43
1:H:355:HIS:CD2	1:H:355:HIS:N	2.82	0.43
1:H:414:GLU:OE2	1:I:412:LYS:HE3	2.18	0.43
1:A:126:TRP:CG	1:A:153:LEU:HD21	2.53	0.43
1:D:146:PHE:CE1	1:D:229:MET:CE	3.01	0.43
1:D:452:ARG:HB2	1:D:467:PHE:HZ	1.83	0.43
1:F:31:THR:C	1:F:32:HIS:CG	2.92	0.43
1:F:42:ASN:HB2	1:F:287:ALA:O	2.18	0.43
1:G:471:HIS:ND1	1:G:472:LYS:O	2.39	0.43
1:H:45:LEU:HD12	1:H:45:LEU:N	2.32	0.43
1:I:422:THR:O	1:I:423:TYR:C	2.57	0.43
1:D:228:ARG:HH22	1:F:206:SER:HA	1.83	0.43
1:D:299:PRO:O	1:D:301:THR:HG23	2.18	0.43
1:D:460:LYS:CG	1:D:468:GLU:HB3	2.48	0.43
1:E:34:GLN:OE1	1:E:381:VAL:HG11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LYS:HD2	1:E:418:LEU:HD23	2.00	0.43
1:F:268:MET:HE3	1:F:302:ILE:HD12	1.99	0.43
1:G:471:HIS:NE2	1:G:486:TYR:OH	2.52	0.43
1:I:140:VAL:HG23	1:I:145:SER:CB	2.49	0.43
1:A:200:TYR:C	1:A:200:TYR:CD2	2.92	0.43
1:A:445:LYS:C	1:A:446:ASN:HD22	2.21	0.43
1:C:320:LEU:HB3	1:C:440:HIS:HB3	1.99	0.43
1:E:11:TYR:CE2	1:E:335:ILE:CA	2.76	0.43
1:F:129:HIS:CD2	1:F:161:PRO:HD2	2.53	0.43
1:F:319:GLY:C	1:F:440:HIS:NE2	2.72	0.43
1:G:36:ILE:O	1:G:292:LEU:HB3	2.17	0.43
1:I:53:PRO:HG3	1:I:82:TYR:CE2	2.53	0.43
1:A:7:ILE:HG21	1:A:451:VAL:HG11	2.01	0.43
1:A:35:ASP:OD1	1:A:314:LEU:O	2.36	0.43
1:A:38:GLU:HB3	1:A:294:PHE:O	2.18	0.43
1:A:283:THR:CG2	1:A:298:HIS:HB3	2.46	0.43
1:C:460:LYS:CG	1:C:468:GLU:HB3	2.48	0.43
1:D:379:ASN:HB2	1:E:24:LEU:HA	2.01	0.43
1:E:45:LEU:CD2	1:E:270:THR:HG21	2.48	0.43
1:G:380:LYS:O	1:G:384:VAL:HG23	2.19	0.43
1:H:294:PHE:HB3	1:H:309:VAL:HG22	1.99	0.43
1:I:278:GLU:O	1:I:279:THR:CB	2.67	0.43
1:A:156:LYS:HE2	1:A:156:LYS:HB3	1.62	0.43
1:A:298:HIS:HA	1:A:299:PRO:HD3	1.74	0.43
1:A:373:ALA:HB1	1:A:440:HIS:HE1	1.84	0.43
1:A:410:ASN:CB	1:B:409:LEU:HD11	2.35	0.43
1:B:452:ARG:HB2	1:B:467:PHE:CZ	2.54	0.43
1:B:460:LYS:HG2	1:B:468:GLU:HB3	2.01	0.43
1:C:451:VAL:HG12	1:C:452:ARG:N	2.34	0.43
1:D:126:TRP:CE3	1:D:153:LEU:HD11	2.53	0.43
1:E:202:SER:HB2	1:F:217:ALA:CB	2.45	0.43
1:G:58:ASP:HA	1:G:86:LYS:HD3	2.00	0.43
1:G:353:TYR:CE2	1:G:482:LYS:HG2	2.52	0.43
1:H:131:THR:HG22	1:H:153:LEU:CD2	2.49	0.43
1:H:295:HIS:HD2	1:H:297:ILE:N	2.09	0.43
1:I:290:THR:OG1	1:I:292:LEU:HG	2.18	0.43
1:I:360:GLY:O	1:I:361:SER:HB2	2.18	0.43
1:A:345:GLY:HA3	1:A:363:TYR:CD2	2.53	0.43
1:A:456:ARG:HB2	1:A:457:ASP:H	1.73	0.43
1:B:12:HIS:CE1	1:B:13:SER:O	2.71	0.43
1:B:404:LYS:HA	1:B:404:LYS:HD2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:CB	1:C:448:TYR:HD1	2.26	0.43
1:D:360:GLY:O	1:D:361:SER:HB2	2.19	0.43
1:F:8:CYS:HA	1:F:466:CYS:HA	1.99	0.43
1:A:23:ILE:HG22	1:A:430:LEU:O	2.18	0.43
1:A:81:SER:O	1:A:111:SER:HB3	2.18	0.43
1:A:338:PHE:CD1	1:A:339:ILE:N	2.87	0.43
1:A:474:ASP:N	1:A:474:ASP:OD2	2.52	0.43
1:B:113:THR:HA	1:B:114:HIS:HA	1.88	0.43
1:D:121:LEU:O	1:D:122:PRO:C	2.58	0.43
1:F:288:ILE:HG12	1:F:297:ILE:HD12	2.00	0.43
1:F:293:PRO:HG3	1:F:385:ILE:HG23	1.99	0.43
1:G:31:THR:C	1:G:32:HIS:CG	2.91	0.43
1:G:80:TRP:CE2	1:G:112:VAL:HG22	2.53	0.43
1:G:294:PHE:HB3	1:G:309:VAL:CG2	2.49	0.43
1:H:80:TRP:CE2	1:H:112:VAL:HG22	2.54	0.43
1:H:155:LYS:HE2	1:H:192:THR:O	2.19	0.43
1:A:23:ILE:O	1:A:23:ILE:CG1	2.66	0.43
1:D:95:TYR:CD2	1:D:229:MET:CG	2.90	0.43
1:E:323:VAL:HG11	1:E:336:ALA:CB	2.47	0.43
1:E:360:GLY:O	1:E:361:SER:HB2	2.18	0.43
1:F:131:THR:HG22	1:F:153:LEU:CD2	2.49	0.43
1:F:174:GLN:O	1:F:259:ILE:HG22	2.18	0.43
1:G:411:LYS:O	1:G:415:ASP:HB2	2.18	0.43
1:H:66:LEU:O	1:H:147:PHE:HB3	2.19	0.43
1:I:12:HIS:CE1	1:I:13:SER:O	2.72	0.43
1:A:381:VAL:HG12	1:A:382:ASN:HD22	1.84	0.42
1:A:436:THR:O	1:A:436:THR:CG2	2.65	0.42
1:C:36:ILE:O	1:C:292:LEU:HB3	2.18	0.42
1:D:202:SER:HG	1:E:217:ALA:HB2	1.81	0.42
1:D:261:LYS:HE2	1:D:261:LYS:HB3	1.84	0.42
1:D:316:LEU:O	1:D:317:ALA:HB2	2.18	0.42
1:E:129:HIS:CD2	1:E:161:PRO:HD2	2.54	0.42
1:F:141:PHE:N	1:F:142:ASP:CA	2.76	0.42
1:F:184:PRO:HD2	1:F:216:ILE:HG12	2.01	0.42
1:G:12:HIS:CE1	1:G:13:SER:O	2.72	0.42
1:G:405:ARG:HE	1:G:405:ARG:HB2	1.48	0.42
1:G:405:ARG:NH1	1:I:399:PHE:HA	2.34	0.42
1:G:427:LEU:CD1	1:G:431:MET:HE2	2.49	0.42
1:H:495:SER:C	1:H:496:LYS:HD2	2.39	0.42
1:D:166:SER:OG	1:D:243:ASN:ND2	2.52	0.42
1:D:284:PRO:O	1:D:285:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ASN:HB2	1:E:409:LEU:CD1	2.50	0.42
1:H:278:GLU:O	1:H:279:THR:CB	2.66	0.42
1:A:366:ASP:OD2	1:A:368:GLU:HB3	2.19	0.42
1:A:462:LEU:N	1:A:462:LEU:CD1	2.82	0.42
1:B:306:PRO:O	1:B:307:LYS:C	2.57	0.42
1:C:31:THR:C	1:C:32:HIS:CG	2.92	0.42
1:D:8:CYS:HB3	1:D:343:TRP:CZ2	2.54	0.42
1:D:308:TYR:CD2	1:D:418:LEU:CD1	3.02	0.42
1:E:42:ASN:HB2	1:E:287:ALA:O	2.20	0.42
1:F:200:TYR:CE1	1:F:247:THR:HG23	2.54	0.42
1:G:320:LEU:HD23	1:G:320:LEU:N	2.32	0.42
1:G:360:GLY:O	1:G:361:SER:CB	2.66	0.42
1:H:360:GLY:O	1:H:361:SER:HB2	2.19	0.42
1:H:361:SER:HA	1:H:362:GLY:HA3	1.73	0.42
1:H:464:ASN:OD1	1:H:466:CYS:HB2	2.18	0.42
1:I:31:THR:C	1:I:32:HIS:CG	2.92	0.42
1:B:490:LYS:C	1:B:492:GLU:H	2.20	0.42
1:D:48:LEU:HD23	1:D:392:PHE:CE1	2.55	0.42
1:D:82:TYR:CD2	1:D:82:TYR:N	2.87	0.42
1:D:452:ARG:HB2	1:D:467:PHE:CZ	2.54	0.42
1:E:9:VAL:HG21	1:E:448:TYR:CD1	2.54	0.42
1:E:451:VAL:HG12	1:E:452:ARG:N	2.33	0.42
1:F:45:LEU:H	1:F:45:LEU:HD12	1.84	0.42
1:F:445:LYS:O	1:F:445:LYS:HG3	2.19	0.42
1:F:452:ARG:HB2	1:F:467:PHE:CZ	2.55	0.42
1:F:452:ARG:HB2	1:F:467:PHE:HZ	1.83	0.42
1:G:202:SER:HB2	1:H:217:ALA:HB2	2.00	0.42
1:G:278:GLU:CG	1:G:279:THR:N	2.81	0.42
1:H:138:CYS:O	1:H:145:SER:HB3	2.20	0.42
1:A:334:ALA:HA	1:A:338:PHE:CE2	2.54	0.42
1:A:452:ARG:HH21	1:A:453:MET:CG	2.33	0.42
1:B:12:HIS:HB2	1:B:350:TRP:HA	2.01	0.42
1:D:293:PRO:HB3	1:D:388:MET:HB2	2.02	0.42
1:F:288:ILE:HD11	1:F:297:ILE:HD12	2.01	0.42
1:F:306:PRO:O	1:F:308:TYR:N	2.51	0.42
1:G:130:THR:HB	1:G:154:THR:OG1	2.19	0.42
1:G:278:GLU:O	1:G:279:THR:HB	2.19	0.42
1:G:409:LEU:HD11	1:I:410:ASN:CG	2.39	0.42
1:G:425:ALA:O	1:G:428:LEU:N	2.53	0.42
1:G:457:ASP:C	1:G:459:VAL:N	2.72	0.42
1:H:8:CYS:HB2	1:H:354:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:THR:HB	1:I:154:THR:OG1	2.20	0.42
1:I:298:HIS:HE1	1:I:300:LEU:HD12	1.85	0.42
1:B:174:GLN:O	1:B:259:ILE:HG22	2.19	0.42
1:D:46:CYS:HB3	1:D:47:LYS:H	1.62	0.42
1:D:283:THR:CB	1:D:286:GLY:O	2.61	0.42
1:E:130:THR:HB	1:E:154:THR:OG1	2.19	0.42
1:E:320:LEU:HD23	1:E:320:LEU:N	2.30	0.42
1:F:360:GLY:O	1:F:361:SER:HB2	2.20	0.42
1:G:294:PHE:HB3	1:G:309:VAL:HG22	2.00	0.42
1:A:48:LEU:O	1:A:49:ASN:C	2.58	0.42
1:A:454:GLN:OE1	1:A:484:GLY:O	2.37	0.42
1:B:141:PHE:N	1:B:142:ASP:CA	2.75	0.42
1:D:117:LYS:HG3	1:D:255:TYR:HB3	2.01	0.42
1:D:169:ASN:O	1:D:239:TRP:HE3	2.03	0.42
1:D:242:ILE:CG1	1:D:243:ASN:N	2.82	0.42
1:E:38:GLU:OE2	1:E:40:THR:HG22	2.19	0.42
1:E:45:LEU:HD12	1:E:45:LEU:H	1.84	0.42
1:F:51:ILE:HB	1:F:81:SER:HB3	2.01	0.42
1:F:77:VAL:HG22	1:F:79:GLU:O	2.19	0.42
1:F:138:CYS:O	1:F:145:SER:HB3	2.19	0.42
1:I:278:GLU:CG	1:I:279:THR:N	2.78	0.42
1:A:28:VAL:HG12	1:A:30:VAL:CG1	2.50	0.42
1:A:48:LEU:HB3	1:A:81:SER:HB3	2.01	0.42
1:A:299:PRO:HG3	1:A:308:TYR:CZ	2.53	0.42
1:A:462:LEU:HD11	1:A:468:GLU:N	2.34	0.42
1:D:58:ASP:HA	1:D:86:LYS:HD3	2.01	0.42
1:D:96:PRO:CG	1:D:222:VAL:O	2.68	0.42
1:D:214:PRO:HG3	1:D:249:ASN:CG	2.38	0.42
1:F:201:VAL:HG22	1:F:250:LEU:HB2	2.01	0.42
1:F:320:LEU:HB3	1:F:440:HIS:HB3	2.00	0.42
1:G:129:HIS:NE2	1:G:161:PRO:HD2	2.34	0.42
1:H:37:LEU:O	1:H:39:LYS:HE2	2.20	0.42
1:I:37:LEU:O	1:I:39:LYS:HE2	2.20	0.42
1:I:250:LEU:HD21	1:I:252:ALA:HB2	2.01	0.42
1:A:96:PRO:HG3	1:A:222:VAL:HG12	2.02	0.42
1:B:348:ASP:N	1:B:348:ASP:OD1	2.53	0.42
1:C:367:LYS:HE2	1:C:367:LYS:HB3	1.95	0.42
1:E:379:ASN:ND2	1:F:26:ARG:CZ	2.79	0.42
1:G:277:CYS:O	1:G:278:GLU:HB2	2.20	0.42
1:G:348:ASP:O	1:G:365:ALA:CB	2.68	0.42
1:H:430:LEU:C	1:H:431:MET:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:400:SER:OG	1:I:403:GLU:HG3	2.19	0.42
1:B:259:ILE:CG2	1:B:260:SER:H	2.07	0.42
1:D:169:ASN:C	1:D:169:ASN:OD1	2.58	0.42
1:E:320:LEU:HD13	1:E:335:ILE:CD1	2.49	0.42
1:F:361:SER:HA	1:F:362:GLY:HA3	1.73	0.42
1:G:348:ASP:N	1:G:348:ASP:OD1	2.53	0.42
1:G:432:GLU:OE2	1:H:23:ILE:HD13	2.20	0.42
1:I:58:ASP:HA	1:I:86:LYS:HD3	2.02	0.42
1:I:67:GLY:O	1:I:68:ASN:C	2.55	0.42
1:A:107:HIS:ND1	1:A:107:HIS:O	2.53	0.41
1:B:45:LEU:HD12	1:B:45:LEU:H	1.85	0.41
1:E:73:ARG:C	1:G:44:LYS:NZ	2.74	0.41
1:E:99:PHE:HE1	1:E:233:TRP:CD1	2.37	0.41
1:E:131:THR:HG22	1:E:153:LEU:CD2	2.49	0.41
1:F:444:VAL:O	1:F:447:LEU:N	2.52	0.41
1:G:45:LEU:CD2	1:G:270:THR:HG21	2.50	0.41
1:G:140:VAL:HG23	1:G:145:SER:CB	2.50	0.41
1:G:471:HIS:CD2	1:G:491:TYR:HB3	2.55	0.41
1:H:120:ILE:HB	1:H:167:TYR:CD1	2.55	0.41
1:H:126:TRP:HB2	1:H:131:THR:HG21	2.02	0.41
1:I:259:ILE:CG2	1:I:260:SER:H	2.12	0.41
1:I:325:GLN:NE2	1:I:325:GLN:C	2.74	0.41
1:A:335:ILE:HG13	1:A:441:ASP:CA	2.38	0.41
1:C:355:HIS:CD2	1:C:355:HIS:N	2.87	0.41
1:D:54:LEU:HB3	1:D:83:ILE:HG12	2.02	0.41
1:D:222:VAL:HG23	1:D:228:ARG:HH12	1.84	0.41
1:E:323:VAL:HA	1:E:324:PRO:HD3	1.79	0.41
1:H:183:HIS:HA	1:H:184:PRO:HD3	1.89	0.41
1:H:348:ASP:N	1:H:348:ASP:OD1	2.53	0.41
1:I:51:ILE:HB	1:I:81:SER:HB3	2.00	0.41
1:I:278:GLU:CG	1:I:279:THR:H	2.32	0.41
1:A:38:GLU:O	1:A:295:HIS:HA	2.20	0.41
1:B:67:GLY:O	1:B:68:ASN:C	2.59	0.41
1:C:140:VAL:HG23	1:C:145:SER:CB	2.50	0.41
1:D:23:ILE:HD11	1:F:380:LYS:HG3	2.02	0.41
1:D:355:HIS:CD2	1:D:355:HIS:N	2.88	0.41
1:E:51:ILE:HB	1:E:81:SER:HB3	2.01	0.41
1:F:306:PRO:O	1:F:307:LYS:C	2.58	0.41
1:G:51:ILE:HB	1:G:81:SER:HB3	2.00	0.41
1:G:462:LEU:CD1	1:G:462:LEU:N	2.84	0.41
1:H:36:ILE:HB	1:H:293:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:CYS:O	1:I:278:GLU:HB2	2.19	0.41
1:I:338:PHE:CE1	1:I:339:ILE:CG1	3.03	0.41
1:A:42:ASN:C	1:A:44:LYS:H	2.22	0.41
1:B:400:SER:OG	1:B:403:GLU:HG3	2.21	0.41
1:C:131:THR:HG22	1:C:153:LEU:CD2	2.50	0.41
1:D:97:GLY:HA3	1:D:229:MET:O	2.20	0.41
1:E:126:TRP:HB2	1:E:131:THR:HG21	2.03	0.41
1:E:295:HIS:CD2	1:E:297:ILE:H	2.21	0.41
1:G:77:VAL:HG22	1:G:79:GLU:H	1.85	0.41
1:H:31:THR:HB	1:H:32:HIS:CE1	2.54	0.41
1:H:298:HIS:HE1	1:H:300:LEU:HD12	1.85	0.41
1:E:12:HIS:CB	1:E:350:TRP:HA	2.50	0.41
1:E:141:PHE:HE2	1:G:274:LEU:CD1	2.33	0.41
1:F:95:TYR:HA	1:F:96:PRO:HD3	1.94	0.41
1:G:346:MET:SD	1:G:352:GLY:CA	3.05	0.41
1:H:105:LEU:O	1:H:109:ILE:HG12	2.20	0.41
1:H:456:ARG:HB2	1:H:457:ASP:H	1.66	0.41
1:I:126:TRP:HB2	1:I:131:THR:HG21	2.02	0.41
1:I:131:THR:HG22	1:I:153:LEU:CD2	2.51	0.41
1:A:57:GLY:O	1:A:86:LYS:HG3	2.21	0.41
1:B:12:HIS:CE1	1:B:14:ASN:HB3	2.55	0.41
1:B:142:ASP:OD2	1:B:142:ASP:N	2.53	0.41
1:C:442:SER:O	1:C:446:ASN:HB2	2.21	0.41
1:D:167:TYR:CE2	1:D:169:ASN:HA	2.56	0.41
1:E:183:HIS:HA	1:E:184:PRO:HD3	1.87	0.41
1:E:299:PRO:O	1:E:395:VAL:HG21	2.19	0.41
1:F:259:ILE:CG2	1:F:260:SER:H	2.10	0.41
1:F:355:HIS:CD2	1:F:355:HIS:N	2.87	0.41
1:G:412:LYS:HD2	1:G:412:LYS:HA	1.71	0.41
1:H:278:GLU:CG	1:H:279:THR:H	2.33	0.41
1:I:399:PHE:CG	1:I:407:GLU:HB2	2.55	0.41
1:A:160:TYR:CE2	1:A:248:GLY:CA	3.03	0.41
1:A:218:THR:HG22	1:C:243:ASN:CB	2.51	0.41
1:A:309:VAL:HA	1:A:418:LEU:HD11	2.03	0.41
1:A:344:GLN:CD	1:A:344:GLN:N	2.74	0.41
1:A:397:LYS:HB3	1:A:397:LYS:HE3	1.86	0.41
1:A:473:CYS:SG	1:A:478:MET:HG2	2.61	0.41
1:B:222:VAL:O	1:B:223:ASN:HB2	2.21	0.41
1:B:282:GLN:HG3	1:B:283:THR:N	2.35	0.41
1:B:293:PRO:HG3	1:B:385:ILE:CA	2.50	0.41
1:B:379:ASN:HB3	1:C:23:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LYS:HB2	1:C:307:LYS:NZ	2.36	0.41
1:D:51:ILE:CG2	1:D:52:PRO:CD	2.99	0.41
1:E:460:LYS:HG2	1:E:468:GLU:HB3	2.02	0.41
1:G:298:HIS:HE1	1:G:300:LEU:HD12	1.85	0.41
1:G:335:ILE:HG13	1:G:441:ASP:HA	2.03	0.41
1:G:346:MET:HA	1:G:346:MET:CE	2.49	0.41
1:G:486:TYR:O	1:G:487:ASP:CB	2.68	0.41
1:H:404:LYS:HA	1:H:404:LYS:HD2	1.69	0.41
1:I:444:VAL:O	1:I:447:LEU:N	2.51	0.41
1:A:56:LEU:HA	1:A:74:LEU:HD11	2.03	0.41
1:B:399:PHE:CG	1:B:407:GLU:HB2	2.56	0.41
1:D:293:PRO:HB2	1:D:294:PHE:CD2	2.55	0.41
1:E:36:ILE:O	1:E:292:LEU:HB3	2.19	0.41
1:G:282:GLN:HG3	1:G:283:THR:N	2.35	0.41
1:H:355:HIS:H	1:H:355:HIS:HD2	1.66	0.41
1:A:13:SER:HA	1:A:322:ASN:OD1	2.21	0.41
1:A:48:LEU:HD23	1:A:392:PHE:HE1	1.86	0.41
1:A:107:HIS:O	1:A:110:SER:HB2	2.21	0.41
1:A:206:SER:OG	1:A:240:ASP:OD1	2.39	0.41
1:A:447:LEU:HD12	1:A:447:LEU:HA	1.68	0.41
1:B:42:ASN:HB2	1:B:287:ALA:O	2.21	0.41
1:B:140:VAL:HG23	1:B:145:SER:CB	2.50	0.41
1:C:400:SER:OG	1:C:403:GLU:HG3	2.20	0.41
1:D:26:ARG:HA	1:D:26:ARG:HD2	1.84	0.41
1:D:114:HIS:HB2	1:D:115:PHE:H	1.52	0.41
1:D:259:ILE:O	1:D:259:ILE:CG2	2.67	0.41
1:D:451:VAL:HG12	1:D:452:ARG:N	2.35	0.41
3:D:1497:SIA:O1A	3:D:1497:SIA:H6	2.21	0.41
1:E:77:VAL:HG22	1:E:79:GLU:O	2.21	0.41
1:E:197:VAL:CG1	1:E:198:GLY:N	2.84	0.41
1:E:317:ALA:O	1:E:436:THR:HG21	2.21	0.41
1:F:22:THR:HG22	1:F:433:ASN:HB3	2.02	0.41
1:F:67:GLY:O	1:F:68:ASN:C	2.59	0.41
1:F:333:GLY:O	1:F:337:GLY:HA3	2.21	0.41
1:F:451:VAL:HG12	1:F:452:ARG:N	2.35	0.41
1:G:10:GLY:HA3	1:G:343:TRP:CH2	2.56	0.41
1:G:354:HIS:HA	1:G:362:GLY:O	2.21	0.41
1:I:42:ASN:HD22	1:I:287:ALA:HB3	1.85	0.41
1:I:197:VAL:CG1	1:I:198:GLY:N	2.84	0.41
1:I:279:THR:OG1	1:I:281:CYS:O	2.33	0.41
1:A:24:LEU:HD22	1:C:376:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:C	1:A:224:GLY:N	2.75	0.41
1:B:51:ILE:HB	1:B:81:SER:HB3	2.03	0.41
1:C:293:PRO:HG3	1:C:385:ILE:HG12	2.03	0.41
1:C:452:ARG:HB2	1:C:467:PHE:HZ	1.84	0.41
1:D:138:CYS:O	1:D:145:SER:HB3	2.21	0.41
1:E:34:GLN:NE2	1:E:381:VAL:HG21	2.36	0.41
1:E:382:ASN:O	1:E:386:GLU:N	2.52	0.41
1:F:37:LEU:O	1:F:39:LYS:HE2	2.21	0.41
1:H:211:ARG:NH1	1:I:216:ILE:HB	2.36	0.41
1:A:469:PHE:HE1	1:A:471:HIS:NE2	2.18	0.40
1:B:333:GLY:O	1:B:337:GLY:HA3	2.21	0.40
1:B:397:LYS:HB3	1:B:397:LYS:HE3	1.86	0.40
1:B:456:ARG:HB2	1:B:457:ASP:H	1.66	0.40
1:C:445:LYS:O	1:C:445:LYS:HG3	2.20	0.40
1:D:12:HIS:ND1	1:D:349:GLY:O	2.53	0.40
1:D:179:TRP:HZ3	1:D:234:THR:HG22	1.86	0.40
1:D:199:ALA:HA	1:D:247:THR:OG1	2.21	0.40
1:D:243:ASN:HD22	1:D:243:ASN:HA	1.73	0.40
1:D:310:LYS:HZ1	1:D:418:LEU:CD2	2.34	0.40
1:E:73:ARG:NH1	1:G:276:ASN:O	2.54	0.40
1:F:45:LEU:HD12	1:F:45:LEU:N	2.36	0.40
1:G:323:VAL:HA	1:G:324:PRO:HD3	1.66	0.40
1:G:332:PHE:N	1:G:441:ASP:OD2	2.53	0.40
1:G:427:LEU:O	1:G:428:LEU:C	2.59	0.40
1:H:24:LEU:HD12	1:H:434:GLU:CD	2.41	0.40
1:A:18:GLU:OE1	1:A:33:ALA:HB3	2.21	0.40
1:A:218:THR:O	1:C:243:ASN:HB2	2.21	0.40
1:D:51:ILE:CG2	1:D:52:PRO:HD2	2.50	0.40
1:D:120:ILE:HG21	1:D:175:MET:SD	2.61	0.40
1:D:200:TYR:CE1	1:D:247:THR:CG2	3.04	0.40
1:D:442:SER:O	1:D:446:ASN:HB2	2.21	0.40
1:E:446:ASN:HD21	1:F:333:GLY:N	2.19	0.40
1:F:135:SER:OG	2:J:2:SIA:O1A	2.33	0.40
1:G:278:GLU:O	1:G:279:THR:CB	2.69	0.40
1:G:355:HIS:HB2	1:G:478:MET:SD	2.61	0.40
1:G:455:LEU:HG	1:G:459:VAL:HG21	2.04	0.40
1:A:105:LEU:HD12	1:A:108:LEU:HD23	2.02	0.40
1:A:167:TYR:O	1:A:241:THR:HA	2.21	0.40
1:A:191:ARG:HG2	1:A:195:GLN:NE2	2.36	0.40
1:A:295:HIS:HD2	1:A:297:ILE:H	1.69	0.40
1:A:475:ASP:O	1:A:479:ASN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:PRO:HD2	1:B:216:ILE:HG12	2.03	0.40
1:C:37:LEU:O	1:C:39:LYS:HE2	2.21	0.40
1:C:105:LEU:O	1:C:109:ILE:HG12	2.21	0.40
1:C:120:ILE:HB	1:C:167:TYR:CD1	2.57	0.40
1:C:197:VAL:CG1	1:C:198:GLY:N	2.85	0.40
1:C:460:LYS:HG2	1:C:468:GLU:HB3	2.03	0.40
1:D:34:GLN:CG	1:D:35:ASP:H	2.35	0.40
1:E:442:SER:CB	1:F:331:LEU:HD13	2.51	0.40
1:F:197:VAL:CG1	1:F:198:GLY:N	2.84	0.40
1:F:298:HIS:HE1	1:F:300:LEU:HD12	1.86	0.40
1:G:129:HIS:CD2	1:G:161:PRO:HD2	2.56	0.40
1:G:380:LYS:HD2	1:G:436:THR:OG1	2.21	0.40
1:G:400:SER:OG	1:G:401:ASN:N	2.53	0.40
1:H:338:PHE:CE1	1:H:339:ILE:CG1	3.05	0.40
1:I:22:THR:HB	1:I:434:GLU:OE2	2.22	0.40
1:A:379:ASN:ND2	1:B:26:ARG:CZ	2.83	0.40
1:A:399:PHE:CB	1:A:407:GLU:HB2	2.52	0.40
1:C:184:PRO:HD2	1:C:216:ILE:HG12	2.04	0.40
1:C:306:PRO:O	1:C:307:LYS:C	2.60	0.40
1:E:9:VAL:N	1:E:465:GLY:O	2.43	0.40
1:E:51:ILE:HA	1:E:52:PRO:HD3	1.94	0.40
1:E:170:THR:HA	1:E:239:TRP:CZ3	2.56	0.40
1:E:184:PRO:HD2	1:E:216:ILE:HG12	2.04	0.40
1:E:318:THR:HB	1:E:377:ILE:HG21	2.02	0.40
1:F:140:VAL:HG23	1:F:145:SER:CB	2.51	0.40
1:F:277:CYS:O	1:F:278:GLU:HB2	2.22	0.40
1:G:126:TRP:HB2	1:G:131:THR:HG21	2.04	0.40
1:G:131:THR:HG22	1:G:153:LEU:CD2	2.52	0.40
1:G:384:VAL:O	1:G:384:VAL:CG1	2.67	0.40
1:G:419:ASP:O	1:G:420:VAL:C	2.59	0.40
1:H:51:ILE:HB	1:H:81:SER:HB3	2.02	0.40
1:H:323:VAL:HA	1:H:324:PRO:HD3	1.87	0.40
1:A:41:HIS:O	1:A:43:GLY:N	2.54	0.40
1:A:297:ILE:O	1:A:298:HIS:HB2	2.20	0.40
1:A:321:ARG:HG3	1:A:322:ASN:N	2.37	0.40
1:A:332:PHE:CE1	1:C:332:PHE:HE1	2.39	0.40
1:B:114:HIS:O	1:B:259:ILE:O	2.38	0.40
1:D:146:PHE:HE1	1:D:229:MET:CE	2.34	0.40
1:D:382:ASN:O	1:D:386:GLU:N	2.50	0.40
1:F:77:VAL:HG22	1:F:79:GLU:H	1.87	0.40
1:F:290:THR:OG1	1:F:292:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:THR:HG22	1:G:153:LEU:HD22	2.04	0.40
1:H:129:HIS:NE2	1:H:161:PRO:HD2	2.37	0.40
1:H:140:VAL:HG23	1:H:145:SER:CB	2.51	0.40
1:H:243:ASN:HB2	1:I:218:THR:O	2.22	0.40
1:H:474:ASP:OD2	1:H:474:ASP:N	2.51	0.40
1:I:474:ASP:OD2	1:I:474:ASP:N	2.54	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	482/507 (95%)	371 (77%)	80 (17%)	31 (6%)	1 8
1	B	482/507 (95%)	408 (85%)	62 (13%)	12 (2%)	5 27
1	C	482/507 (95%)	407 (84%)	63 (13%)	12 (2%)	5 27
1	D	482/507 (95%)	384 (80%)	74 (15%)	24 (5%)	2 13
1	E	482/507 (95%)	411 (85%)	60 (12%)	11 (2%)	6 28
1	F	482/507 (95%)	407 (84%)	63 (13%)	12 (2%)	5 27
1	G	482/507 (95%)	393 (82%)	61 (13%)	28 (6%)	1 10
1	H	482/507 (95%)	406 (84%)	64 (13%)	12 (2%)	5 27
1	I	482/507 (95%)	403 (84%)	69 (14%)	10 (2%)	7 30
All	All	4338/4563 (95%)	3590 (83%)	596 (14%)	152 (4%)	3 20

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	155	LYS

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	276	ASN
1	A	306	PRO
1	A	357	ASN
1	A	396	GLY
1	A	432	GLU
1	A	452	ARG
1	A	479	ASN
1	A	494	GLU
1	B	260	SER
1	B	307	LYS
1	B	494	GLU
1	C	260	SER
1	C	307	LYS
1	C	494	GLU
1	D	42	ASN
1	D	113	THR
1	D	196	ASN
1	D	238	ILE
1	D	239	TRP
1	D	320	LEU
1	D	494	GLU
1	E	260	SER
1	E	307	LYS
1	E	494	GLU
1	F	260	SER
1	F	307	LYS
1	F	494	GLU
1	G	260	SER
1	G	307	LYS
1	G	425	ALA
1	G	426	GLU
1	G	433	ASN
1	G	490	LYS
1	G	494	GLU
1	H	260	SER
1	H	307	LYS
1	I	260	SER
1	I	307	LYS
1	A	42	ASN
1	A	49	ASN
1	A	57	GLY

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Mol	Chain	Res	Type
1	A	87	GLU
1	A	140	VAL
1	A	368	GLU
1	A	369	SER
1	A	431	MET
1	A	436	THR
1	A	474	ASP
1	B	113	THR
1	B	279	THR
1	B	495	SER
1	C	279	THR
1	D	13	SER
1	D	64	TRP
1	D	125	ARG
1	D	127	THR
1	D	276	ASN
1	D	277	CYS
1	E	279	THR
1	F	113	THR
1	F	279	THR
1	G	113	THR
1	G	279	THR
1	G	367	LYS
1	G	418	LEU
1	G	458	ASN
1	H	279	THR
1	I	113	THR
1	I	262	ARG
1	I	279	THR
1	I	324	PRO
1	A	209	ASN
1	A	220	PRO
1	A	425	ALA
1	B	262	ARG
1	C	113	THR
1	C	259	ILE
1	C	262	ARG
1	C	324	PRO
1	D	15	ASN
1	E	113	THR
1	E	262	ARG
1	F	262	ARG

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Mol	Chain	Res	Type
1	G	262	ARG
1	G	361	SER
1	G	400	SER
1	G	420	VAL
1	G	456	ARG
1	G	483	ASN
1	G	487	ASP
1	G	489	SER
1	H	113	THR
1	H	262	ARG
1	I	430	LEU
1	A	89	PRO
1	A	361	SER
1	A	458	ASN
1	B	195	GLN
1	B	259	ILE
1	C	195	GLN
1	C	430	LEU
1	D	27	ASN
1	D	49	ASN
1	D	317	ALA
1	D	430	LEU
1	E	195	GLN
1	E	259	ILE
1	E	430	LEU
1	F	195	GLN
1	F	259	ILE
1	G	195	GLN
1	G	259	ILE
1	H	195	GLN
1	H	259	ILE
1	H	430	LEU
1	H	494	GLU
1	I	195	GLN
1	I	259	ILE
1	A	445	LYS
1	A	456	ARG
1	B	334	ALA
1	B	340	GLU
1	D	12	HIS
1	D	73	ARG
1	D	297	ILE

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Mol	Chain	Res	Type
1	D	316	LEU
1	D	334	ALA
1	F	334	ALA
1	F	430	LEU
1	G	324	PRO
1	G	455	LEU
1	H	324	PRO
1	H	487	ASP
1	A	323	VAL
1	B	430	LEU
1	C	334	ALA
1	C	487	ASP
1	E	487	ASP
1	G	397	LYS
1	F	324	PRO
1	G	360	GLY
1	G	109	ILE
1	D	28	VAL
1	E	109	ILE
1	G	306	PRO
1	I	109	ILE
1	A	298	HIS
1	F	109	ILE
1	H	109	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	422/444 (95%)	347 (82%)	75 (18%)	2 8
1	B	422/444 (95%)	389 (92%)	33 (8%)	12 40
1	C	421/444 (95%)	392 (93%)	29 (7%)	15 45
1	D	422/444 (95%)	361 (86%)	61 (14%)	3 13
1	E	422/444 (95%)	391 (93%)	31 (7%)	14 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	421/444 (95%)	391 (93%)	30 (7%)	14	44
1	G	422/444 (95%)	374 (89%)	48 (11%)	5	23
1	H	422/444 (95%)	391 (93%)	31 (7%)	14	43
1	I	421/444 (95%)	389 (92%)	32 (8%)	13	41
All	All	3795/3996 (95%)	3425 (90%)	370 (10%)	8	30

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	19	LYS
1	A	21	ASP
1	A	23	ILE
1	A	26	ARG
1	A	29	THR
1	A	36	ILE
1	A	45	LEU
1	A	51	ILE
1	A	65	LEU
1	A	70	GLU
1	A	73	ARG
1	A	74	LEU
1	A	77	VAL
1	A	79	GLU
1	A	81	SER
1	A	93	LEU
1	A	94	CYS
1	A	98	SER
1	A	99	PHE
1	A	108	LEU
1	A	114	HIS
1	A	132	THR
1	A	136	GLN
1	A	141	PHE
1	A	145	SER
1	A	151	VAL
1	A	154	THR
1	A	158	SER
1	A	159	ASN
1	A	173	GLU
1	A	186	ASP

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Mol	Chain	Res	Type
1	A	188	THR
1	A	193	LEU
1	A	196	ASN
1	A	201	VAL
1	A	206	SER
1	A	207	THR
1	A	212	SER
1	A	219	ARG
1	A	234	THR
1	A	259	ILE
1	A	273	THR
1	A	274	LEU
1	A	280	LYS
1	A	281	CYS
1	A	282	GLN
1	A	309	VAL
1	A	315	VAL
1	A	320	LEU
1	A	323	VAL
1	A	331	LEU
1	A	335	ILE
1	A	343	TRP
1	A	348	ASP
1	A	350	TRP
1	A	351	TYR
1	A	359	GLN
1	A	366	ASP
1	A	371	GLN
1	A	375	ASP
1	A	380	LYS
1	A	382	ASN
1	A	389	ASN
1	A	390	THR
1	A	395	VAL
1	A	407	GLU
1	A	410	ASN
1	A	428	LEU
1	A	452	ARG
1	A	457	ASP
1	A	460	LYS
1	A	469	PHE
1	A	494	GLU

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Mol	Chain	Res	Type
1	A	496	LYS
1	B	19	LYS
1	B	23	ILE
1	B	55	GLU
1	B	61	ILE
1	B	70	GLU
1	B	73	ARG
1	B	86	LYS
1	B	110	SER
1	B	113	THR
1	B	141	PHE
1	B	142	ASP
1	B	143	ASN
1	B	154	THR
1	B	188	THR
1	B	241	THR
1	B	273	THR
1	B	275	GLU
1	B	277	CYS
1	B	283	THR
1	B	307	LYS
1	B	309	VAL
1	B	323	VAL
1	B	325	GLN
1	B	331	LEU
1	B	389	ASN
1	B	397	LYS
1	B	404	LYS
1	B	410	ASN
1	B	426	GLU
1	B	437	LEU
1	B	456	ARG
1	B	473	CYS
1	B	496	LYS
1	C	19	LYS
1	C	23	ILE
1	C	55	GLU
1	C	61	ILE
1	C	70	GLU
1	C	73	ARG
1	C	86	LYS
1	C	110	SER

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Mol	Chain	Res	Type
1	C	113	THR
1	C	141	PHE
1	C	142	ASP
1	C	143	ASN
1	C	154	THR
1	C	188	THR
1	C	241	THR
1	C	273	THR
1	C	275	GLU
1	C	277	CYS
1	C	283	THR
1	C	307	LYS
1	C	323	VAL
1	C	331	LEU
1	C	389	ASN
1	C	397	LYS
1	C	404	LYS
1	C	410	ASN
1	C	426	GLU
1	C	437	LEU
1	C	473	CYS
1	D	17	THR
1	D	19	LYS
1	D	21	ASP
1	D	23	ILE
1	D	26	ARG
1	D	39	LYS
1	D	40	THR
1	D	52	PRO
1	D	56	LEU
1	D	58	ASP
1	D	74	LEU
1	D	77	VAL
1	D	82	TYR
1	D	86	LYS
1	D	88	ASN
1	D	90	ARG
1	D	91	ASN
1	D	94	CYS
1	D	98	SER
1	D	108	LEU
1	D	111	SER

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Mol	Chain	Res	Type
1	D	114	HIS
1	D	118	VAL
1	D	148	ARG
1	D	162	VAL
1	D	170	THR
1	D	173	GLU
1	D	176	LEU
1	D	177	ILE
1	D	188	THR
1	D	195	GLN
1	D	196	ASN
1	D	197	VAL
1	D	202	SER
1	D	208	LEU
1	D	211	ARG
1	D	212	SER
1	D	219	ARG
1	D	230	GLU
1	D	239	TRP
1	D	241	THR
1	D	259	ILE
1	D	260	SER
1	D	273	THR
1	D	274	LEU
1	D	281	CYS
1	D	295	HIS
1	D	307	LYS
1	D	310	LYS
1	D	316	LEU
1	D	321	ARG
1	D	323	VAL
1	D	331	LEU
1	D	389	ASN
1	D	397	LYS
1	D	404	LYS
1	D	410	ASN
1	D	426	GLU
1	D	437	LEU
1	D	473	CYS
1	D	495	SER
1	E	19	LYS
1	E	23	ILE

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Mol	Chain	Res	Type
1	E	55	GLU
1	E	61	ILE
1	E	70	GLU
1	E	73	ARG
1	E	86	LYS
1	E	110	SER
1	E	113	THR
1	E	141	PHE
1	E	142	ASP
1	E	143	ASN
1	E	154	THR
1	E	188	THR
1	E	241	THR
1	E	260	SER
1	E	273	THR
1	E	275	GLU
1	E	277	CYS
1	E	283	THR
1	E	307	LYS
1	E	323	VAL
1	E	331	LEU
1	E	389	ASN
1	E	397	LYS
1	E	404	LYS
1	E	410	ASN
1	E	426	GLU
1	E	437	LEU
1	E	456	ARG
1	E	473	CYS
1	F	19	LYS
1	F	23	ILE
1	F	55	GLU
1	F	61	ILE
1	F	70	GLU
1	F	73	ARG
1	F	86	LYS
1	F	110	SER
1	F	113	THR
1	F	141	PHE
1	F	142	ASP
1	F	143	ASN
1	F	154	THR

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Mol	Chain	Res	Type
1	F	188	THR
1	F	241	THR
1	F	273	THR
1	F	275	GLU
1	F	277	CYS
1	F	283	THR
1	F	307	LYS
1	F	309	VAL
1	F	323	VAL
1	F	331	LEU
1	F	389	ASN
1	F	397	LYS
1	F	404	LYS
1	F	410	ASN
1	F	426	GLU
1	F	437	LEU
1	F	473	CYS
1	G	19	LYS
1	G	23	ILE
1	G	55	GLU
1	G	61	ILE
1	G	70	GLU
1	G	73	ARG
1	G	86	LYS
1	G	110	SER
1	G	113	THR
1	G	141	PHE
1	G	142	ASP
1	G	143	ASN
1	G	154	THR
1	G	188	THR
1	G	241	THR
1	G	273	THR
1	G	275	GLU
1	G	277	CYS
1	G	283	THR
1	G	307	LYS
1	G	323	VAL
1	G	346	MET
1	G	347	VAL
1	G	351	TYR
1	G	355	HIS

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Mol	Chain	Res	Type
1	G	356	SER
1	G	357	ASN
1	G	358	ASP
1	G	359	GLN
1	G	367	LYS
1	G	381	VAL
1	G	389	ASN
1	G	390	THR
1	G	398	GLU
1	G	404	LYS
1	G	407	GLU
1	G	408	ASN
1	G	409	LEU
1	G	410	ASN
1	G	411	LYS
1	G	426	GLU
1	G	427	LEU
1	G	430	LEU
1	G	459	VAL
1	G	466	CYS
1	G	483	ASN
1	G	494	GLU
1	G	496	LYS
1	H	19	LYS
1	H	23	ILE
1	H	55	GLU
1	H	61	ILE
1	H	70	GLU
1	H	73	ARG
1	H	86	LYS
1	H	110	SER
1	H	113	THR
1	H	141	PHE
1	H	142	ASP
1	H	143	ASN
1	H	154	THR
1	H	188	THR
1	H	241	THR
1	H	273	THR
1	H	275	GLU
1	H	277	CYS
1	H	283	THR

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Mol	Chain	Res	Type
1	H	307	LYS
1	H	323	VAL
1	H	325	GLN
1	H	389	ASN
1	H	397	LYS
1	H	404	LYS
1	H	410	ASN
1	H	426	GLU
1	H	437	LEU
1	H	456	ARG
1	H	473	CYS
1	H	493	GLU
1	I	19	LYS
1	I	23	ILE
1	I	55	GLU
1	I	61	ILE
1	I	70	GLU
1	I	73	ARG
1	I	86	LYS
1	I	110	SER
1	I	113	THR
1	I	141	PHE
1	I	142	ASP
1	I	143	ASN
1	I	154	THR
1	I	188	THR
1	I	241	THR
1	I	273	THR
1	I	275	GLU
1	I	277	CYS
1	I	283	THR
1	I	307	LYS
1	I	309	VAL
1	I	323	VAL
1	I	325	GLN
1	I	351	TYR
1	I	389	ASN
1	I	397	LYS
1	I	404	LYS
1	I	410	ASN
1	I	426	GLU
1	I	437	LEU

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Mol	Chain	Res	Type
1	I	456	ARG
1	I	473	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	88	ASN
1	A	129	HIS
1	A	182	HIS
1	A	196	ASN
1	A	225	GLN
1	A	243	ASN
1	A	249	ASN
1	A	282	GLN
1	A	354	HIS
1	A	359	GLN
1	A	371	GLN
1	A	379	ASN
1	A	382	ASN
1	A	389	ASN
1	A	391	GLN
1	A	440	HIS
1	A	446	ASN
1	B	34	GLN
1	B	91	ASN
1	B	136	GLN
1	B	143	ASN
1	B	159	ASN
1	B	182	HIS
1	B	185	ASN
1	B	243	ASN
1	B	249	ASN
1	B	295	HIS
1	B	354	HIS
1	B	355	HIS
1	B	371	GLN
1	B	379	ASN
1	B	389	ASN
1	B	391	GLN
1	B	408	ASN
1	C	34	GLN

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Mol	Chain	Res	Type
1	C	91	ASN
1	C	136	GLN
1	C	143	ASN
1	C	159	ASN
1	C	182	HIS
1	C	185	ASN
1	C	243	ASN
1	C	249	ASN
1	C	295	HIS
1	C	354	HIS
1	C	355	HIS
1	C	371	GLN
1	C	379	ASN
1	C	389	ASN
1	C	391	GLN
1	C	446	ASN
1	D	12	HIS
1	D	41	HIS
1	D	42	ASN
1	D	49	ASN
1	D	88	ASN
1	D	100	ASN
1	D	159	ASN
1	D	182	HIS
1	D	195	GLN
1	D	243	ASN
1	D	249	ASN
1	D	295	HIS
1	D	354	HIS
1	D	355	HIS
1	D	371	GLN
1	D	379	ASN
1	D	389	ASN
1	D	391	GLN
1	E	34	GLN
1	E	91	ASN
1	E	136	GLN
1	E	143	ASN
1	E	159	ASN
1	E	182	HIS
1	E	185	ASN
1	E	243	ASN

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Mol	Chain	Res	Type
1	E	249	ASN
1	E	295	HIS
1	E	354	HIS
1	E	355	HIS
1	E	371	GLN
1	E	379	ASN
1	E	389	ASN
1	E	391	GLN
1	E	446	ASN
1	F	34	GLN
1	F	91	ASN
1	F	143	ASN
1	F	159	ASN
1	F	182	HIS
1	F	185	ASN
1	F	243	ASN
1	F	249	ASN
1	F	295	HIS
1	F	354	HIS
1	F	355	HIS
1	F	371	GLN
1	F	379	ASN
1	F	389	ASN
1	F	391	GLN
1	G	34	GLN
1	G	91	ASN
1	G	136	GLN
1	G	143	ASN
1	G	159	ASN
1	G	182	HIS
1	G	185	ASN
1	G	243	ASN
1	G	249	ASN
1	G	295	HIS
1	G	408	ASN
1	H	34	GLN
1	H	91	ASN
1	H	136	GLN
1	H	143	ASN
1	H	159	ASN
1	H	182	HIS
1	H	185	ASN

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Mol	Chain	Res	Type
1	H	243	ASN
1	H	249	ASN
1	H	295	HIS
1	H	355	HIS
1	H	371	GLN
1	H	379	ASN
1	H	389	ASN
1	H	391	GLN
1	I	15	ASN
1	I	34	GLN
1	I	91	ASN
1	I	136	GLN
1	I	143	ASN
1	I	159	ASN
1	I	182	HIS
1	I	185	ASN
1	I	243	ASN
1	I	249	ASN
1	I	295	HIS
1	I	325	GLN
1	I	344	GLN
1	I	354	HIS
1	I	355	HIS
1	I	371	GLN
1	I	379	ASN
1	I	389	ASN
1	I	408	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 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	$\#\|Z\| > 2$
2	GAL	J	1	2	12,12,12	0.50	0	17,17,17	1.14	2 (11%)
2	SIA	J	2	2	20,20,21	0.70	0	21,28,31	1.61	3 (14%)

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	GAL	J	1	2	-	2/2/22/22	0/1/1/1
2	SIA	J	2	2	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	SIA	C6-C5-N5	3.74	116.87	110.91
2	J	2	SIA	C8-C7-C6	-3.49	106.49	113.05
2	J	2	SIA	O1B-C1-C2	2.61	119.50	112.71
2	J	1	GAL	C1-C2-C3	2.52	115.49	110.36
2	J	1	GAL	O5-C1-C2	2.09	113.98	110.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

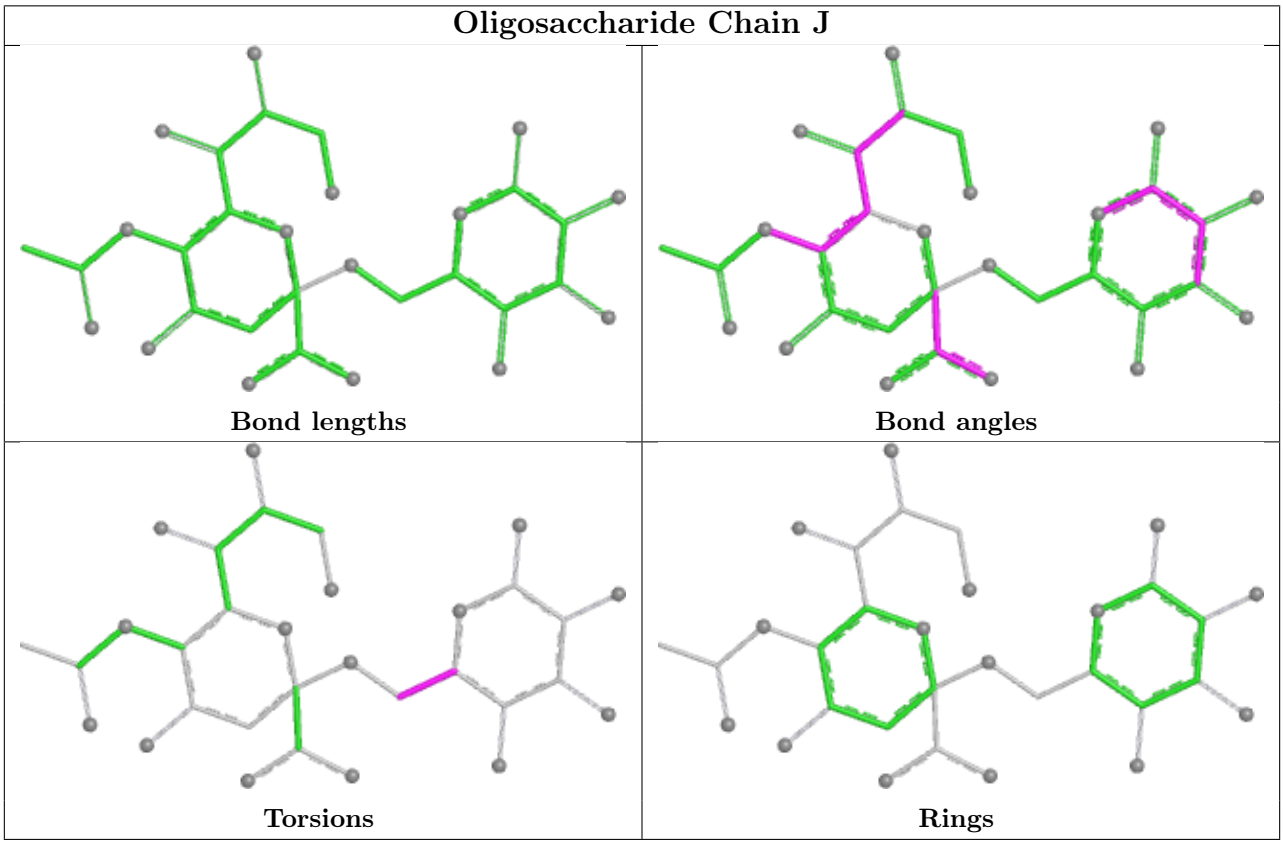
Mol	Chain	Res	Type	Atoms
2	J	1	GAL	O5-C5-C6-O6
2	J	1	GAL	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	SIA	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 oligosaccharide.



5.6 Ligand geometry (i)

1 ligand is 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	SIA	D	1497	-	21,21,21	0.77	0	24,31,31	1.30	2 (8%)

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	SIA	D	1497	-	-	2/20/38/38	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1497	SIA	C3-C2-C1	-3.19	106.92	112.84
3	D	1497	SIA	O6-C6-C5	2.74	112.35	109.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1497	SIA	O8-C8-C9-O9
3	D	1497	SIA	O1B-C1-C2-O2

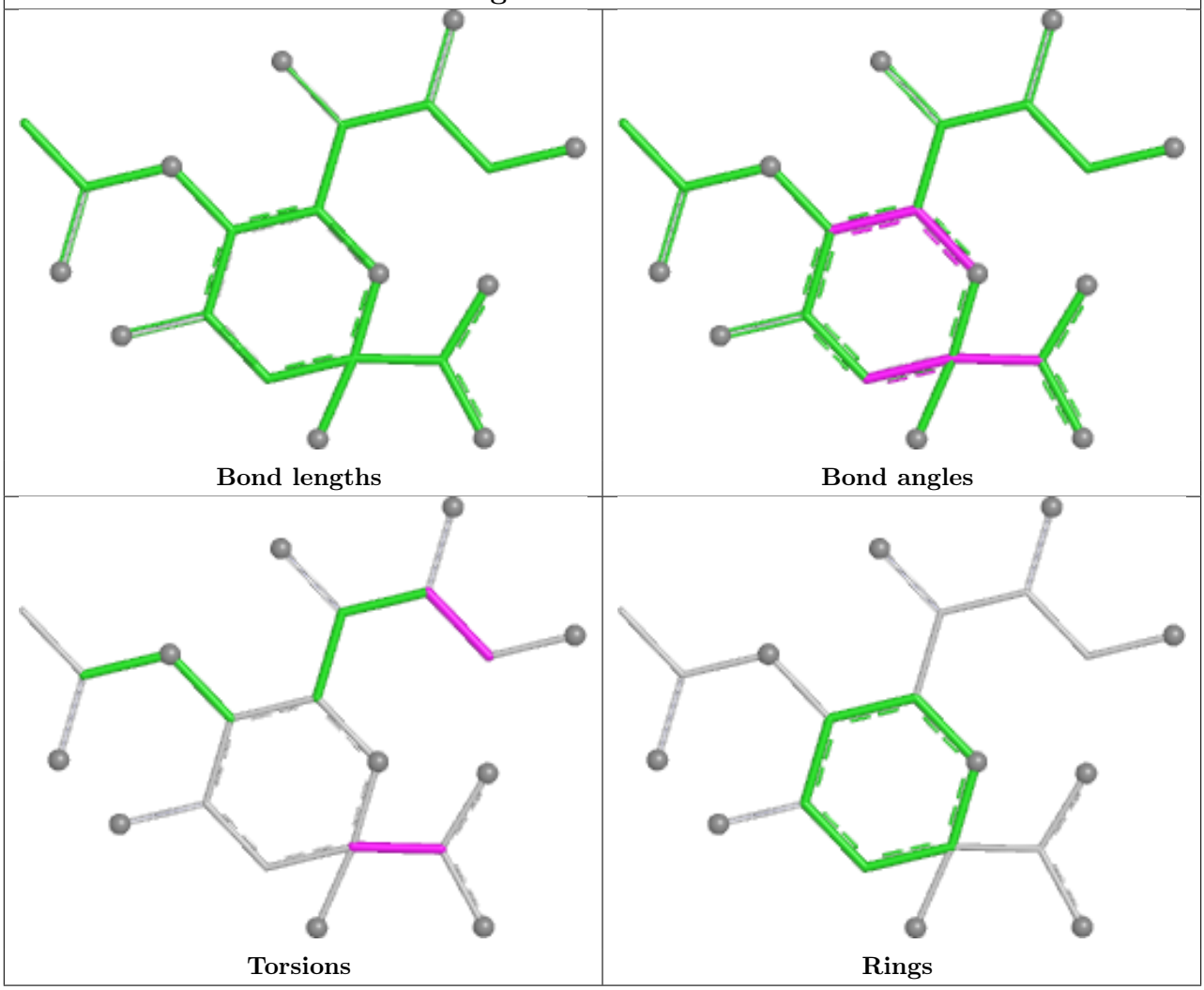
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1497	SIA	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 SIA D 1497



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	486/507 (95%)	-0.09	20 (4%)	37	18	23, 64, 148, 275	0
1	B	486/507 (95%)	0.09	23 (4%)	31	15	27, 66, 148, 278	0
1	C	486/507 (95%)	0.19	31 (6%)	19	8	24, 78, 160, 298	0
1	D	486/507 (95%)	0.22	43 (8%)	10	4	26, 71, 222, 378	0
1	E	486/507 (95%)	0.50	59 (12%)	4	1	31, 94, 232, 308	0
1	F	486/507 (95%)	0.39	39 (8%)	12	5	40, 96, 188, 258	0
1	G	486/507 (95%)	0.24	45 (9%)	8	3	20, 70, 182, 365	0
1	H	486/507 (95%)	0.51	50 (10%)	6	2	20, 73, 179, 367	0
1	I	486/507 (95%)	0.32	37 (7%)	13	5	26, 73, 195, 376	0
All	All	4374/4563 (95%)	0.26	347 (7%)	12	5	20, 76, 188, 378	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	263	GLY	14.6
1	G	265	SER	13.0
1	I	391	GLN	10.3
1	H	75	LEU	9.9
1	D	486	TYR	9.3
1	G	390	THR	9.1
1	I	390	THR	8.9
1	H	276	ASN	8.1
1	I	392	PHE	8.1
1	I	265	SER	7.7
1	I	276	ASN	7.6
1	D	348	ASP	7.3
1	H	265	SER	7.0
1	D	356	SER	6.7
1	F	460	LYS	6.7

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Mol	Chain	Res	Type	RSRZ
1	F	351	TYR	6.7
1	H	304	GLU	6.6
1	H	392	PHE	6.6
1	D	361	SER	6.3
1	G	221	GLU	6.3
1	H	262	ARG	6.3
1	D	460	LYS	6.3
1	G	111	SER	6.3
1	G	195	GLN	6.2
1	H	141	PHE	6.2
1	I	264	SER	6.1
1	I	51	ILE	6.1
1	F	469	PHE	5.9
1	B	358	ASP	5.8
1	G	264	SER	5.5
1	E	9	VAL	5.5
1	F	349	GLY	5.5
1	H	157	GLY	5.4
1	D	468	GLU	5.3
1	A	10	GLY	5.2
1	E	27	ASN	5.1
1	H	142	ASP	5.0
1	F	459	VAL	5.0
1	I	75	LEU	5.0
1	F	325	GLN	5.0
1	G	304	GLU	4.9
1	B	275	GLU	4.9
1	D	470	TYR	4.8
1	C	460	LYS	4.8
1	D	355	HIS	4.8
1	H	391	GLN	4.7
1	E	356	SER	4.7
1	F	478	MET	4.7
1	D	354	HIS	4.7
1	A	486	TYR	4.7
1	D	360	GLY	4.6
1	G	391	GLN	4.6
1	H	111	SER	4.6
1	G	263	GLY	4.5
1	I	15	ASN	4.5
1	D	456	ARG	4.5
1	B	475	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	261	LYS	4.4
1	D	455	LEU	4.4
1	G	49	ASN	4.4
1	E	8	CYS	4.4
1	E	10	GLY	4.4
1	E	352	GLY	4.3
1	H	303	GLY	4.3
1	E	355	HIS	4.3
1	D	487	ASP	4.3
1	I	49	ASN	4.2
1	C	141	PHE	4.2
1	H	49	ASN	4.2
1	E	467	PHE	4.2
1	I	111	SER	4.2
1	H	81	SER	4.1
1	I	472	LYS	4.1
1	F	350	TRP	4.1
1	F	348	ASP	4.1
1	F	159	ASN	4.1
1	E	90	ARG	4.1
1	E	359	GLN	4.0
1	H	389	ASN	4.0
1	I	262	ARG	4.0
1	G	325	GLN	3.9
1	C	487	ASP	3.9
1	A	276	ASN	3.9
1	F	27	ASN	3.9
1	H	394	ALA	3.9
1	A	15	ASN	3.8
1	H	8	CYS	3.8
1	C	10	GLY	3.8
1	G	266	GLY	3.8
1	E	477	CYS	3.8
1	H	390	THR	3.8
1	C	262	ARG	3.7
1	B	271	GLU	3.7
1	E	73	ARG	3.7
1	E	40	THR	3.7
1	G	276	ASN	3.6
1	F	10	GLY	3.6
1	E	275	GLU	3.6
1	E	325	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	345	GLY	3.6
1	E	461	GLU	3.5
1	I	48	LEU	3.5
1	G	389	ASN	3.5
1	D	353	TYR	3.4
1	E	478	MET	3.4
1	H	46	CYS	3.4
1	B	272	GLY	3.4
1	F	473	CYS	3.4
1	H	112	VAL	3.3
1	D	457	ASP	3.3
1	H	489	SER	3.3
1	E	493	GLU	3.3
1	E	358	ASP	3.3
1	E	289	ASN	3.3
1	F	187	GLU	3.3
1	F	458	ASN	3.2
1	E	141	PHE	3.2
1	B	460	LYS	3.2
1	D	371	GLN	3.2
1	H	137	GLY	3.2
1	D	340	GLU	3.2
1	G	81	SER	3.2
1	H	264	SER	3.2
1	E	473	CYS	3.2
1	F	476	GLU	3.2
1	E	7	ILE	3.2
1	E	463	GLY	3.2
1	H	360	GLY	3.2
1	D	15	ASN	3.2
1	A	358	ASP	3.2
1	A	16	SER	3.2
1	D	480	SER	3.2
1	F	474	ASP	3.2
1	G	194	TYR	3.2
1	H	395	VAL	3.1
1	D	484	GLY	3.1
1	F	470	TYR	3.1
1	A	487	ASP	3.1
1	H	114	HIS	3.1
1	I	172	GLY	3.1
1	C	277	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	303	GLY	3.1
1	B	472	LYS	3.1
1	C	8	CYS	3.1
1	F	276	ASN	3.1
1	G	305	CYS	3.1
1	B	359	GLN	3.1
1	B	50	GLY	3.0
1	G	79	GLU	3.0
1	I	393	GLU	3.0
1	E	466	CYS	3.0
1	E	353	TYR	3.0
1	D	459	VAL	3.0
1	D	489	SER	3.0
1	G	128	GLN	3.0
1	F	369	SER	3.0
1	H	47	LYS	3.0
1	H	487	ASP	3.0
1	E	492	GLU	3.0
1	H	7	ILE	3.0
1	A	352	GLY	3.0
1	D	362	GLY	3.0
1	D	322	ASN	2.9
1	G	196	ASN	2.9
1	I	290	THR	2.9
1	H	44	LYS	2.9
1	E	271	GLU	2.9
1	I	358	ASP	2.9
1	H	386	GLU	2.9
1	B	192	THR	2.9
1	C	364	ALA	2.9
1	G	32	HIS	2.9
1	D	338	PHE	2.9
1	I	136	GLN	2.9
1	H	53	PRO	2.9
1	C	475	ASP	2.9
1	D	90	ARG	2.9
1	I	489	SER	2.9
1	I	291	THR	2.9
1	A	489	SER	2.9
1	E	354	HIS	2.9
1	G	394	ALA	2.9
1	I	394	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	2.9
1	G	489	SER	2.8
1	D	477	CYS	2.8
1	H	280	LYS	2.8
1	D	471	HIS	2.8
1	E	246	SER	2.8
1	B	476	GLU	2.8
1	E	472	LYS	2.8
1	F	34	GLN	2.8
1	F	280	LYS	2.8
1	E	156	LYS	2.8
1	F	468	GLU	2.8
1	E	361	SER	2.8
1	G	303	GLY	2.8
1	D	347	VAL	2.8
1	I	280	LYS	2.8
1	H	325	GLN	2.8
1	D	364	ALA	2.7
1	H	195	GLN	2.7
1	E	11	TYR	2.7
1	F	471	HIS	2.7
1	G	114	HIS	2.7
1	G	140	VAL	2.7
1	G	190	GLN	2.7
1	I	388	MET	2.7
1	D	352	GLY	2.7
1	G	26	ARG	2.7
1	B	195	GLN	2.7
1	A	485	THR	2.7
1	E	128	GLN	2.7
1	D	381	VAL	2.7
1	B	311	SER	2.7
1	A	350	TRP	2.7
1	C	9	VAL	2.7
1	C	346	MET	2.6
1	D	481	VAL	2.6
1	B	467	PHE	2.6
1	C	136	GLN	2.6
1	H	359	GLN	2.6
1	F	375	ASP	2.6
1	C	340	GLU	2.6
1	E	21	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	387	LYS	2.6
1	C	351	TYR	2.6
1	F	456	ARG	2.6
1	G	222	VAL	2.6
1	E	475	ASP	2.6
1	G	42	ASN	2.6
1	H	42	ASN	2.6
1	F	58	ASP	2.6
1	A	324	PRO	2.6
1	G	220	PRO	2.6
1	D	345	GLY	2.5
1	H	159	ASN	2.5
1	E	465	GLY	2.5
1	E	487	ASP	2.5
1	B	289	ASN	2.5
1	C	454	GLN	2.5
1	E	351	TYR	2.5
1	E	239	TRP	2.5
1	F	461	GLU	2.5
1	D	142	ASP	2.5
1	E	158	SER	2.5
1	G	395	VAL	2.5
1	C	486	TYR	2.5
1	C	289	ASN	2.4
1	A	325	GLN	2.4
1	C	355	HIS	2.4
1	F	67	GLY	2.4
1	D	485	THR	2.4
1	E	155	LYS	2.4
1	B	273	THR	2.4
1	H	222	VAL	2.4
1	D	16	SER	2.4
1	D	491	TYR	2.4
1	E	12	HIS	2.4
1	I	79	GLU	2.4
1	F	90	ARG	2.4
1	G	191	ARG	2.4
1	D	323	VAL	2.4
1	B	474	ASP	2.4
1	A	17	THR	2.4
1	G	223	ASN	2.4
1	G	290	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	353	TYR	2.4
1	E	460	LYS	2.3
1	I	386	GLU	2.3
1	I	42	ASN	2.3
1	C	15	ASN	2.3
1	E	468	GLU	2.3
1	B	356	SER	2.3
1	D	49	ASN	2.3
1	B	141	PHE	2.3
1	E	28	VAL	2.3
1	E	191	ARG	2.3
1	C	361	SER	2.3
1	I	109	ILE	2.3
1	C	347	VAL	2.3
1	F	370	THR	2.3
1	I	266	GLY	2.3
1	E	462	LEU	2.3
1	A	29	THR	2.3
1	E	364	ALA	2.2
1	I	395	VAL	2.2
1	G	157	GLY	2.2
1	B	361	SER	2.2
1	G	288	ILE	2.2
1	I	191	ARG	2.2
1	E	311	SER	2.2
1	E	247	THR	2.2
1	F	277	CYS	2.2
1	D	472	LYS	2.2
1	I	110	SER	2.2
1	H	128	GLN	2.2
1	H	73	ARG	2.2
1	I	81	SER	2.2
1	C	7	ILE	2.2
1	G	112	VAL	2.1
1	H	310	LYS	2.1
1	H	393	GLU	2.1
1	I	53	PRO	2.1
1	A	362	GLY	2.1
1	A	472	LYS	2.1
1	C	125	ARG	2.1
1	H	260	SER	2.1
1	C	470	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	273	THR	2.1
1	C	137	GLY	2.1
1	I	256	GLY	2.1
1	G	143	ASN	2.1
1	H	305	CYS	2.1
1	C	360	GLY	2.1
1	F	330	GLY	2.1
1	H	388	MET	2.1
1	F	340	GLU	2.1
1	B	34	GLN	2.1
1	E	319	GLY	2.1
1	C	348	ASP	2.1
1	G	73	ARG	2.1
1	G	110	SER	2.1
1	A	124	ASP	2.1
1	G	186	ASP	2.1
1	B	9	VAL	2.1
1	G	75	LEU	2.1
1	G	392	PHE	2.1
1	C	321	ARG	2.1
1	H	300	LEU	2.1
1	E	39	LYS	2.0
1	C	344	GLN	2.0
1	G	158	SER	2.0
1	E	481	VAL	2.0
1	F	143	ASN	2.0
1	A	456	ARG	2.0
1	C	221	GLU	2.0
1	D	325	GLN	2.0
1	E	41	HIS	2.0
1	D	324	PRO	2.0
1	H	400	SER	2.0
1	E	127	THR	2.0
1	A	491	TYR	2.0
1	F	486	TYR	2.0
1	E	165	GLY	2.0
1	F	26	ARG	2.0
1	F	191	ARG	2.0

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

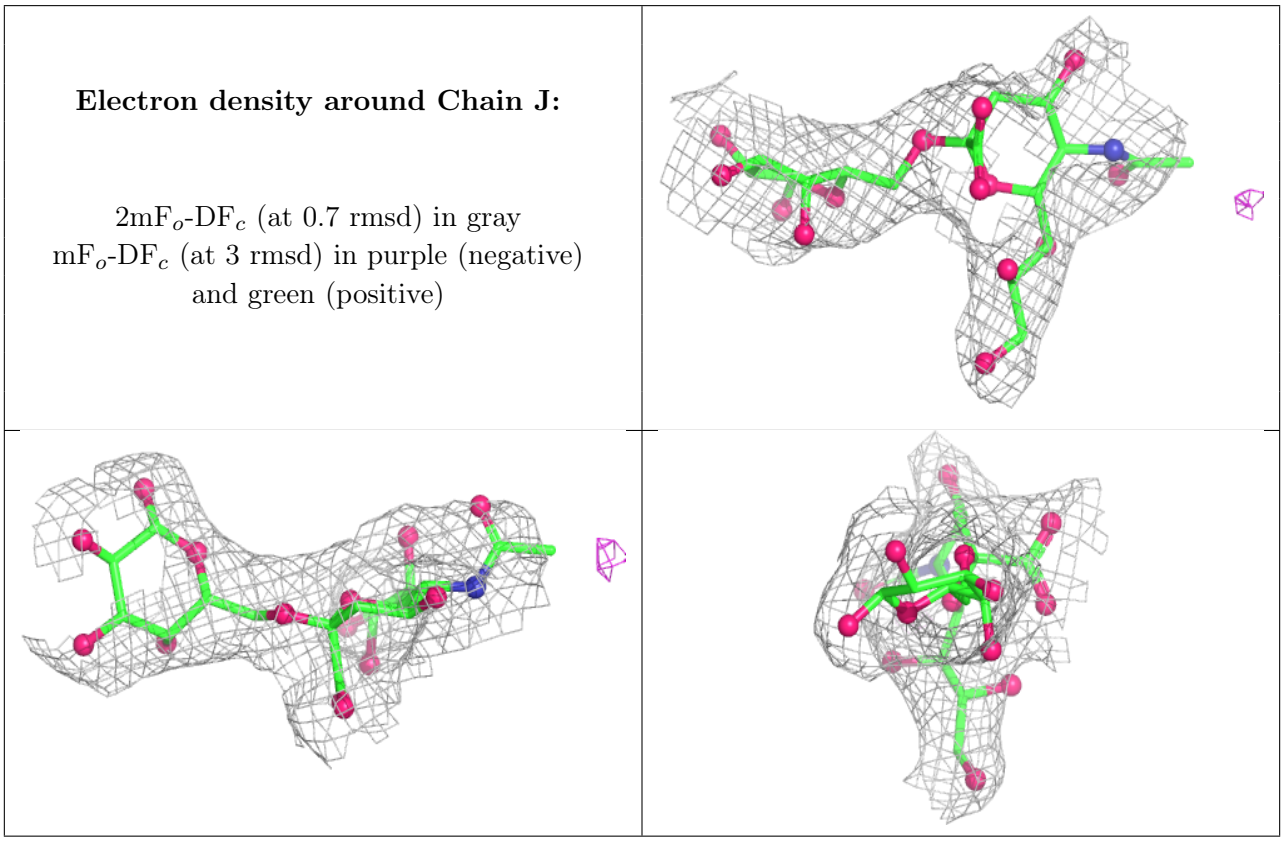
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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^2)	Q<0.9
2	GAL	J	1	12/12	0.88	0.16	89,89,89,89	0
2	SIA	J	2	20/21	0.90	0.16	89,89,89,89	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.

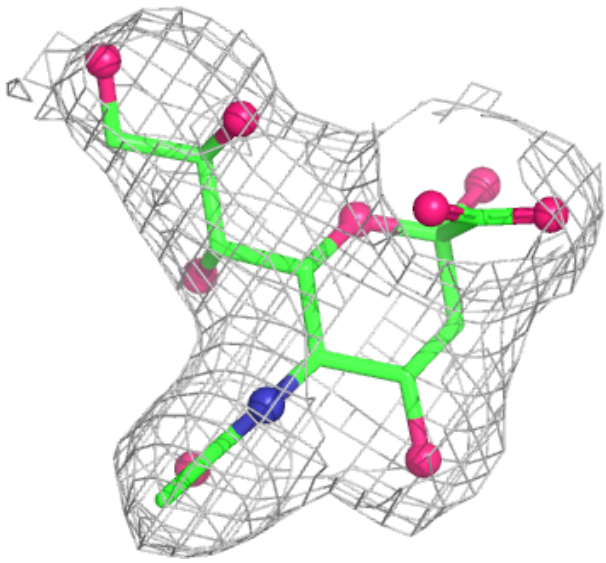
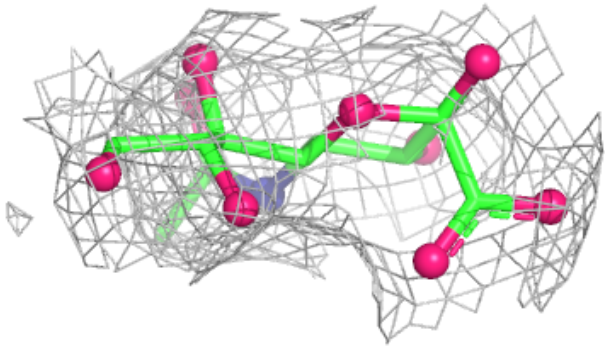
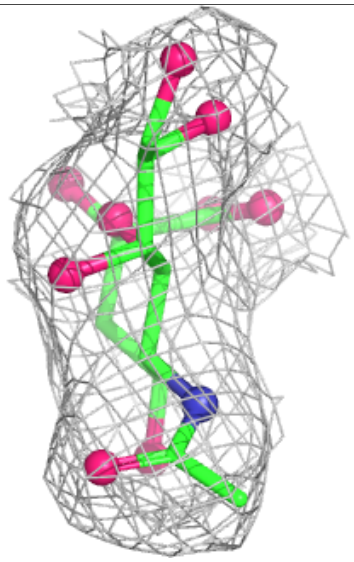


6.4 Ligands (i)

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, 95th 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^2)	Q<0.9
3	SIA	D	1497	21/21	0.92	0.17	52,52,52,52	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.

Electron density around SIA D 1497: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.