



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:56 AM GMT

PDB ID : 3GHG
Title : Crystal Structure of Human Fibrinogen
Authors : Doolittle, R.F.; Kollman, J.M.; Sawaya, M.R.; Pandi, L.; Riley, M.
Deposited on : 2009-03-03
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

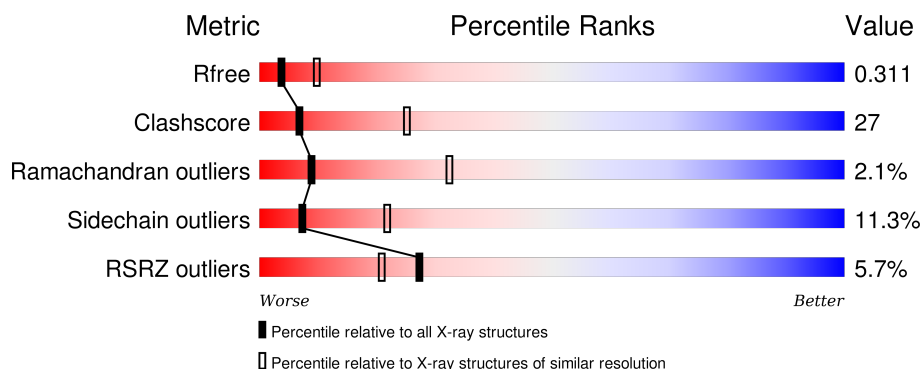
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	562	<div> <div>18% 12% . 69%</div> <div>6%</div> </div>
1	D	562	<div> <div>18% 12% . 69%</div> <div>6%</div> </div>
1	G	562	<div> <div>20% 10% . 69%</div> <div>2%</div> </div>
1	J	562	<div> <div>16% 15% . 67%</div> <div>4%</div> </div>
2	B	461	<div> <div>46% 34% 6% . 13%</div> <div>0%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	461	
2	H	461	
2	K	461	
3	C	411	
3	F	411	
3	I	411	
3	L	411	
4	M	4	
4	N	4	
4	Q	4	
4	R	4	
5	O	4	
5	P	4	
5	S	4	
5	T	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	B	470	-	-	X	-
6	GAL	B	478	X	-	-	-
6	NAG	E	470	X	-	-	-
6	GAL	E	478	X	-	-	-
6	NAG	K	470	-	-	X	-
6	GAL	K	478	X	-	-	-
7	NAG	H	470	X	-	-	-
8	NAG	L	570	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31833 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	D	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	G	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	J	186	Total	C	N	O	S	0	0	0
			1527	941	284	292	10			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	E	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	H	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	K	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	381	Total	C	N	O	S	0	0	0
			3050	1931	510	593	16			
3	F	382	Total	C	N	O	S	0	0	0
			3054	1933	511	594	16			
3	I	394	Total	C	N	O	S	0	0	0
			3145	1986	527	614	18			
3	L	391	Total	C	N	O	S	0	0	0
			3126	1974	524	610	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	408	ALA	-	SEE REMARK 999	UNP P02679
C	409	GLY	-	SEE REMARK 999	UNP P02679
C	410	ASP	-	SEE REMARK 999	UNP P02679
F	408	ALA	-	SEE REMARK 999	UNP P02679
F	409	GLY	-	SEE REMARK 999	UNP P02679
F	410	ASP	-	SEE REMARK 999	UNP P02679
I	408	ALA	-	SEE REMARK 999	UNP P02679
I	409	GLY	-	SEE REMARK 999	UNP P02679
I	410	ASP	-	SEE REMARK 999	UNP P02679
L	408	ALA	-	SEE REMARK 999	UNP P02679
L	409	GLY	-	SEE REMARK 999	UNP P02679
L	410	ASP	-	SEE REMARK 999	UNP P02679

- Molecule 4 is a protein called A knob.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	N	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	Q	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	R	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is a protein called B knob.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	P	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	S	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	T	4	Total	C	N	O	0	0	0
			33	19	9	5			

- Molecule 6 is a polymer of unknown type called SUGAR (11-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	11	Total	C	N	O	0	0
			151	84	6	61		
6	E	11	Total	C	N	O	0	0
			151	84	6	61		
6	K	11	Total	C	N	O	0	0
			151	84	6	61		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

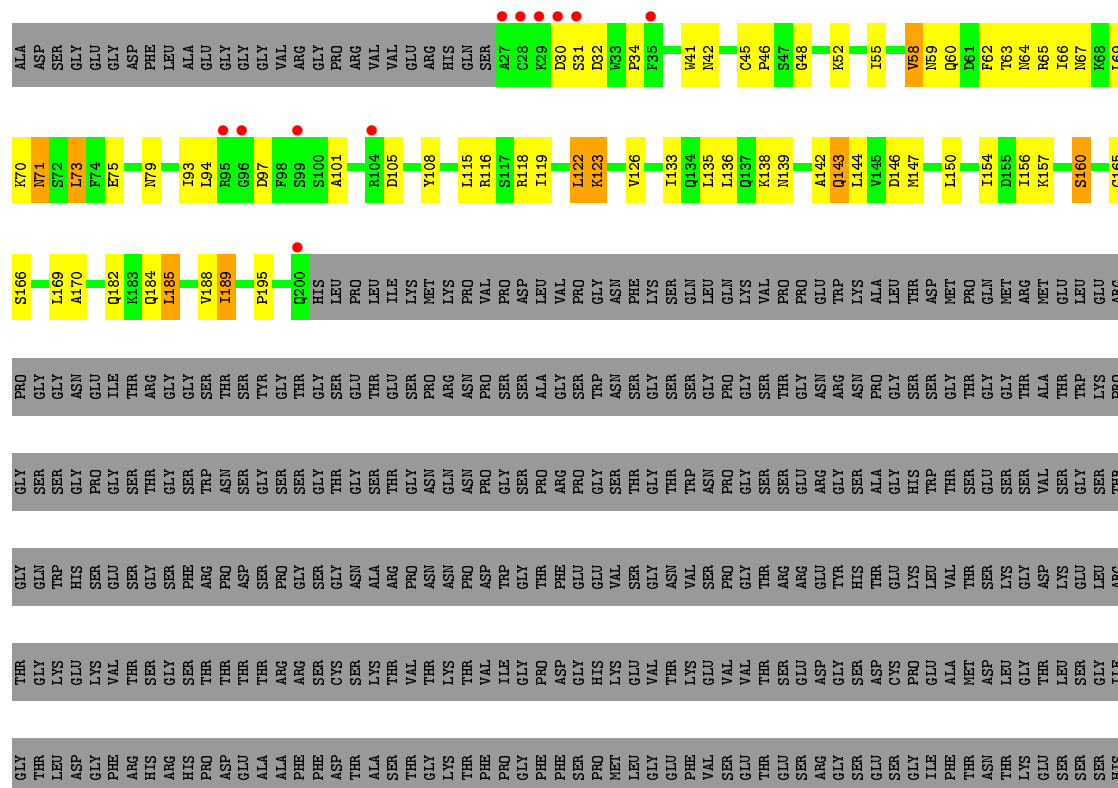
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

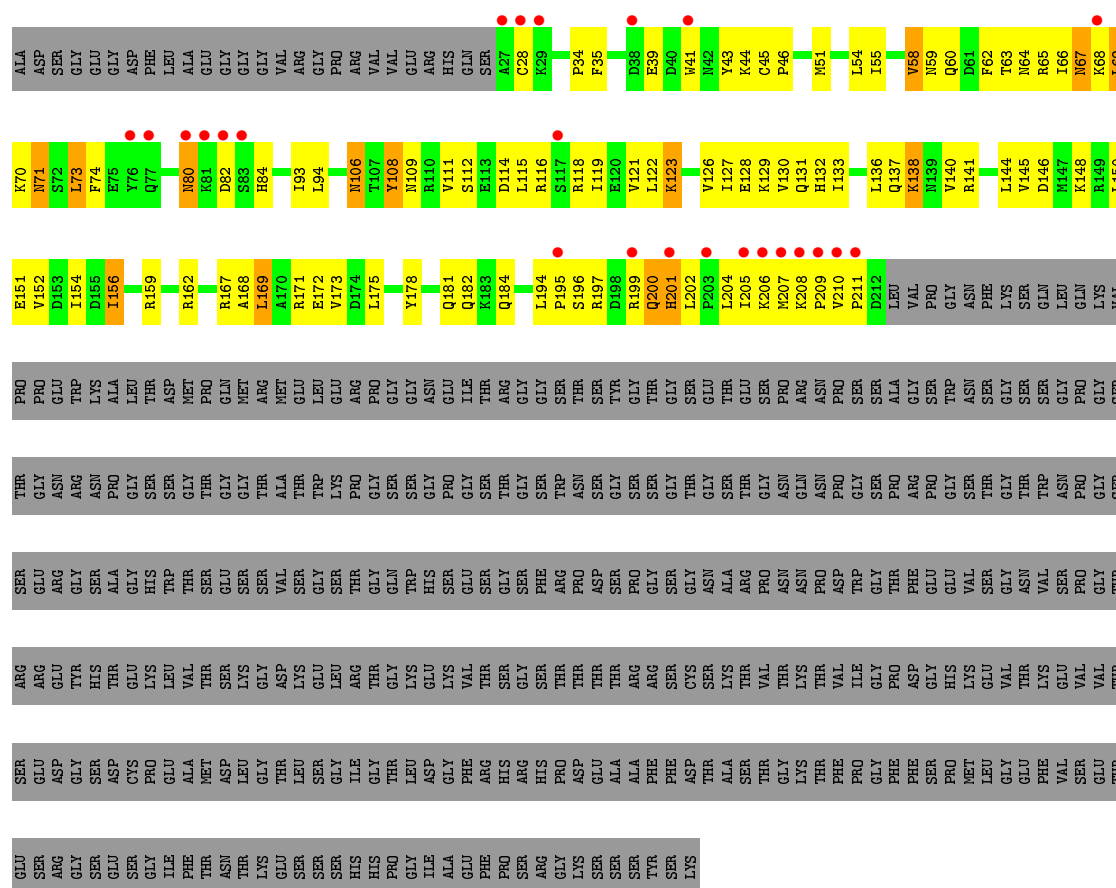
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	K	1	Total	Ca	0	0
			1	1		
9	E	1	Total	Ca	0	0
			1	1		
9	H	1	Total	Ca	0	0
			1	1		
9	B	1	Total	Ca	0	0
			1	1		
9	I	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		
9	L	1	Total	Ca	0	0
			1	1		
9	F	1	Total	Ca	0	0
			1	1		



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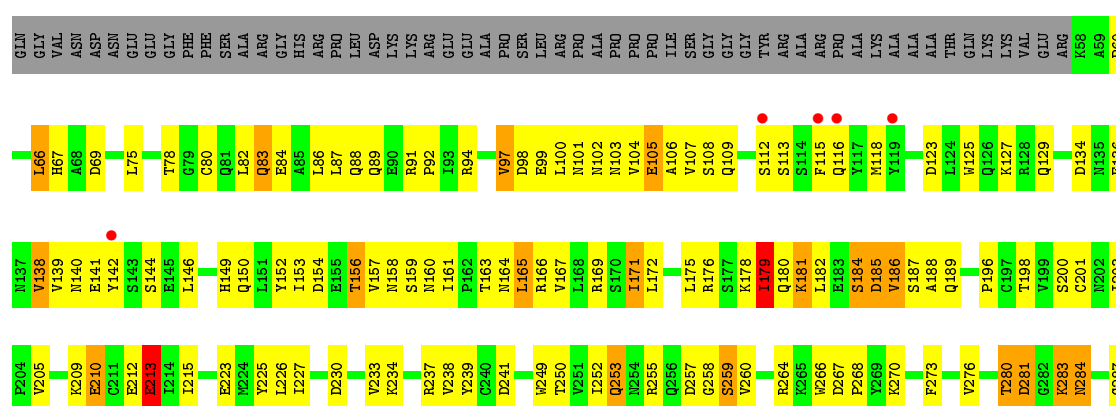
- Molecule 1: Fibrinogen alpha chain

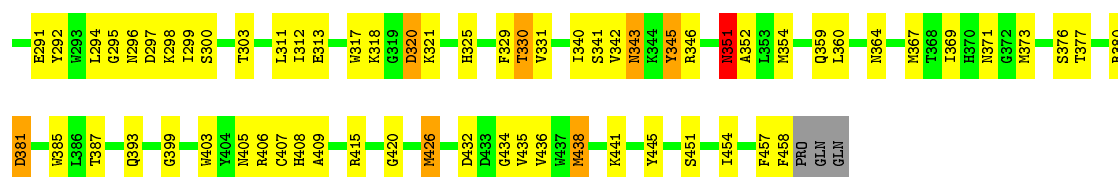
Chain J: 



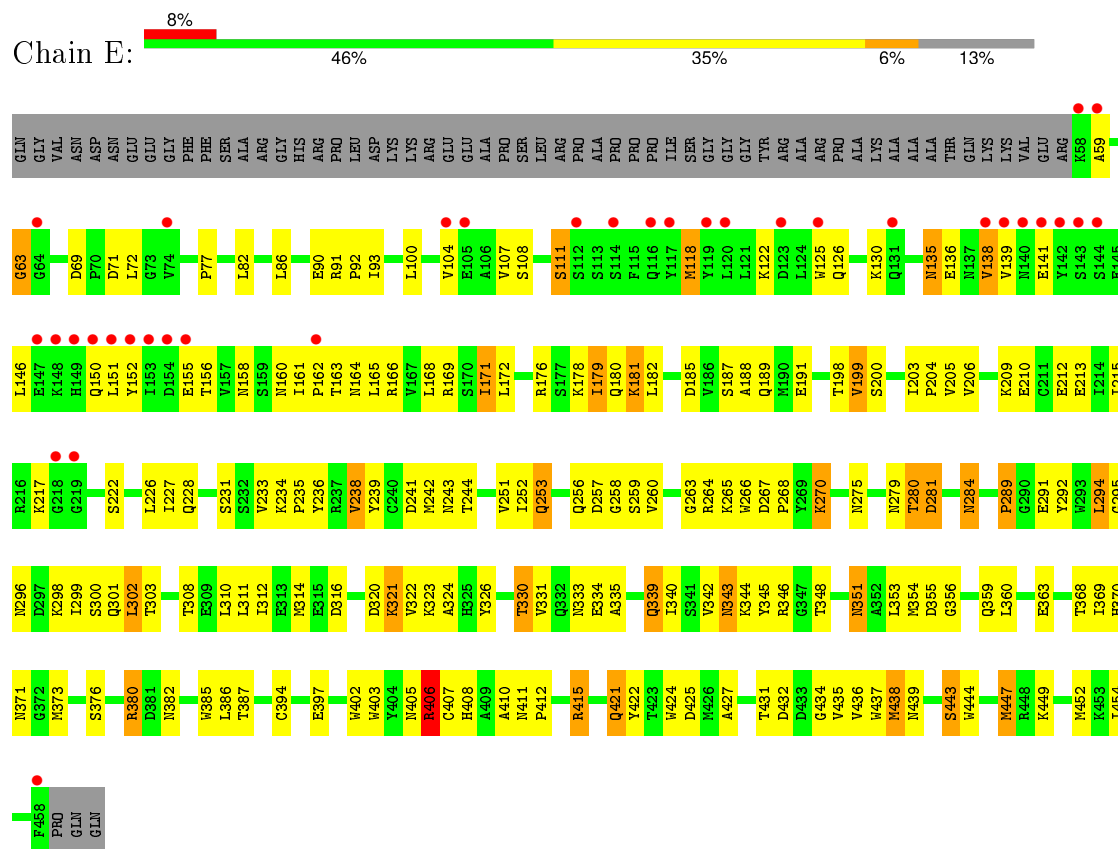
- Molecule 2: Fibrinogen beta chain

Chain B:  46% 34% 6% 13%

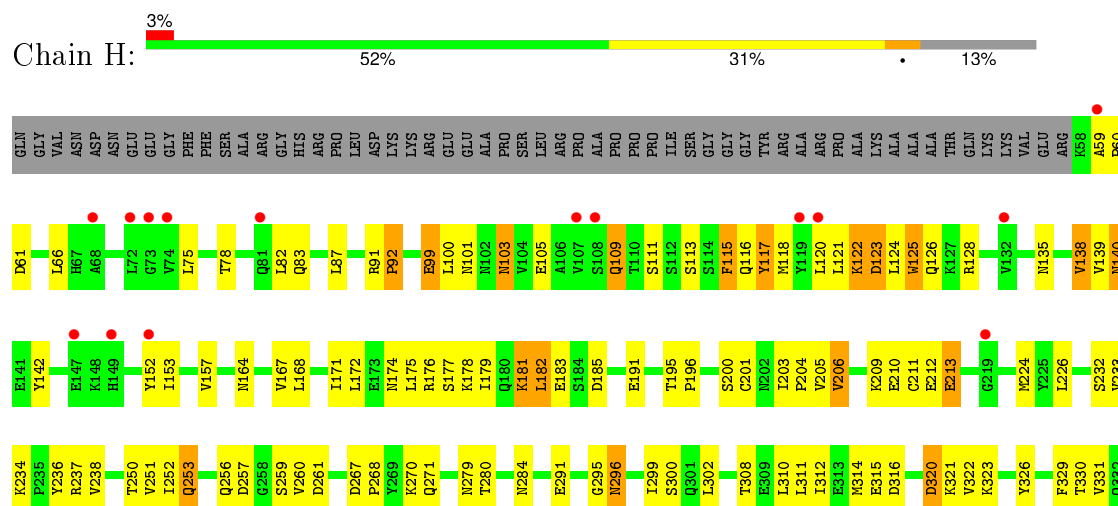


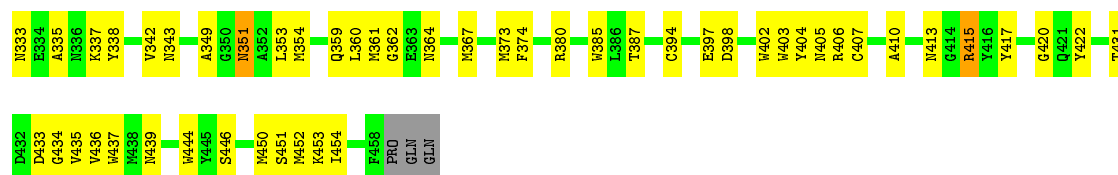


• Molecule 2: Fibrinogen beta chain

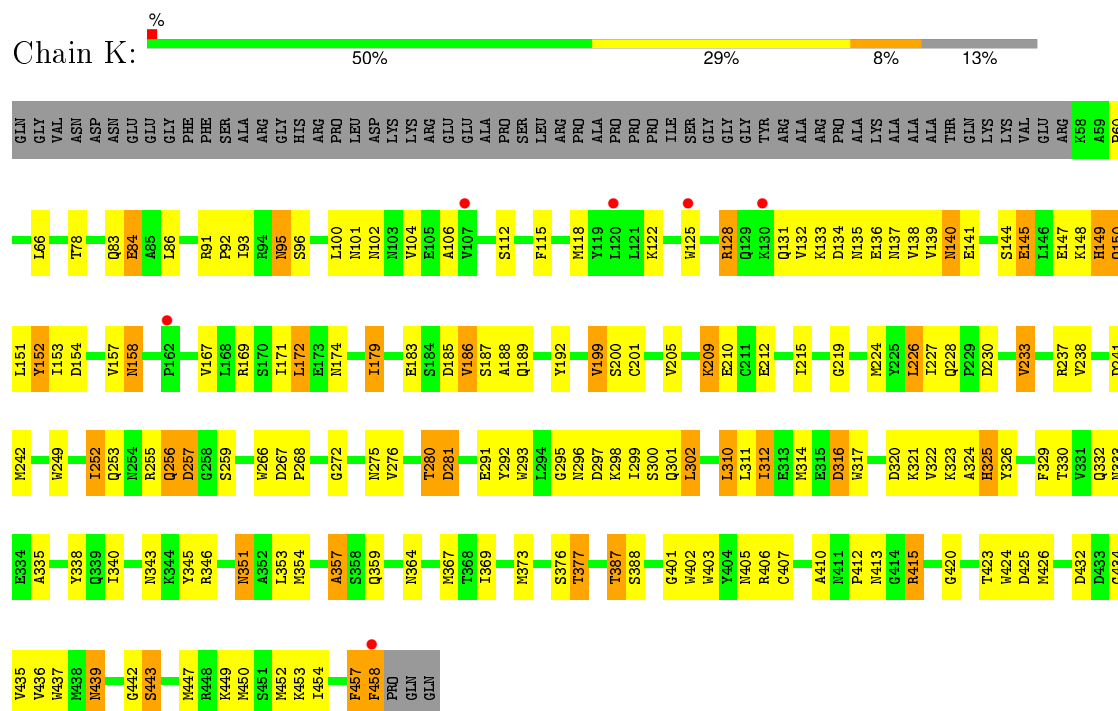


• Molecule 2: Fibrinogen beta chain

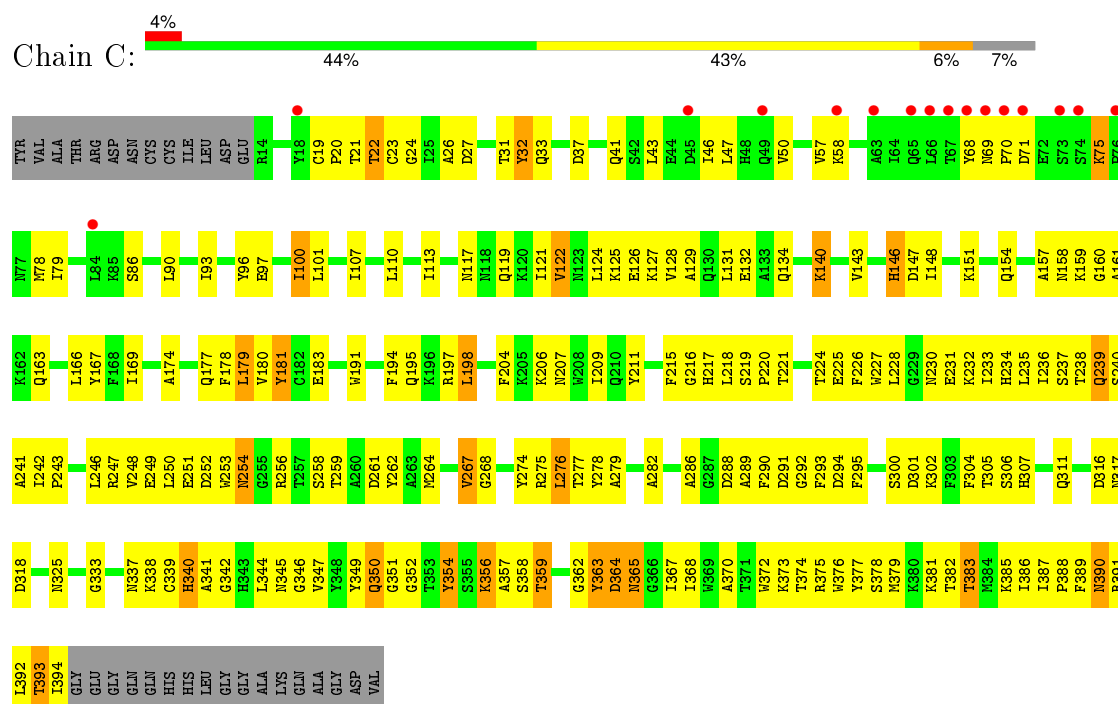




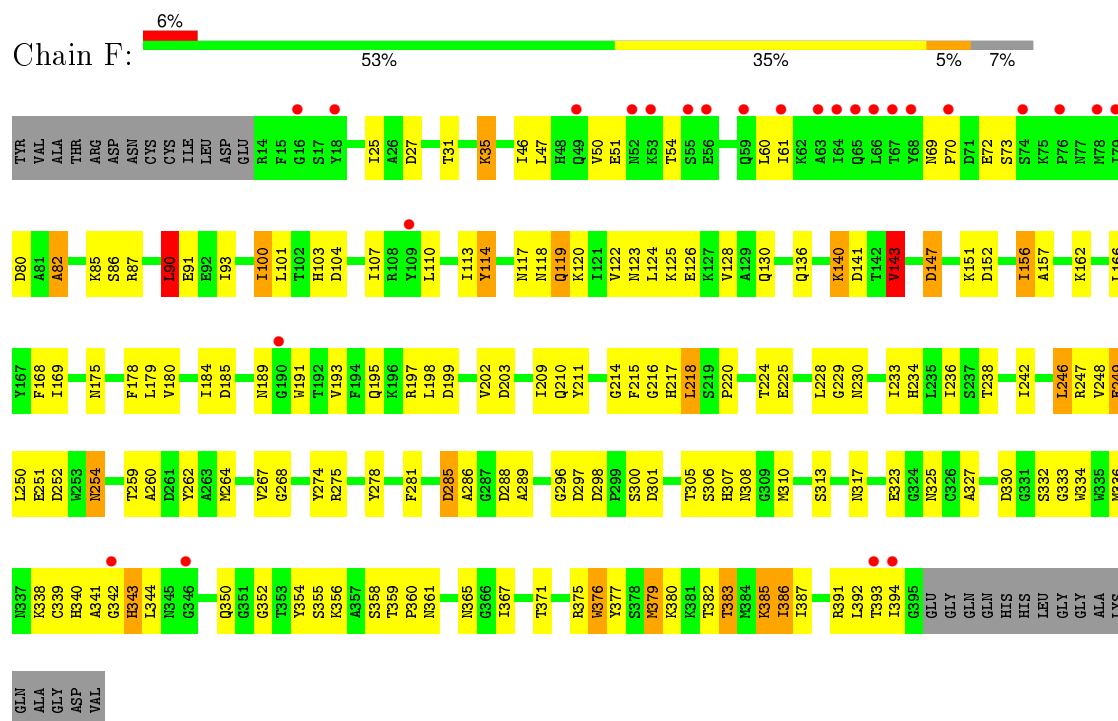
• Molecule 2: Fibrinogen beta chain



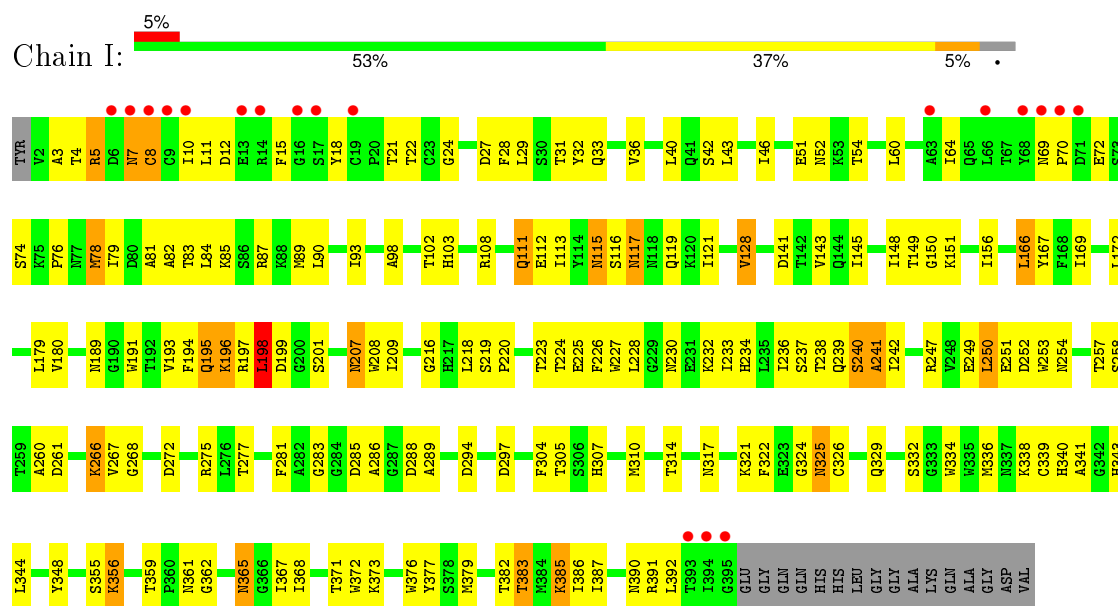
• Molecule 3: Fibrinogen gamma chain



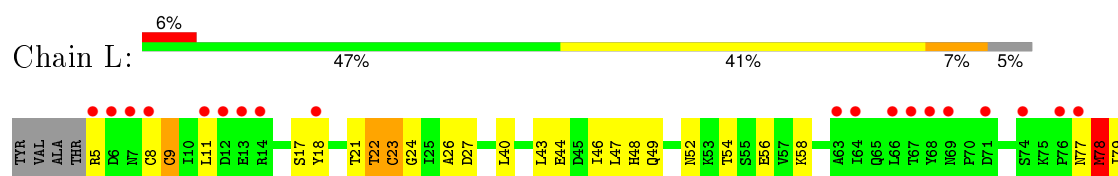
• Molecule 3: Fibrinogen gamma chain

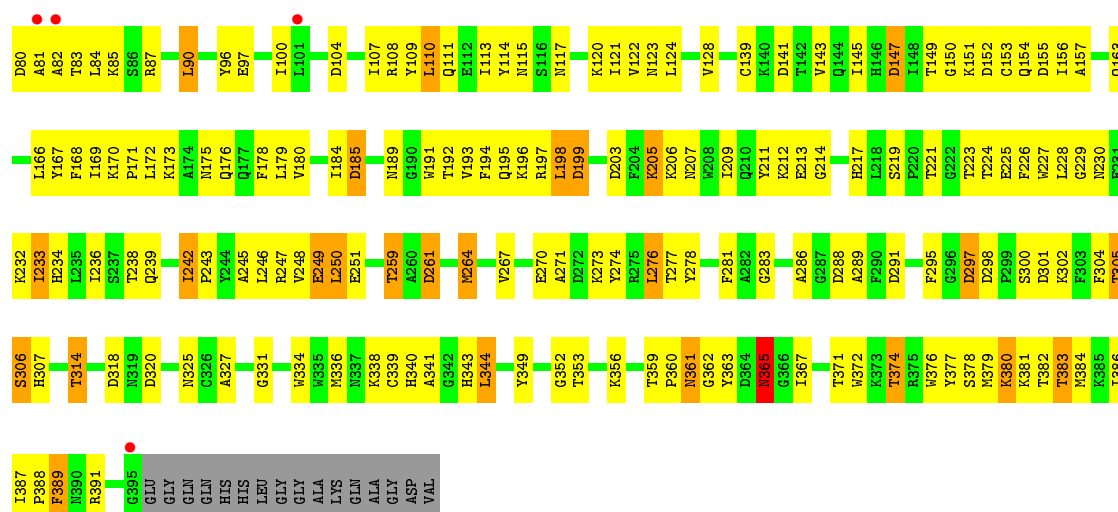


• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain





- Molecule 4: A knob

Chain M: 25% 50% 25%



- Molecule 4: A knob

Chain N: 75% 25%



- Molecule 4: A knob

Chain Q: 75% 25%



- Molecule 4: A knob

Chain R: 50% 50%



- Molecule 5: B knob

Chain O: 25% 75%



- Molecule 5: B knob

Chain P: 50% 50%



- Molecule 5: B knob



- Molecule 5: B knob



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.24Å 94.87Å 300.81Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.90) 69.4 (19.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.4.0061	Depositor
R, R_{free}	0.252 , 0.309 0.259 , 0.311	Depositor DCC
R_{free} test set	5820 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 75.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	23 of 116461 reflections (0.020%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31833	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2228e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, NDG, SIA, GAL, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/1447	0.61	0/1939
1	D	0.44	0/1447	0.56	0/1939
1	G	0.40	0/1447	0.54	0/1939
1	J	0.46	0/1547	0.62	0/2076
2	B	0.59	0/3283	0.73	0/4438
2	E	0.52	0/3283	0.62	0/4438
2	H	0.52	0/3283	0.65	0/4438
2	K	0.51	0/3283	0.65	0/4438
3	C	0.83	2/3125 (0.1%)	0.84	2/4224 (0.0%)
3	F	0.46	0/3129	0.57	1/4229 (0.0%)
3	I	0.53	0/3220	0.63	0/4353
3	L	0.55	0/3201	0.65	0/4326
4	M	0.80	0/31	0.89	0/40
4	N	0.46	0/31	0.62	0/40
4	Q	0.74	0/31	0.62	0/40
4	R	0.74	0/31	0.59	0/40
5	O	0.57	0/34	0.72	0/43
5	P	0.48	0/34	0.67	0/43
5	S	0.47	0/34	0.59	0/43
5	T	0.56	0/34	0.86	0/43
All	All	0.55	2/31955 (0.0%)	0.66	3/43109 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B	1	0
6	E	2	0
6	K	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	H	1	0
All	All	5	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	TYR	CG-CD1	-5.83	1.31	1.39
3	C	181	TYR	CG-CD2	-5.10	1.32	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	90	LEU	CA-CB-CG	5.60	128.18	115.30
3	C	364	ASP	CB-CG-OD1	5.47	123.22	118.30
3	C	363	TYR	CA-CB-CG	5.25	123.38	113.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	478	GAL	C1
6	E	470	NAG	C1
6	E	478	GAL	C1
7	H	470	NAG	C1
6	K	478	GAL	C1

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	1431	0	1424	104	0
1	D	1431	0	1424	72	0
1	G	1431	0	1424	78	0
1	J	1527	0	1533	140	1
2	B	3209	0	3042	210	0
2	E	3209	0	3042	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	3209	0	3041	159	0
2	K	3209	0	3043	192	0
3	C	3050	0	2906	209	0
3	F	3054	0	2909	157	0
3	I	3145	0	2993	186	1
3	L	3126	0	2972	239	0
4	M	30	0	32	2	0
4	N	30	0	32	0	0
4	Q	30	0	32	0	0
4	R	30	0	32	1	0
5	O	33	0	32	3	0
5	P	33	0	32	2	0
5	S	33	0	32	4	0
5	T	33	0	32	4	0
6	B	151	0	126	25	0
6	E	151	0	126	16	0
6	K	151	0	126	18	0
7	H	61	0	52	8	0
8	L	28	0	25	12	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
All	All	31833	0	30464	1667	1

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 27.

All (1667) 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)
2:K:364:ASN:HD21	6:K:470:NAG:C1	1.17	1.55
2:B:364:ASN:ND2	6:B:470:NAG:C1	1.70	1.52
2:K:364:ASN:ND2	6:K:470:NAG:C1	1.85	1.38
3:L:56:GLU:HB2	8:L:570:NAG:O3	1.20	1.32
2:H:172:LEU:HD21	3:I:113:ILE:CG2	1.70	1.19
1:J:108:TYR:OH	3:L:83:THR:C	1.85	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:115:LEU:CD2	3:L:90:LEU:HD21	1.78	1.14
1:A:115:LEU:HD21	3:C:90:LEU:HD13	1.23	1.13
3:I:10:ILE:O	3:I:18:TYR:OH	1.65	1.12
2:K:302:LEU:HD22	2:K:454:ILE:HD11	1.31	1.11
1:G:108:TYR:CE2	3:I:82:ALA:HB1	1.86	1.11
3:I:12:ASP:HB3	3:I:15:PHE:HD1	0.99	1.09
3:I:12:ASP:CB	3:I:15:PHE:HD1	1.65	1.08
6:K:471:NDG:H6C2	6:K:477:NDG:H8C2	1.17	1.07
1:G:154:ILE:HD11	3:I:128:VAL:HG21	1.28	1.07
1:J:108:TYR:OH	3:L:84:LEU:N	1.87	1.07
3:I:12:ASP:HB3	3:I:15:PHE:CD1	1.90	1.06
1:A:55:ILE:HG23	2:B:86:LEU:HD21	1.35	1.06
3:I:27:ASP:O	3:I:31:THR:HG23	1.56	1.06
1:J:115:LEU:HD21	3:L:90:LEU:HD21	1.12	1.06
1:A:108:TYR:O	1:A:112:SER:OG	1.74	1.05
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.34	1.04
3:L:49:GLN:NE2	8:L:570:NAG:H81	1.72	1.02
3:L:359:THR:HG21	3:L:363:TYR:O	1.59	1.02
1:G:119:ILE:HD11	3:I:93:ILE:CD1	1.89	1.01
1:A:119:ILE:HD13	3:C:93:ILE:HD13	1.43	1.01
2:B:252:ILE:HD11	2:B:454:ILE:HD13	1.02	1.01
2:H:172:LEU:HD21	3:I:113:ILE:HG21	1.39	1.01
3:L:52:ASN:ND2	8:L:570:NAG:C1	2.24	1.01
1:G:154:ILE:CD1	3:I:128:VAL:HG21	1.90	0.99
1:D:135:LEU:HD22	1:D:136:LEU:HD22	1.43	0.99
1:G:105:ASP:OD1	3:I:79:ILE:HD11	1.63	0.98
1:J:60:GLN:O	1:J:64:ASN:OD1	1.81	0.98
2:B:154:ASP:OD1	3:C:96:TYR:OH	1.79	0.98
1:A:115:LEU:CD2	3:C:90:LEU:HD13	1.94	0.97
1:J:108:TYR:CE1	3:L:83:THR:HB	1.99	0.97
1:J:207:MET:HB2	2:K:135:ASN:HD21	1.21	0.97
1:G:55:ILE:HD12	2:H:82:LEU:HD22	1.44	0.97
3:I:8:CYS:SG	3:I:18:TYR:CE2	2.58	0.97
3:I:8:CYS:SG	3:I:18:TYR:CD2	2.58	0.97
1:G:119:ILE:HD11	3:I:93:ILE:HD11	1.48	0.95
3:L:56:GLU:HB2	8:L:570:NAG:HO3	1.21	0.95
3:L:219:SER:H	3:L:224:THR:HG21	1.29	0.95
2:B:159:SER:O	2:B:163:THR:HG23	1.67	0.95
3:L:56:GLU:CB	8:L:570:NAG:O3	2.15	0.94
2:E:241:ASP:OD1	2:E:244:THR:OG1	1.85	0.94
1:J:115:LEU:HD13	3:L:90:LEU:HD11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:ILE:HD11	2:B:454:ILE:CD1	1.97	0.93
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.51	0.92
2:H:310:LEU:HD12	2:H:311:LEU:N	1.85	0.92
2:E:222:SER:OG	2:E:242:MET:N	2.01	0.92
2:H:252:ILE:HD12	2:H:454:ILE:HG23	1.50	0.92
2:B:239:TYR:OH	2:B:287:GLY:O	1.85	0.91
2:B:230:ASP:O	2:B:233:VAL:HG12	1.69	0.91
3:I:12:ASP:CB	3:I:15:PHE:CD1	2.51	0.90
3:C:390:ASN:HD22	3:C:391:ARG:N	1.69	0.90
1:J:115:LEU:HD21	3:L:90:LEU:CD2	2.00	0.90
2:B:252:ILE:CD1	2:B:454:ILE:HD13	1.96	0.89
2:H:172:LEU:CD2	3:I:113:ILE:HG21	2.02	0.89
3:F:323:GLU:N	3:F:323:GLU:OE2	2.05	0.89
3:C:307:HIS:HE1	3:C:342:GLY:H	1.21	0.88
3:L:52:ASN:ND2	8:L:570:NAG:O5	2.07	0.88
1:A:55:ILE:HD12	2:B:82:LEU:HD22	1.53	0.88
1:J:108:TYR:HH	3:L:84:LEU:N	1.69	0.88
1:A:144:LEU:HD13	2:B:175:LEU:HD11	1.54	0.88
2:H:135:ASN:O	2:H:139:VAL:HG23	1.74	0.87
2:B:172:LEU:HB3	3:C:113:ILE:HG21	1.57	0.87
1:J:184:GLN:HE21	2:K:167:VAL:HG23	1.37	0.87
3:L:219:SER:OG	3:L:224:THR:HG22	1.74	0.86
2:K:201:CYS:O	3:L:143:VAL:HG21	1.74	0.86
1:A:55:ILE:HG23	2:B:86:LEU:CD2	2.04	0.85
1:J:169:LEU:HB2	2:K:189:GLN:HE22	1.41	0.85
1:J:148:LYS:HZ1	2:K:425:ASP:CG	1.79	0.85
2:E:222:SER:HG	2:E:242:MET:H	1.19	0.85
3:L:49:GLN:NE2	8:L:570:NAG:C8	2.39	0.85
3:I:219:SER:OG	3:I:224:THR:HG22	1.77	0.85
2:H:210:GLU:OE2	2:H:212:GLU:N	2.09	0.84
1:J:69:LEU:HD11	2:K:100:LEU:HD13	1.56	0.84
1:A:122:LEU:HD11	2:B:153:ILE:HG21	1.60	0.83
1:A:73:LEU:HD23	2:B:104:VAL:HG22	1.60	0.83
3:F:246:LEU:HD11	3:F:248:VAL:HG23	1.59	0.83
2:H:172:LEU:HD21	3:I:113:ILE:CB	2.08	0.83
2:E:172:LEU:CD2	3:F:113:ILE:HG23	2.07	0.83
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.61	0.83
2:H:302:LEU:HD22	2:H:454:ILE:CD1	2.09	0.82
2:K:310:LEU:HD12	2:K:311:LEU:N	1.94	0.82
3:L:52:ASN:HD22	8:L:570:NAG:C1	1.91	0.82
3:C:194:PHE:CD1	3:C:233:ILE:CD1	2.63	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ASN:CG	6:B:470:NAG:C1	2.46	0.82
1:A:59:ASN:HD21	2:B:86:LEU:HD23	1.41	0.82
2:H:252:ILE:HD11	2:H:454:ILE:HD13	1.60	0.82
1:J:207:MET:HB2	2:K:135:ASN:ND2	1.95	0.82
2:K:133:LYS:O	2:K:136:GLU:HG2	1.79	0.82
2:K:343:ASN:HA	2:K:354:MET:SD	2.21	0.81
1:J:115:LEU:HD13	3:L:90:LEU:CD1	2.11	0.80
2:E:212:GLU:O	2:E:215:ILE:HG22	1.81	0.80
2:H:310:LEU:HD12	2:H:311:LEU:H	1.46	0.80
3:C:254:ASN:N	3:C:254:ASN:HD22	1.79	0.80
2:K:423:THR:OG1	2:K:425:ASP:OD1	1.99	0.80
1:A:123:LYS:HA	1:A:126:VAL:HG12	1.62	0.80
1:G:93:ILE:HG22	1:G:94:LEU:HD12	1.62	0.80
3:C:215:PHE:CE2	3:C:227:TRP:HB3	2.17	0.80
3:C:179:LEU:HD22	3:C:218:LEU:HD13	1.63	0.79
3:I:208:TRP:HA	3:I:314:THR:HG21	1.64	0.79
3:F:234:HIS:ND1	3:F:267:VAL:O	2.11	0.79
2:B:354:MET:O	2:B:369:ILE:HD13	1.81	0.79
1:D:119:ILE:HD11	3:F:93:ILE:HD13	1.64	0.79
3:C:253:TRP:C	3:C:254:ASN:HD22	1.85	0.79
6:K:471:NDG:H6C2	6:K:477:NDG:C8	2.09	0.79
2:K:295:GLY:O	2:K:299:ILE:HG13	1.83	0.79
2:H:252:ILE:CD1	2:H:454:ILE:HG23	2.12	0.79
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.62	0.79
3:F:46:ILE:O	3:F:50:VAL:HG22	1.83	0.79
1:A:119:ILE:HD13	3:C:93:ILE:CD1	2.14	0.78
3:C:307:HIS:CE1	3:C:342:GLY:H	2.02	0.78
1:G:58:VAL:HG21	3:I:29:LEU:HD11	1.66	0.78
2:B:179:ILE:HG23	2:B:180:GLN:N	1.98	0.78
1:J:108:TYR:CZ	3:L:83:THR:HB	2.18	0.78
1:J:205:ILE:HG13	2:K:138:VAL:HG11	1.65	0.78
2:B:351:ASN:C	2:B:351:ASN:HD22	1.87	0.78
2:E:343:ASN:HA	2:E:354:MET:SD	2.24	0.78
1:A:69:LEU:HD12	2:B:100:LEU:HD13	1.67	0.77
2:E:326:TYR:CE1	2:E:353:LEU:HD12	2.19	0.77
2:E:165:LEU:HD21	3:F:107:ILE:HD12	1.64	0.77
1:A:71:ASN:HD22	1:A:72:SER:N	1.82	0.77
3:F:296:GLY:N	3:F:301:ASP:OD2	2.18	0.77
2:B:252:ILE:HD12	2:B:454:ILE:HG23	1.67	0.77
1:J:46:PRO:O	3:L:22:THR:HG21	1.85	0.77
2:E:203:ILE:HG22	2:E:204:PRO:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:210:GLU:OE2	2:K:212:GLU:N	2.14	0.76
2:H:78:THR:HG23	1:J:43:TYR:O	1.84	0.76
3:I:8:CYS:SG	3:I:18:TYR:HD2	2.06	0.76
2:B:165:LEU:HD11	3:C:107:ILE:CD1	2.15	0.76
1:A:55:ILE:CD1	2:B:82:LEU:HD22	2.16	0.76
3:C:246:LEU:HD21	3:C:248:VAL:CG2	2.16	0.76
3:C:364:ASP:O	3:C:364:ASP:OD1	2.04	0.76
3:I:8:CYS:SG	3:I:18:TYR:HE2	2.06	0.76
3:I:281:PHE:CE2	3:I:283:GLY:HA2	2.20	0.76
3:F:246:LEU:HD12	3:F:247:ARG:N	2.00	0.76
2:K:312:ILE:HB	2:K:324:ALA:HB3	1.67	0.76
3:I:143:VAL:O	3:I:143:VAL:HG23	1.84	0.76
1:A:122:LEU:HD11	2:B:153:ILE:CG2	2.16	0.76
2:H:434:GLY:O	2:H:436:VAL:HG23	1.85	0.75
3:I:260:ALA:HB2	3:I:286:ALA:HB3	1.66	0.75
1:J:63:THR:HA	1:J:66:ILE:HG22	1.68	0.75
1:G:69:LEU:HD12	2:H:100:LEU:HD13	1.68	0.75
3:L:246:LEU:HD12	3:L:247:ARG:N	2.02	0.75
2:K:149:HIS:C	2:K:149:HIS:ND1	2.39	0.75
3:F:90:LEU:HD22	3:F:91:GLU:N	2.02	0.75
2:B:320:ASP:N	2:B:320:ASP:OD2	2.16	0.74
2:K:252:ILE:HD12	2:K:452:MET:C	2.08	0.74
1:A:122:LEU:CD1	2:B:153:ILE:HG21	2.17	0.74
3:L:77:ASN:HA	3:L:82:ALA:HB2	1.69	0.74
1:J:69:LEU:HD13	1:J:69:LEU:C	2.08	0.74
2:H:367:MET:SD	2:H:406:ARG:HD3	2.28	0.74
3:C:90:LEU:O	3:C:93:ILE:HG22	1.87	0.74
3:I:207:ASN:HD21	3:I:209:ILE:HD13	1.51	0.74
1:J:128:GLU:O	1:J:132:HIS:ND1	2.21	0.74
2:K:439:ASN:HD22	2:K:439:ASN:N	1.86	0.74
2:B:205:VAL:O	2:B:205:VAL:HG12	1.87	0.73
3:I:141:ASP:CG	3:I:143:VAL:HG22	2.07	0.73
2:E:181:LYS:O	2:E:185:ASP:HB2	1.87	0.73
3:L:198:LEU:HD13	3:L:199:ASP:N	2.02	0.73
1:D:55:ILE:HG23	2:E:86:LEU:HD13	1.69	0.73
2:B:381:ASP:HB2	2:B:393:GLN:HE21	1.54	0.73
2:B:169:ARG:HA	3:C:110:LEU:HD21	1.69	0.73
1:J:66:ILE:HG23	1:J:67:ASN:HD22	1.54	0.73
2:K:412:PRO:HG3	2:K:450:MET:HE3	1.71	0.73
6:K:470:NAG:O3	6:K:471:NDG:H2	1.90	0.72
2:H:172:LEU:CD2	3:I:113:ILE:CG2	2.58	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:ALA:HB1	2:H:60:PRO:HD2	1.70	0.72
2:H:201:CYS:O	3:I:143:VAL:HG21	1.88	0.72
3:F:218:LEU:N	3:F:218:LEU:HD23	2.04	0.72
3:C:368:ILE:CG2	3:C:377:TYR:O	2.37	0.72
3:I:219:SER:OG	3:I:224:THR:CG2	2.37	0.72
3:L:203:ASP:O	3:L:206:LYS:NZ	2.23	0.72
1:D:86:LEU:HD23	3:F:61:ILE:HD12	1.71	0.72
2:K:364:ASN:ND2	6:K:470:NAG:C2	2.52	0.71
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.72	0.71
3:L:334:TRP:HH2	3:L:344:LEU:HD12	1.54	0.71
3:L:344:LEU:HA	3:L:367:ILE:HG23	1.72	0.71
1:J:129:LYS:O	1:J:133:ILE:HD13	1.91	0.71
2:K:172:LEU:HD22	3:L:113:ILE:HG23	1.70	0.71
3:L:213:GLU:O	3:L:232:LYS:NZ	2.20	0.71
1:J:127:ILE:HA	1:J:130:VAL:HG12	1.70	0.71
3:L:318:ASP:OD1	3:L:325:ASN:ND2	2.22	0.71
3:C:194:PHE:CD1	3:C:233:ILE:HD13	2.25	0.71
3:C:295:PHE:CE1	3:C:305:THR:HG21	2.25	0.71
1:J:148:LYS:NZ	2:K:425:ASP:CG	2.42	0.71
1:J:169:LEU:HB2	2:K:189:GLN:NE2	2.06	0.71
2:E:316:ASP:OD2	2:E:320:ASP:N	2.23	0.71
1:J:67:ASN:HA	1:J:70:LYS:HE2	1.73	0.71
3:F:301:ASP:O	3:F:305:THR:HG23	1.89	0.71
2:E:406:ARG:H	2:E:407:CYS:HA	1.56	0.71
1:G:55:ILE:CD1	2:H:82:LEU:HD22	2.20	0.70
2:K:149:HIS:ND1	2:K:150:GLN:N	2.39	0.70
1:A:175:LEU:HD12	2:B:426:MET:CE	2.21	0.70
3:C:194:PHE:CG	3:C:233:ILE:HD13	2.27	0.70
3:I:3:ALA:HB2	3:L:11:LEU:HD12	1.73	0.70
2:H:302:LEU:HD22	2:H:454:ILE:HD11	1.73	0.70
3:F:147:ASP:OD1	3:F:147:ASP:N	2.23	0.70
1:G:123:LYS:HA	1:G:126:VAL:HG12	1.72	0.70
1:A:71:ASN:C	1:A:71:ASN:HD22	1.95	0.70
3:L:195:GLN:NE2	3:L:197:ARG:HG3	2.06	0.70
2:E:169:ARG:HA	3:F:110:LEU:HD11	1.74	0.70
3:F:169:ILE:HD11	3:F:180:VAL:HG21	1.74	0.70
3:C:75:LYS:HB3	3:C:78:MET:HE3	1.72	0.70
1:A:129:LYS:O	1:A:133:ILE:HD13	1.91	0.70
3:L:9:CYS:O	3:L:17:SER:HA	1.92	0.70
3:C:276:LEU:C	3:C:276:LEU:HD23	2.12	0.70
2:B:101:ASN:OD1	3:C:43:LEU:HD21	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:470:NAG:H62	5:S:4:PRO:HB3	1.73	0.69
2:B:364:ASN:HD22	6:B:470:NAG:C1	1.96	0.69
1:A:119:ILE:CD1	3:C:93:ILE:HD13	2.18	0.69
3:L:219:SER:OG	3:L:224:THR:CG2	2.38	0.69
2:E:168:LEU:HD22	3:F:110:LEU:CD2	2.21	0.69
2:K:118:MET:O	2:K:122:LYS:HB3	1.93	0.69
3:C:100:ILE:HG23	3:C:101:LEU:HD23	1.74	0.69
1:A:59:ASN:HD21	2:B:86:LEU:CD2	2.05	0.69
2:E:351:ASN:HD21	2:E:354:MET:H	1.39	0.69
1:D:118:ARG:HH22	3:F:90:LEU:HD23	1.56	0.69
1:J:207:MET:O	1:J:211:PRO:HD3	1.93	0.69
2:H:224:MET:HE2	2:H:237:ARG:HD3	1.75	0.69
3:I:81:ALA:O	3:I:85:LYS:N	2.23	0.69
6:B:479:SIA:H7	6:B:479:SIA:O10	1.93	0.69
1:J:115:LEU:O	1:J:119:ILE:HG12	1.93	0.69
3:C:368:ILE:HG22	3:C:377:TYR:O	1.92	0.69
2:K:179:ILE:HD11	3:L:121:ILE:HG13	1.75	0.69
2:B:253:GLN:C	2:B:253:GLN:HE21	1.96	0.69
1:A:111:VAL:O	1:A:115:LEU:HD12	1.93	0.69
6:B:476:GAL:H5	6:B:480:SIA:H32	1.74	0.69
1:J:71:ASN:HA	1:J:74:PHE:CD2	2.28	0.68
3:F:246:LEU:HD11	3:F:248:VAL:CG2	2.23	0.68
2:B:252:ILE:CD1	2:B:454:ILE:HG23	2.23	0.68
3:C:166:LEU:HB3	3:C:179:LEU:HD21	1.75	0.68
2:K:212:GLU:O	2:K:215:ILE:HG22	1.92	0.68
2:H:342:VAL:HG11	2:H:353:LEU:HD13	1.74	0.68
1:J:145:VAL:HG13	1:J:146:ASP:N	2.07	0.68
3:C:197:ARG:NH1	3:C:367:ILE:HD11	2.08	0.68
2:K:432:ASP:OD1	2:K:443:SER:OG	2.10	0.68
3:C:248:VAL:HG12	3:C:250:LEU:HD11	1.73	0.68
1:A:115:LEU:HD21	3:C:90:LEU:CD1	2.14	0.68
2:E:436:VAL:HG11	2:E:443:SER:HA	1.75	0.68
1:G:115:LEU:HD11	3:I:89:MET:HB2	1.75	0.68
3:F:27:ASP:O	3:F:31:THR:HB	1.94	0.68
2:K:345:TYR:HB2	2:K:354:MET:HE2	1.74	0.68
3:C:291:ASP:O	3:C:302:LYS:NZ	2.27	0.68
1:A:63:THR:HA	1:A:66:ILE:HG22	1.75	0.68
2:H:172:LEU:HD21	3:I:113:ILE:HB	1.75	0.67
3:F:260:ALA:HB2	3:F:286:ALA:CB	2.20	0.67
1:J:144:LEU:HD22	2:K:171:ILE:HD11	1.75	0.67
1:J:69:LEU:HD11	2:K:100:LEU:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:102:ASN:O	2:K:106:ALA:HB3	1.94	0.67
3:L:379:MET:HE3	3:L:379:MET:HA	1.75	0.67
1:J:121:VAL:HG12	1:J:122:LEU:HD22	1.74	0.67
2:B:406:ARG:N	2:B:407:CYS:HA	2.08	0.67
1:D:55:ILE:CG2	2:E:86:LEU:HD13	2.24	0.67
3:L:288:ASP:C	3:L:371:THR:HG21	2.14	0.67
3:L:314:THR:C	3:L:327:ALA:HB1	2.15	0.67
2:K:364:ASN:CG	6:K:470:NAG:C1	2.61	0.67
2:B:408:HIS:O	5:O:1:GLY:N	2.24	0.67
3:C:350:GLN:O	3:C:352:GLY:N	2.21	0.67
1:A:115:LEU:HD11	3:C:90:LEU:HB2	1.76	0.67
3:C:181:TYR:HE1	3:C:220:PRO:O	1.77	0.67
1:A:175:LEU:HD12	2:B:426:MET:HE2	1.76	0.67
2:H:398:ASP:HA	2:H:433:ASP:HB3	1.77	0.67
3:I:79:ILE:HA	3:I:82:ALA:HB3	1.76	0.67
2:H:135:ASN:HA	2:H:138:VAL:HG12	1.77	0.67
2:K:351:ASN:HD21	2:K:354:MET:HG3	1.59	0.66
3:I:199:ASP:OD1	3:I:201:SER:N	2.27	0.66
2:B:367:MET:SD	2:B:406:ARG:HD3	2.35	0.66
2:H:361:MET:HB2	7:H:470:NAG:H81	1.78	0.66
3:C:225:GLU:O	3:C:226:PHE:HB3	1.96	0.66
3:L:185:ASP:OD2	3:L:189:ASN:N	2.25	0.66
2:H:360:LEU:HD11	5:S:2:HIS:ND1	2.10	0.66
3:I:11:LEU:HD23	3:I:12:ASP:N	2.11	0.66
6:B:477:NDG:H4	6:B:478:GAL:O2	1.95	0.66
2:E:406:ARG:N	2:E:407:CYS:HA	2.10	0.66
3:C:276:LEU:HD21	3:C:278:TYR:CD2	2.31	0.66
3:L:242:ILE:HG23	3:L:243:PRO:HD2	1.76	0.66
6:B:471:NDG:O6	6:B:477:NDG:H2	1.94	0.66
3:C:365:ASN:H	3:C:365:ASN:HD22	1.43	0.66
1:J:208:LYS:HB2	1:J:209:PRO:HD3	1.78	0.66
3:C:194:PHE:CD1	3:C:233:ILE:HD11	2.29	0.66
1:J:51:MET:HG3	3:L:22:THR:HG22	1.77	0.66
3:L:11:LEU:HB3	3:L:18:TYR:CE1	2.31	0.66
1:G:119:ILE:HD11	3:I:93:ILE:HD13	1.78	0.66
3:C:179:LEU:HD23	3:C:180:VAL:N	2.10	0.66
3:C:364:ASP:OD2	4:M:1:GLY:N	2.28	0.66
1:D:109:ASN:OD1	1:D:110:ARG:N	2.29	0.65
2:H:182:LEU:O	2:H:185:ASP:N	2.29	0.65
2:H:257:ASP:OD1	2:H:259:SER:OG	2.10	0.65
2:B:294:LEU:HD12	2:B:295:GLY:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:LYS:NZ	2:H:153:ILE:HG21	2.10	0.65
3:F:27:ASP:O	3:F:31:THR:CB	2.45	0.65
2:B:354:MET:O	2:B:369:ILE:HG23	1.96	0.65
3:C:197:ARG:HD2	3:C:344:LEU:O	1.97	0.65
2:H:302:LEU:HD22	2:H:454:ILE:HD12	1.77	0.65
3:L:236:ILE:HG21	3:L:386:ILE:HD11	1.77	0.65
2:E:340:ILE:HD12	2:E:403:TRP:CZ3	2.31	0.65
3:I:42:SER:O	3:I:46:ILE:HD13	1.96	0.65
8:L:570:NAG:H62	8:L:571:NAG:H61	1.77	0.65
3:L:264:MET:O	3:L:278:TYR:HA	1.96	0.65
2:K:276:VAL:HA	2:K:292:TYR:CD2	2.32	0.65
6:B:473:MAN:H4	6:B:475:NDG:N2	2.12	0.65
2:E:205:VAL:HG22	3:F:218:LEU:HD21	1.78	0.65
3:I:193:VAL:HG22	3:I:385:LYS:HB3	1.77	0.65
3:L:169:ILE:CD1	3:L:180:VAL:HG11	2.27	0.64
3:C:146:HIS:HD2	3:C:167:TYR:CZ	2.14	0.64
1:D:144:LEU:HD21	1:D:182:GLN:HA	1.78	0.64
2:H:252:ILE:CD1	2:H:454:ILE:CG2	2.75	0.64
2:E:296:ASN:O	2:E:299:ILE:N	2.28	0.64
1:A:134:GLN:NE2	1:A:193:LEU:HD23	2.12	0.64
2:B:154:ASP:CG	3:C:96:TYR:OH	2.34	0.64
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.31	0.64
3:L:246:LEU:HD12	3:L:247:ARG:H	1.63	0.64
2:H:316:ASP:OD2	2:H:320:ASP:N	2.20	0.64
2:E:227:ILE:HD11	2:E:236:TYR:CE2	2.33	0.64
3:L:219:SER:N	3:L:224:THR:HG21	2.09	0.64
2:B:171:ILE:HG22	2:B:172:LEU:HD13	1.80	0.64
1:J:69:LEU:HD13	1:J:70:LYS:N	2.13	0.64
2:B:205:VAL:HG22	3:C:218:LEU:HG	1.79	0.64
6:B:470:NAG:O3	6:B:471:NDG:H2	1.98	0.64
1:J:71:ASN:HA	1:J:74:PHE:CE2	2.33	0.64
7:H:471:NDG:H3	7:H:471:NDG:O7	1.98	0.64
2:H:66:LEU:N	1:J:34:PRO:O	2.31	0.64
2:E:160:ASN:O	2:E:164:ASN:N	2.20	0.64
3:L:152:ASP:OD1	3:L:155:ASP:N	2.30	0.64
1:G:97:ASP:O	1:G:101:ALA:CB	2.46	0.64
2:B:165:LEU:HD11	3:C:107:ILE:HD12	1.79	0.64
3:C:365:ASN:N	3:C:365:ASN:HD22	1.96	0.64
2:E:199:VAL:O	3:F:141:ASP:OD2	2.16	0.63
3:C:174:ALA:HB2	3:C:235:LEU:HD13	1.79	0.63
3:L:209:ILE:H	3:L:209:ILE:HD12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:340:HIS:ND1	3:C:340:HIS:O	2.30	0.63
2:H:153:ILE:HG22	2:H:153:ILE:O	1.97	0.63
3:I:189:ASN:HB3	3:I:387:ILE:HD11	1.78	0.63
3:F:250:LEU:HD23	3:F:379:MET:CE	2.28	0.63
1:A:134:GLN:HE22	1:A:193:LEU:HD23	1.63	0.63
3:I:5:ARG:HB2	3:I:11:LEU:HD13	1.80	0.63
2:K:199:VAL:HG23	3:L:141:ASP:HA	1.80	0.63
1:A:169:LEU:HD23	1:A:171:ARG:HD2	1.80	0.63
3:I:12:ASP:OD2	3:I:15:PHE:CD1	2.52	0.63
3:L:197:ARG:NH1	3:L:367:ILE:HD11	2.14	0.63
1:J:132:HIS:CB	3:L:107:ILE:HD11	2.28	0.63
2:K:332:GLN:O	2:K:338:TYR:HA	1.98	0.63
2:E:172:LEU:HD21	3:F:113:ILE:HG23	1.79	0.63
3:C:261:ASP:HB3	3:C:282:ALA:HB3	1.81	0.63
2:K:436:VAL:HG11	2:K:442:GLY:O	1.99	0.63
3:C:121:ILE:HG22	3:C:122:VAL:N	2.12	0.63
2:B:238:VAL:HG11	2:B:250:THR:HG23	1.81	0.63
2:E:314:MET:CG	2:E:322:VAL:HG23	2.28	0.63
2:B:172:LEU:HB3	3:C:113:ILE:CG2	2.27	0.63
1:D:50:ARG:HD3	2:E:59:ALA:HB1	1.81	0.63
3:I:356:LYS:HA	3:I:359:THR:HG23	1.80	0.63
1:G:118:ARG:NH2	3:I:90:LEU:HD21	2.14	0.63
1:G:184:GLN:HE21	2:H:167:VAL:HG23	1.64	0.62
3:I:242:ILE:O	3:I:242:ILE:HD12	1.98	0.62
6:B:477:NDG:H3	6:B:477:NDG:H8C1	1.81	0.62
1:J:115:LEU:CD2	3:L:90:LEU:CD2	2.66	0.62
2:K:172:LEU:CD2	3:L:113:ILE:HG23	2.29	0.62
2:E:226:LEU:HD11	2:E:235:PRO:HB2	1.80	0.62
2:E:385:TRP:O	2:E:387:THR:N	2.29	0.62
2:B:281:ASP:O	2:B:281:ASP:OD2	2.18	0.62
3:C:246:LEU:HA	3:C:386:ILE:HG22	1.80	0.62
3:C:349:TYR:CE1	3:C:354:TYR:CE1	2.88	0.62
2:H:87:LEU:HD23	2:H:87:LEU:O	2.00	0.62
1:G:62:PHE:CE1	3:I:36:VAL:HG12	2.35	0.62
1:J:137:GLN:O	1:J:140:VAL:HG22	1.99	0.62
2:K:373:MET:SD	2:K:405:ASN:HB2	2.38	0.62
2:K:406:ARG:N	2:K:407:CYS:HA	2.13	0.62
1:J:156:ILE:O	1:J:159:ARG:N	2.32	0.62
2:E:171:ILE:CG2	2:E:172:LEU:N	2.62	0.62
1:D:118:ARG:NH2	3:F:90:LEU:HD23	2.13	0.62
1:D:86:LEU:CD2	3:F:61:ILE:HG21	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:VAL:HG23	3:F:216:GLY:O	1.98	0.62
3:I:169:ILE:HD11	3:I:180:VAL:HG11	1.80	0.62
2:K:376:SER:O	2:K:401:GLY:HA2	1.99	0.62
3:C:248:VAL:HG12	3:C:250:LEU:CD1	2.29	0.62
2:H:171:ILE:HG23	2:H:172:LEU:N	2.15	0.61
3:C:261:ASP:CB	3:C:282:ALA:HB3	2.30	0.61
1:J:106:ASN:ND2	1:J:106:ASN:C	2.54	0.61
2:E:340:ILE:HD12	2:E:403:TRP:CE3	2.36	0.61
3:C:333:GLY:O	3:C:345:ASN:ND2	2.32	0.61
1:J:154:ILE:HD11	3:L:128:VAL:HG21	1.80	0.61
2:K:326:TYR:CE1	2:K:353:LEU:HD12	2.35	0.61
2:E:165:LEU:HD21	3:F:107:ILE:CD1	2.30	0.61
3:C:295:PHE:HE1	3:C:305:THR:HG21	1.63	0.61
2:H:122:LYS:HZ3	3:I:60:LEU:HB3	1.66	0.61
1:D:137:GLN:O	1:D:140:VAL:HG22	1.99	0.61
2:B:102:ASN:O	2:B:106:ALA:HB3	2.00	0.61
2:K:137:ASN:HA	2:K:140:ASN:HD21	1.64	0.61
3:F:124:LEU:O	3:F:128:VAL:HG23	1.99	0.61
3:C:240:SER:O	3:C:242:ILE:N	2.28	0.61
2:H:253:GLN:C	2:H:253:GLN:HE21	2.03	0.61
1:G:185:LEU:HD11	1:G:189:ILE:HD11	1.82	0.61
3:L:56:GLU:CB	8:L:570:NAG:HO3	2.03	0.61
2:B:172:LEU:HD22	3:C:110:LEU:HD22	1.81	0.61
2:E:176:ARG:O	2:E:179:ILE:HG22	2.01	0.61
1:D:135:LEU:HD22	1:D:136:LEU:CD2	2.24	0.61
3:I:141:ASP:OD2	3:I:143:VAL:HG22	2.01	0.61
2:K:410:ALA:HB1	2:K:437:TRP:CE3	2.36	0.61
3:I:116:SER:O	3:I:119:GLN:N	2.33	0.61
1:J:118:ARG:O	1:J:122:LEU:HD23	2.01	0.61
3:L:143:VAL:HG23	3:L:143:VAL:O	2.00	0.60
1:J:63:THR:HA	1:J:66:ILE:CG2	2.31	0.60
2:H:75:LEU:HD22	1:J:46:PRO:N	2.16	0.60
2:E:226:LEU:HD11	2:E:235:PRO:CB	2.30	0.60
2:E:199:VAL:HG23	3:F:141:ASP:HA	1.82	0.60
3:L:21:THR:HG23	3:L:24:GLY:H	1.66	0.60
1:G:154:ILE:HD11	3:I:128:VAL:CG2	2.19	0.60
2:E:312:ILE:HD11	2:E:452:MET:HE2	1.83	0.60
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.35	0.60
3:L:236:ILE:CG2	3:L:386:ILE:HD11	2.30	0.60
2:B:260:VAL:HG21	2:B:291:GLU:O	2.01	0.60
2:H:172:LEU:HD21	3:I:113:ILE:HG22	1.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:209:ILE:H	3:I:209:ILE:HD12	1.66	0.60
1:G:58:VAL:HG12	1:G:59:ASN:N	2.16	0.60
3:C:367:ILE:O	3:C:378:SER:HA	2.01	0.60
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.82	0.60
3:C:359:THR:HG21	3:C:363:TYR:O	2.01	0.60
6:K:471:NDG:C6	6:K:477:NDG:H8C2	2.11	0.60
2:H:406:ARG:N	2:H:407:CYS:HA	2.16	0.60
3:L:153:CYS:HB2	3:L:192:THR:OG1	2.02	0.60
3:C:191:TRP:CH2	3:C:387:ILE:HG21	2.37	0.60
1:J:207:MET:HE2	2:K:131:GLN:HE22	1.66	0.60
1:A:139:ASN:O	1:A:142:ALA:HB3	2.00	0.60
2:B:75:LEU:HD13	1:D:44:LYS:O	2.00	0.60
3:F:246:LEU:CD1	3:F:248:VAL:HG23	2.30	0.60
2:B:238:VAL:HG11	2:B:250:THR:CG2	2.32	0.60
2:H:312:ILE:HG23	2:H:451:SER:O	2.02	0.60
2:K:412:PRO:HG3	2:K:450:MET:CE	2.31	0.60
3:F:298:ASP:OD2	3:F:300:SER:N	2.35	0.60
2:H:374:PHE:O	2:H:403:TRP:HA	2.02	0.60
2:K:139:VAL:HG21	3:L:79:ILE:HG21	1.84	0.60
2:K:169:ARG:HA	3:L:110:LEU:HD11	1.84	0.60
3:I:387:ILE:O	3:I:387:ILE:HG23	2.02	0.60
2:K:199:VAL:HG23	3:L:141:ASP:CA	2.31	0.60
1:J:132:HIS:HB3	3:L:107:ILE:HD11	1.83	0.60
2:E:126:GLN:O	2:E:130:LYS:N	2.31	0.60
3:I:79:ILE:O	3:I:83:THR:N	2.25	0.59
3:C:293:PHE:CD1	3:C:370:ALA:HB1	2.37	0.59
6:E:477:NDG:H6C2	6:E:478:GAL:C1	2.32	0.59
3:L:349:TYR:OH	3:L:365:ASN:ND2	2.32	0.59
2:B:179:ILE:CG2	2:B:180:GLN:N	2.64	0.59
2:E:405:ASN:O	2:E:406:ARG:CB	2.50	0.59
1:G:166:SER:HB3	2:H:195:THR:OG1	2.02	0.59
2:E:253:GLN:HE21	2:E:253:GLN:C	2.06	0.59
2:K:266:TRP:HA	2:K:377:THR:HG21	1.84	0.59
3:I:98:ALA:O	3:I:102:THR:HG23	2.02	0.59
2:K:171:ILE:HG23	2:K:172:LEU:N	2.17	0.59
6:K:480:SIA:O10	6:K:480:SIA:H7	2.01	0.59
3:I:51:GLU:O	3:I:54:THR:OG1	2.16	0.59
3:F:197:ARG:NH2	3:F:367:ILE:HD11	2.18	0.59
3:I:227:TRP:HE1	3:I:230:ASN:HD22	1.50	0.59
2:K:139:VAL:HG21	3:L:79:ILE:CG2	2.33	0.59
3:L:219:SER:HG	3:L:224:THR:HG22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:390:ASN:C	3:C:390:ASN:HD22	2.05	0.59
1:G:188:VAL:HG11	2:H:164:ASN:ND2	2.18	0.59
2:B:210:GLU:OE2	2:B:212:GLU:N	2.31	0.59
2:E:238:VAL:HG13	2:E:239:TYR:O	2.02	0.59
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.03	0.59
2:E:146:LEU:O	2:E:150:GLN:N	2.25	0.59
2:H:333:ASN:OD1	2:H:335:ALA:HB3	2.03	0.59
3:I:11:LEU:HA	3:I:18:TYR:OH	2.02	0.59
2:E:432:ASP:OD1	2:E:443:SER:OG	2.19	0.59
1:A:185:LEU:O	1:A:185:LEU:HD22	2.01	0.59
2:H:211:CYS:SG	2:H:250:THR:HG23	2.43	0.59
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.51	0.59
1:G:30:ASP:O	1:G:32:ASP:N	2.35	0.59
2:B:257:ASP:OD1	2:B:257:ASP:N	2.35	0.59
1:G:75:GLU:O	1:G:79:ASN:HB2	2.03	0.59
2:B:351:ASN:HD21	2:B:354:MET:H	1.50	0.59
1:D:55:ILE:HG23	2:E:86:LEU:CD1	2.32	0.59
1:J:127:ILE:O	1:J:130:VAL:HG12	2.03	0.59
3:C:126:GLU:O	3:C:129:ALA:HB3	2.03	0.59
3:L:224:THR:O	3:L:224:THR:HG23	2.02	0.58
3:C:246:LEU:HG	3:C:247:ARG:N	2.17	0.58
2:B:434:GLY:O	2:B:436:VAL:N	2.36	0.58
3:L:44:GLU:O	3:L:48:HIS:HB2	2.03	0.58
3:C:367:ILE:HG21	3:C:382:THR:HG21	1.85	0.58
2:E:171:ILE:HG22	2:E:172:LEU:N	2.19	0.58
1:G:115:LEU:HD11	3:I:89:MET:CB	2.33	0.58
1:A:169:LEU:HD21	2:B:185:ASP:OD2	2.04	0.58
3:C:206:LYS:HB2	3:C:211:TYR:CE1	2.38	0.58
2:H:176:ARG:NH1	3:I:113:ILE:HG23	2.18	0.58
1:A:147:MET:SD	3:C:121:ILE:HD11	2.43	0.58
3:I:84:LEU:HD12	3:I:87:ARG:HD2	1.84	0.58
1:A:119:ILE:O	1:A:122:LEU:HB3	2.04	0.58
2:B:351:ASN:C	2:B:351:ASN:ND2	2.56	0.58
2:E:185:ASP:O	2:E:188:ALA:HB3	2.03	0.58
2:K:141:GLU:O	2:K:145:GLU:HB2	2.04	0.58
3:I:166:LEU:HD23	3:I:218:LEU:HB3	1.85	0.58
3:L:367:ILE:HG21	3:L:382:THR:HG21	1.85	0.58
1:A:115:LEU:CD1	3:C:90:LEU:HB2	2.33	0.58
1:J:207:MET:HA	1:J:210:VAL:HG12	1.86	0.58
3:C:179:LEU:HD23	3:C:180:VAL:H	1.69	0.58
1:J:123:LYS:HA	1:J:126:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:236:ILE:HG21	3:F:386:ILE:HD11	1.86	0.58
1:J:73:LEU:HD13	1:J:73:LEU:C	2.24	0.58
2:K:215:ILE:HD12	2:K:219:GLY:O	2.04	0.58
3:F:393:THR:HG23	3:F:394:ILE:HD12	1.85	0.58
2:B:66:LEU:HD12	1:D:31:SER:HB3	1.86	0.58
1:G:105:ASP:OD1	3:I:79:ILE:CD1	2.46	0.58
2:E:213:GLU:OE2	2:E:217:LYS:HE3	2.03	0.58
1:G:122:LEU:HB3	1:G:123:LYS:HZ2	1.69	0.58
3:L:169:ILE:HD13	3:L:180:VAL:HG11	1.85	0.58
3:C:121:ILE:O	3:C:124:LEU:N	2.37	0.58
2:K:144:SER:HB3	2:K:148:LYS:HZ1	1.68	0.58
2:B:325:HIS:HB3	2:B:346:ARG:HG2	1.85	0.58
2:B:186:VAL:HG12	2:B:187:SER:N	2.18	0.58
2:K:345:TYR:CB	2:K:354:MET:HE2	2.33	0.57
3:F:90:LEU:C	3:F:90:LEU:HD22	2.24	0.57
1:A:91:MET:O	1:A:95:ARG:N	2.37	0.57
2:H:178:LYS:O	2:H:181:LYS:HG3	2.03	0.57
2:B:142:TYR:O	2:B:146:LEU:HG	2.04	0.57
2:H:205:VAL:HG23	3:I:216:GLY:O	2.04	0.57
1:J:133:ILE:O	1:J:137:GLN:HG3	2.04	0.57
1:A:149:ARG:O	1:A:152:VAL:CG1	2.52	0.57
1:J:184:GLN:HE21	2:K:167:VAL:CG2	2.14	0.57
2:H:415:ARG:O	2:H:434:GLY:HA2	2.05	0.57
1:J:210:VAL:HG21	2:K:131:GLN:HG3	1.86	0.57
2:E:394:CYS:SG	2:E:406:ARG:HA	2.45	0.57
3:C:97:GLU:O	3:C:100:ILE:HG22	2.05	0.57
3:I:289:ALA:HA	3:I:371:THR:HG23	1.87	0.57
2:B:205:VAL:O	2:B:205:VAL:CG1	2.53	0.57
1:G:150:LEU:O	1:G:154:ILE:HD13	2.04	0.57
3:F:197:ARG:CZ	3:F:367:ILE:HD11	2.35	0.57
1:D:122:LEU:HD12	1:D:123:LYS:HE3	1.86	0.57
2:H:251:VAL:HG22	2:H:453:LYS:HE2	1.86	0.57
1:G:108:TYR:CZ	3:I:82:ALA:HB1	2.38	0.57
2:E:312:ILE:HD11	2:E:452:MET:CE	2.35	0.57
1:J:58:VAL:HG22	1:J:62:PHE:CE1	2.39	0.57
2:K:312:ILE:HD13	2:K:452:MET:HG2	1.86	0.57
1:A:70:LYS:HG2	2:B:100:LEU:HD21	1.86	0.57
2:E:210:GLU:OE1	2:E:213:GLU:N	2.30	0.57
2:B:179:ILE:HG23	2:B:180:GLN:H	1.70	0.57
2:H:373:MET:HG3	2:H:405:ASN:HB2	1.85	0.57
1:J:136:LEU:O	1:J:140:VAL:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:140:ASN:OD1	2:K:140:ASN:N	2.38	0.57
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.53	0.57
2:E:310:LEU:HD12	2:E:311:LEU:N	2.19	0.57
1:D:111:VAL:HG11	3:F:87:ARG:HB2	1.85	0.57
2:K:333:ASN:ND2	2:K:335:ALA:HB3	2.20	0.57
3:L:143:VAL:CG2	3:L:143:VAL:O	2.53	0.57
3:F:250:LEU:HD23	3:F:379:MET:HE2	1.86	0.57
2:B:311:LEU:HD12	2:B:312:ILE:N	2.20	0.57
1:D:94:LEU:HD13	2:E:125:TRP:CD1	2.40	0.57
2:B:153:ILE:O	2:B:153:ILE:HG22	2.05	0.56
3:I:10:ILE:O	3:I:18:TYR:CZ	2.57	0.56
6:K:473:MAN:C1	6:K:475:NDG:O	2.53	0.56
3:I:334:TRP:HB3	3:I:336:MET:HE1	1.87	0.56
2:B:296:ASN:O	2:B:299:ILE:N	2.34	0.56
6:K:479:SIA:O6	6:K:478:GAL:H5	2.04	0.56
6:E:473:MAN:H62	6:E:476:GAL:H2	1.86	0.56
2:B:115:PHE:CE2	3:C:50:VAL:HG13	2.40	0.56
3:L:228:LEU:HD11	3:L:232:LYS:HD2	1.87	0.56
3:F:217:HIS:C	3:F:218:LEU:HD23	2.26	0.56
2:E:340:ILE:HG22	2:E:373:MET:O	2.05	0.56
6:B:473:MAN:C3	6:B:475:NDG:HA	2.17	0.56
3:C:228:LEU:HD11	3:C:232:LYS:HD2	1.85	0.56
3:I:338:LYS:N	3:I:339:CYS:HA	2.20	0.56
2:K:209:LYS:HA	2:K:228:GLN:O	2.04	0.56
3:C:246:LEU:HD21	3:C:248:VAL:HG22	1.88	0.56
1:A:169:LEU:H	2:B:189:GLN:NE2	2.04	0.56
1:D:94:LEU:HD22	2:E:125:TRP:NE1	2.20	0.56
3:L:259:THR:O	3:L:286:ALA:HB3	2.06	0.56
1:J:69:LEU:CD1	2:K:100:LEU:CD1	2.83	0.56
2:H:224:MET:CE	2:H:237:ARG:HD3	2.36	0.56
2:H:351:ASN:HD21	2:H:354:MET:HG3	1.70	0.56
6:E:479:SIA:H112	6:E:479:SIA:H7	1.88	0.56
3:L:78:MET:O	3:L:81:ALA:N	2.38	0.56
1:A:122:LEU:HD13	1:A:122:LEU:C	2.26	0.56
1:A:70:LYS:HG3	2:B:100:LEU:HD11	1.87	0.56
3:I:209:ILE:HD12	3:I:209:ILE:N	2.21	0.56
1:G:58:VAL:HG13	1:G:62:PHE:CE2	2.40	0.56
2:E:345:TYR:CG	2:E:351:ASN:HB2	2.40	0.56
1:D:169:LEU:HB2	2:E:189:GLN:HE22	1.70	0.56
3:F:289:ALA:HA	3:F:371:THR:HG23	1.87	0.56
2:K:101:ASN:OD1	3:L:43:LEU:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:249:GLU:C	3:F:250:LEU:HD12	2.26	0.56
1:J:162:ARG:HA	1:J:168:ALA:HB2	1.85	0.56
2:B:112:SER:HA	2:B:115:PHE:CD2	2.41	0.56
2:E:402:TRP:CZ3	2:E:412:PRO:HG2	2.41	0.56
3:I:297:ASP:N	3:I:297:ASP:OD1	2.38	0.56
1:J:108:TYR:CE1	3:L:83:THR:CB	2.84	0.56
3:I:143:VAL:CG2	3:I:143:VAL:O	2.53	0.56
2:E:402:TRP:CH2	2:E:412:PRO:HG3	2.41	0.56
3:I:344:LEU:HA	3:I:367:ILE:HG23	1.86	0.56
2:K:185:ASP:O	2:K:188:ALA:HB3	2.05	0.56
2:B:104:VAL:HG12	2:B:105:GLU:OE2	2.06	0.55
2:K:171:ILE:CG2	2:K:172:LEU:N	2.69	0.55
1:J:108:TYR:OH	3:L:83:THR:CA	2.53	0.55
2:H:252:ILE:HD11	2:H:454:ILE:CG2	2.36	0.55
2:B:179:ILE:HD13	2:B:179:ILE:C	2.26	0.55
3:I:7:ASN:O	3:L:9:CYS:HA	2.07	0.55
3:C:197:ARG:HH11	3:C:367:ILE:HD11	1.70	0.55
2:E:303:THR:HG22	2:E:308:THR:HG21	1.88	0.55
2:H:402:TRP:HB3	2:H:404:TYR:CE2	2.41	0.55
2:K:157:VAL:C	2:K:158:ASN:HD22	2.10	0.55
1:J:66:ILE:O	1:J:70:LYS:HG3	2.07	0.55
3:C:295:PHE:HB3	3:C:375:ARG:NH2	2.22	0.55
1:G:123:LYS:HZ3	2:H:153:ILE:HG21	1.70	0.55
1:A:137:GLN:HB3	1:A:189:ILE:HD13	1.89	0.55
3:I:310:MET:CE	3:I:321:LYS:HZ1	2.19	0.55
2:K:415:ARG:O	2:K:434:GLY:HA2	2.06	0.55
1:A:105:ASP:O	1:A:109:ASN:N	2.35	0.55
1:A:184:GLN:NE2	2:B:167:VAL:HG23	2.21	0.55
6:K:471:NDG:H5	6:K:472:BMA:C2	2.37	0.55
3:I:387:ILE:CG2	3:I:387:ILE:O	2.55	0.55
2:E:227:ILE:HD11	2:E:236:TYR:HE2	1.70	0.55
3:I:179:LEU:HD23	3:I:218:LEU:HD12	1.89	0.55
3:C:276:LEU:HD21	3:C:278:TYR:HD2	1.68	0.55
2:B:156:THR:HG22	2:B:157:VAL:N	2.22	0.55
3:I:151:LYS:HE2	3:I:172:LEU:HD13	1.89	0.55
1:J:207:MET:HE1	2:K:131:GLN:OE1	2.06	0.55
3:F:218:LEU:CD2	3:F:218:LEU:N	2.70	0.55
3:L:189:ASN:HD22	3:L:391:ARG:HE	1.54	0.55
3:L:334:TRP:CH2	3:L:344:LEU:HD12	2.40	0.55
2:H:117:TYR:CD1	2:H:120:LEU:HD12	2.42	0.55
3:C:390:ASN:ND2	3:C:391:ARG:N	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:191:TRP:CH2	3:F:247:ARG:HB2	2.42	0.54
2:K:340:ILE:HG22	2:K:403:TRP:CD1	2.42	0.54
1:A:149:ARG:O	1:A:152:VAL:HG12	2.08	0.54
3:L:79:ILE:H	3:L:79:ILE:HD12	1.73	0.54
2:B:176:ARG:O	2:B:179:ILE:HG22	2.07	0.54
2:E:182:LEU:O	2:E:185:ASP:N	2.40	0.54
1:J:140:VAL:HG23	1:J:141:ARG:N	2.23	0.54
1:D:169:LEU:HB2	2:E:189:GLN:NE2	2.23	0.54
3:F:289:ALA:HB1	3:F:341:ALA:O	2.08	0.54
2:B:123:ASP:O	2:B:127:LYS:N	2.40	0.54
3:L:338:LYS:N	3:L:339:CYS:HA	2.21	0.54
2:B:311:LEU:HD11	2:B:313:GLU:HG2	1.88	0.54
1:G:46:PRO:O	3:I:22:THR:CB	2.56	0.54
3:C:23:CYS:O	3:C:26:ALA:N	2.40	0.54
3:L:110:LEU:HA	3:L:113:ILE:CG2	2.36	0.54
2:H:315:GLU:HA	2:H:320:ASP:O	2.06	0.54
3:C:121:ILE:O	3:C:122:VAL:C	2.46	0.54
2:E:376:SER:OG	2:E:382:ASN:N	2.34	0.54
3:L:276:LEU:HD23	3:L:277:THR:N	2.22	0.54
1:J:129:LYS:HE2	3:L:104:ASP:HB3	1.89	0.54
3:F:189:ASN:HB3	3:F:387:ILE:HD11	1.90	0.54
2:B:300:SER:HB2	2:B:331:VAL:O	2.07	0.54
3:C:148:ILE:HD12	3:C:161:ALA:HB2	1.90	0.54
3:F:233:ILE:CG2	3:F:267:VAL:HG21	2.37	0.54
1:G:46:PRO:O	3:I:22:THR:OG1	2.21	0.54
3:L:352:GLY:O	3:L:377:TYR:HA	2.08	0.54
3:L:234:HIS:HB2	3:L:267:VAL:HG12	1.88	0.54
3:C:364:ASP:OD2	3:C:375:ARG:HG3	2.07	0.54
1:J:132:HIS:CG	3:L:107:ILE:HD11	2.43	0.54
2:H:59:ALA:HB1	2:H:60:PRO:CD	2.36	0.54
2:H:398:ASP:OD1	5:S:3:ARG:NH1	2.40	0.54
3:C:372:TRP:HZ3	3:C:379:MET:CE	2.21	0.54
1:D:89:ASN:O	1:D:93:ILE:HG23	2.06	0.54
2:K:135:ASN:O	2:K:139:VAL:HG23	2.08	0.54
1:A:181:GLN:HB3	2:B:171:ILE:HD11	1.90	0.54
2:B:299:ILE:O	2:B:303:THR:HG23	2.07	0.54
2:E:424:TRP:CH2	6:E:479:SIA:H31	2.43	0.54
3:I:238:THR:HG22	3:I:266:LYS:HG3	1.88	0.54
1:J:115:LEU:CD1	3:L:90:LEU:HD11	2.30	0.54
2:K:252:ILE:HG21	2:K:299:ILE:HG23	1.89	0.54
3:L:314:THR:C	3:L:327:ALA:CB	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:479:SIA:H7	6:B:479:SIA:C10	2.39	0.53
3:L:84:LEU:C	3:L:84:LEU:HD23	2.28	0.53
3:L:152:ASP:OD1	3:L:154:GLN:N	2.40	0.53
3:C:349:TYR:CE1	3:C:354:TYR:CD1	2.96	0.53
1:A:94:LEU:HD13	2:B:125:TRP:CZ3	2.43	0.53
2:E:275:ASN:N	2:E:291:GLU:O	2.41	0.53
3:I:10:ILE:C	3:I:18:TYR:HH	1.93	0.53
2:H:351:ASN:C	2:H:351:ASN:HD22	2.10	0.53
6:E:472:BMA:H5	6:E:477:NDG:H8C3	1.90	0.53
1:J:65:ARG:NH2	3:L:44:GLU:OE2	2.38	0.53
1:A:188:VAL:CG1	2:B:164:ASN:ND2	2.71	0.53
1:G:73:LEU:HD22	1:G:73:LEU:O	2.08	0.53
6:K:471:NDG:H5	6:K:472:BMA:H2	1.90	0.53
1:J:127:ILE:O	1:J:131:GLN:N	2.34	0.53
2:E:405:ASN:O	2:E:406:ARG:HB3	2.07	0.53
1:A:135:LEU:CD2	1:A:136:LEU:HD22	2.38	0.53
3:L:150:GLY:HA3	3:L:155:ASP:OD1	2.09	0.53
1:J:106:ASN:HD22	1:J:106:ASN:C	2.12	0.53
2:K:310:LEU:HD22	2:K:329:PHE:CE2	2.43	0.53
2:H:326:TYR:OH	2:H:351:ASN:ND2	2.41	0.53
1:G:166:SER:CB	2:H:195:THR:OG1	2.56	0.53
2:B:317:TRP:HB2	2:B:445:TYR:OH	2.08	0.53
2:E:135:ASN:HA	2:E:138:VAL:HG12	1.91	0.53
2:K:252:ILE:HG21	2:K:299:ILE:CG2	2.37	0.53
1:J:210:VAL:N	1:J:211:PRO:CD	2.72	0.53
1:J:145:VAL:CG1	1:J:146:ASP:N	2.71	0.53
3:I:191:TRP:CE3	3:I:385:LYS:HD2	2.43	0.53
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.90	0.53
3:L:23:CYS:O	3:L:26:ALA:N	2.37	0.53
3:I:249:GLU:HB2	3:I:383:THR:HG23	1.89	0.53
2:H:118:MET:O	2:H:123:ASP:N	2.40	0.53
2:E:435:VAL:HG12	2:E:435:VAL:O	2.09	0.53
3:F:193:VAL:CG1	3:F:195:GLN:O	2.56	0.53
3:F:233:ILE:HG22	3:F:267:VAL:HG21	1.91	0.53
1:A:71:ASN:C	1:A:71:ASN:ND2	2.62	0.53
1:G:97:ASP:O	1:G:101:ALA:HB3	2.08	0.53
3:F:288:ASP:C	3:F:371:THR:HG21	2.29	0.53
3:C:217:HIS:O	3:C:224:THR:CG2	2.56	0.53
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.90	0.53
3:L:120:LYS:O	3:L:123:ASN:HB2	2.09	0.53
3:L:166:LEU:HB3	3:L:179:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:GLU:C	3:C:250:LEU:HD12	2.29	0.53
3:L:229:GLY:O	3:L:233:ILE:HG13	2.08	0.53
2:H:405:ASN:O	2:H:406:ARG:HB3	2.09	0.53
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.91	0.53
1:D:64:ASN:C	1:D:64:ASN:HD22	2.12	0.53
2:E:369:ILE:H	2:E:405:ASN:HD22	1.55	0.53
2:H:122:LYS:NZ	3:I:60:LEU:HB3	2.23	0.53
2:K:137:ASN:HA	2:K:140:ASN:ND2	2.24	0.53
3:C:354:TYR:CE2	3:C:376:TRP:HA	2.44	0.53
2:H:115:PHE:CZ	3:I:54:THR:HG22	2.43	0.53
3:C:372:TRP:CZ3	3:C:379:MET:HE2	2.44	0.53
2:E:421:GLN:HE21	2:E:421:GLN:HA	1.74	0.53
2:B:373:MET:CG	2:B:405:ASN:HB2	2.35	0.52
2:K:351:ASN:C	2:K:351:ASN:HD22	2.11	0.52
3:I:191:TRP:CE3	3:I:387:ILE:HB	2.44	0.52
6:K:473:MAN:H4	6:K:475:NDG:HA	1.72	0.52
3:C:251:GLU:HA	3:C:256:ARG:O	2.09	0.52
4:M:3:ARG:HG3	4:M:4:PRO:O	2.08	0.52
3:L:167:TYR:O	3:L:179:LEU:HD12	2.09	0.52
3:C:340:HIS:HD1	3:C:340:HIS:C	2.13	0.52
3:C:191:TRP:CZ3	3:C:387:ILE:CG2	2.92	0.52
3:F:189:ASN:ND2	3:F:391:ARG:HE	2.07	0.52
3:C:46:ILE:HG22	3:C:46:ILE:O	2.10	0.52
2:E:168:LEU:HD22	3:F:110:LEU:HD23	1.90	0.52
2:B:187:SER:OG	3:C:127:LYS:NZ	2.39	0.52
3:F:285:ASP:OD1	3:F:285:ASP:N	2.26	0.52
2:K:354:MET:O	2:K:369:ILE:HD13	2.10	0.52
2:B:87:LEU:HD23	2:B:87:LEU:C	2.29	0.52
1:A:73:LEU:O	1:A:73:LEU:HD22	2.10	0.52
3:L:195:GLN:OE1	3:L:384:MET:HG3	2.09	0.52
2:K:280:THR:HG22	2:K:281:ASP:H	1.75	0.52
2:E:172:LEU:HD23	3:F:113:ILE:HG23	1.88	0.52
2:K:325:HIS:O	2:K:345:TYR:HA	2.09	0.52
2:H:75:LEU:HD13	1:J:44:LYS:O	2.10	0.52
3:L:246:LEU:HA	3:L:386:ILE:HG22	1.91	0.52
3:F:355:SER:O	3:F:359:THR:HG23	2.10	0.52
2:E:280:THR:HG22	2:E:281:ASP:OD2	2.08	0.52
3:F:268:GLY:N	3:F:275:ARG:O	2.39	0.52
1:A:55:ILE:HG12	2:B:86:LEU:HD11	1.91	0.52
2:K:136:GLU:HB2	3:L:79:ILE:HD11	1.92	0.52
1:G:59:ASN:O	1:G:63:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:VAL:HG23	2:H:354:MET:HG2	1.91	0.52
3:F:340:HIS:ND1	3:F:343:HIS:HB2	2.24	0.52
3:I:209:ILE:H	3:I:209:ILE:CD1	2.23	0.52
6:E:471:NDG:H5	6:E:472:BMA:O2	2.10	0.52
2:B:317:TRP:CD1	2:B:420:GLY:HA3	2.45	0.52
1:J:59:ASN:OD1	2:K:93:ILE:HD12	2.10	0.52
2:E:270:LYS:NZ	2:E:334:GLU:OE1	2.24	0.52
1:J:138:LYS:C	1:J:138:LYS:HD3	2.30	0.52
2:E:168:LEU:C	2:E:168:LEU:HD23	2.31	0.52
2:B:253:GLN:C	2:B:253:GLN:NE2	2.62	0.52
2:K:200:SER:HA	3:L:141:ASP:OD2	2.10	0.52
2:H:174:ASN:O	2:H:177:SER:OG	2.24	0.52
2:B:203:ILE:N	2:B:203:ILE:HD12	2.25	0.52
6:E:480:SIA:C10	6:E:480:SIA:H7	2.39	0.52
3:F:209:ILE:H	3:F:209:ILE:HD12	1.74	0.52
1:J:209:PRO:C	1:J:211:PRO:HD2	2.30	0.52
1:D:48:GLY:HA2	2:E:82:LEU:HD11	1.92	0.52
3:L:288:ASP:O	3:L:371:THR:HG21	2.09	0.52
2:B:94:ARG:O	2:B:97:VAL:HG12	2.09	0.52
2:E:264:ARG:HG2	3:F:136:GLN:HE22	1.73	0.52
2:E:82:LEU:CB	3:F:25:ILE:HD13	2.40	0.51
2:B:212:GLU:O	2:B:213:GLU:C	2.48	0.51
2:E:260:VAL:HG23	2:E:291:GLU:HB2	1.92	0.51
2:E:251:VAL:HB	2:E:292:TYR:OH	2.10	0.51
3:F:268:GLY:O	3:F:274:TYR:HA	2.10	0.51
3:L:356:LYS:HG2	3:L:362:GLY:O	2.09	0.51
2:K:151:LEU:HD23	2:K:151:LEU:C	2.30	0.51
3:L:261:ASP:OD2	3:L:261:ASP:N	2.43	0.51
6:B:479:SIA:O6	6:B:478:GAL:H4	2.10	0.51
2:K:252:ILE:HD11	2:K:454:ILE:HG23	1.93	0.51
2:B:171:ILE:CG2	2:B:172:LEU:N	2.74	0.51
1:D:181:GLN:HB3	2:E:171:ILE:HD11	1.91	0.51
3:F:110:LEU:HD12	3:F:113:ILE:HG21	1.91	0.51
6:E:479:SIA:O4	6:E:478:GAL:H4	2.11	0.51
3:I:233:ILE:HA	3:I:236:ILE:HD12	1.92	0.51
3:F:156:ILE:HG22	3:F:157:ALA:N	2.25	0.51
2:K:302:LEU:HD22	2:K:454:ILE:CD1	2.22	0.51
1:A:48:GLY:CA	2:B:82:LEU:HD11	2.40	0.51
1:D:86:LEU:HD23	3:F:61:ILE:HG21	1.91	0.51
2:E:340:ILE:CD1	2:E:403:TRP:CE3	2.93	0.51
1:A:175:LEU:HD12	2:B:426:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:252:ILE:HG21	2:E:299:ILE:HG23	1.92	0.51
3:I:179:LEU:HD23	3:I:218:LEU:CD1	2.39	0.51
2:B:150:GLN:O	2:B:153:ILE:N	2.43	0.51
1:J:63:THR:CA	1:J:66:ILE:HG22	2.37	0.51
2:E:168:LEU:HD22	3:F:110:LEU:HD21	1.93	0.51
2:E:82:LEU:HB2	3:F:25:ILE:HD13	1.92	0.51
2:K:314:MET:CG	2:K:322:VAL:HG23	2.40	0.51
2:H:99:GLU:O	2:H:103:ASN:N	2.43	0.51
3:I:196:LYS:HG3	3:I:197:ARG:N	2.25	0.51
1:A:175:LEU:HD23	1:A:176:LYS:H	1.76	0.51
3:C:372:TRP:HZ3	3:C:379:MET:HE2	1.75	0.51
3:L:389:PHE:CD1	3:L:389:PHE:C	2.83	0.51
1:J:196:SER:C	1:J:197:ARG:HD3	2.31	0.51
2:H:252:ILE:HD11	2:H:454:ILE:CD1	2.35	0.51
3:F:141:ASP:OD2	3:F:143:VAL:HG13	2.10	0.51
1:D:69:LEU:HD13	3:F:47:LEU:CD1	2.41	0.51
1:D:63:THR:CG2	2:E:93:ILE:HD11	2.40	0.51
2:B:360:LEU:HD22	5:O:2:HIS:CE1	2.46	0.51
1:A:70:LYS:CG	2:B:100:LEU:HD11	2.40	0.51
3:L:81:ALA:O	3:L:85:LYS:HG2	2.10	0.51
2:B:441:LYS:HB3	2:B:445:TYR:HB3	1.92	0.51
2:H:397:GLU:HG3	2:H:431:THR:HG21	1.93	0.51
3:L:191:TRP:CE3	3:L:387:ILE:HB	2.46	0.51
3:C:158:ASN:C	3:C:160:GLY:H	2.12	0.51
1:G:52:LYS:HB2	2:H:82:LEU:HD21	1.92	0.51
1:D:86:LEU:HD23	3:F:61:ILE:CD1	2.40	0.51
3:L:124:LEU:O	3:L:128:VAL:HG23	2.10	0.51
2:B:146:LEU:HA	2:B:149:HIS:HB3	1.93	0.51
3:C:207:ASN:OD1	3:C:209:ILE:N	2.44	0.51
2:B:340:ILE:HB	2:B:403:TRP:CD1	2.45	0.51
3:I:11:LEU:C	3:I:11:LEU:HD23	2.32	0.51
2:H:296:ASN:O	2:H:299:ILE:N	2.44	0.51
1:G:184:GLN:NE2	2:H:167:VAL:HG23	2.26	0.51
3:I:238:THR:O	3:I:238:THR:OG1	2.28	0.51
2:K:257:ASP:O	2:K:291:GLU:OE2	2.29	0.51
3:I:365:ASN:HD22	3:I:365:ASN:H	1.57	0.51
2:B:364:ASN:ND2	6:B:470:NAG:C2	2.66	0.51
3:I:5:ARG:CB	3:I:11:LEU:HD13	2.40	0.51
1:A:48:GLY:O	1:A:52:LYS:N	2.28	0.51
1:D:135:LEU:C	1:D:135:LEU:HD23	2.32	0.51
1:J:69:LEU:CD1	1:J:69:LEU:C	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:70:LYS:HB3	1:J:74:PHE:CZ	2.46	0.51
2:K:104:VAL:HG11	3:L:47:LEU:HB2	1.93	0.51
1:A:104:ARG:HD3	3:C:79:ILE:HG21	1.92	0.51
2:E:437:TRP:O	2:E:438:MET:C	2.49	0.51
2:E:314:MET:HA	2:E:449:LYS:O	2.11	0.51
3:C:356:LYS:HG3	3:C:362:GLY:O	2.11	0.51
2:B:78:THR:HG23	1:D:43:TYR:O	2.11	0.51
6:K:480:SIA:C10	6:K:480:SIA:H7	2.41	0.50
3:L:172:LEU:HB2	3:L:239:GLN:HB2	1.92	0.50
1:A:111:VAL:O	1:A:115:LEU:CD1	2.60	0.50
2:B:104:VAL:O	2:B:108:SER:HB3	2.11	0.50
3:C:254:ASN:ND2	3:C:254:ASN:N	2.50	0.50
1:A:136:LEU:O	1:A:140:VAL:HG13	2.10	0.50
2:K:145:GLU:HA	2:K:145:GLU:OE2	2.12	0.50
3:C:228:LEU:CD1	3:C:232:LYS:HD2	2.41	0.50
3:L:340:HIS:CE1	4:R:1:GLY:H2	2.29	0.50
1:G:64:ASN:OD1	1:G:65:ARG:N	2.44	0.50
2:B:171:ILE:HG22	2:B:172:LEU:N	2.26	0.50
3:C:246:LEU:HD12	3:C:386:ILE:HG22	1.93	0.50
2:K:169:ARG:HE	3:L:110:LEU:HD21	1.76	0.50
1:J:167:ARG:HB3	2:K:192:TYR:HB3	1.92	0.50
3:I:272:ASP:OD1	3:I:275:ARG:NH1	2.45	0.50
3:I:27:ASP:O	3:I:31:THR:CG2	2.43	0.50
3:L:219:SER:CB	3:L:224:THR:HG21	2.42	0.50
2:B:223:GLU:HG2	2:B:225:TYR:CE2	2.46	0.50
1:A:94:LEU:HD22	2:B:125:TRP:CZ3	2.47	0.50
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.94	0.50
3:C:69:ASN:O	3:C:71:ASP:N	2.44	0.50
1:G:147:MET:SD	3:I:121:ILE:HD11	2.52	0.50
3:I:251:GLU:HB2	3:I:257:THR:HG22	1.94	0.50
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.46	0.50
1:J:108:TYR:HH	3:L:84:LEU:H	1.55	0.50
2:K:252:ILE:HD12	2:K:452:MET:O	2.12	0.50
3:F:224:THR:HG23	3:F:224:THR:O	2.12	0.50
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.92	0.50
2:K:257:ASP:OD1	2:K:259:SER:CB	2.60	0.50
2:K:230:ASP:O	2:K:233:VAL:HG12	2.11	0.50
1:D:115:LEU:HD13	3:F:86:SER:HA	1.93	0.50
1:A:48:GLY:HA2	2:B:82:LEU:HD11	1.94	0.50
3:L:251:GLU:CD	3:L:381:LYS:NZ	2.65	0.50
2:K:257:ASP:OD1	2:K:259:SER:OG	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:360:LEU:HD13	5:P:2:HIS:ND1	2.26	0.50
3:I:5:ARG:HG2	3:I:11:LEU:HB3	1.93	0.50
2:E:295:GLY:O	2:E:298:LYS:HB2	2.12	0.50
3:I:195:GLN:OE1	3:I:382:THR:HG22	2.11	0.50
3:F:330:ASP:OD2	3:F:340:HIS:NE2	2.44	0.50
3:I:250:LEU:CD1	3:I:250:LEU:N	2.74	0.50
1:J:208:LYS:HB2	1:J:209:PRO:CD	2.41	0.50
1:J:210:VAL:N	1:J:211:PRO:HD2	2.27	0.50
3:I:356:LYS:HA	3:I:359:THR:CG2	2.41	0.50
1:D:111:VAL:HG11	3:F:87:ARG:CB	2.42	0.50
3:F:80:ASP:O	3:F:82:ALA:N	2.45	0.50
3:F:69:ASN:HB2	3:F:70:PRO:HD2	1.93	0.50
2:E:257:ASP:OD1	2:E:259:SER:OG	2.24	0.50
2:B:284:ASN:HD22	2:B:284:ASN:H	1.59	0.50
3:I:252:ASP:HB2	3:I:377:TYR:OH	2.12	0.50
5:T:2:HIS:CD2	5:T:4:PRO:HD3	2.47	0.49
1:A:59:ASN:ND2	2:B:86:LEU:HD23	2.20	0.49
3:C:262:TYR:CE2	3:C:290:PHE:HB2	2.47	0.49
3:I:3:ALA:HB2	3:L:11:LEU:CD1	2.42	0.49
2:B:87:LEU:HD23	2:B:87:LEU:O	2.12	0.49
1:D:63:THR:HG23	2:E:93:ILE:HD11	1.94	0.49
1:D:143:GLN:NE2	3:F:118:ASN:OD1	2.45	0.49
2:B:171:ILE:HG22	2:B:172:LEU:CD1	2.42	0.49
2:K:351:ASN:ND2	2:K:354:MET:H	2.09	0.49
2:H:326:TYR:CE1	2:H:353:LEU:HD12	2.48	0.49
3:L:291:ASP:OD1	3:L:302:LYS:NZ	2.44	0.49
3:L:297:ASP:N	3:L:297:ASP:OD1	2.45	0.49
3:L:194:PHE:CD1	3:L:233:ILE:HD13	2.47	0.49
3:C:276:LEU:O	3:C:276:LEU:HD23	2.13	0.49
1:A:136:LEU:HD13	1:A:139:ASN:HD22	1.76	0.49
3:C:304:PHE:O	3:C:337:ASN:CG	2.51	0.49
3:C:289:ALA:O	3:C:292:GLY:N	2.35	0.49
3:L:248:VAL:HG12	3:L:249:GLU:N	2.27	0.49
2:E:314:MET:HG3	2:E:322:VAL:HG23	1.95	0.49
3:L:193:VAL:O	3:L:226:PHE:HZ	1.95	0.49
1:J:115:LEU:CD1	3:L:90:LEU:HD21	2.42	0.49
3:I:208:TRP:CE3	3:I:317:ASN:HB3	2.48	0.49
3:F:166:LEU:HD11	3:F:220:PRO:N	2.28	0.49
2:H:402:TRP:CE3	2:H:413:ASN:ND2	2.81	0.49
3:L:295:PHE:HE1	3:L:305:THR:HG21	1.77	0.49
2:K:215:ILE:CD1	2:K:242:MET:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:281:PHE:CD2	3:I:283:GLY:HA2	2.46	0.49
2:K:255:ARG:NH1	2:K:412:PRO:O	2.43	0.49
3:L:379:MET:HA	3:L:379:MET:CE	2.41	0.49
3:L:264:MET:N	3:L:264:MET:SD	2.86	0.49
1:J:93:ILE:HD12	1:J:94:LEU:HD23	1.93	0.49
3:F:246:LEU:HD12	3:F:246:LEU:C	2.33	0.49
2:B:385:TRP:CD1	2:B:406:ARG:HG3	2.48	0.49
3:L:197:ARG:O	3:L:381:LYS:HA	2.13	0.49
2:E:205:VAL:HG22	3:F:218:LEU:CD2	2.43	0.49
1:D:86:LEU:HD21	3:F:61:ILE:HG21	1.93	0.49
1:J:127:ILE:CA	1:J:130:VAL:HG12	2.39	0.49
1:G:97:ASP:O	1:G:101:ALA:HB2	2.13	0.49
3:F:375:ARG:HG3	3:F:376:TRP:N	2.27	0.49
2:E:108:SER:HA	2:E:111:SER:HB3	1.95	0.49
2:H:329:PHE:HE2	2:H:454:ILE:HG21	1.77	0.49
2:H:210:GLU:OE1	2:H:213:GLU:N	2.45	0.49
1:D:115:LEU:HD13	3:F:86:SER:HB2	1.94	0.49
3:L:225:GLU:O	3:L:226:PHE:HB3	2.12	0.49
3:C:258:SER:HB2	3:C:286:ALA:HB2	1.94	0.49
1:J:152:VAL:HG11	2:K:426:MET:HB3	1.95	0.49
1:A:133:ILE:HD11	3:C:107:ILE:CG1	2.42	0.49
3:L:367:ILE:O	3:L:378:SER:HA	2.13	0.49
2:E:178:LYS:O	2:E:181:LYS:HG3	2.13	0.49
1:J:129:LYS:CE	3:L:104:ASP:HB3	2.43	0.49
1:A:200:GLN:NE2	2:B:149:HIS:NE2	2.61	0.49
3:I:288:ASP:C	3:I:371:THR:HG21	2.33	0.49
2:E:439:ASN:HD22	2:E:439:ASN:H	1.59	0.49
2:H:308:THR:CG2	2:H:454:ILE:HB	2.43	0.49
2:B:179:ILE:CG2	2:B:180:GLN:H	2.26	0.49
2:H:326:TYR:CZ	2:H:353:LEU:HD12	2.48	0.49
2:E:179:ILE:HD12	3:F:120:LYS:HD3	1.95	0.49
2:E:351:ASN:C	2:E:351:ASN:HD22	2.16	0.48
3:C:301:ASP:O	3:C:305:THR:OG1	2.30	0.48
3:L:214:GLY:HA3	3:L:228:LEU:O	2.13	0.48
2:H:343:ASN:HA	2:H:354:MET:SD	2.53	0.48
2:K:410:ALA:CB	2:K:437:TRP:CE3	2.96	0.48
2:E:330:THR:O	2:E:331:VAL:HG22	2.12	0.48
1:D:149:ARG:NE	2:E:427:ALA:O	2.45	0.48
2:E:161:ILE:HG21	3:F:103:HIS:CG	2.47	0.48
3:F:191:TRP:CE3	3:F:385:LYS:CG	2.96	0.48
3:F:166:LEU:CD2	3:F:218:LEU:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:VAL:HG13	1:J:146:ASP:H	1.76	0.48
2:E:199:VAL:HG23	3:F:141:ASP:CA	2.42	0.48
1:G:46:PRO:O	3:I:22:THR:HG21	2.13	0.48
1:G:116:ARG:HD3	2:H:142:TYR:OH	2.13	0.48
2:K:122:LYS:O	2:K:125:TRP:HB3	2.13	0.48
3:I:355:SER:O	3:I:359:THR:HG23	2.14	0.48
1:D:65:ARG:O	1:D:69:LEU:HD23	2.13	0.48
3:F:352:GLY:O	3:F:354:TYR:HD2	1.95	0.48
3:I:305:THR:HB	3:I:341:ALA:HB2	1.96	0.48
1:A:46:PRO:O	3:C:22:THR:HG21	2.13	0.48
2:E:152:TYR:O	2:E:156:THR:HG22	2.13	0.48
3:L:46:ILE:O	3:L:46:ILE:HG22	2.12	0.48
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.95	0.48
6:B:471:NDG:H5	6:B:472:BMA:C2	2.43	0.48
2:B:252:ILE:HD11	2:B:454:ILE:CG2	2.43	0.48
3:C:246:LEU:HD12	3:C:386:ILE:CG2	2.44	0.48
3:C:292:GLY:HA2	3:C:341:ALA:CB	2.43	0.48
3:F:169:ILE:HD11	3:F:180:VAL:CG2	2.41	0.48
3:C:340:HIS:C	3:C:340:HIS:ND1	2.67	0.48
2:E:321:LYS:O	2:E:322:VAL:HG13	2.13	0.48
6:E:479:SIA:H6	6:E:479:SIA:O1B	2.13	0.48
6:B:471:NDG:H3	6:B:472:BMA:O2	2.13	0.48
3:C:246:LEU:CD2	3:C:248:VAL:CG2	2.89	0.48
2:E:205:VAL:HG21	3:F:215:PHE:O	2.14	0.48
2:K:148:LYS:HD3	2:K:148:LYS:N	2.28	0.48
3:C:387:ILE:O	3:C:387:ILE:HG23	2.13	0.48
3:I:365:ASN:N	3:I:365:ASN:HD22	2.12	0.48
3:L:172:LEU:H	3:L:239:GLN:HE21	1.61	0.48
2:E:422:TYR:CE1	2:E:444:TRP:HA	2.48	0.48
3:L:207:ASN:OD1	3:L:207:ASN:C	2.52	0.48
3:C:347:VAL:CG2	3:C:349:TYR:CE1	2.97	0.48
3:I:236:ILE:HA	3:I:239:GLN:HE21	1.78	0.48
3:L:259:THR:N	3:L:286:ALA:HB2	2.29	0.48
3:F:327:ALA:HB1	3:F:332:SER:O	2.13	0.48
1:J:138:LYS:C	1:J:138:LYS:CD	2.82	0.48
3:L:307:HIS:CE1	3:L:341:ALA:H	2.31	0.48
1:J:169:LEU:HD22	1:J:171:ARG:HG2	1.96	0.48
2:B:178:LYS:O	2:B:179:ILE:C	2.52	0.48
2:K:212:GLU:HA	2:K:215:ILE:HG22	1.95	0.48
1:A:185:LEU:HD11	1:A:189:ILE:HD11	1.95	0.48
2:K:300:SER:OG	2:K:301:GLN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:ALA:HB1	2:B:409:ALA:HB3	1.95	0.48
3:I:253:TRP:C	3:I:254:ASN:HD22	2.16	0.48
1:A:165:CYS:HA	2:B:196:PRO:HA	1.96	0.48
3:I:15:PHE:O	3:L:24:GLY:HA3	2.14	0.48
1:J:62:PHE:O	1:J:66:ILE:HB	2.13	0.48
2:K:353:LEU:O	2:K:369:ILE:HG23	2.14	0.48
3:L:110:LEU:HA	3:L:113:ILE:HG22	1.96	0.48
2:B:101:ASN:CG	3:C:43:LEU:HD11	2.34	0.48
6:B:473:MAN:O5	6:B:475:NDG:H3	2.13	0.48
6:E:472:BMA:H3	6:E:474:MAN:O2	2.13	0.48
2:B:115:PHE:HE2	3:C:50:VAL:HG13	1.78	0.48
2:E:266:TRP:CD1	2:E:380:ARG:NH2	2.82	0.48
1:G:157:LYS:HD2	3:I:128:VAL:HG13	1.96	0.48
2:E:370:HIS:O	2:E:373:MET:N	2.36	0.48
1:G:123:LYS:HE3	1:G:123:LYS:HA	1.96	0.48
2:B:101:ASN:OD1	3:C:43:LEU:CD2	2.61	0.48
3:L:154:GLN:O	3:L:157:ALA:HB3	2.14	0.48
2:E:322:VAL:HG12	2:E:348:THR:HB	1.95	0.48
2:E:424:TRP:CZ2	6:E:479:SIA:H31	2.49	0.48
2:B:125:TRP:O	2:B:129:GLN:HB3	2.13	0.48
3:C:252:ASP:HB2	3:C:373:LYS:NZ	2.29	0.48
1:J:111:VAL:HG11	3:L:87:ARG:HD2	1.95	0.48
2:K:435:VAL:O	2:K:435:VAL:HG12	2.12	0.48
3:I:247:ARG:NE	3:I:261:ASP:OD1	2.47	0.48
3:I:234:HIS:HB2	3:I:267:VAL:HG12	1.95	0.48
1:G:63:THR:O	1:G:66:ILE:HG22	2.14	0.47
2:B:281:ASP:O	2:B:283:LYS:NZ	2.46	0.47
3:I:169:ILE:CD1	3:I:180:VAL:HG11	2.43	0.47
3:C:238:THR:O	3:C:238:THR:OG1	2.24	0.47
2:E:228:GLN:NE2	2:E:231:SER:HA	2.29	0.47
1:J:194:LEU:HD12	2:K:152:TYR:CD2	2.49	0.47
2:B:113:SER:O	2:B:116:GLN:NE2	2.46	0.47
2:B:295:GLY:O	2:B:299:ILE:HG13	2.13	0.47
1:A:135:LEU:HD22	1:A:136:LEU:HD22	1.97	0.47
2:K:249:TRP:HB3	2:K:453:LYS:HD3	1.96	0.47
3:C:90:LEU:HD12	3:C:90:LEU:O	2.12	0.47
3:C:215:PHE:CE2	3:C:227:TRP:CB	2.95	0.47
1:D:86:LEU:HD23	3:F:61:ILE:CG2	2.44	0.47
3:F:31:THR:HG22	3:F:35:LYS:NZ	2.28	0.47
2:K:199:VAL:HG23	3:L:141:ASP:CB	2.44	0.47
1:G:169:LEU:HD23	1:G:170:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:298:ASP:OD2	3:L:300:SER:N	2.44	0.47
2:E:351:ASN:C	2:E:351:ASN:ND2	2.68	0.47
3:L:247:ARG:HG3	3:L:248:VAL:O	2.14	0.47
3:C:216:GLY:HA3	3:C:226:PHE:CB	2.44	0.47
2:B:210:GLU:C	2:B:210:GLU:OE2	2.52	0.47
3:F:262:TYR:OH	3:F:288:ASP:OD1	2.16	0.47
3:L:389:PHE:HD1	3:L:389:PHE:C	2.16	0.47
2:B:409:ALA:O	2:B:438:MET:HB2	2.14	0.47
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.96	0.47
2:B:67:HIS:CD2	2:B:69:ASP:HB3	2.50	0.47
2:B:342:VAL:C	2:B:343:ASN:HD22	2.17	0.47
2:K:179:ILE:O	2:K:183:GLU:HB2	2.14	0.47
2:B:255:ARG:HA	2:B:291:GLU:HG2	1.96	0.47
3:F:281:PHE:HB2	3:F:288:ASP:OD2	2.14	0.47
3:C:252:ASP:OD2	3:C:256:ARG:NH1	2.47	0.47
2:K:257:ASP:OD1	2:K:259:SER:HB3	2.15	0.47
2:H:226:LEU:HD12	2:H:236:TYR:C	2.35	0.47
2:K:112:SER:HA	2:K:115:PHE:HD2	1.79	0.47
3:L:289:ALA:HA	3:L:371:THR:HG23	1.96	0.47
1:A:188:VAL:HG12	2:B:164:ASN:ND2	2.29	0.47
2:B:80:CYS:O	2:B:84:GLU:N	2.30	0.47
6:K:470:NAG:H62	5:T:4:PRO:CG	2.45	0.47
1:A:58:VAL:CG1	1:A:59:ASN:N	2.78	0.47
2:H:415:ARG:N	2:H:434:GLY:HA2	2.30	0.47
1:G:60:GLN:HE22	1:G:64:ASN:HD22	1.61	0.47
3:L:304:PHE:O	3:L:306:SER:N	2.48	0.47
1:D:160:SER:HA	2:E:258:GLY:O	2.15	0.47
3:L:147:ASP:OD1	3:L:147:ASP:N	2.47	0.47
3:I:228:LEU:O	3:I:232:LYS:HD2	2.15	0.47
3:C:27:ASP:O	3:C:31:THR:HG23	2.15	0.47
3:I:325:ASN:HD22	3:I:325:ASN:C	2.18	0.47
3:L:90:LEU:HD23	3:L:90:LEU:C	2.35	0.47
2:K:147:GLU:O	2:K:150:GLN:HG3	2.15	0.47
3:L:153:CYS:O	3:L:156:ILE:HB	2.15	0.47
1:A:148:LYS:O	1:A:152:VAL:HG12	2.15	0.47
2:E:402:TRP:CZ3	2:E:412:PRO:CG	2.98	0.47
1:D:59:ASN:O	1:D:63:THR:HG23	2.14	0.47
6:K:470:NAG:H62	5:T:4:PRO:HG3	1.97	0.47
3:L:219:SER:HG	3:L:224:THR:CG2	2.26	0.47
3:I:286:ALA:O	3:I:372:TRP:HB2	2.14	0.47
2:K:172:LEU:HD11	3:L:114:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:VAL:CG2	2:H:354:MET:HG2	2.45	0.47
1:G:166:SER:CB	2:H:195:THR:HG1	2.28	0.47
1:J:123:LYS:HA	1:J:123:LYS:HE3	1.97	0.47
3:C:178:PHE:CD1	3:C:232:LYS:HD3	2.50	0.47
1:D:162:ARG:HA	1:D:168:ALA:HB2	1.96	0.47
3:I:115:ASN:C	3:I:115:ASN:HD22	2.18	0.47
3:L:219:SER:CB	3:L:224:THR:CG2	2.93	0.47
2:B:163:THR:HG22	2:B:166:ARG:HH22	1.80	0.47
3:L:169:ILE:HD11	3:L:180:VAL:HG11	1.97	0.47
2:B:212:GLU:HA	2:B:215:ILE:HG22	1.96	0.47
3:C:206:LYS:HB2	3:C:211:TYR:HE1	1.78	0.47
2:E:402:TRP:CH2	2:E:412:PRO:CG	2.97	0.47
2:H:314:MET:HB3	2:H:314:MET:HE2	1.82	0.47
2:H:314:MET:HE2	2:H:450:MET:SD	2.55	0.47
2:H:101:ASN:OD1	3:I:43:LEU:HD11	2.14	0.47
2:E:233:VAL:HG22	2:E:234:LYS:O	2.14	0.47
1:J:108:TYR:HE1	3:L:83:THR:CG2	2.28	0.46
3:C:179:LEU:CD2	3:C:180:VAL:O	2.63	0.46
3:F:51:GLU:HA	3:F:54:THR:HG22	1.97	0.46
2:E:410:ALA:HB2	2:E:437:TRP:CE3	2.49	0.46
1:A:147:MET:O	1:A:148:LYS:C	2.53	0.46
1:D:134:GLN:OE1	1:D:193:LEU:HD22	2.15	0.46
2:K:312:ILE:CB	2:K:324:ALA:HB3	2.41	0.46
2:H:329:PHE:CE2	2:H:454:ILE:HG21	2.51	0.46
2:B:343:ASN:HA	2:B:354:MET:SD	2.55	0.46
3:C:374:THR:OG1	3:C:375:ARG:N	2.48	0.46
3:C:163:GLN:O	3:C:167:TYR:OH	2.30	0.46
3:C:183:GLU:O	3:C:191:TRP:HB2	2.16	0.46
2:E:435:VAL:O	2:E:447:MET:HG2	2.14	0.46
2:H:200:SER:O	2:H:279:ASN:ND2	2.48	0.46
2:H:260:VAL:HG12	2:H:261:ASP:O	2.14	0.46
2:H:171:ILE:HG23	2:H:172:LEU:H	1.78	0.46
2:B:329:PHE:HD1	2:B:342:VAL:HG12	1.79	0.46
3:F:332:SER:CB	3:F:343:HIS:NE2	2.78	0.46
2:H:420:GLY:HA2	2:H:446:SER:O	2.16	0.46
3:C:264:MET:HB2	3:C:279:ALA:CB	2.45	0.46
3:F:211:TYR:CE1	3:F:333:GLY:HA3	2.50	0.46
3:L:96:TYR:O	3:L:100:ILE:HD13	2.15	0.46
3:I:304:PHE:CG	3:I:338:LYS:HE3	2.51	0.46
2:E:91:ARG:N	2:E:92:PRO:HD2	2.30	0.46
2:B:252:ILE:CD1	2:B:454:ILE:CG2	2.91	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:302:LEU:HD13	2:H:454:ILE:HD11	1.98	0.46
3:C:179:LEU:HD23	3:C:180:VAL:O	2.16	0.46
1:J:140:VAL:CG2	1:J:141:ARG:N	2.78	0.46
2:K:172:LEU:HD22	3:L:113:ILE:CG2	2.41	0.46
3:L:109:TYR:O	3:L:113:ILE:HG22	2.15	0.46
2:K:340:ILE:HG21	2:K:403:TRP:CG	2.50	0.46
1:J:111:VAL:HG21	3:L:87:ARG:CZ	2.45	0.46
1:A:41:TRP:O	1:A:42:ASN:HB2	2.15	0.46
3:F:122:VAL:HG13	3:F:123:ASN:ND2	2.30	0.46
2:H:140:ASN:HD22	2:H:140:ASN:C	2.19	0.46
1:G:135:LEU:HD23	1:G:136:LEU:HD22	1.98	0.46
3:C:113:ILE:O	3:C:117:ASN:HB2	2.15	0.46
2:H:210:GLU:OE2	2:H:212:GLU:HB3	2.15	0.46
2:H:364:ASN:HA	2:H:367:MET:HE3	1.98	0.46
2:B:253:GLN:NE2	2:B:451:SER:HA	2.30	0.46
2:K:436:VAL:HG12	2:K:437:TRP:N	2.30	0.46
3:F:143:VAL:HG22	3:F:143:VAL:O	2.16	0.46
2:B:345:TYR:CG	2:B:346:ARG:N	2.82	0.46
3:F:334:TRP:HB3	3:F:336:MET:HE2	1.96	0.46
1:J:206:LYS:O	1:J:210:VAL:N	2.47	0.46
2:K:424:TRP:CG	2:K:425:ASP:N	2.84	0.46
3:I:240:SER:O	3:I:241:ALA:C	2.54	0.46
1:J:159:ARG:HB2	1:J:159:ARG:CZ	2.45	0.46
1:D:151:GLU:CG	1:D:173:VAL:HG11	2.45	0.46
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.98	0.46
3:C:290:PHE:HA	3:C:307:HIS:HD1	1.79	0.46
3:I:29:LEU:HD12	3:I:33:GLN:HB2	1.97	0.46
1:G:122:LEU:HD12	1:G:123:LYS:NZ	2.31	0.46
3:I:60:LEU:O	3:I:64:ILE:HD13	2.16	0.46
3:C:219:SER:H	3:C:224:THR:HG21	1.81	0.46
3:C:304:PHE:O	3:C:337:ASN:ND2	2.49	0.46
3:C:264:MET:HB2	3:C:279:ALA:HB2	1.98	0.46
3:C:21:THR:HG23	3:C:24:GLY:H	1.81	0.46
3:L:205:LYS:HD2	3:L:331:GLY:CA	2.46	0.46
2:B:364:ASN:ND2	6:B:470:NAG:N2	2.64	0.46
3:L:49:GLN:HE21	8:L:570:NAG:C8	2.28	0.46
2:B:172:LEU:CD2	3:C:110:LEU:HD22	2.46	0.46
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.13	0.46
3:L:198:LEU:HD13	3:L:199:ASP:HB3	1.98	0.46
2:E:435:VAL:HG12	2:E:447:MET:CG	2.46	0.46
3:C:132:GLU:C	3:C:134:GLN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:LYS:HD3	2:B:182:LEU:HD12	1.97	0.46
3:F:210:GLN:O	3:F:214:GLY:N	2.43	0.46
3:C:246:LEU:CD2	3:C:248:VAL:HG23	2.45	0.46
6:B:473:MAN:H4	6:B:475:NDG:HA	1.79	0.46
2:E:226:LEU:HD12	2:E:236:TYR:C	2.37	0.46
2:B:345:TYR:C	2:B:345:TYR:CD2	2.90	0.46
2:E:376:SER:HG	2:E:382:ASN:H	1.62	0.46
1:G:73:LEU:HD11	2:H:103:ASN:OD1	2.16	0.46
1:A:96:GLY:O	1:A:99:SER:N	2.44	0.46
1:A:160:SER:O	2:B:259:SER:O	2.33	0.46
3:F:254:ASN:N	3:F:254:ASN:HD22	2.15	0.46
3:C:169:ILE:HD13	3:C:180:VAL:HG21	1.98	0.45
3:F:168:PHE:CE2	3:F:179:LEU:HD13	2.51	0.45
2:H:105:GLU:OE2	3:I:46:ILE:HG21	2.16	0.45
2:E:298:LYS:O	2:E:302:LEU:HB2	2.16	0.45
1:G:185:LEU:CD1	1:G:189:ILE:HD11	2.44	0.45
2:K:259:SER:OG	2:K:291:GLU:HG3	2.16	0.45
1:G:65:ARG:CD	3:I:40:LEU:HD23	2.47	0.45
2:B:136:GLU:O	2:B:140:ASN:O	2.34	0.45
3:I:225:GLU:O	3:I:226:PHE:HB3	2.16	0.45
1:D:55:ILE:HD11	3:F:25:ILE:CG2	2.46	0.45
2:K:436:VAL:HG21	2:K:443:SER:O	2.16	0.45
2:H:66:LEU:HD22	1:J:35:PHE:CE1	2.51	0.45
1:A:169:LEU:H	2:B:189:GLN:HE22	1.63	0.45
1:A:149:ARG:O	1:A:152:VAL:HG13	2.16	0.45
2:H:167:VAL:HG13	2:H:168:LEU:N	2.31	0.45
1:A:188:VAL:HG12	2:B:164:ASN:HD21	1.81	0.45
2:H:417:TYR:HB2	2:H:446:SER:HB3	1.98	0.45
2:B:134:ASP:O	2:B:138:VAL:HG12	2.16	0.45
3:I:148:ILE:HG22	3:I:149:THR:N	2.32	0.45
2:B:364:ASN:ND2	6:B:470:NAG:O5	2.42	0.45
1:J:73:LEU:HD13	1:J:74:PHE:N	2.31	0.45
2:K:150:GLN:O	2:K:153:ILE:N	2.47	0.45
3:L:343:HIS:CG	3:L:343:HIS:O	2.70	0.45
3:L:295:PHE:CE1	3:L:305:THR:HG21	2.50	0.45
2:K:84:GLU:OE1	3:L:5:ARG:NH1	2.50	0.45
3:I:5:ARG:HD3	3:I:5:ARG:O	2.17	0.45
2:B:329:PHE:C	2:B:330:THR:CG2	2.85	0.45
1:G:66:ILE:HG23	1:G:70:LYS:HE2	1.98	0.45
1:D:52:LYS:HB2	2:E:82:LEU:HD21	1.97	0.45
3:L:305:THR:HB	3:L:341:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:TRP:O	1:D:42:ASN:CB	2.65	0.45
3:I:108:ARG:O	3:I:111:GLN:HG2	2.16	0.45
3:C:231:GLU:OE1	3:C:274:TYR:OH	2.16	0.45
2:B:198:THR:HG22	3:C:140:LYS:HB2	1.97	0.45
2:B:118:MET:HG3	3:C:57:VAL:HG13	1.99	0.45
1:J:69:LEU:HD12	2:K:100:LEU:HD11	1.99	0.45
1:A:73:LEU:CD2	2:B:104:VAL:HG22	2.40	0.45
2:H:367:MET:SD	2:H:406:ARG:CD	3.00	0.45
3:C:216:GLY:HA3	3:C:226:PHE:HB2	1.97	0.45
3:F:218:LEU:C	3:F:224:THR:HG21	2.37	0.45
1:A:104:ARG:HH22	3:C:78:MET:CE	2.30	0.45
3:C:181:TYR:CE1	3:C:220:PRO:O	2.64	0.45
3:L:152:ASP:OD1	3:L:152:ASP:C	2.54	0.45
1:G:185:LEU:O	1:G:185:LEU:HD22	2.17	0.45
2:E:300:SER:HB2	2:E:331:VAL:O	2.16	0.45
2:K:230:ASP:O	2:K:233:VAL:CG1	2.64	0.45
3:I:267:VAL:CG1	3:I:268:GLY:N	2.80	0.45
3:F:342:GLY:O	3:F:344:LEU:N	2.48	0.45
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.99	0.45
3:I:21:THR:HG23	3:I:24:GLY:H	1.82	0.45
2:E:163:THR:HG23	2:E:166:ARG:HH12	1.81	0.45
2:K:326:TYR:CZ	2:K:353:LEU:HD12	2.52	0.45
3:C:166:LEU:HD21	3:C:218:LEU:HB3	1.99	0.45
6:E:470:NAG:H62	5:P:4:PRO:HB3	1.99	0.45
1:D:29:LYS:O	1:D:31:SER:N	2.50	0.45
1:A:94:LEU:HD22	2:B:125:TRP:HZ3	1.80	0.45
3:F:251:GLU:O	3:F:380:LYS:HB3	2.17	0.45
2:K:256:GLN:O	2:K:449:LYS:NZ	2.44	0.45
3:C:97:GLU:C	3:C:100:ILE:HG22	2.36	0.45
2:E:253:GLN:NE2	2:E:253:GLN:C	2.69	0.45
2:H:402:TRP:HB3	2:H:404:TYR:CD2	2.52	0.45
2:E:435:VAL:HG12	2:E:447:MET:HG2	1.99	0.45
3:L:340:HIS:ND1	3:L:343:HIS:HB3	2.32	0.45
1:A:150:LEU:HD22	3:C:125:LYS:HE3	1.99	0.45
3:I:10:ILE:HG13	2:K:83:GLN:HE22	1.82	0.45
1:A:58:VAL:HG12	1:A:59:ASN:N	2.32	0.45
3:I:224:THR:O	3:I:224:THR:HG23	2.17	0.45
3:L:372:TRP:HZ3	3:L:379:MET:HE1	1.81	0.45
3:L:291:ASP:OD1	3:L:302:LYS:CE	2.65	0.45
1:J:115:LEU:HD11	3:L:90:LEU:HD21	1.99	0.45
2:K:357:ALA:HA	2:K:439:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:140:ASN:O	2:K:144:SER:OG	2.22	0.45
3:I:166:LEU:HD11	3:I:220:PRO:N	2.31	0.45
1:D:45:CYS:HB3	1:D:46:PRO:HD2	1.98	0.45
1:G:116:ARG:NE	2:H:142:TYR:OH	2.50	0.45
2:K:128:ARG:O	2:K:132:VAL:HG22	2.17	0.45
1:J:151:GLU:HG2	1:J:173:VAL:HG13	1.99	0.45
2:K:272:GLY:HA3	2:K:295:GLY:N	2.32	0.44
7:H:470:NAG:C6	5:S:4:PRO:HB3	2.46	0.44
2:B:253:GLN:HE22	2:B:451:SER:HA	1.81	0.44
1:D:63:THR:O	1:D:66:ILE:HG22	2.16	0.44
2:E:415:ARG:O	2:E:434:GLY:HA2	2.17	0.44
1:D:150:LEU:HD11	3:F:125:LYS:NZ	2.32	0.44
3:L:221:THR:OG1	3:L:223:THR:CG2	2.64	0.44
3:L:11:LEU:HB3	3:L:18:TYR:CZ	2.52	0.44
2:K:401:GLY:O	2:K:413:ASN:ND2	2.51	0.44
3:C:183:GLU:HB3	3:C:191:TRP:HB2	1.99	0.44
2:E:424:TRP:CG	2:E:425:ASP:N	2.85	0.44
1:D:122:LEU:HD12	1:D:123:LYS:CE	2.47	0.44
1:G:135:LEU:HD23	1:G:139:ASN:HD22	1.82	0.44
3:F:202:VAL:HG12	3:F:203:ASP:O	2.17	0.44
2:E:104:VAL:O	2:E:104:VAL:HG12	2.17	0.44
3:I:12:ASP:CG	3:I:15:PHE:CD1	2.90	0.44
1:J:55:ILE:HG23	2:K:86:LEU:CD2	2.47	0.44
1:J:55:ILE:O	1:J:58:VAL:HG12	2.18	0.44
3:F:246:LEU:HD12	3:F:247:ARG:CA	2.46	0.44
3:I:208:TRP:HB3	3:I:209:ILE:HD12	1.99	0.44
3:I:156:ILE:HD13	3:I:167:TYR:CD2	2.53	0.44
2:K:95:ASN:C	2:K:95:ASN:ND2	2.70	0.44
1:J:66:ILE:HD11	2:K:100:LEU:HD12	1.99	0.44
2:E:212:GLU:O	2:E:213:GLU:C	2.56	0.44
6:K:476:GAL:H4	6:K:480:SIA:H31	1.98	0.44
3:I:310:MET:CE	3:I:321:LYS:NZ	2.80	0.44
2:B:156:THR:HG22	2:B:157:VAL:HG23	2.00	0.44
1:D:69:LEU:HD13	3:F:47:LEU:HD11	2.00	0.44
3:L:173:LYS:NZ	3:L:238:THR:O	2.49	0.44
2:E:63:GLY:O	2:E:77:PRO:HD3	2.18	0.44
2:H:121:LEU:HD23	2:H:124:LEU:HD23	1.99	0.44
6:B:471:NDG:H5	6:B:472:BMA:H2	1.99	0.44
2:H:295:GLY:O	2:H:299:ILE:HG13	2.17	0.44
2:H:201:CYS:HB3	2:H:224:MET:HE3	1.99	0.44
3:L:318:ASP:OD1	3:L:320:ASP:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:GLY:O	2:B:260:VAL:N	2.51	0.44
6:E:471:NDG:H5	6:E:472:BMA:C2	2.48	0.44
3:C:207:ASN:C	3:C:207:ASN:OD1	2.56	0.44
3:C:68:TYR:O	3:C:69:ASN:HB2	2.18	0.44
2:E:161:ILE:HB	2:E:162:PRO:HD3	2.00	0.44
2:H:337:LYS:O	2:H:338:TYR:C	2.55	0.44
1:J:63:THR:C	1:J:66:ILE:HG22	2.37	0.44
2:K:314:MET:HE2	2:K:314:MET:HB3	1.79	0.44
2:B:294:LEU:HD12	2:B:295:GLY:N	2.29	0.44
3:F:236:ILE:CG2	3:F:386:ILE:HD11	2.46	0.44
2:E:291:GLU:O	2:E:292:TYR:HB3	2.16	0.44
3:I:251:GLU:CB	3:I:257:THR:HG22	2.48	0.44
2:H:314:MET:HG3	2:H:322:VAL:CG2	2.48	0.44
1:A:99:SER:HA	1:A:102:ASN:HD22	1.83	0.44
1:D:30:ASP:O	1:D:32:ASP:N	2.51	0.44
3:I:10:ILE:CD1	2:K:83:GLN:HE22	2.30	0.44
1:A:105:ASP:O	1:A:108:TYR:N	2.51	0.44
1:J:69:LEU:CD1	2:K:100:LEU:HD11	2.47	0.44
1:G:166:SER:N	2:H:195:THR:O	2.40	0.44
3:F:289:ALA:CA	3:F:371:THR:HG23	2.46	0.44
1:D:115:LEU:HD13	3:F:86:SER:CA	2.48	0.44
3:L:193:VAL:O	3:L:226:PHE:CZ	2.71	0.44
2:H:233:VAL:HG22	2:H:234:LYS:O	2.18	0.44
1:J:201:HIS:CE1	1:J:202:LEU:HD23	2.53	0.44
3:C:275:ARG:HA	3:C:311:GLN:HA	1.99	0.44
1:A:194:LEU:HG	2:B:152:TYR:CD2	2.52	0.44
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.33	0.44
3:L:80:ASP:OD1	3:L:80:ASP:N	2.51	0.44
3:F:230:ASN:HA	3:F:233:ILE:HD12	1.99	0.44
1:D:119:ILE:HD11	3:F:93:ILE:CD1	2.40	0.44
3:L:248:VAL:HG12	3:L:250:LEU:HD13	2.00	0.44
6:E:471:NDG:O7	6:E:471:NDG:H3	2.17	0.44
3:I:166:LEU:HD23	3:I:218:LEU:CB	2.47	0.44
3:I:151:LYS:CE	3:I:172:LEU:HD13	2.47	0.44
1:D:151:GLU:HG3	1:D:173:VAL:HG11	1.98	0.44
3:F:254:ASN:ND2	3:F:254:ASN:N	2.65	0.44
2:H:135:ASN:O	2:H:139:VAL:N	2.50	0.44
2:B:405:ASN:CG	2:B:405:ASN:O	2.55	0.44
2:H:75:LEU:HD22	1:J:46:PRO:CD	2.48	0.44
3:L:197:ARG:CZ	3:L:367:ILE:HD11	2.48	0.44
3:L:367:ILE:CG2	3:L:382:THR:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:198:LEU:CD1	3:L:199:ASP:N	2.75	0.44
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.99	0.44
3:C:167:TYR:CD1	3:C:167:TYR:N	2.86	0.44
3:L:156:ILE:HG22	3:L:157:ALA:N	2.32	0.44
3:I:240:SER:HB2	3:I:242:ILE:HG13	1.99	0.44
2:K:373:MET:HG3	2:K:405:ASN:HB2	2.00	0.44
2:K:151:LEU:HA	2:K:154:ASP:HB3	2.00	0.44
3:C:288:ASP:O	3:C:289:ALA:C	2.54	0.43
2:H:373:MET:HA	2:H:373:MET:CE	2.48	0.43
3:C:197:ARG:NH2	3:C:204:PHE:CD2	2.83	0.43
2:E:410:ALA:HA	2:E:436:VAL:O	2.18	0.43
2:H:99:GLU:O	2:H:103:ASN:HB2	2.17	0.43
1:D:115:LEU:HD13	3:F:86:SER:CB	2.48	0.43
3:F:100:ILE:HG22	3:F:101:LEU:HD12	1.99	0.43
2:E:241:ASP:OD2	2:E:243:ASN:N	2.42	0.43
2:E:351:ASN:ND2	2:E:354:MET:H	2.12	0.43
3:L:380:LYS:HG2	3:L:381:LYS:HE2	2.00	0.43
3:F:281:PHE:CB	3:F:288:ASP:OD2	2.66	0.43
2:B:203:ILE:H	2:B:203:ILE:HD12	1.82	0.43
3:C:338:LYS:N	3:C:339:CYS:HA	2.32	0.43
6:B:470:NAG:H62	5:O:4:PRO:HG3	2.00	0.43
2:B:163:THR:HG22	2:B:166:ARG:HH12	1.82	0.43
2:H:252:ILE:HG23	2:H:299:ILE:HD13	2.01	0.43
3:F:193:VAL:HA	3:F:385:LYS:HB3	2.00	0.43
2:E:212:GLU:HA	2:E:215:ILE:HG22	2.00	0.43
3:F:50:VAL:O	3:F:54:THR:HB	2.18	0.43
2:H:434:GLY:O	2:H:436:VAL:N	2.51	0.43
2:E:302:LEU:HD22	2:E:454:ILE:HD11	1.99	0.43
3:L:207:ASN:OD1	3:L:209:ILE:N	2.51	0.43
1:J:154:ILE:HD11	3:L:128:VAL:CG2	2.46	0.43
3:L:196:LYS:O	3:L:225:GLU:HA	2.18	0.43
3:L:300:SER:O	3:L:301:ASP:C	2.56	0.43
1:G:143:GLN:O	1:G:146:ASP:N	2.51	0.43
1:J:175:LEU:O	1:J:178:TYR:N	2.52	0.43
2:K:139:VAL:HG11	3:L:79:ILE:HG23	2.01	0.43
2:K:100:LEU:O	2:K:104:VAL:HG23	2.18	0.43
2:B:105:GLU:O	2:B:109:GLN:HB2	2.18	0.43
2:K:310:LEU:C	2:K:310:LEU:HD12	2.38	0.43
1:J:145:VAL:CG1	1:J:146:ASP:H	2.31	0.43
3:I:199:ASP:OD1	3:I:201:SER:CB	2.66	0.43
2:B:294:LEU:HD11	2:B:298:LYS:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ALA:CB	3:C:235:LEU:HD13	2.47	0.43
2:K:338:TYR:O	2:K:403:TRP:NE1	2.46	0.43
3:C:387:ILE:O	3:C:388:PRO:C	2.56	0.43
3:I:145:ILE:HD13	3:I:179:LEU:HD13	2.00	0.43
3:L:307:HIS:HE1	3:L:341:ALA:H	1.64	0.43
3:F:119:GLN:O	3:F:122:VAL:HG12	2.18	0.43
3:L:281:PHE:CZ	3:L:283:GLY:HA2	2.54	0.43
2:B:264:ARG:HD2	2:B:273:PHE:CD2	2.54	0.43
2:K:91:ARG:N	2:K:92:PRO:HD2	2.34	0.43
3:C:300:SER:O	3:C:301:ASP:C	2.56	0.43
3:I:372:TRP:HZ3	3:I:379:MET:CE	2.32	0.43
3:L:228:LEU:CD1	3:L:232:LYS:HD2	2.48	0.43
1:A:63:THR:HA	1:A:66:ILE:CG2	2.47	0.43
2:H:115:PHE:CZ	3:I:54:THR:CG2	3.02	0.43
3:I:289:ALA:HA	3:I:371:THR:CG2	2.48	0.43
1:G:60:GLN:NE2	1:G:64:ASN:HD22	2.16	0.43
3:L:359:THR:HG22	3:L:365:ASN:ND2	2.33	0.43
1:J:169:LEU:HD12	2:K:188:ALA:HB3	2.00	0.43
3:C:295:PHE:HZ	3:C:341:ALA:HA	1.84	0.43
2:H:394:CYS:SG	2:H:406:ARG:HA	2.59	0.43
2:E:226:LEU:HD12	2:E:236:TYR:O	2.19	0.43
3:L:156:ILE:HD13	3:L:167:TYR:CD2	2.53	0.43
2:E:330:THR:O	2:E:331:VAL:CG2	2.66	0.43
3:L:172:LEU:H	3:L:239:GLN:NE2	2.17	0.43
2:E:257:ASP:OD1	2:E:259:SER:CB	2.66	0.43
3:C:267:VAL:HG13	3:C:268:GLY:N	2.34	0.43
3:I:5:ARG:HA	3:I:11:LEU:CD1	2.48	0.43
3:F:234:HIS:CE1	3:F:238:THR:HG21	2.54	0.43
3:F:90:LEU:C	3:F:90:LEU:CD2	2.85	0.43
7:H:470:NAG:O3	7:H:471:NDG:H2	2.17	0.43
2:B:280:THR:O	2:B:281:ASP:C	2.57	0.43
3:C:191:TRP:CD2	3:C:385:LYS:HE3	2.54	0.43
1:D:100:SER:HB3	3:F:80:ASP:CG	2.39	0.43
2:B:80:CYS:HA	2:B:83:GLN:HG3	1.99	0.43
3:C:31:THR:OG1	3:C:32:TYR:N	2.52	0.43
1:D:156:ILE:HD13	2:E:415:ARG:NH1	2.34	0.43
3:L:211:TYR:O	3:L:230:ASN:OD1	2.36	0.43
3:I:5:ARG:HA	3:I:11:LEU:HD12	2.01	0.43
2:H:211:CYS:HB2	2:H:250:THR:OG1	2.18	0.43
2:E:330:THR:C	2:E:331:VAL:CG2	2.87	0.43
3:L:387:ILE:HG23	3:L:388:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:457:PHE:C	2:K:458:PHE:CG	2.92	0.43
3:L:49:GLN:HE21	8:L:570:NAG:H81	1.73	0.43
1:J:69:LEU:CD1	2:K:100:LEU:HD13	2.36	0.43
2:E:210:GLU:OE1	2:E:213:GLU:HB2	2.18	0.43
3:C:166:LEU:CD2	3:C:218:LEU:HB3	2.49	0.43
2:K:134:ASP:O	2:K:138:VAL:HG23	2.18	0.43
2:E:410:ALA:CB	2:E:437:TRP:CE3	3.02	0.43
3:I:326:CYS:HB2	3:I:336:MET:HG3	2.00	0.43
3:I:195:GLN:OE1	3:I:382:THR:CG2	2.67	0.43
3:I:382:THR:CG2	3:I:383:THR:N	2.82	0.43
3:F:275:ARG:HA	3:F:310:MET:O	2.18	0.43
3:L:191:TRP:CZ3	3:L:387:ILE:HB	2.53	0.43
3:L:270:GLU:O	3:L:273:LYS:N	2.40	0.43
3:L:217:HIS:O	3:L:224:THR:OG1	2.33	0.43
1:J:205:ILE:CG1	2:K:138:VAL:HG11	2.42	0.43
3:F:168:PHE:O	3:F:169:ILE:HG23	2.19	0.43
2:H:361:MET:CB	7:H:470:NAG:H81	2.47	0.43
7:H:471:NDG:H3	7:H:472:BMA:O2	2.19	0.43
2:K:183:GLU:OE1	3:L:120:LYS:NZ	2.27	0.43
3:F:249:GLU:O	3:F:250:LEU:HD12	2.18	0.43
3:I:116:SER:O	3:I:117:ASN:C	2.57	0.43
2:B:352:ALA:HB1	2:B:409:ALA:CB	2.48	0.43
1:G:156:ILE:O	1:G:160:SER:N	2.42	0.43
1:J:112:SER:HB3	1:J:116:ARG:NH2	2.34	0.43
1:G:67:ASN:O	1:G:71:ASN:HB2	2.19	0.43
3:I:27:ASP:OD1	3:I:28:PHE:N	2.51	0.42
2:B:160:ASN:O	2:B:163:THR:OG1	2.19	0.42
3:L:100:ILE:O	3:L:104:ASP:HB2	2.18	0.42
3:C:100:ILE:HG23	3:C:101:LEU:CD2	2.44	0.42
2:E:295:GLY:O	2:E:296:ASN:C	2.58	0.42
3:L:150:GLY:CA	3:L:155:ASP:OD1	2.66	0.42
2:B:185:ASP:O	2:B:188:ALA:HB3	2.19	0.42
2:K:137:ASN:O	2:K:141:GLU:HG2	2.19	0.42
2:E:135:ASN:O	2:E:139:VAL:HG12	2.18	0.42
2:K:435:VAL:HG12	2:K:447:MET:HG2	2.01	0.42
3:C:236:ILE:O	3:C:239:GLN:HG2	2.19	0.42
3:I:329:GLN:HA	3:I:361:ASN:HD21	1.83	0.42
2:K:215:ILE:HD13	2:K:242:MET:HB3	2.01	0.42
2:K:439:ASN:ND2	2:K:439:ASN:N	2.57	0.42
2:E:355:ASP:O	2:E:369:ILE:HD11	2.19	0.42
2:E:303:THR:HB	2:E:330:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:260:VAL:CG2	2:H:291:GLU:HB2	2.49	0.42
1:G:42:ASN:O	2:K:78:THR:HG21	2.18	0.42
2:H:203:ILE:HG22	2:H:204:PRO:O	2.19	0.42
3:C:47:LEU:HD23	3:C:47:LEU:C	2.39	0.42
3:F:242:ILE:HD12	3:F:242:ILE:H	1.83	0.42
2:E:284:ASN:HD22	2:E:284:ASN:C	2.21	0.42
3:L:361:ASN:HD22	3:L:361:ASN:H	1.68	0.42
1:D:73:LEU:HD13	1:D:73:LEU:C	2.40	0.42
1:J:210:VAL:HG11	2:K:131:GLN:NE2	2.34	0.42
1:J:184:GLN:NE2	2:K:167:VAL:HG23	2.18	0.42
2:B:342:VAL:O	2:B:371:ASN:ND2	2.52	0.42
3:L:145:ILE:CD1	3:L:179:LEU:HD22	2.49	0.42
6:E:474:MAN:O3	6:E:477:NDG:C1	2.67	0.42
3:I:334:TRP:CB	3:I:336:MET:HE1	2.48	0.42
1:D:66:ILE:HG13	2:E:100:LEU:HD11	2.00	0.42
2:B:276:VAL:HA	2:B:292:TYR:CD2	2.54	0.42
2:H:139:VAL:HG11	3:I:78:MET:HG2	2.01	0.42
3:C:247:ARG:HB2	3:C:261:ASP:OD2	2.19	0.42
3:L:229:GLY:O	3:L:233:ILE:N	2.43	0.42
1:J:144:LEU:HD23	1:J:182:GLN:HG3	2.01	0.42
3:C:276:LEU:C	3:C:276:LEU:CD2	2.82	0.42
3:I:307:HIS:CE1	3:I:341:ALA:H	2.37	0.42
2:K:293:TRP:HZ2	2:K:296:ASN:HD21	1.66	0.42
2:B:226:LEU:HA	2:B:226:LEU:HD12	1.71	0.42
1:J:115:LEU:HD11	3:L:90:LEU:CD2	2.49	0.42
2:E:345:TYR:CG	2:E:346:ARG:N	2.88	0.42
3:L:382:THR:C	3:L:383:THR:HG22	2.39	0.42
2:H:253:GLN:C	2:H:253:GLN:NE2	2.73	0.42
3:C:393:THR:O	3:C:394:ILE:HD13	2.20	0.42
3:C:243:PRO:HG2	3:C:389:PHE:HB3	2.02	0.42
2:H:267:ASP:HB3	2:H:268:PRO:HD3	2.00	0.42
6:B:479:SIA:H32	6:B:478:GAL:H62	1.87	0.42
3:L:194:PHE:CZ	3:L:384:MET:HB3	2.55	0.42
2:B:381:ASP:C	2:B:381:ASP:OD2	2.58	0.42
2:K:172:LEU:HD23	3:L:113:ILE:HD13	2.00	0.42
3:L:178:PHE:CE1	3:L:180:VAL:HG12	2.54	0.42
2:E:179:ILE:HD11	3:F:120:LYS:HG2	2.02	0.42
2:K:367:MET:SD	5:T:2:HIS:HB2	2.60	0.42
3:I:12:ASP:OD2	3:I:15:PHE:CE1	2.73	0.42
2:H:167:VAL:CG1	2:H:168:LEU:N	2.83	0.42
3:I:334:TRP:HB3	3:I:336:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:275:ASN:OD1	3:L:139:CYS:N	2.47	0.42
2:E:356:GLY:HA2	2:E:368:THR:O	2.19	0.42
6:B:470:NAG:O3	6:B:471:NDG:C2	2.66	0.42
2:H:171:ILE:CG2	2:H:172:LEU:N	2.81	0.42
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.20	0.42
2:H:410:ALA:HA	2:H:436:VAL:O	2.19	0.42
3:L:367:ILE:HG21	3:L:382:THR:CG2	2.47	0.42
2:K:172:LEU:HD23	3:L:113:ILE:CD1	2.50	0.42
3:I:3:ALA:CB	3:L:11:LEU:HD12	2.45	0.42
2:K:402:TRP:CG	2:K:403:TRP:N	2.88	0.42
3:F:262:TYR:HD2	3:F:278:TYR:CD1	2.37	0.42
2:E:303:THR:HA	2:E:308:THR:OG1	2.19	0.42
3:I:332:SER:HG	3:I:343:HIS:CE1	2.30	0.42
3:F:338:LYS:N	3:F:339:CYS:HA	2.35	0.42
1:J:108:TYR:CE2	3:L:80:ASP:O	2.73	0.42
3:I:10:ILE:HD11	2:K:83:GLN:NE2	2.34	0.42
1:G:93:ILE:HG22	1:G:94:LEU:CD1	2.42	0.42
1:G:66:ILE:HD11	2:H:100:LEU:HD12	2.02	0.42
1:A:135:LEU:HD23	1:A:136:LEU:HD22	2.00	0.42
1:J:200:GLN:NE2	2:K:145:GLU:HB3	2.35	0.42
3:F:307:HIS:O	3:F:310:MET:HG2	2.19	0.42
3:L:304:PHE:C	3:L:306:SER:H	2.23	0.42
1:G:144:LEU:HD21	1:G:182:GLN:HA	2.02	0.42
2:B:405:ASN:O	2:B:406:ARG:CB	2.68	0.42
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.88	0.42
1:A:104:ARG:HD3	3:C:79:ILE:CG2	2.49	0.42
3:C:346:GLY:HA3	3:C:367:ILE:HG13	2.02	0.42
3:I:191:TRP:CD2	3:I:385:LYS:HD2	2.55	0.42
3:I:322:PHE:HB2	3:I:338:LYS:HG3	2.02	0.42
3:L:270:GLU:O	3:L:271:ALA:C	2.57	0.42
1:G:45:CYS:HB2	2:K:78:THR:HG22	2.02	0.42
2:H:91:ARG:N	2:H:92:PRO:HD2	2.35	0.42
2:H:109:GLN:O	2:H:113:SER:N	2.50	0.42
2:K:316:ASP:OD2	2:K:320:ASP:N	2.53	0.42
6:B:479:SIA:O7	6:B:478:GAL:H3	2.19	0.41
1:A:107:THR:O	1:A:111:VAL:HB	2.20	0.41
1:J:210:VAL:HG21	2:K:131:GLN:CG	2.49	0.41
1:G:48:GLY:HA2	2:H:82:LEU:HD11	2.02	0.41
3:F:193:VAL:HG13	3:F:195:GLN:O	2.19	0.41
1:G:188:VAL:HG11	2:H:164:ASN:HD21	1.85	0.41
3:F:307:HIS:O	3:F:308:ASN:C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:SER:OG	3:C:238:THR:HG23	2.20	0.41
3:L:281:PHE:CE2	3:L:283:GLY:HA2	2.55	0.41
2:H:267:ASP:O	2:H:271:GLN:HG2	2.20	0.41
2:H:422:TYR:CE1	2:H:444:TRP:HA	2.55	0.41
3:L:212:LYS:HE3	3:L:274:TYR:OH	2.20	0.41
2:B:201:CYS:O	3:C:143:VAL:HG21	2.18	0.41
2:B:223:GLU:HA	2:B:287:GLY:HA2	2.02	0.41
2:B:354:MET:O	2:B:369:ILE:CG2	2.66	0.41
3:F:90:LEU:HD22	3:F:91:GLU:CA	2.50	0.41
2:H:253:GLN:NE2	2:H:452:MET:HG3	2.35	0.41
2:B:415:ARG:O	2:B:434:GLY:HA2	2.20	0.41
1:G:143:GLN:O	1:G:144:LEU:C	2.59	0.41
1:J:54:LEU:HD23	2:K:60:PRO:HG2	2.02	0.41
2:K:226:LEU:HD12	2:K:227:ILE:H	1.84	0.41
2:K:317:TRP:CD1	2:K:420:GLY:HA3	2.55	0.41
3:C:316:ASP:OD1	3:C:316:ASP:N	2.52	0.41
3:F:228:LEU:O	3:F:228:LEU:HD12	2.20	0.41
2:K:329:PHE:C	2:K:329:PHE:CD1	2.92	0.41
6:E:470:NAG:O3	6:E:471:NDG:N2	2.54	0.41
2:H:175:LEU:O	2:H:178:LYS:N	2.54	0.41
2:K:186:VAL:CG1	2:K:187:SER:N	2.83	0.41
2:B:457:PHE:O	2:B:458:PHE:HB2	2.21	0.41
2:H:125:TRP:CD1	2:H:126:GLN:N	2.88	0.41
3:F:31:THR:HG22	3:F:35:LYS:HZ2	1.86	0.41
3:L:221:THR:O	3:L:223:THR:HG23	2.20	0.41
3:C:267:VAL:CG1	3:C:268:GLY:N	2.80	0.41
2:E:69:ASP:HB3	2:E:72:LEU:HB2	2.02	0.41
2:K:224:MET:SD	2:K:237:ARG:HB3	2.60	0.41
3:C:19:CYS:HB3	3:C:20:PRO:HD2	2.02	0.41
3:C:119:GLN:NE2	3:C:119:GLN:HA	2.34	0.41
2:B:184:SER:O	2:B:185:ASP:C	2.58	0.41
1:A:200:GLN:HB3	2:B:146:LEU:HD11	2.03	0.41
1:G:139:ASN:O	1:G:142:ALA:HB3	2.21	0.41
3:L:205:LYS:HD2	3:L:331:GLY:HA2	2.01	0.41
3:C:154:GLN:O	3:C:157:ALA:HB3	2.20	0.41
1:D:185:LEU:HD22	1:D:189:ILE:HG13	2.02	0.41
1:J:148:LYS:NZ	2:K:425:ASP:OD1	2.53	0.41
3:F:246:LEU:HD12	3:F:247:ARG:C	2.40	0.41
2:K:205:VAL:HG12	3:L:232:LYS:HZ2	1.85	0.41
1:A:156:ILE:HD13	2:B:415:ARG:CZ	2.50	0.41
3:I:108:ARG:O	3:I:112:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:340:HIS:ND1	3:I:343:HIS:HB2	2.35	0.41
2:B:91:ARG:HB3	2:B:92:PRO:HD3	2.03	0.41
3:F:184:ILE:HG22	3:F:185:ASP:O	2.21	0.41
2:E:118:MET:O	2:E:122:LYS:CB	2.68	0.41
1:A:86:LEU:HD12	1:A:89:ASN:HD22	1.85	0.41
3:C:390:ASN:ND2	3:C:390:ASN:C	2.74	0.41
3:C:75:LYS:HB3	3:C:78:MET:CE	2.46	0.41
2:E:294:LEU:O	2:E:299:ILE:HD11	2.21	0.41
1:A:137:GLN:O	1:A:140:VAL:HG22	2.21	0.41
1:G:188:VAL:O	1:G:189:ILE:C	2.59	0.41
3:C:191:TRP:CE3	3:C:387:ILE:HB	2.56	0.41
1:D:116:ARG:NH2	2:E:146:LEU:HD21	2.35	0.41
3:C:206:LYS:HB2	3:C:211:TYR:CD1	2.55	0.41
3:L:245:ALA:HB3	3:L:387:ILE:CG2	2.51	0.41
3:C:356:LYS:O	3:C:362:GLY:HA2	2.20	0.41
2:B:160:ASN:HA	2:B:163:THR:OG1	2.21	0.41
2:B:329:PHE:O	2:B:330:THR:HG22	2.21	0.41
1:J:127:ILE:HA	1:J:130:VAL:CG1	2.46	0.41
3:L:168:PHE:CD2	3:L:179:LEU:HD13	2.56	0.41
2:K:199:VAL:HG23	3:L:141:ASP:HB2	2.02	0.41
2:K:340:ILE:HB	2:K:403:TRP:CE2	2.56	0.41
1:D:122:LEU:HD12	1:D:123:LYS:HZ1	1.86	0.41
2:B:340:ILE:CG1	2:B:341:SER:N	2.84	0.41
2:E:118:MET:SD	3:F:60:LEU:HD23	2.60	0.41
3:L:54:THR:O	3:L:58:LYS:HB2	2.21	0.41
2:E:198:THR:HG22	3:F:140:LYS:O	2.21	0.41
1:J:210:VAL:HG21	2:K:131:GLN:CD	2.41	0.41
2:B:163:THR:O	2:B:167:VAL:HG12	2.21	0.41
2:E:172:LEU:HD23	3:F:113:ILE:CG2	2.51	0.41
3:I:207:ASN:ND2	3:I:209:ILE:HD13	2.26	0.41
3:C:292:GLY:HA2	3:C:341:ALA:HB2	2.02	0.41
3:I:372:TRP:CE3	3:I:373:LYS:HG2	2.56	0.41
3:L:229:GLY:O	3:L:232:LYS:N	2.53	0.41
3:L:251:GLU:OE1	3:L:381:LYS:HE3	2.21	0.41
2:H:405:ASN:O	2:H:406:ARG:CB	2.68	0.41
2:E:432:ASP:O	2:E:432:ASP:CG	2.59	0.41
1:G:133:ILE:HG21	2:H:164:ASN:OD1	2.21	0.41
2:B:212:GLU:O	2:B:215:ILE:N	2.53	0.41
2:K:151:LEU:HD23	2:K:151:LEU:O	2.20	0.41
2:B:78:THR:HG22	1:D:45:CYS:SG	2.60	0.41
3:C:234:HIS:O	3:C:238:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:458:PHE:CD1	2:K:458:PHE:N	2.87	0.41
3:I:69:ASN:N	3:I:70:PRO:CD	2.84	0.41
2:B:103:ASN:HA	2:B:107:VAL:HG23	2.03	0.41
2:H:439:ASN:N	2:H:439:ASN:HD22	2.19	0.41
2:B:141:GLU:HG3	2:B:144:SER:OG	2.21	0.41
2:B:100:LEU:O	2:B:104:VAL:HG23	2.21	0.41
1:A:104:ARG:HH22	3:C:78:MET:HE2	1.86	0.41
3:C:294:ASP:OD2	3:C:302:LYS:HB2	2.21	0.41
1:G:165:CYS:HA	2:H:196:PRO:HA	2.02	0.41
1:J:80:ASN:C	1:J:80:ASN:OD1	2.59	0.41
3:L:115:ASN:HD22	3:L:115:ASN:HA	1.76	0.41
3:L:227:TRP:C	3:L:227:TRP:CD1	2.93	0.41
3:C:305:THR:HB	3:C:341:ALA:HB2	2.03	0.40
2:H:349:ALA:HB1	2:H:437:TRP:NE1	2.36	0.40
3:L:334:TRP:HB3	3:L:336:MET:SD	2.61	0.40
2:E:205:VAL:CG2	3:F:215:PHE:O	2.69	0.40
3:C:365:ASN:N	3:C:365:ASN:ND2	2.66	0.40
2:E:227:ILE:O	2:E:235:PRO:HA	2.21	0.40
3:C:124:LEU:O	3:C:128:VAL:HG12	2.21	0.40
1:A:46:PRO:O	3:C:22:THR:CG2	2.70	0.40
3:I:194:PHE:HA	3:I:228:LEU:HB2	2.03	0.40
1:D:193:LEU:N	1:D:193:LEU:HD23	2.36	0.40
3:I:340:HIS:CE1	3:I:368:ILE:HD11	2.56	0.40
1:D:102:ASN:OD1	1:D:103:ASN:N	2.54	0.40
2:E:256:GLN:NE2	2:E:289:PRO:O	2.54	0.40
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.22	0.40
2:E:200:SER:O	2:E:279:ASN:ND2	2.54	0.40
1:D:139:ASN:HB3	3:F:114:TYR:CE1	2.56	0.40
1:D:141:ARG:NH1	1:D:186:GLU:OE2	2.54	0.40
2:B:432:ASP:OD2	2:B:432:ASP:N	2.54	0.40
3:I:5:ARG:CA	3:I:11:LEU:HD13	2.51	0.40
2:B:159:SER:O	2:B:163:THR:CG2	2.55	0.40
3:L:249:GLU:O	3:L:383:THR:HG23	2.20	0.40
2:H:152:TYR:O	2:H:153:ILE:HD13	2.22	0.40
3:I:230:ASN:HA	3:I:233:ILE:HD12	2.01	0.40
1:J:111:VAL:HG21	3:L:87:ARG:NH1	2.36	0.40
2:K:387:THR:HG22	2:K:388:SER:H	1.86	0.40
1:J:115:LEU:HD22	3:L:90:LEU:HD11	2.03	0.40
1:A:184:GLN:HE21	2:B:167:VAL:HG23	1.85	0.40
1:A:73:LEU:HD13	1:A:73:LEU:C	2.41	0.40
2:B:373:MET:HE3	2:B:373:MET:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:LEU:N	1:J:195:PRO:HD3	2.37	0.40
3:I:149:THR:CG2	3:I:150:GLY:N	2.84	0.40
3:I:198:LEU:O	3:I:348:TYR:OH	2.39	0.40
2:B:266:TRP:HA	2:B:377:THR:HG21	2.02	0.40
2:H:157:VAL:HG12	2:H:157:VAL:O	2.21	0.40
1:J:45:CYS:HB3	1:J:46:PRO:HD2	2.03	0.40
2:H:410:ALA:CB	2:H:437:TRP:CE3	3.04	0.40
3:L:168:PHE:CE2	3:L:179:LEU:HB2	2.55	0.40
3:F:211:TYR:O	3:F:229:GLY:HA2	2.22	0.40
2:E:151:LEU:O	2:E:155:GLU:HB2	2.21	0.40
3:I:10:ILE:C	3:I:18:TYR:OH	2.52	0.40
2:B:405:ASN:O	2:B:406:ARG:HB3	2.22	0.40
2:K:314:MET:HE1	2:K:450:MET:SD	2.62	0.40
7:H:471:NDG:H5	7:H:472:BMA:HO2	1.87	0.40
2:K:340:ILE:CG2	2:K:403:TRP:CG	3.05	0.40
2:K:241:ASP:HB3	2:K:249:TRP:HB2	2.04	0.40
2:B:138:VAL:CG1	2:B:139:VAL:N	2.84	0.40
3:F:202:VAL:HG23	3:F:225:GLU:HB2	2.03	0.40
1:A:76:TYR:HA	1:A:79:ASN:HB3	2.03	0.40
2:E:107:VAL:O	2:E:107:VAL:HG12	2.22	0.40
2:H:300:SER:HB2	2:H:331:VAL:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:72:GLU:OE2	1:J:84:HIS:NE2[1_455]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/562 (31%)	150 (87%)	20 (12%)	2 (1%)	16	48
1	D	172/562 (31%)	158 (92%)	8 (5%)	6 (4%)	4	18
1	G	172/562 (31%)	150 (87%)	18 (10%)	4 (2%)	8	30
1	J	184/562 (33%)	164 (89%)	18 (10%)	2 (1%)	17	51
2	B	399/461 (87%)	344 (86%)	46 (12%)	9 (2%)	8	30
2	E	399/461 (87%)	337 (84%)	48 (12%)	14 (4%)	4	18
2	H	399/461 (87%)	354 (89%)	38 (10%)	7 (2%)	11	37
2	K	399/461 (87%)	348 (87%)	45 (11%)	6 (2%)	13	42
3	C	379/411 (92%)	322 (85%)	48 (13%)	9 (2%)	7	29
3	F	380/411 (92%)	320 (84%)	54 (14%)	6 (2%)	12	40
3	I	392/411 (95%)	347 (88%)	39 (10%)	6 (2%)	13	42
3	L	389/411 (95%)	338 (87%)	42 (11%)	9 (2%)	8	30
4	M	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	N	2/4 (50%)	2 (100%)	0	0	100	100
4	Q	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	R	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
5	O	2/4 (50%)	2 (100%)	0	0	100	100
5	P	2/4 (50%)	2 (100%)	0	0	100	100
5	S	2/4 (50%)	2 (100%)	0	0	100	100
5	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	3852/5768 (67%)	3345 (87%)	427 (11%)	80 (2%)	9	32

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	195	PRO
2	B	259	SER
3	C	70	PRO
3	C	350	GLN
3	C	357	ALA
1	D	30	ASP
2	E	265	LYS
2	E	406	ARG
1	G	31	SER
1	G	189	ILE

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Mol	Chain	Res	Type
1	J	199	ARG
2	K	233	VAL
3	L	360	PRO
3	L	374	THR
2	B	281	ASP
2	B	351	ASN
2	B	399	GLY
3	C	198	LEU
3	C	351	GLY
1	D	42	ASN
2	E	263	GLY
2	E	339	GLN
2	E	443	SER
2	E	447	MET
3	F	198	LEU
3	F	199	ASP
2	H	362	GLY
3	I	74	SER
1	J	200	GLN
2	K	316	ASP
3	L	9	CYS
3	L	305	THR
2	B	435	VAL
1	D	195	PRO
2	E	111	SER
2	E	371	ASN
2	E	386	LEU
3	F	82	ALA
3	F	360	PRO
2	H	183	GLU
2	H	206	VAL
2	H	256	GLN
3	I	241	ALA
2	K	281	ASP
3	L	23	CYS
3	L	205	LYS
3	L	365	ASN
2	B	213	GLU
3	C	159	LYS
2	E	281	ASP
2	E	344	LYS
2	E	363	GLU

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Mol	Chain	Res	Type
2	H	435	VAL
3	I	198	LEU
2	K	357	ALA
2	B	60	PRO
2	B	185	ASP
3	C	146	HIS
1	D	31	SER
1	D	34	PRO
2	H	92	PRO
3	I	362	GLY
2	K	256	GLN
2	K	298	LYS
3	L	78	MET
3	C	122	VAL
3	C	241	ALA
3	F	343	HIS
1	G	34	PRO
2	H	280	THR
2	B	179	ILE
1	G	195	PRO
3	F	143	VAL
3	I	324	GLY
1	D	194	LEU
2	E	63	GLY
3	I	76	PRO
2	E	289	PRO
3	L	171	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/479 (34%)	150 (92%)	14 (8%)	13	37
1	D	164/479 (34%)	150 (92%)	14 (8%)	13	37
1	G	164/479 (34%)	154 (94%)	10 (6%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	176/479 (37%)	152 (86%)	24 (14%)	5	13
2	B	350/396 (88%)	306 (87%)	44 (13%)	5	16
2	E	350/396 (88%)	312 (89%)	38 (11%)	8	23
2	H	350/396 (88%)	313 (89%)	37 (11%)	8	25
2	K	350/396 (88%)	309 (88%)	41 (12%)	7	19
3	C	328/350 (94%)	290 (88%)	38 (12%)	7	20
3	F	328/350 (94%)	284 (87%)	44 (13%)	5	13
3	I	339/350 (97%)	303 (89%)	36 (11%)	8	25
3	L	337/350 (96%)	294 (87%)	43 (13%)	5	16
4	M	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	N	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	Q	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	R	3/3 (100%)	2 (67%)	1 (33%)	0	1
5	O	3/3 (100%)	3 (100%)	0	100	100
5	P	3/3 (100%)	3 (100%)	0	100	100
5	S	3/3 (100%)	3 (100%)	0	100	100
5	T	3/3 (100%)	3 (100%)	0	100	100
All	All	3424/4924 (70%)	3037 (89%)	387 (11%)	7	22

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	TRP
1	A	58	VAL
1	A	64	ASN
1	A	66	ILE
1	A	71	ASN
1	A	105	ASP
1	A	129	LYS
1	A	135	LEU
1	A	162	ARG
1	A	175	LEU
1	A	185	LEU
1	A	192	ASP
1	A	197	ARG

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Mol	Chain	Res	Type
2	B	66	LEU
2	B	83	GLN
2	B	88	GLN
2	B	89	GLN
2	B	97	VAL
2	B	98	ASP
2	B	99	GLU
2	B	105	GLU
2	B	138	VAL
2	B	156	THR
2	B	158	ASN
2	B	161	ILE
2	B	165	LEU
2	B	171	ILE
2	B	179	ILE
2	B	181	LYS
2	B	184	SER
2	B	186	VAL
2	B	200	SER
2	B	209	LYS
2	B	210	GLU
2	B	213	GLU
2	B	227	ILE
2	B	234	LYS
2	B	237	ARG
2	B	253	GLN
2	B	280	THR
2	B	283	LYS
2	B	284	ASN
2	B	297	ASP
2	B	318	LYS
2	B	320	ASP
2	B	321	LYS
2	B	330	THR
2	B	343	ASN
2	B	345	TYR
2	B	351	ASN
2	B	359	GLN
2	B	376	SER
2	B	380	ARG
2	B	381	ASP
2	B	387	THR

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Mol	Chain	Res	Type
2	B	426	MET
2	B	438	MET
3	C	22	THR
3	C	32	TYR
3	C	33	GLN
3	C	37	ASP
3	C	41	GLN
3	C	58	LYS
3	C	75	LYS
3	C	86	SER
3	C	100	ILE
3	C	131	LEU
3	C	140	LYS
3	C	147	ASP
3	C	151	LYS
3	C	177	GLN
3	C	179	LEU
3	C	195	GLN
3	C	198	LEU
3	C	221	THR
3	C	239	GLN
3	C	254	ASN
3	C	259	THR
3	C	267	VAL
3	C	276	LEU
3	C	277	THR
3	C	306	SER
3	C	317	ASN
3	C	318	ASP
3	C	325	ASN
3	C	340	HIS
3	C	354	TYR
3	C	356	LYS
3	C	358	SER
3	C	359	THR
3	C	365	ASN
3	C	383	THR
3	C	390	ASN
3	C	392	LEU
3	C	393	THR
1	D	37	SER
1	D	47	SER

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Mol	Chain	Res	Type
1	D	64	ASN
1	D	68	LYS
1	D	123	LYS
1	D	131	GLN
1	D	136	LEU
1	D	138	LYS
1	D	153	ASP
1	D	171	ARG
1	D	174	ASP
1	D	185	LEU
1	D	191	LYS
1	D	200	GLN
2	E	71	ASP
2	E	90	GLU
2	E	118	MET
2	E	135	ASN
2	E	136	GLU
2	E	138	VAL
2	E	141	GLU
2	E	158	ASN
2	E	171	ILE
2	E	179	ILE
2	E	180	GLN
2	E	181	LYS
2	E	187	SER
2	E	191	GLU
2	E	199	VAL
2	E	206	VAL
2	E	209	LYS
2	E	238	VAL
2	E	253	GLN
2	E	270	LYS
2	E	280	THR
2	E	284	ASN
2	E	294	LEU
2	E	301	GLN
2	E	302	LEU
2	E	321	LYS
2	E	323	LYS
2	E	330	THR
2	E	339	GLN
2	E	342	VAL

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Mol	Chain	Res	Type
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	380	ARG
2	E	406	ARG
2	E	415	ARG
2	E	421	GLN
2	E	438	MET
3	F	35	LYS
3	F	72	GLU
3	F	73	SER
3	F	85	LYS
3	F	90	LEU
3	F	100	ILE
3	F	104	ASP
3	F	114	TYR
3	F	117	ASN
3	F	119	GLN
3	F	126	GLU
3	F	130	GLN
3	F	140	LYS
3	F	143	VAL
3	F	147	ASP
3	F	151	LYS
3	F	152	ASP
3	F	156	ILE
3	F	162	LYS
3	F	175	ASN
3	F	178	PHE
3	F	218	LEU
3	F	246	LEU
3	F	249	GLU
3	F	254	ASN
3	F	259	THR
3	F	264	MET
3	F	285	ASP
3	F	297	ASP
3	F	306	SER
3	F	313	SER
3	F	317	ASN
3	F	325	ASN
3	F	350	GLN

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Mol	Chain	Res	Type
3	F	356	LYS
3	F	358	SER
3	F	361	ASN
3	F	365	ASN
3	F	376	TRP
3	F	379	MET
3	F	383	THR
3	F	385	LYS
3	F	386	ILE
3	F	392	LEU
1	G	41	TRP
1	G	58	VAL
1	G	71	ASN
1	G	73	LEU
1	G	122	LEU
1	G	123	LYS
1	G	138	LYS
1	G	143	GLN
1	G	160	SER
1	G	185	LEU
2	H	61	ASP
2	H	83	GLN
2	H	99	GLU
2	H	103	ASN
2	H	109	GLN
2	H	111	SER
2	H	115	PHE
2	H	116	GLN
2	H	117	TYR
2	H	122	LYS
2	H	123	ASP
2	H	125	TRP
2	H	128	ARG
2	H	138	VAL
2	H	140	ASN
2	H	179	ILE
2	H	181	LYS
2	H	182	LEU
2	H	191	GLU
2	H	206	VAL
2	H	209	LYS
2	H	213	GLU

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Mol	Chain	Res	Type
2	H	232	SER
2	H	238	VAL
2	H	253	GLN
2	H	284	ASN
2	H	296	ASN
2	H	320	ASP
2	H	321	LYS
2	H	323	LYS
2	H	330	THR
2	H	351	ASN
2	H	359	GLN
2	H	380	ARG
2	H	385	TRP
2	H	387	THR
2	H	415	ARG
3	I	4	THR
3	I	5	ARG
3	I	7	ASN
3	I	8	CYS
3	I	32	TYR
3	I	52	ASN
3	I	78	MET
3	I	103	HIS
3	I	111	GLN
3	I	115	ASN
3	I	117	ASN
3	I	128	VAL
3	I	166	LEU
3	I	195	GLN
3	I	196	LYS
3	I	198	LEU
3	I	207	ASN
3	I	223	THR
3	I	237	SER
3	I	240	SER
3	I	250	LEU
3	I	258	SER
3	I	266	LYS
3	I	277	THR
3	I	285	ASP
3	I	294	ASP
3	I	325	ASN

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Mol	Chain	Res	Type
3	I	356	LYS
3	I	365	ASN
3	I	376	TRP
3	I	383	THR
3	I	385	LYS
3	I	386	ILE
3	I	390	ASN
3	I	391	ARG
3	I	392	LEU
1	J	28	CYS
1	J	39	GLU
1	J	41	TRP
1	J	58	VAL
1	J	67	ASN
1	J	68	LYS
1	J	69	LEU
1	J	71	ASN
1	J	73	LEU
1	J	80	ASN
1	J	82	ASP
1	J	106	ASN
1	J	108	TYR
1	J	109	ASN
1	J	114	ASP
1	J	123	LYS
1	J	138	LYS
1	J	150	LEU
1	J	156	ILE
1	J	169	LEU
1	J	172	GLU
1	J	181	GLN
1	J	201	HIS
1	J	204	LEU
2	K	66	LEU
2	K	84	GLU
2	K	95	ASN
2	K	96	SER
2	K	128	ARG
2	K	140	ASN
2	K	145	GLU
2	K	149	HIS
2	K	150	GLN

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Mol	Chain	Res	Type
2	K	152	TYR
2	K	158	ASN
2	K	172	LEU
2	K	174	ASN
2	K	179	ILE
2	K	186	VAL
2	K	199	VAL
2	K	209	LYS
2	K	226	LEU
2	K	238	VAL
2	K	252	ILE
2	K	253	GLN
2	K	257	ASP
2	K	280	THR
2	K	297	ASP
2	K	302	LEU
2	K	310	LEU
2	K	312	ILE
2	K	321	LYS
2	K	323	LYS
2	K	325	HIS
2	K	330	THR
2	K	346	ARG
2	K	351	ASN
2	K	359	GLN
2	K	377	THR
2	K	387	THR
2	K	415	ARG
2	K	439	ASN
2	K	443	SER
2	K	457	PHE
2	K	458	PHE
3	L	8	CYS
3	L	22	THR
3	L	27	ASP
3	L	40	LEU
3	L	78	MET
3	L	90	LEU
3	L	97	GLU
3	L	108	ARG
3	L	110	LEU
3	L	111	GLN

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Mol	Chain	Res	Type
3	L	117	ASN
3	L	122	VAL
3	L	147	ASP
3	L	149	THR
3	L	151	LYS
3	L	163	GLN
3	L	170	LYS
3	L	175	ASN
3	L	176	GLN
3	L	184	ILE
3	L	185	ASP
3	L	198	LEU
3	L	199	ASP
3	L	233	ILE
3	L	242	ILE
3	L	249	GLU
3	L	250	LEU
3	L	259	THR
3	L	261	ASP
3	L	264	MET
3	L	276	LEU
3	L	297	ASP
3	L	306	SER
3	L	314	THR
3	L	344	LEU
3	L	353	THR
3	L	361	ASN
3	L	365	ASN
3	L	374	THR
3	L	376	TRP
3	L	380	LYS
3	L	383	THR
3	L	389	PHE
4	M	3	ARG
4	N	3	ARG
4	Q	3	ARG
4	R	3	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	71	ASN
1	A	79	ASN
1	A	80	ASN
1	A	84	HIS
1	A	89	ASN
1	A	103	ASN
1	A	134	GLN
1	A	139	ASN
1	A	181	GLN
1	A	184	GLN
1	A	200	GLN
2	B	67	HIS
2	B	88	GLN
2	B	89	GLN
2	B	129	GLN
2	B	150	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN
2	B	180	GLN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	284	ASN
2	B	296	ASN
2	B	343	ASN
2	B	351	ASN
2	B	393	GLN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	69	ASN
3	C	117	ASN
3	C	144	GLN
3	C	146	HIS
3	C	189	ASN
3	C	230	ASN
3	C	254	ASN
3	C	307	HIS
3	C	319	ASN
3	C	325	ASN
3	C	350	GLN

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Mol	Chain	Res	Type
3	C	365	ASN
3	C	390	ASN
1	D	64	ASN
1	D	131	GLN
1	D	137	GLN
1	D	143	GLN
1	D	200	GLN
2	E	67	HIS
2	E	149	HIS
2	E	158	ASN
2	E	253	GLN
2	E	256	GLN
2	E	284	ASN
2	E	296	ASN
2	E	351	ASN
2	E	405	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	33	GLN
3	F	118	ASN
3	F	123	ASN
3	F	130	GLN
3	F	136	GLN
3	F	158	ASN
3	F	189	ASN
3	F	210	GLN
3	F	230	ASN
3	F	254	ASN
3	F	317	ASN
3	F	350	GLN
3	F	365	ASN
1	G	59	ASN
1	G	60	GLN
1	G	71	ASN
1	G	131	GLN
1	G	134	GLN
1	G	143	GLN
1	G	181	GLN
1	G	184	GLN
2	H	89	GLN
2	H	95	ASN

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Mol	Chain	Res	Type
2	H	102	ASN
2	H	140	ASN
2	H	150	GLN
2	H	158	ASN
2	H	160	ASN
2	H	180	GLN
2	H	253	GLN
2	H	256	GLN
2	H	284	ASN
2	H	296	ASN
2	H	301	GLN
2	H	325	HIS
2	H	351	ASN
2	H	413	ASN
2	H	421	GLN
2	H	439	ASN
3	I	59	GLN
3	I	115	ASN
3	I	117	ASN
3	I	119	GLN
3	I	144	GLN
3	I	207	ASN
3	I	230	ASN
3	I	239	GLN
3	I	254	ASN
3	I	319	ASN
3	I	325	ASN
3	I	365	ASN
3	I	390	ASN
1	J	59	ASN
1	J	67	ASN
1	J	106	ASN
1	J	131	GLN
1	J	181	GLN
1	J	182	GLN
1	J	184	GLN
2	K	83	GLN
2	K	89	GLN
2	K	95	ASN
2	K	135	ASN
2	K	158	ASN
2	K	160	ASN

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Mol	Chain	Res	Type
2	K	189	GLN
2	K	253	GLN
2	K	256	GLN
2	K	296	ASN
2	K	301	GLN
2	K	351	ASN
2	K	364	ASN
2	K	421	GLN
2	K	439	ASN
3	L	33	GLN
3	L	49	GLN
3	L	52	ASN
3	L	115	ASN
3	L	117	ASN
3	L	144	GLN
3	L	177	GLN
3	L	189	ASN
3	L	239	GLN
3	L	317	ASN
3	L	325	ASN
3	L	361	ASN
3	L	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

40 carbohydrates 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
6	NAG	B	470	6	14,14,15	0.92	0	15,19,21	1.63	1 (6%)
6	NDG	B	471	6	14,14,15	0.78	0	15,19,21	1.09	1 (6%)
6	BMA	B	472	6	11,11,12	1.09	2 (18%)	14,15,17	1.26	1 (7%)
6	MAN	B	473	6	11,11,12	1.68	3 (27%)	14,15,17	1.45	1 (7%)
6	MAN	B	474	6	11,11,12	1.15	1 (9%)	14,15,17	0.97	1 (7%)
6	NDG	B	475	6	14,14,15	1.05	1 (7%)	15,19,21	0.87	0
6	GAL	B	476	6	11,11,12	0.95	0	14,15,17	0.80	0
6	NDG	B	477	6	14,14,15	1.10	1 (7%)	15,19,21	1.02	1 (6%)
6	GAL	B	478	6	11,11,12	0.62	0	14,15,17	0.58	0
6	SIA	B	479	6	16,20,21	1.32	3 (18%)	18,28,31	0.85	0
6	SIA	B	480	6	16,20,21	1.48	1 (6%)	18,28,31	0.81	0
6	NAG	E	470	2,6	14,14,15	0.74	0	15,19,21	1.30	3 (20%)
6	NDG	E	471	6	14,14,15	0.93	1 (7%)	15,19,21	0.90	0
6	BMA	E	472	6	11,11,12	1.17	1 (9%)	14,15,17	1.45	1 (7%)
6	MAN	E	473	6	11,11,12	0.95	0	14,15,17	1.74	3 (21%)
6	MAN	E	474	6	11,11,12	1.44	2 (18%)	14,15,17	1.24	3 (21%)
6	NDG	E	475	6	14,14,15	1.10	1 (7%)	15,19,21	0.97	1 (6%)
6	GAL	E	476	6	11,11,12	0.98	1 (9%)	14,15,17	0.96	1 (7%)
6	NDG	E	477	6	14,14,15	1.19	1 (7%)	15,19,21	0.92	0
6	GAL	E	478	6	11,11,12	1.15	0	14,15,17	0.75	0
6	SIA	E	479	6	16,20,21	0.67	0	18,28,31	1.27	2 (11%)
6	SIA	E	480	6	16,20,21	0.91	0	18,28,31	0.84	0
7	NAG	H	470	2,7	14,14,15	0.66	0	15,19,21	1.17	1 (6%)
7	NDG	H	471	7	14,14,15	0.79	1 (7%)	15,19,21	1.16	1 (6%)
7	BMA	H	472	7	11,11,12	0.74	0	14,15,17	1.24	1 (7%)
7	MAN	H	473	7	11,11,12	0.63	0	14,15,17	0.74	0
7	MAN	H	474	7	11,11,12	1.17	2 (18%)	14,15,17	1.20	1 (7%)
6	NAG	K	470	6	14,14,15	0.95	0	15,19,21	1.39	3 (20%)
6	NDG	K	471	6	14,14,15	1.22	2 (14%)	15,19,21	1.00	0
6	BMA	K	472	6	11,11,12	1.28	1 (9%)	14,15,17	1.10	2 (14%)
6	MAN	K	473	6	11,11,12	1.14	2 (18%)	14,15,17	1.45	3 (21%)
6	MAN	K	474	6	11,11,12	1.04	0	14,15,17	1.35	2 (14%)
6	NDG	K	475	6	14,14,15	1.09	1 (7%)	15,19,21	1.24	2 (13%)
6	GAL	K	476	6	11,11,12	1.24	1 (9%)	14,15,17	0.76	1 (7%)
6	NDG	K	477	6	14,14,15	1.06	1 (7%)	15,19,21	1.01	0
6	GAL	K	478	6	11,11,12	1.00	0	14,15,17	1.05	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SIA	K	479	6	16,20,21	1.09	2 (12%)	18,28,31	1.55	4 (22%)
6	SIA	K	480	6	16,20,21	0.77	0	18,28,31	0.86	0
8	NAG	L	570	8	14,14,15	0.99	0	15,19,21	1.12	2 (13%)
8	NAG	L	571	8	14,14,15	1.18	1 (7%)	15,19,21	0.93	1 (6%)

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
6	NAG	B	470	6	-	0/6/23/26	0/1/1/1
6	NDG	B	471	6	-	0/6/23/26	0/1/1/1
6	BMA	B	472	6	-	0/2/19/22	0/1/1/1
6	MAN	B	473	6	-	0/2/19/22	0/1/1/1
6	MAN	B	474	6	-	0/2/19/22	0/1/1/1
6	NDG	B	475	6	-	0/6/23/26	0/1/1/1
6	GAL	B	476	6	-	0/2/19/22	0/1/1/1
6	NDG	B	477	6	-	2/6/23/26	0/1/1/1
6	GAL	B	478	6	1/1/4/5	0/2/19/22	0/1/1/1
6	SIA	B	479	6	-	0/14/34/38	0/1/1/1
6	SIA	B	480	6	-	0/14/34/38	0/1/1/1
6	NAG	E	470	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NDG	E	471	6	-	0/6/23/26	0/1/1/1
6	BMA	E	472	6	-	0/2/19/22	0/1/1/1
6	MAN	E	473	6	-	0/2/19/22	0/1/1/1
6	MAN	E	474	6	-	0/2/19/22	0/1/1/1
6	NDG	E	475	6	-	0/6/23/26	0/1/1/1
6	GAL	E	476	6	-	0/2/19/22	0/1/1/1
6	NDG	E	477	6	-	0/6/23/26	0/1/1/1
6	GAL	E	478	6	1/1/4/5	0/2/19/22	0/1/1/1
6	SIA	E	479	6	-	0/14/34/38	0/1/1/1
6	SIA	E	480	6	-	0/14/34/38	0/1/1/1
7	NAG	H	470	2,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NDG	H	471	7	-	0/6/23/26	0/1/1/1
7	BMA	H	472	7	-	0/2/19/22	0/1/1/1
7	MAN	H	473	7	-	0/2/19/22	0/1/1/1
7	MAN	H	474	7	-	0/2/19/22	0/1/1/1
6	NAG	K	470	6	-	0/6/23/26	0/1/1/1
6	NDG	K	471	6	-	0/6/23/26	0/1/1/1
6	BMA	K	472	6	-	0/2/19/22	0/1/1/1
6	MAN	K	473	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	K	474	6	-	0/2/19/22	0/1/1/1
6	NDG	K	475	6	-	0/6/23/26	0/1/1/1
6	GAL	K	476	6	-	0/2/19/22	0/1/1/1
6	NDG	K	477	6	-	1/6/23/26	0/1/1/1
6	GAL	K	478	6	1/1/4/5	0/2/19/22	0/1/1/1
6	SIA	K	479	6	-	0/14/34/38	0/1/1/1
6	SIA	K	480	6	-	0/14/34/38	0/1/1/1
8	NAG	L	570	8	-	0/6/23/26	0/1/1/1
8	NAG	L	571	8	-	0/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	474	MAN	C2-C3	2.01	1.55	1.52
6	B	473	MAN	C1-C2	2.01	1.57	1.52
6	B	479	SIA	C6-C5	2.04	1.56	1.53
6	B	472	BMA	C2-C3	2.05	1.55	1.52
6	B	472	BMA	O3-C3	2.08	1.47	1.43
6	B	473	MAN	O2-C2	2.09	1.48	1.43
6	K	476	GAL	C1-C2	2.14	1.57	1.52
6	K	479	SIA	C3-C2	2.15	1.56	1.52
6	K	473	MAN	C1-C2	2.18	1.57	1.52
6	K	471	NDG	O-C5	2.20	1.48	1.43
6	B	475	NDG	C1-C2	2.20	1.55	1.52
7	H	471	NDG	C1-C2	2.23	1.55	1.52
6	K	472	BMA	C2-C3	2.23	1.55	1.52
6	E	477	NDG	O-C5	2.24	1.48	1.43
6	B	479	SIA	C3-C2	2.24	1.56	1.52
6	K	475	NDG	C1-C2	2.27	1.55	1.52
6	K	473	MAN	C2-C3	2.39	1.55	1.52
7	H	474	MAN	C4-C5	2.41	1.58	1.53
6	E	476	GAL	C1-C2	2.42	1.58	1.52
6	B	479	SIA	C7-C6	2.47	1.56	1.52
6	K	477	NDG	C1-C2	2.50	1.55	1.52
6	B	477	NDG	C1-C2	2.54	1.56	1.52
6	K	471	NDG	C1-C2	2.56	1.56	1.52
7	H	474	MAN	C4-C3	2.57	1.59	1.52
6	E	474	MAN	C2-C3	2.58	1.56	1.52
6	K	479	SIA	C3-C4	2.59	1.56	1.52
6	E	471	NDG	C1-C2	2.66	1.56	1.52
6	E	475	NDG	C1-C2	2.81	1.56	1.52
6	E	474	MAN	C4-C5	2.89	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	571	NAG	C1-C2	3.10	1.56	1.52
6	E	472	BMA	C2-C3	3.48	1.57	1.52
6	B	473	MAN	C2-C3	4.37	1.58	1.52
6	B	480	SIA	C3-C2	4.39	1.60	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	470	NAG	C2-N2-C7	-5.76	115.64	123.04
6	E	472	BMA	C1-C2-C3	-4.25	104.52	109.54
7	H	472	BMA	C1-C2-C3	-4.00	104.81	109.54
7	H	470	NAG	C2-N2-C7	-3.50	118.55	123.04
6	K	475	NDG	C2-N2-C7	-3.49	118.55	123.04
6	K	470	NAG	C2-N2-C7	-3.33	118.76	123.04
7	H	471	NDG	C2-N2-C7	-2.87	119.35	123.04
6	E	470	NAG	C2-N2-C7	-2.67	119.61	123.04
6	B	471	NDG	C2-N2-C7	-2.63	119.66	123.04
6	E	470	NAG	C4-C3-C2	-2.55	107.27	111.23
6	K	479	SIA	C8-C7-C6	-2.52	107.95	113.01
6	K	472	BMA	C2-C3-C4	-2.44	106.90	111.04
6	K	472	BMA	C1-C2-C3	-2.32	106.79	109.54
8	L	570	NAG	C2-N2-C7	-2.25	120.15	123.04
6	E	475	NDG	C2-N2-C7	-2.24	120.16	123.04
6	E	479	SIA	C7-C6-C5	-2.21	110.98	114.32
6	K	479	SIA	C5-N5-C10	-2.18	117.52	123.10
6	K	479	SIA	C7-C6-C5	-2.12	111.11	114.32
6	E	474	MAN	C1-C2-C3	-2.04	107.13	109.54
6	K	475	NDG	C6-C5-C4	2.01	117.98	113.02
6	K	476	GAL	C1-C2-C3	2.07	111.99	109.54
6	E	474	MAN	O2-C2-C1	2.08	113.37	109.21
6	K	470	NAG	C6-C5-C4	2.12	118.25	113.02
6	K	478	GAL	C1-C2-C3	2.19	112.13	109.54
6	K	478	GAL	O2-C2-C1	2.21	113.63	109.21
6	K	473	MAN	O2-C2-C1	2.30	113.82	109.21
6	B	474	MAN	C2-C3-C4	2.31	114.97	111.04
6	E	473	MAN	C2-C3-C4	2.34	115.02	111.04
6	E	474	MAN	C1-O5-C5	2.38	115.26	112.25
8	L	570	NAG	C4-C3-C2	2.45	115.04	111.23
8	L	571	NAG	C1-O5-C5	2.56	115.50	112.25
6	K	473	MAN	C6-C5-C4	2.56	119.34	113.02
6	B	477	NDG	C3-C4-C5	2.60	114.73	110.20
6	K	470	NAG	C1-O5-C5	2.69	115.67	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	473	MAN	O2-C2-C1	2.71	114.63	109.21
6	K	474	MAN	C2-C3-C4	2.90	115.97	111.04
6	B	472	BMA	C3-C4-C5	2.93	115.30	110.20
6	E	476	GAL	C1-C2-C3	2.97	113.05	109.54
6	E	470	NAG	C1-O5-C5	3.00	116.06	112.25
7	H	474	MAN	C3-C4-C5	3.57	116.41	110.20
6	K	473	MAN	C1-C2-C3	3.71	113.92	109.54
6	K	474	MAN	C3-C4-C5	3.75	116.73	110.20
6	E	479	SIA	C3-C4-C5	3.77	115.67	111.47
6	K	479	SIA	C3-C4-C5	3.90	115.82	111.47
6	B	473	MAN	C1-C2-C3	4.24	114.56	109.54
6	E	473	MAN	C1-C2-C3	4.92	115.36	109.54

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	478	GAL	C1
6	K	478	GAL	C1
6	E	470	NAG	C1
7	H	470	NAG	C1
6	B	478	GAL	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	477	NDG	O7-C7-N2-C2
6	B	477	NDG	C8-C7-N2-C2
6	B	477	NDG	O7-C7-N2-C2

There are no ring outliers.

35 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	470	NAG	9	0
6	B	471	NDG	6	0
6	B	472	BMA	3	0
6	B	473	MAN	4	0
6	B	475	NDG	4	0
6	B	476	GAL	1	0
6	B	477	NDG	3	0
6	B	478	GAL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	479	SIA	5	0
6	B	480	SIA	1	0
6	E	470	NAG	2	0
6	E	471	NDG	4	0
6	E	472	BMA	4	0
6	E	473	MAN	1	0
6	E	474	MAN	2	0
6	E	476	GAL	1	0
6	E	477	NDG	3	0
6	E	478	GAL	2	0
6	E	479	SIA	5	0
6	E	480	SIA	1	0
7	H	470	NAG	5	0
7	H	471	NDG	4	0
7	H	472	BMA	2	0
6	K	470	NAG	7	0
6	K	471	NDG	6	0
6	K	472	BMA	2	0
6	K	473	MAN	2	0
6	K	475	NDG	2	0
6	K	476	GAL	1	0
6	K	477	NDG	3	0
6	K	478	GAL	1	0
6	K	479	SIA	1	0
6	K	480	SIA	3	0
8	L	570	NAG	12	0
8	L	571	NAG	1	0

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	174/562 (30%)	0.06	8 (4%) 36 30	21, 106, 173, 187	0
1	D	174/562 (30%)	0.86	34 (19%) 1 1	62, 137, 231, 238	0
1	G	174/562 (30%)	0.15	11 (6%) 23 17	51, 120, 163, 173	0
1	J	186/562 (33%)	0.48	24 (12%) 5 3	64, 135, 224, 246	0
2	B	401/461 (86%)	-0.30	5 (1%) 81 78	21, 53, 151, 184	0
2	E	401/461 (86%)	0.10	35 (8%) 13 8	40, 64, 211, 226	0
2	H	401/461 (86%)	-0.11	15 (3%) 45 38	30, 62, 168, 195	0
2	K	401/461 (86%)	-0.23	6 (1%) 76 74	40, 64, 156, 164	0
3	C	381/411 (92%)	-0.45	16 (4%) 40 33	8, 39, 189, 232	0
3	F	382/411 (92%)	0.14	26 (6%) 20 14	52, 89, 208, 221	0
3	I	394/411 (95%)	-0.16	19 (4%) 34 28	29, 69, 179, 207	0
3	L	391/411 (95%)	-0.08	23 (5%) 26 19	35, 70, 177, 203	0
4	M	4/4 (100%)	0.42	0 100 100	63, 64, 103, 108	0
4	N	4/4 (100%)	0.26	0 100 100	119, 131, 149, 154	0
4	Q	4/4 (100%)	-0.54	0 100 100	78, 89, 90, 115	0
4	R	4/4 (100%)	0.39	0 100 100	92, 105, 106, 118	0
5	O	4/4 (100%)	-0.53	0 100 100	66, 68, 73, 93	0
5	P	4/4 (100%)	-0.27	0 100 100	90, 99, 106, 113	0
5	S	4/4 (100%)	-1.03	0 100 100	58, 69, 75, 95	0
5	T	4/4 (100%)	-0.10	0 100 100	75, 91, 98, 108	0
All	All	3892/5768 (67%)	-0.04	222 (5%) 27 21	8, 75, 189, 246	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	73	GLY	9.4
3	I	9	CYS	8.1
1	J	206	LYS	7.9
1	D	117	SER	7.5
2	H	107	VAL	7.5
1	J	27	ALA	6.3
1	J	28	CYS	6.3
3	L	8	CYS	6.2
1	D	118	ARG	6.1
1	J	29	LYS	6.0
1	D	96	GLY	5.9
3	L	6	ASP	5.9
2	E	116	GLN	5.9
3	C	66	LEU	5.8
3	F	52	ASN	5.8
3	F	53	LYS	5.8
3	F	394	ILE	5.7
3	F	68	TYR	5.6
1	D	116	ARG	5.6
1	G	28	CYS	5.6
1	A	28	CYS	5.5
3	L	76	PRO	5.2
3	L	5	ARG	5.1
1	D	195	PRO	5.1
3	L	63	ALA	5.1
3	I	8	CYS	5.1
3	L	66	LEU	5.1
3	F	66	LEU	5.0
3	C	68	TYR	5.0
1	D	85	SER	4.8
2	E	147	GLU	4.7
3	F	59	GLN	4.6
3	I	70	PRO	4.6
1	G	200	GLN	4.5
1	D	102	ASN	4.5
1	G	27	ALA	4.5
3	L	67	THR	4.5
1	J	41	TRP	4.5
1	J	210	VAL	4.5
3	F	63	ALA	4.4
2	E	139	VAL	4.3
3	I	395	GLY	4.3
1	J	201	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	88	THR	4.3
3	F	65	GLN	4.2
3	F	76	PRO	4.2
1	D	98	PHE	4.2
1	A	29	LYS	4.0
2	E	153	ILE	4.0
3	F	67	THR	4.0
3	F	49	GLN	4.0
2	E	119	TYR	4.0
1	D	196	SER	4.0
1	G	29	LYS	3.9
1	J	76	TYR	3.9
3	F	70	PRO	3.9
1	D	101	ALA	3.9
3	C	67	THR	3.9
1	G	31	SER	3.9
3	C	76	PRO	3.8
1	D	27	ALA	3.8
1	D	95	ARG	3.8
1	D	114	ASP	3.7
2	E	142	TYR	3.7
3	I	13	GLU	3.7
3	I	7	ASN	3.7
3	I	14	ARG	3.6
1	D	28	CYS	3.6
2	E	152	TYR	3.6
3	L	11	LEU	3.6
2	E	218	GLY	3.6
3	I	17	SER	3.5
3	I	393	THR	3.5
1	A	93	ILE	3.5
1	D	110	ARG	3.5
3	C	18	TYR	3.5
3	C	71	ASP	3.5
1	D	91	MET	3.5
1	A	83	SER	3.5
1	D	83	SER	3.5
1	G	99	SER	3.5
1	A	82	ASP	3.5
2	H	68	ALA	3.5
2	K	130	LYS	3.4
1	J	199	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	112	SER	3.3
2	E	144	SER	3.3
3	L	13	GLU	3.3
1	D	97	ASP	3.3
3	L	77	ASN	3.2
1	D	74	PHE	3.2
3	L	7	ASN	3.2
2	H	108	SER	3.2
2	B	119	TYR	3.2
2	E	143	SER	3.2
1	G	95	ARG	3.2
1	D	81	LYS	3.1
3	I	19	CYS	3.1
1	A	84	HIS	3.1
2	H	149	HIS	3.1
3	C	74	SER	3.1
3	L	12	ASP	3.0
2	E	64	GLY	3.0
2	E	120	LEU	3.0
3	I	16	GLY	3.0
1	D	107	THR	3.0
2	E	131	GLN	3.0
3	F	61	ILE	3.0
1	J	83	SER	3.0
3	F	55	SER	3.0
1	D	106	ASN	2.9
1	G	104	ARG	2.9
1	D	162	ARG	2.9
3	F	78	MET	2.9
2	K	107	VAL	2.9
2	E	123	ASP	2.9
2	E	151	LEU	2.9
2	E	59	ALA	2.9
2	E	138	VAL	2.9
2	H	59	ALA	2.9
2	E	117	TYR	2.9
2	H	81	GLN	2.9
3	C	69	ASN	2.9
3	C	65	GLN	2.8
2	B	115	PHE	2.8
2	E	141	GLU	2.8
1	D	194	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	K	120	LEU	2.8
1	D	80	ASN	2.8
1	D	127	ILE	2.8
1	G	30	ASP	2.8
1	D	41	TRP	2.8
2	E	154	ASP	2.8
1	D	82	ASP	2.8
2	B	142	TYR	2.8
1	J	205	ILE	2.7
3	C	70	PRO	2.7
2	K	458	PHE	2.7
1	J	81	LYS	2.7
3	I	10	ILE	2.7
3	C	63	ALA	2.7
3	C	73	SER	2.7
2	E	219	GLY	2.7
1	J	82	ASP	2.6
2	E	155	GLU	2.6
2	E	140	ASN	2.6
3	F	56	GLU	2.6
3	I	394	ILE	2.6
3	L	69	ASN	2.6
3	L	82	ALA	2.6
1	J	195	PRO	2.6
2	E	112	SER	2.6
2	H	72	LEU	2.6
2	H	74	VAL	2.6
3	L	71	ASP	2.5
1	A	81	LYS	2.5
1	A	76	TYR	2.5
1	J	80	ASN	2.5
1	J	208	LYS	2.5
3	C	45	ASP	2.5
2	H	147	GLU	2.5
2	E	105	GLU	2.4
3	L	68	TYR	2.4
1	J	209	PRO	2.4
1	J	38	ASP	2.4
2	H	132	VAL	2.4
1	J	203	PRO	2.4
2	H	119	TYR	2.4
2	E	162	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	68	TYR	2.4
3	I	66	LEU	2.4
2	B	116	GLN	2.4
3	F	18	TYR	2.4
3	I	69	ASN	2.4
1	D	113	GLU	2.3
1	G	96	GLY	2.3
3	F	79	ILE	2.3
3	L	64	ILE	2.3
3	F	190	GLY	2.3
2	E	74	VAL	2.3
2	E	148	LYS	2.3
3	I	71	ASP	2.3
2	H	152	TYR	2.3
3	F	74	SER	2.3
2	E	149	HIS	2.3
3	F	109	TYR	2.3
3	I	63	ALA	2.3
3	L	18	TYR	2.3
2	H	219	GLY	2.3
2	E	114	SER	2.3
1	J	207	MET	2.3
2	K	162	PRO	2.3
1	D	79	ASN	2.2
3	C	84	LEU	2.2
3	F	393	THR	2.2
3	I	6	ASP	2.2
2	E	58	LYS	2.2
2	K	125	TRP	2.2
3	F	346	GLY	2.2
3	L	395	GLY	2.2
3	L	101	LEU	2.2
2	E	104	VAL	2.2
3	L	81	ALA	2.2
2	H	120	LEU	2.2
2	E	458	PHE	2.1
1	J	211	PRO	2.1
3	F	64	ILE	2.1
2	E	150	GLN	2.1
1	J	117	SER	2.1
1	D	56	ASP	2.1
3	L	74	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	76	TYR	2.1
3	F	16	GLY	2.1
3	F	342	GLY	2.1
2	E	125	TRP	2.1
1	D	92	GLU	2.1
1	J	77	GLN	2.0
3	C	49	GLN	2.0
3	L	14	ARG	2.0
1	J	68	LYS	2.0
1	G	35	PHE	2.0
3	C	58	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	B	470	14/15	0.85	0.18	1.71	83,89,92,95	0
7	NAG	H	470	14/15	0.83	0.19	0.30	83,87,91,93	0
6	NAG	K	470	14/15	0.82	0.18	0.07	83,87,92,96	0
6	NAG	E	470	14/15	0.84	0.15	-0.46	80,85,89,92	0
6	BMA	E	472	11/12	0.72	0.34	-	98,103,106,108	0
6	MAN	B	474	11/12	0.70	0.50	-	109,111,112,113	0
6	SIA	B	479	20/21	0.46	0.51	-	99,104,108,108	0
7	MAN	H	473	11/12	0.65	0.70	-	104,108,110,110	0
6	SIA	B	480	20/21	0.56	0.61	-	97,103,109,111	0
6	GAL	K	478	11/12	0.65	0.59	-	105,110,111,111	0
6	MAN	B	473	11/12	0.75	0.48	-	104,108,109,109	0
6	NDG	B	475	14/15	0.75	0.56	-	104,107,109,110	0
8	NAG	L	571	14/15	0.65	0.75	-	105,108,109,109	0
8	NAG	L	570	14/15	0.67	0.62	-	106,109,110,111	0
6	MAN	K	473	11/12	0.80	0.32	-	99,101,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BMA	B	472	11/12	0.83	0.46	-	99,105,108,109	0
7	MAN	H	474	11/12	0.33	0.50	-	100,103,105,107	0
6	NDG	B	477	14/15	0.74	0.46	-	104,111,112,113	0
6	NDG	E	475	14/15	0.77	0.62	-	105,109,111,115	0
6	NDG	K	477	14/15	0.74	0.55	-	97,105,107,109	0
6	GAL	B	476	11/12	0.59	0.61	-	106,107,108,112	0
6	NDG	E	477	14/15	0.70	0.59	-	103,110,115,117	0
6	SIA	E	480	20/21	0.62	0.66	-	109,114,119,125	0
6	NDG	B	471	14/15	0.82	0.31	-	96,98,101,102	0
6	NDG	K	475	14/15	0.76	0.44	-	106,111,112,115	0
6	SIA	E	479	20/21	0.80	0.46	-	103,107,111,112	0
6	NDG	K	471	14/15	0.62	0.47	-	97,100,102,104	0
6	NDG	E	471	14/15	0.87	0.28	-	95,97,101,101	0
6	SIA	K	479	20/21	0.64	0.41	-	102,107,109,109	0
6	BMA	K	472	11/12	0.61	0.43	-	101,104,107,107	0
6	GAL	B	478	11/12	0.84	0.51	-	98,104,107,108	0
6	GAL	E	478	11/12	0.64	0.48	-	109,112,115,116	0
6	MAN	E	473	11/12	0.68	0.74	-	99,104,107,107	0
6	GAL	E	476	11/12	0.74	0.47	-	115,118,118,119	0
6	SIA	K	480	20/21	0.46	0.69	-	105,113,116,116	0
7	NDG	H	471	14/15	0.83	0.28	-	94,97,102,103	0
6	GAL	K	476	11/12	0.58	0.90	-	113,116,117,117	0
6	MAN	E	474	11/12	0.57	0.56	-	106,108,109,112	0
6	MAN	K	474	11/12	0.71	0.42	-	93,103,105,105	0
7	BMA	H	472	11/12	0.72	0.32	-	100,104,108,110	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
9	CA	H	501	1/1	0.99	0.05	-1.30	51,51,51,51	0
9	CA	E	501	1/1	0.93	0.09	-1.53	47,47,47,47	0
9	CA	L	601	1/1	0.96	0.06	-1.68	51,51,51,51	0
9	CA	I	601	1/1	0.97	0.05	-1.90	56,56,56,56	0
9	CA	F	601	1/1	0.98	0.05	-1.95	49,49,49,49	0
9	CA	K	501	1/1	0.91	0.07	-1.95	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	CA	C	601	1/1	0.98	0.06	-2.20	31,31,31,31	0
9	CA	B	501	1/1	0.99	0.08	-	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.