



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:08 PM UTC

PDB ID : 6L9J / pdb_00006l9j
Title : Structure of yeast Snf5 and Swi3 subcomplex
Authors : Long, J.; Zhou, H.
Deposited on : 2019-11-10
Resolution : 2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

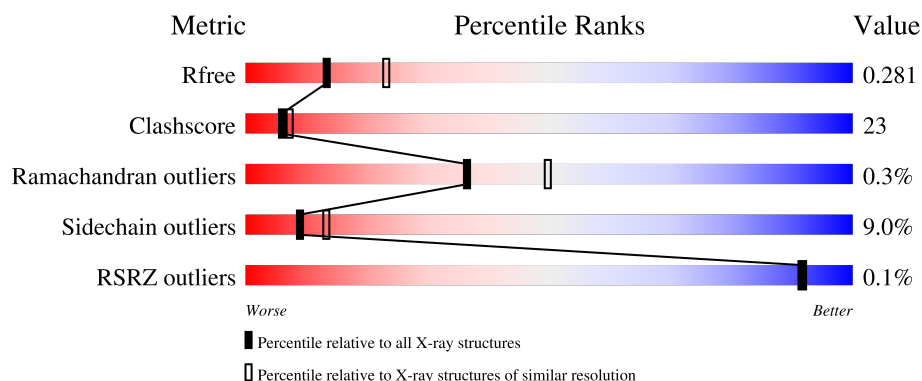
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	227	
1	D	227	
1	G	227	
1	J	227	
2	B	187	

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Mol	Chain	Length	Quality of chain
2	C	187	 26% 22% . 48%
2	E	187	 33% 18% . 47%
2	F	187	 25% 24% . 49%
2	H	187	 35% 16% . 48%
2	I	187	 29% 19% . 49%
2	K	187	 35% 11% . 50%
2	L	187	 34% 16% . 49%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13745 atoms, of which 72 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 SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1722	1078	293	344	7			
1	D	213	Total	C	N	O	S	0	0	0
			1760	1102	300	351	7			
1	G	210	Total	C	N	O	S	0	0	0
			1739	1090	297	345	7			
1	J	207	Total	C	N	O	S	0	0	0
			1706	1068	290	341	7			

- Molecule 2 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	0	0	0
			793	516	138	137	2			
2	C	97	Total	C	N	O	S	0	0	0
			817	530	142	143	2			
2	E	99	Total	C	N	O	S	0	0	0
			832	539	145	146	2			
2	F	95	Total	C	N	O	S	0	0	0
			801	520	139	140	2			
2	H	97	Total	C	N	O	S	0	0	0
			816	529	142	143	2			
2	I	95	Total	C	N	O	S	0	0	0
			801	520	139	140	2			
2	K	94	Total	C	N	O	S	0	0	0
			793	516	138	137	2			
2	L	95	Total	C	N	O	S	0	0	0
			801	520	139	140	2			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		
3	K	1	Total	C	H	O	0	0
			14	3	8	3		
3	L	1	Total	C	H	O	0	0
			14	3	8	3		
3	L	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is water.

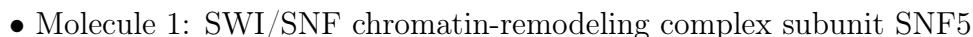
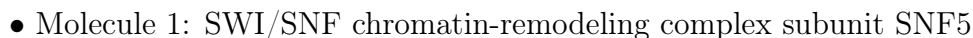
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	20	Total	O	0	0
			20	20		
4	C	14	Total	O	0	0
			14	14		

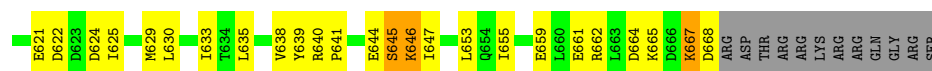
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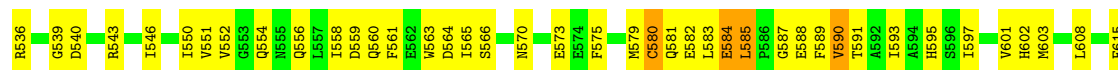
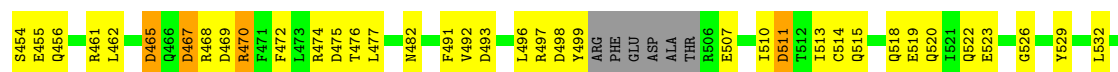
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	28	Total 28	O 28	0	0
4	E	14	Total 14	O 14	0	0
4	F	15	Total 15	O 15	0	0
4	G	25	Total 25	O 25	0	0
4	H	16	Total 16	O 16	0	0
4	I	13	Total 13	O 13	0	0
4	J	34	Total 34	O 34	0	0
4	K	19	Total 19	O 19	0	0
4	L	13	Total 13	O 13	0	0

- Molecule 1: SWI/SNF chromatin-remodeling complex subunit SNF5

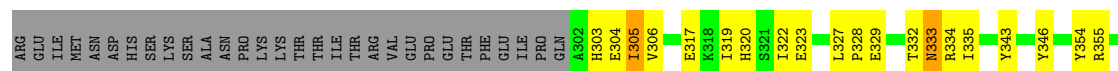
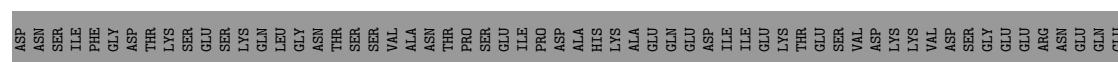
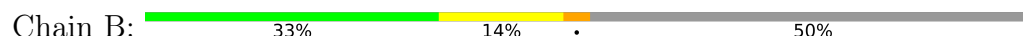




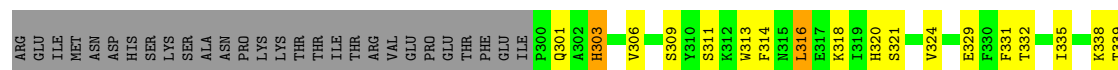
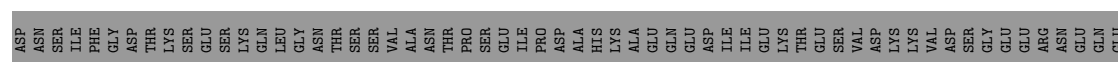
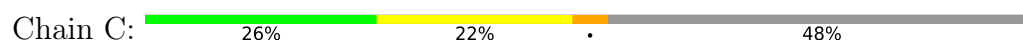
- Molecule 1: SWI/SNF chromatin-remodeling complex subunit SNF5



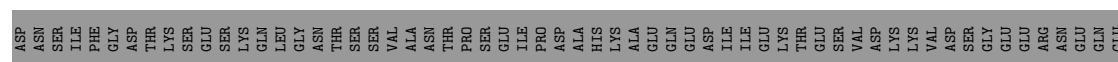
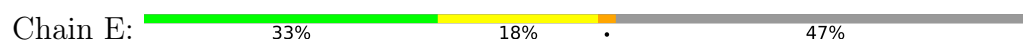
- Molecule 2: SWI/SNF complex subunit SWI3

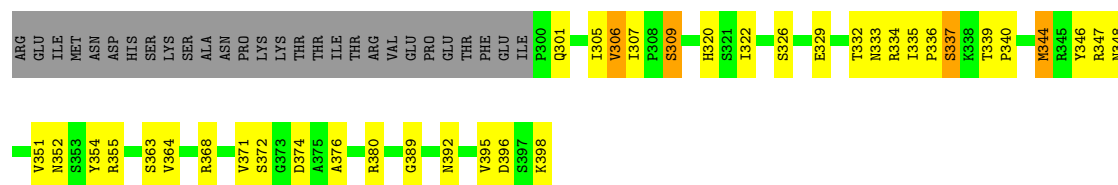


- Molecule 2: SWI/SNF complex subunit SWI3

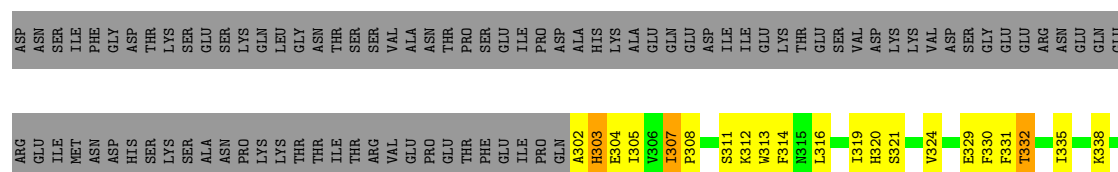


- Molecule 2: SWI/SNF complex subunit SWI3

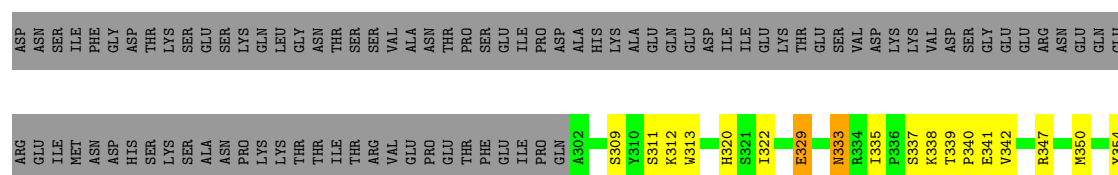
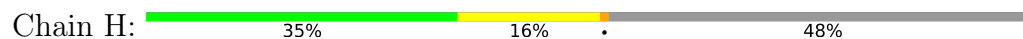




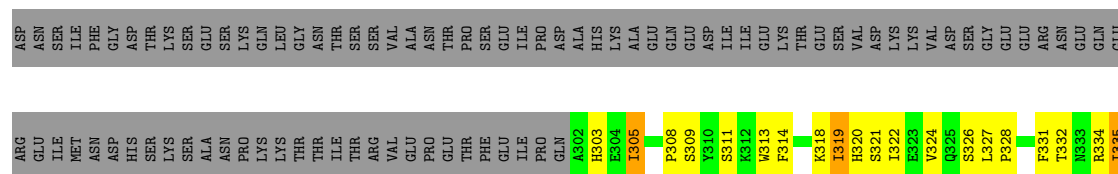
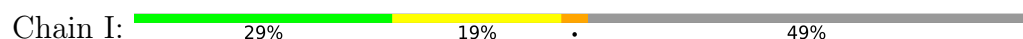
• Molecule 2: SWI/SNF complex subunit SWI3



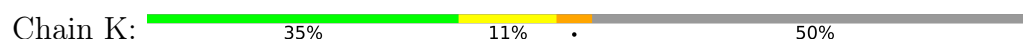
• Molecule 2: SWI/SNF complex subunit SWI3

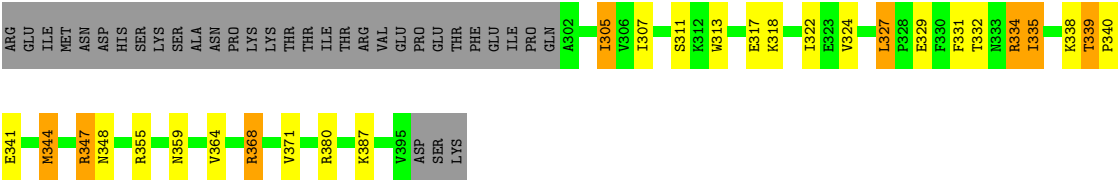


• Molecule 2: SWI/SNF complex subunit SWI3

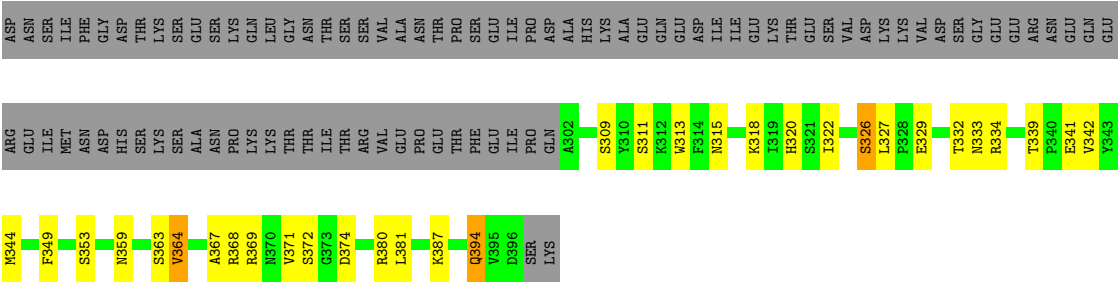
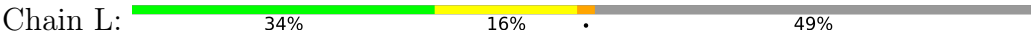


• Molecule 2: SWI/SNF complex subunit SWI3





● Molecule 2: SWI/SNF complex subunit SWI3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.52Å 146.46Å 154.33Å 90.00° 131.20° 90.00°	Depositor
Resolution (Å)	48.62 – 2.64 48.62 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.62-2.64) 96.9 (48.62-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.229 , 0.280 0.230 , 0.281	Depositor DCC
R_{free} test set	4879 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.096 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13745	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.35	0/1750	0.50	0/2363
1	D	0.38	0/1790	0.53	1/2418 (0.0%)
1	G	0.38	0/1768	0.53	0/2386
1	J	0.39	0/1734	0.52	0/2342
2	B	0.43	0/817	0.55	0/1108
2	C	0.40	0/842	0.62	0/1142
2	E	0.45	0/857	0.56	0/1161
2	F	0.41	0/825	0.52	0/1119
2	H	0.46	0/840	0.52	0/1138
2	I	0.39	0/825	0.56	0/1119
2	K	0.40	0/817	0.53	0/1108
2	L	0.39	0/825	0.50	0/1119
All	All	0.40	0/13690	0.53	1/18523 (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
1	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	526	GLY	N-CA-C	-5.70	105.59	112.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	616	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1722	0	1661	92	0
1	D	1760	0	1694	85	0
1	G	1739	0	1675	120	0
1	J	1706	0	1641	87	0
2	B	793	0	782	26	2
2	C	817	0	802	46	0
2	E	832	0	820	25	2
2	F	801	0	786	51	0
2	H	816	0	804	25	1
2	I	801	0	786	48	0
2	K	793	0	782	26	1
2	L	801	0	786	37	0
3	E	24	32	32	2	0
3	F	6	8	8	0	0
3	H	6	8	8	2	0
3	K	6	8	8	2	0
3	L	12	16	16	0	0
4	A	27	0	0	1	0
4	B	20	0	0	6	0
4	C	14	0	0	1	0
4	D	28	0	0	2	0
4	E	14	0	0	2	0
4	F	15	0	0	2	0
4	G	25	0	0	2	0
4	H	16	0	0	1	0
4	I	13	0	0	1	0
4	J	34	0	0	3	0
4	K	19	0	0	4	0
4	L	13	0	0	1	0
All	All	13673	72	13091	605	3

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 23.

All (605) 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:I:369:ARG:NH1	1:J:659:GLU:OE1	1.88	1.06
1:G:541:ASP:HB2	2:I:335:ILE:HD11	1.36	1.05
1:J:570:ASN:OD1	2:L:380:ARG:NH2	1.95	1.00
1:D:460:ILE:HB	1:D:477:LEU:HD22	1.45	0.98
1:G:570:ASN:OD1	2:I:380:ARG:NH2	1.96	0.98
2:I:321:SER:HA	2:I:324:VAL:HG12	1.46	0.94
2:K:329:GLU:OE2	2:K:338:LYS:NZ	2.00	0.93
1:A:534:GLN:NE2	1:A:615:PHE:O	2.03	0.92
1:G:662:ARG:NH2	1:J:645:SER:OG	2.04	0.91
1:D:577:GLU:HG3	1:D:590:VAL:HG21	1.52	0.91
3:H:401:GOL:O3	3:H:401:GOL:O1	1.88	0.89
1:G:588:GLU:OE1	1:G:588:GLU:N	2.05	0.88
1:G:460:ILE:HB	1:G:477:LEU:CD1	2.03	0.88
1:A:483:ASP:OD1	2:B:380:ARG:NH2	2.07	0.87
2:I:365:THR:HG22	2:I:368:ARG:NH1	1.91	0.86
1:G:460:ILE:HB	1:G:477:LEU:HD12	1.58	0.85
1:G:581:GLN:NE2	4:G:701:HOH:O	2.09	0.84
1:A:654:GLN:O	1:A:655:ILE:HD12	1.77	0.84
1:D:562:GLU:HG2	1:D:630:LEU:CD1	2.08	0.83
1:G:537:LEU:HD11	2:I:328:PRO:HB2	1.61	0.83
1:G:661:GLU:O	1:G:665:LYS:HB2	1.79	0.83
2:C:324:VAL:HA	2:C:331:PHE:CE2	2.15	0.82
1:G:461:ARG:NH2	1:G:599:GLU:OE1	2.13	0.81
1:A:544:ILE:HD11	1:A:604:TYR:CE2	2.14	0.81
1:D:559:ASP:OD1	1:D:560:GLN:N	2.12	0.81
1:G:573:GLU:O	1:G:577:GLU:HG3	1.81	0.81
1:D:570:ASN:OD1	2:F:380:ARG:NH2	2.14	0.80
1:G:511:ASP:O	1:G:515:GLN:HG3	1.81	0.80
1:D:467:ASP:OD1	1:D:468:ARG:N	2.14	0.80
1:D:479:TRP:CD1	1:D:521:ILE:HD11	2.17	0.79
1:J:520:GLN:O	4:J:701:HOH:O	1.99	0.79
1:D:494:ASP:OD2	4:D:701:HOH:O	1.99	0.78
2:E:335:ILE:HG22	2:E:337:SER:H	1.47	0.78
1:G:638:VAL:HG11	2:I:345:ARG:HG2	1.65	0.78
1:A:543:ARG:NH1	1:A:562:GLU:OE2	2.17	0.77
1:D:529:TYR:CZ	1:D:566:SER:HB2	2.20	0.77
1:J:597:ILE:O	1:J:601:VAL:HG23	1.85	0.76
2:L:332:THR:HG22	2:L:334:ARG:HB3	1.68	0.76
1:D:625:ILE:HD12	1:D:629:MET:HE1	1.68	0.76
1:D:460:ILE:HB	1:D:477:LEU:CD2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:THR:HB	1:A:595:HIS:CD2	2.22	0.75
2:C:350:MET:HE1	2:C:382:HIS:HA	1.69	0.74
1:J:539:GLY:O	2:L:334:ARG:NH2	2.21	0.74
2:F:313:TRP:O	4:F:501:HOH:O	2.04	0.74
1:J:608:LEU:HD11	1:J:625:ILE:HG21	1.70	0.73
2:C:329:GLU:OE1	2:C:338:LYS:NZ	2.21	0.73
1:J:640:ARG:NH2	2:L:368:ARG:O	2.21	0.73
1:G:646:LYS:HB2	1:G:646:LYS:NZ	2.02	0.73
2:L:332:THR:C	2:L:334:ARG:H	1.97	0.73
1:D:577:GLU:HG3	1:D:590:VAL:CG2	2.19	0.72
1:G:543:ARG:HH12	1:G:633:ILE:HD11	1.53	0.72
2:I:321:SER:CA	2:I:324:VAL:HG12	2.19	0.72
1:A:594:ALA:O	1:A:598:ARG:HG3	1.90	0.72
2:H:333:ASN:O	2:H:333:ASN:ND2	2.21	0.72
1:A:646:LYS:HG2	1:D:558:ILE:HD12	1.71	0.72
2:L:394:GLN:HB3	4:L:501:HOH:O	1.90	0.71
1:D:611:LEU:HD13	1:D:622:ASP:OD2	1.90	0.71
1:G:577:GLU:HG2	1:G:590:VAL:CG2	2.19	0.71
2:I:305:ILE:HD13	2:I:355:ARG:HD3	1.72	0.71
2:L:381:LEU:HD12	2:L:381:LEU:O	1.90	0.71
1:G:515:GLN:O	1:G:519:GLU:HG3	1.90	0.71
1:G:545:ARG:HD2	1:G:560:GLN:OE1	1.90	0.71
1:A:623:ASP:HA	1:A:626:ARG:HH11	1.54	0.71
2:K:344:MET:O	2:K:348:ASN:HB2	1.91	0.70
1:G:664:ASP:O	1:G:667:LYS:HD2	1.92	0.70
1:A:587:GLY:O	1:A:590:VAL:HG12	1.92	0.70
1:G:467:ASP:HB2	1:G:468:ARG:HH11	1.56	0.70
1:G:496:LEU:HD21	1:G:513:ILE:HD12	1.74	0.70
1:D:606:LYS:O	1:D:610:LEU:HD23	1.91	0.70
1:A:467:ASP:OD1	1:A:468:ARG:N	2.24	0.69
1:G:525:GLN:HE21	1:G:528:PRO:HG3	1.58	0.69
2:I:332:THR:OG1	2:I:335:ILE:HG22	1.92	0.69
2:H:354:TYR:CE2	2:H:392:ASN:HA	2.28	0.69
2:E:335:ILE:HG23	2:E:336:PRO:HD2	1.73	0.68
1:G:456:GLN:HA	1:G:456:GLN:OE1	1.91	0.68
1:J:559:ASP:OD1	2:L:368:ARG:NH2	2.26	0.68
1:G:621:GLU:OE1	1:G:621:GLU:N	2.20	0.68
1:J:580:CYS:HA	1:J:585:LEU:HB2	1.75	0.68
2:C:354:TYR:OH	2:C:394:GLN:HG3	1.94	0.68
1:G:531:GLU:O	1:G:532:LEU:HD12	1.94	0.68
2:C:350:MET:CE	2:C:391:ILE:HD11	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:329:GLU:OE1	2:L:380:ARG:NH1	2.26	0.67
1:G:543:ARG:HH22	1:G:633:ILE:HG13	1.59	0.67
1:J:515:GLN:O	1:J:519:GLU:HG3	1.95	0.67
2:K:339:THR:HG21	4:K:516:HOH:O	1.93	0.67
2:E:352:ASN:O	4:E:501:HOH:O	2.12	0.67
2:I:365:THR:HG22	2:I:368:ARG:HH12	1.57	0.67
1:J:640:ARG:HG2	1:J:644:GLU:HB2	1.76	0.66
2:C:382:HIS:ND1	2:C:383:LYS:HE2	2.10	0.66
2:L:315:ASN:HD22	2:L:318:LYS:HE3	1.60	0.66
2:C:346:TYR:O	2:C:350:MET:HG3	1.95	0.66
2:H:312:LYS:HD2	3:H:401:GOL:H32	1.78	0.66
1:G:541:ASP:CB	2:I:335:ILE:HD11	2.19	0.66
1:J:582:GLU:OE2	2:L:364:VAL:HG23	1.96	0.66
2:B:329:GLU:HG3	4:B:415:HOH:O	1.95	0.66
1:A:511:ASP:O	1:A:515:GLN:HG3	1.94	0.65
1:A:597:ILE:O	1:A:601:VAL:HG23	1.96	0.65
1:G:645:SER:OG	1:J:662:ARG:NH2	2.28	0.65
1:A:544:ILE:HD11	1:A:604:TYR:CD2	2.31	0.65
1:J:587:GLY:O	1:J:590:VAL:HG23	1.96	0.65
1:J:589:PHE:O	1:J:593:ILE:HG13	1.96	0.65
2:K:368:ARG:NH1	4:K:501:HOH:O	2.28	0.65
2:C:311:SER:HA	2:C:313:TRP:NE1	2.11	0.65
1:J:469:ASP:O	1:J:470:ARG:HB2	1.94	0.65
1:G:543:ARG:HH22	1:G:633:ILE:CD1	2.10	0.65
1:G:606:LYS:O	1:G:610:LEU:HD13	1.96	0.65
1:A:534:GLN:HB3	1:A:536:ARG:NH1	2.12	0.65
1:D:479:TRP:CH2	2:E:376:ALA:HB2	2.32	0.65
2:C:391:ILE:HG22	2:C:392:ASN:HB2	1.79	0.64
2:E:339:THR:OG1	2:E:340:PRO:HD2	1.97	0.64
2:F:351:VAL:O	2:F:355:ARG:HG3	1.97	0.64
1:G:541:ASP:OD2	2:I:337:SER:OG	2.12	0.64
1:A:458:VAL:HG22	1:A:524:PHE:CG	2.32	0.64
2:E:364:VAL:O	2:E:368:ARG:HG3	1.97	0.64
1:G:543:ARG:NH1	1:G:633:ILE:HD11	2.13	0.64
2:B:303:HIS:HB2	4:B:406:HOH:O	1.97	0.64
2:I:326:SER:C	2:I:328:PRO:HD3	2.23	0.64
2:B:306:VAL:HG12	2:B:394:GLN:CD	2.23	0.63
2:I:347:ARG:NH1	2:I:348:ASN:OD1	2.31	0.63
1:G:541:ASP:HB2	2:I:335:ILE:CD1	2.20	0.63
2:L:367:ALA:O	2:L:371:VAL:HG22	1.97	0.63
2:C:324:VAL:HG13	2:C:331:PHE:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:354:TYR:CE1	2:E:392:ASN:HA	2.34	0.63
1:D:493:ASP:OD1	1:D:506:ARG:HD3	1.98	0.63
2:F:302:ALA:HB1	2:F:305:ILE:HD11	1.80	0.63
2:C:311:SER:HA	2:C:313:TRP:CD1	2.34	0.63
1:J:583:LEU:HB2	1:J:585:LEU:HD22	1.79	0.63
2:F:324:VAL:HA	2:F:331:PHE:CE2	2.34	0.63
2:I:337:SER:O	2:I:342:VAL:HG21	1.98	0.63
1:J:454:SER:O	1:J:482:ASN:ND2	2.32	0.62
1:A:650:PRO:HG3	2:C:365:THR:HG21	1.81	0.62
1:A:499:TYR:HB2	1:A:506:ARG:HD2	1.81	0.62
1:G:536:ARG:NH1	1:G:616:ASP:O	2.33	0.62
1:J:559:ASP:CG	2:L:368:ARG:HH22	2.08	0.62
1:D:640:ARG:HB2	2:F:370:ASN:O	2.00	0.62
2:H:350:MET:HE1	2:H:382:HIS:HA	1.82	0.62
2:I:334:ARG:O	2:I:334:ARG:HG2	1.99	0.62
2:C:356:LEU:HD13	1:D:657:ALA:HB3	1.81	0.62
1:D:640:ARG:NH1	2:F:368:ARG:O	2.33	0.62
2:H:350:MET:HE1	2:H:382:HIS:CB	2.30	0.62
2:I:321:SER:HA	2:I:324:VAL:CG1	2.23	0.62
1:J:476:THR:HB	1:J:595:HIS:CD2	2.35	0.62
2:C:324:VAL:HA	2:C:331:PHE:CD2	2.35	0.61
2:F:382:HIS:O	2:F:386:THR:OG1	2.15	0.61
2:L:332:THR:CG2	2:L:334:ARG:HB3	2.29	0.61
2:H:337:SER:O	2:H:338:LYS:HD3	2.00	0.61
1:A:542:LEU:HB3	1:A:629:MET:HE1	1.82	0.61
1:D:608:LEU:HD21	1:D:625:ILE:HG12	1.81	0.61
2:E:332:THR:O	2:E:333:ASN:HB2	1.98	0.61
1:D:573:GLU:N	1:D:573:GLU:OE1	2.34	0.61
1:G:508:GLN:O	1:G:508:GLN:HG2	2.00	0.61
1:G:530:ILE:CD1	1:G:531:GLU:HG2	2.31	0.61
2:L:332:THR:HG22	2:L:334:ARG:CB	2.30	0.61
1:D:551:VAL:HG22	1:D:556:GLN:HG3	1.83	0.60
1:G:559:ASP:OD1	1:G:560:GLN:N	2.34	0.60
1:J:543:ARG:CZ	1:J:633:ILE:HD11	2.31	0.60
1:D:529:TYR:CE1	1:D:566:SER:HB2	2.37	0.60
2:H:350:MET:HE1	2:H:382:HIS:HB2	1.83	0.60
1:A:508:GLN:O	1:A:512:THR:HG23	2.02	0.60
1:J:543:ARG:NH2	1:J:633:ILE:HD11	2.17	0.60
2:K:327:LEU:CD2	2:K:380:ARG:HG2	2.32	0.60
1:A:640:ARG:NH1	2:C:368:ARG:O	2.34	0.60
2:E:329:GLU:OE1	2:E:380:ARG:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:496:LEU:HD11	1:J:513:ILE:HD12	1.83	0.60
1:A:461:ARG:NH1	1:A:599:GLU:OE1	2.34	0.59
2:I:318:LYS:O	2:I:347:ARG:NH2	2.36	0.59
2:I:369:ARG:NH2	4:I:401:HOH:O	2.35	0.59
1:A:638:VAL:HG11	2:C:345:ARG:HG2	1.85	0.59
2:C:370:ASN:OD1	1:D:662:ARG:NE	2.33	0.59
1:J:496:LEU:HD11	1:J:513:ILE:CD1	2.32	0.59
2:F:324:VAL:HA	2:F:331:PHE:CD2	2.37	0.59
1:A:640:ARG:HD2	2:C:369:ARG:O	2.02	0.59
2:F:347:ARG:O	2:F:351:VAL:HG23	2.03	0.59
1:G:543:ARG:HH22	1:G:633:ILE:CG1	2.16	0.59
2:H:320:HIS:CE1	2:H:322:ILE:HG13	2.38	0.58
2:B:354:TYR:CE1	2:B:392:ASN:HA	2.38	0.58
2:F:312:LYS:NZ	4:F:502:HOH:O	2.28	0.58
1:G:640:ARG:HG3	1:G:644:GLU:HB2	1.85	0.58
1:J:467:ASP:OD2	1:J:467:ASP:N	2.35	0.58
2:H:337:SER:C	2:H:338:LYS:HD3	2.28	0.58
1:D:613:TYR:CE1	1:D:615:PHE:HA	2.39	0.58
2:C:320:HIS:CG	2:C:321:SER:H	2.21	0.58
1:A:635:LEU:O	1:A:635:LEU:HG	2.02	0.58
1:J:556:GLN:OE1	1:J:558:ILE:HD11	2.03	0.58
2:H:329:GLU:CD	2:H:329:GLU:H	2.12	0.58
1:D:458:VAL:HG22	1:D:524:PHE:CD2	2.38	0.58
2:F:311:SER:HA	2:F:313:TRP:CD1	2.38	0.58
2:H:350:MET:HE1	2:H:382:HIS:CA	2.34	0.58
1:J:608:LEU:CD1	1:J:625:ILE:HG21	2.34	0.58
1:J:620:ILE:HD11	1:J:625:ILE:HB	1.85	0.58
1:A:496:LEU:HD21	1:A:513:ILE:HD12	1.86	0.57
1:A:462:LEU:HD12	1:A:495:MET:HE1	1.85	0.57
2:B:364:VAL:O	2:B:368:ARG:HG2	2.04	0.57
1:J:655:ILE:HB	1:J:659:GLU:CB	2.33	0.57
2:L:315:ASN:HD22	2:L:318:LYS:CE	2.17	0.57
2:L:322:ILE:O	2:L:326:SER:OG	2.17	0.57
1:A:611:LEU:HD13	1:A:622:ASP:HB2	1.86	0.57
2:I:320:HIS:CE1	2:I:322:ILE:HG13	2.40	0.57
1:A:470:ARG:HG3	1:A:509:HIS:NE2	2.19	0.57
1:J:507:GLU:HB2	4:J:729:HOH:O	2.04	0.57
2:C:350:MET:HE2	2:C:391:ILE:HD11	1.86	0.57
1:D:479:TRP:CD1	1:D:521:ILE:CD1	2.87	0.57
2:F:321:SER:HA	2:F:324:VAL:HG12	1.87	0.57
2:C:316:LEU:HD12	2:C:348:ASN:CG	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:501:PHE:O	1:G:506:ARG:HD3	2.05	0.56
2:I:308:PRO:HG3	2:I:393:TYR:CE1	2.39	0.56
1:G:463:GLU:HB3	1:G:474:ARG:NH1	2.20	0.56
2:H:340:PRO:HG2	2:H:341:GLU:OE2	2.05	0.56
1:A:460:ILE:HB	1:A:477:LEU:HD12	1.88	0.56
1:A:653:LEU:HD12	1:A:653:LEU:N	2.20	0.56
1:A:458:VAL:HG22	1:A:524:PHE:CD2	2.39	0.56
1:D:489:GLU:CD	1:D:489:GLU:H	2.12	0.56
1:D:608:LEU:CD2	1:D:625:ILE:HG12	2.36	0.56
1:J:514:CYS:O	1:J:518:GLN:HG3	2.06	0.56
1:J:565:ILE:HG22	1:J:601:VAL:HG13	1.88	0.56
1:G:463:GLU:HG2	1:G:474:ARG:NE	2.20	0.56
1:G:463:GLU:HG2	1:G:474:ARG:HE	1.71	0.56
2:F:307:ILE:HG23	2:F:308:PRO:HD2	1.88	0.56
1:A:649:THR:OG1	1:A:650:PRO:HD2	2.05	0.56
1:D:647:ILE:O	1:D:647:ILE:HD12	2.06	0.56
1:G:595:HIS:O	1:G:595:HIS:ND1	2.38	0.55
2:H:368:ARG:HA	2:H:378:LEU:HD13	1.89	0.55
1:G:527:ASN:O	1:G:530:ILE:HG13	2.05	0.55
3:E:401:GOL:O1	3:E:401:GOL:O3	2.21	0.55
1:D:562:GLU:HG2	1:D:630:LEU:HD13	1.88	0.55
1:G:530:ILE:HD11	1:G:531:GLU:HG2	1.88	0.55
1:D:498:ASP:OD2	2:E:363:SER:HB2	2.07	0.55
2:L:332:THR:O	2:L:334:ARG:N	2.40	0.55
1:A:589:PHE:O	1:A:593:ILE:HG13	2.06	0.55
1:A:559:ASP:OD1	1:A:560:GLN:N	2.38	0.55
1:A:659:GLU:HG3	2:F:370:ASN:OD1	2.06	0.55
1:J:477:LEU:HD22	1:J:491:PHE:CZ	2.42	0.55
1:G:476:THR:HB	1:G:595:HIS:CD2	2.42	0.55
2:I:364:VAL:O	2:I:368:ARG:HG2	2.07	0.54
2:K:339:THR:HG23	2:K:340:PRO:HD2	1.87	0.54
2:E:305:ILE:O	2:E:305:ILE:HG13	2.06	0.54
2:F:319:ILE:HD13	2:F:347:ARG:NH2	2.22	0.54
2:L:320:HIS:CE1	2:L:322:ILE:HG13	2.43	0.54
2:F:332:THR:HG21	2:F:335:ILE:HD12	1.90	0.54
2:I:339:THR:OG1	2:I:342:VAL:HG13	2.07	0.54
2:L:315:ASN:ND2	2:L:318:LYS:HE3	2.22	0.54
1:A:543:ARG:NH2	1:A:631:PRO:O	2.37	0.54
1:G:667:LYS:HG2	1:G:667:LYS:O	2.08	0.54
1:A:578:SER:O	1:A:582:GLU:HG3	2.07	0.54
1:A:542:LEU:HG	1:A:629:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:LEU:HA	4:B:415:HOH:O	2.08	0.54
1:D:638:VAL:HB	2:F:345:ARG:HD2	1.89	0.54
2:F:346:TYR:HB3	2:F:381:LEU:CD2	2.37	0.54
1:J:461:ARG:NH1	1:J:461:ARG:HG3	2.21	0.54
1:A:635:LEU:HG	2:C:345:ARG:NH1	2.23	0.53
2:E:340:PRO:O	2:E:344:MET:HE2	2.08	0.53
1:A:483:ASP:CG	2:B:380:ARG:HH22	2.16	0.53
2:B:334:ARG:HD2	2:B:334:ARG:O	2.09	0.53
1:G:541:ASP:OD1	1:G:543:ARG:HD2	2.08	0.53
2:E:380:ARG:HD3	4:E:503:HOH:O	2.07	0.53
2:F:307:ILE:HG23	2:F:308:PRO:CD	2.39	0.53
2:B:381:LEU:O	2:B:381:LEU:HD12	2.08	0.53
1:A:638:VAL:HG11	2:C:345:ARG:CG	2.38	0.53
2:B:320:HIS:CE1	2:B:322:ILE:HG13	2.43	0.53
1:G:622:ASP:OD1	1:G:624:ASP:HB3	2.08	0.53
2:I:342:VAL:HG23	2:I:342:VAL:O	2.07	0.53
1:G:457:LEU:O	1:G:459:PRO:HD3	2.08	0.53
2:L:311:SER:C	2:L:313:TRP:H	2.17	0.53
1:G:536:ARG:HD2	2:I:334:ARG:NH1	2.24	0.53
1:J:573:GLU:OE2	1:J:573:GLU:N	2.40	0.53
1:D:559:ASP:OD2	2:F:368:ARG:NH2	2.42	0.53
1:J:454:SER:N	4:J:703:HOH:O	2.42	0.53
2:L:332:THR:C	2:L:334:ARG:N	2.64	0.53
1:G:644:GLU:OE2	4:G:702:HOH:O	2.19	0.53
1:G:638:VAL:HG11	2:I:345:ARG:CG	2.38	0.52
2:C:324:VAL:HG13	2:C:331:PHE:CG	2.44	0.52
1:D:462:LEU:CD1	1:D:495:MET:HE1	2.39	0.52
1:A:461:ARG:NH1	1:A:599:GLU:OE2	2.42	0.52
1:D:625:ILE:HD12	1:D:625:ILE:O	2.10	0.52
2:F:314:PHE:CZ	2:F:347:ARG:HD3	2.44	0.52
1:G:509:HIS:HA	1:G:512:THR:HG22	1.91	0.52
2:C:316:LEU:HD12	2:C:348:ASN:OD1	2.09	0.52
1:D:544:ILE:HD13	1:D:604:TYR:CD1	2.44	0.52
2:L:364:VAL:O	2:L:368:ARG:HG2	2.09	0.52
1:A:529:TYR:C	1:A:531:GLU:H	2.17	0.52
1:G:528:PRO:O	1:G:532:LEU:HB2	2.10	0.52
2:C:367:ALA:O	2:C:371:VAL:HG22	2.10	0.52
2:F:321:SER:O	2:F:324:VAL:HG12	2.10	0.52
1:G:604:TYR:HD1	1:G:629:MET:HE1	1.75	0.52
1:A:534:GLN:HG2	1:A:536:ARG:HH12	1.75	0.52
1:A:621:GLU:CD	1:A:621:GLU:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:640:ARG:HD3	2:L:372:SER:HB2	1.91	0.52
2:C:383:LYS:HD3	2:C:383:LYS:N	2.23	0.52
1:G:635:LEU:HG	1:G:635:LEU:O	2.10	0.52
1:A:489:GLU:HG2	4:A:711:HOH:O	2.11	0.51
2:F:319:ILE:HD11	2:F:344:MET:HG3	1.91	0.51
2:E:346:TYR:CE1	2:E:371:VAL:HG13	2.46	0.51
2:F:314:PHE:HZ	2:F:347:ARG:HD3	1.76	0.51
2:H:368:ARG:NH1	4:H:503:HOH:O	2.44	0.51
2:K:327:LEU:HD23	2:K:380:ARG:HG2	1.92	0.51
2:C:320:HIS:ND1	2:C:321:SER:N	2.59	0.51
2:E:309:SER:OG	3:E:401:GOL:O2	2.16	0.51
2:E:335:ILE:CG2	2:E:336:PRO:HD2	2.40	0.51
1:G:646:LYS:HB2	1:G:646:LYS:HZ3	1.74	0.51
1:J:582:GLU:CD	2:L:363:SER:HB2	2.36	0.51
1:A:529:TYR:HA	1:A:534:GLN:OE1	2.11	0.51
1:J:621:GLU:HG3	1:J:621:GLU:O	2.11	0.51
1:A:505:THR:HG22	1:A:508:GLN:HB2	1.92	0.51
1:J:532:LEU:HD12	1:J:615:PHE:HD1	1.76	0.51
1:G:606:LYS:O	1:G:606:LYS:HG2	2.10	0.51
1:G:475:ASP:CG	2:H:368:ARG:HH22	2.19	0.50
2:K:332:THR:OG1	2:K:334:ARG:HG3	2.11	0.50
1:A:541:ASP:HB2	2:C:335:ILE:CG2	2.40	0.50
2:I:335:ILE:HD12	2:I:336:PRO:CD	2.41	0.50
2:L:339:THR:OG1	2:L:341:GLU:HG2	2.10	0.50
1:A:659:GLU:OE2	2:F:369:ARG:HD2	2.11	0.50
2:H:366:THR:O	2:H:370:ASN:ND2	2.32	0.50
2:K:364:VAL:O	2:K:368:ARG:HG3	2.10	0.50
1:A:460:ILE:HB	1:A:477:LEU:CD1	2.40	0.50
2:C:303:HIS:ND1	2:C:303:HIS:N	2.59	0.50
2:C:306:VAL:HG12	2:C:306:VAL:O	2.11	0.50
1:D:544:ILE:HG22	1:D:629:MET:HE2	1.93	0.50
1:G:541:ASP:OD1	1:G:541:ASP:O	2.29	0.50
1:J:554:GLN:HB2	1:J:655:ILE:O	2.12	0.50
1:D:562:GLU:HG2	1:D:630:LEU:HD11	1.91	0.50
2:F:316:LEU:HD22	2:F:348:ASN:OD1	2.12	0.50
2:F:329:GLU:OE1	2:F:380:ARG:NH1	2.44	0.50
1:G:519:GLU:O	1:G:523:GLU:HB2	2.11	0.50
1:G:542:LEU:O	1:G:565:ILE:HG12	2.12	0.50
2:I:347:ARG:HG3	2:I:348:ASN:N	2.23	0.50
2:C:314:PHE:CE1	2:C:347:ARG:NH1	2.79	0.50
1:A:546:ILE:HD12	1:A:563:TRP:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:461:ARG:HG3	1:J:461:ARG:HH11	1.77	0.50
1:G:463:GLU:HB3	1:G:474:ARG:HH11	1.77	0.50
1:A:560:GLN:HG2	1:A:648:PHE:CE2	2.47	0.50
2:B:328:PRO:O	2:B:332:THR:HG23	2.12	0.50
1:G:622:ASP:OD1	1:G:624:ASP:N	2.44	0.50
1:J:456:GLN:HE21	1:J:526:GLY:HA3	1.75	0.50
1:A:659:GLU:HG3	1:A:662:ARG:HH21	1.77	0.49
2:F:346:TYR:O	2:F:350:MET:HG3	2.12	0.49
1:G:476:THR:HB	1:G:595:HIS:NE2	2.27	0.49
1:G:604:TYR:CD1	1:G:629:MET:HE1	2.47	0.49
2:H:339:THR:HB	2:H:340:PRO:HD2	1.94	0.49
2:I:367:ALA:O	2:I:371:VAL:HG22	2.12	0.49
1:G:667:LYS:O	1:G:667:LYS:CG	2.60	0.49
1:D:560:GLN:NE2	1:D:647:ILE:HD11	2.27	0.49
2:K:305:ILE:HG21	2:K:355:ARG:CZ	2.41	0.49
1:J:492:VAL:HG12	1:J:510:ILE:HG13	1.94	0.49
1:J:575:PHE:CE2	1:J:579:MET:HE3	2.48	0.49
1:G:571:CYS:HB3	1:G:574:GLU:HB3	1.95	0.49
1:D:664:ASP:O	1:D:666:ASP:N	2.43	0.49
1:J:493:ASP:O	1:J:497:ARG:HG3	2.12	0.49
2:K:317:GLU:C	2:K:318:LYS:HD3	2.37	0.49
1:A:577:GLU:O	1:A:581:GLN:HG2	2.12	0.49
2:H:311:SER:C	2:H:313:TRP:H	2.21	0.49
1:J:476:THR:HB	1:J:595:HIS:NE2	2.27	0.49
1:J:519:GLU:O	1:J:523:GLU:HG3	2.12	0.49
1:A:555:ASN:OD1	1:A:654:GLN:NE2	2.39	0.49
1:D:625:ILE:HD12	1:D:629:MET:CE	2.40	0.49
2:F:330:PHE:HA	2:F:338:LYS:HB3	1.94	0.49
1:G:552:VAL:HG11	1:G:588:GLU:HB2	1.95	0.49
1:J:641:PRO:HG2	1:J:644:GLU:HG2	1.95	0.49
2:K:335:ILE:HB	2:K:338:LYS:HB2	1.95	0.49
2:K:339:THR:HG22	2:K:341:GLU:H	1.76	0.49
2:B:323:GLU:OE2	2:B:343:TYR:OH	2.12	0.48
1:G:577:GLU:HG2	1:G:590:VAL:HG21	1.93	0.48
1:A:562:GLU:OE1	1:A:640:ARG:NH2	2.46	0.48
2:C:350:MET:HE1	2:C:382:HIS:CA	2.42	0.48
2:I:335:ILE:HD12	2:I:336:PRO:HD2	1.94	0.48
2:L:315:ASN:ND2	2:L:318:LYS:HG3	2.29	0.48
1:D:551:VAL:CG2	1:D:556:GLN:HG3	2.44	0.48
1:J:565:ILE:CG2	1:J:601:VAL:HG13	2.43	0.48
1:A:537:LEU:HD12	1:A:538:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:320:HIS:CG	2:C:321:SER:N	2.80	0.48
1:D:457:LEU:CD2	2:E:374:ASP:HB3	2.44	0.48
1:D:638:VAL:HG11	2:F:345:ARG:CB	2.43	0.48
2:L:311:SER:HA	2:L:313:TRP:CD1	2.49	0.48
1:G:547:LYS:HG2	1:G:560:GLN:HG3	1.95	0.48
1:J:552:VAL:HG11	1:J:588:GLU:HB2	1.96	0.48
2:K:339:THR:HG22	2:K:341:GLU:N	2.29	0.48
1:D:659:GLU:OE2	1:D:662:ARG:NH2	2.47	0.48
2:E:348:ASN:O	2:E:352:ASN:HB2	2.14	0.48
1:J:559:ASP:OD1	1:J:560:GLN:N	2.46	0.48
1:G:467:ASP:N	1:G:467:ASP:OD2	2.46	0.47
1:G:510:ILE:HG13	1:G:511:ASP:N	2.29	0.47
1:G:638:VAL:CG1	2:I:345:ARG:HG2	2.39	0.47
2:C:361:TYR:HA	2:C:392:ASN:OD1	2.15	0.47
1:G:481:LYS:HG3	1:G:521:ILE:CG2	2.44	0.47
1:A:461:ARG:NH1	1:A:599:GLU:CD	2.72	0.47
1:D:635:LEU:HG	2:F:345:ARG:HH21	1.78	0.47
2:C:355:ARG:HD3	4:C:404:HOH:O	2.13	0.47
1:G:478:LEU:HD12	1:G:478:LEU:HA	1.62	0.47
1:G:639:TYR:OH	2:I:345:ARG:HD2	2.15	0.47
1:D:649:THR:OG1	1:D:650:PRO:HD2	2.15	0.47
2:F:367:ALA:O	2:F:371:VAL:HG22	2.14	0.47
1:G:509:HIS:HA	1:G:512:THR:CG2	2.45	0.47
1:G:591:THR:HG21	2:H:369:ARG:O	2.15	0.47
1:J:579:MET:HE2	2:L:368:ARG:NH1	2.28	0.47
2:K:311:SER:C	2:K:313:TRP:H	2.22	0.47
1:A:633:ILE:HG22	1:A:633:ILE:O	2.15	0.47
2:F:346:TYR:HB3	2:F:381:LEU:HD21	1.96	0.47
1:A:476:THR:HB	1:A:595:HIS:NE2	2.29	0.47
2:B:306:VAL:O	2:B:306:VAL:HG13	2.15	0.47
1:D:624:ASP:HB3	1:D:628:ARG:HH21	1.80	0.47
1:G:625:ILE:N	1:G:625:ILE:HD12	2.30	0.47
1:J:498:ASP:C	1:J:499:TYR:HD2	2.23	0.47
2:B:354:TYR:OH	2:B:394:GLN:HG3	2.15	0.46
1:D:610:LEU:N	1:D:610:LEU:HD22	2.30	0.46
1:J:465:ASP:O	1:J:469:ASP:HB2	2.15	0.46
1:J:529:TYR:CE2	1:J:566:SER:HB2	2.50	0.46
1:G:529:TYR:CZ	1:G:566:SER:HB2	2.50	0.46
2:C:339:THR:HB	2:C:340:PRO:CD	2.45	0.46
2:I:321:SER:O	2:I:324:VAL:HG12	2.15	0.46
1:A:540:ASP:OD1	1:A:540:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:543:ARG:HA	1:J:563:TRP:O	2.16	0.46
1:A:546:ILE:HD12	1:A:563:TRP:HB2	1.98	0.46
2:E:395:VAL:HG12	2:E:396:ASP:OD1	2.16	0.46
1:G:640:ARG:HG3	1:G:641:PRO:HD2	1.98	0.46
1:A:664:ASP:C	1:A:666:ASP:H	2.23	0.46
2:I:311:SER:C	2:I:313:TRP:H	2.24	0.46
2:I:321:SER:C	2:I:324:VAL:HG12	2.40	0.46
1:J:550:ILE:O	1:J:556:GLN:HA	2.16	0.46
1:D:629:MET:HE3	1:D:629:MET:N	2.30	0.46
2:B:346:TYR:CE1	2:B:371:VAL:HG13	2.50	0.46
2:F:307:ILE:HD11	2:F:355:ARG:NH2	2.31	0.46
1:J:511:ASP:OD1	1:J:511:ASP:N	2.49	0.46
1:J:559:ASP:OD2	1:J:650:PRO:HB3	2.16	0.46
1:J:655:ILE:HB	1:J:659:GLU:HB3	1.98	0.46
1:A:625:ILE:O	1:A:629:MET:HG2	2.16	0.46
1:D:555:ASN:HB3	1:D:652:LEU:HD11	1.98	0.46
1:G:497:ARG:HA	1:G:497:ARG:HD3	1.73	0.46
2:E:322:ILE:O	2:E:326:SER:OG	2.27	0.45
1:D:650:PRO:HG3	2:F:365:THR:HG21	1.98	0.45
1:J:536:ARG:HG3	1:J:536:ARG:NH1	2.31	0.45
2:B:363:SER:HB2	4:B:408:HOH:O	2.14	0.45
1:D:565:ILE:O	1:D:605:HIS:NE2	2.42	0.45
1:G:456:GLN:O	1:G:480:ASN:HA	2.16	0.45
1:G:595:HIS:ND1	1:G:595:HIS:C	2.75	0.45
2:K:387:LYS:HE2	3:K:401:GOL:H11	1.98	0.45
1:G:455:GLU:HG2	1:G:457:LEU:HG	1.97	0.45
2:I:311:SER:HA	2:I:313:TRP:CD1	2.51	0.45
1:A:475:ASP:OD2	1:A:495:MET:CE	2.65	0.45
2:I:305:ILE:HG21	2:I:355:ARG:NE	2.31	0.45
1:J:532:LEU:HD12	1:J:615:PHE:CD1	2.52	0.45
1:A:478:LEU:HD23	1:A:478:LEU:HA	1.71	0.45
1:A:547:LYS:O	1:A:600:GLN:NE2	2.47	0.45
1:G:474:ARG:CG	1:G:474:ARG:HH21	2.29	0.45
2:F:374:ASP:OD2	2:F:376:ALA:HB3	2.17	0.45
2:B:306:VAL:O	2:B:306:VAL:CG1	2.65	0.45
1:G:508:GLN:O	1:G:512:THR:HG22	2.16	0.45
1:J:602:HIS:O	1:J:603:MET:C	2.60	0.45
1:J:640:ARG:HG3	1:J:641:PRO:HD2	1.98	0.45
1:A:583:LEU:HB2	1:A:585:LEU:HG	1.98	0.45
1:D:465:ASP:O	1:D:469:ASP:HB2	2.17	0.45
2:E:335:ILE:HG22	2:E:337:SER:N	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:VAL:HG11	2:F:345:ARG:HB3	1.98	0.44
1:G:638:VAL:O	2:I:371:VAL:HA	2.16	0.44
1:D:666:ASP:OD1	1:D:667:LYS:N	2.48	0.44
1:G:645:SER:CB	1:J:662:ARG:NH2	2.80	0.44
1:D:634:THR:OG1	1:D:637:ASP:OD2	2.12	0.44
1:G:639:TYR:CZ	2:I:345:ARG:HD2	2.52	0.44
1:J:529:TYR:HE2	1:J:540:ASP:OD2	2.00	0.44
1:A:586:PRO:HD2	1:A:589:PHE:CD2	2.52	0.44
1:A:623:ASP:HA	1:A:626:ARG:NH1	2.27	0.44
2:C:311:SER:C	2:C:313:TRP:H	2.25	0.44
1:D:543:ARG:HG3	1:D:543:ARG:HH11	1.82	0.44
1:G:541:ASP:OD1	1:G:541:ASP:C	2.61	0.44
1:G:541:ASP:OD2	2:I:337:SER:CB	2.64	0.44
1:J:492:VAL:CG1	1:J:510:ILE:HG13	2.46	0.44
1:D:493:ASP:HB2	1:D:510:ILE:HD11	1.99	0.44
1:D:608:LEU:O	1:D:611:LEU:N	2.38	0.44
1:J:579:MET:HE2	2:L:368:ARG:HH12	1.83	0.44
2:K:387:LYS:HE2	3:K:401:GOL:H31	2.00	0.44
1:G:499:TYR:CD1	1:G:499:TYR:N	2.86	0.44
1:J:477:LEU:C	1:J:477:LEU:HD12	2.43	0.44
1:D:489:GLU:HG3	1:D:514:CYS:SG	2.58	0.44
1:D:482:ASN:O	1:D:484:LYS:HG2	2.18	0.43
1:G:545:ARG:HG3	1:G:630:LEU:HD21	1.99	0.43
2:I:319:ILE:HD11	2:I:331:PHE:CE1	2.53	0.43
1:J:561:PHE:CE2	1:J:579:MET:HE1	2.53	0.43
1:A:475:ASP:OD2	1:A:495:MET:HE2	2.19	0.43
2:I:347:ARG:O	2:I:351:VAL:HG23	2.18	0.43
2:K:317:GLU:O	2:K:318:LYS:HD3	2.17	0.43
2:K:311:SER:C	2:K:313:TRP:N	2.77	0.43
2:B:333:ASN:HA	4:B:405:HOH:O	2.18	0.43
2:L:311:SER:C	2:L:313:TRP:N	2.74	0.43
1:G:475:ASP:OD2	2:H:368:ARG:NH2	2.45	0.43
1:J:472:PHE:HE1	1:J:474:ARG:HH11	1.67	0.43
1:J:583:LEU:O	1:J:584:GLU:C	2.60	0.43
1:A:581:GLN:OE1	1:A:581:GLN:HA	2.18	0.43
1:D:644:GLU:OE1	1:D:644:GLU:HA	2.19	0.43
2:K:339:THR:HG23	2:K:340:PRO:CD	2.49	0.43
1:A:537:LEU:HD12	1:A:538:GLY:H	1.83	0.43
1:A:541:ASP:HB2	2:C:335:ILE:HG23	1.99	0.43
1:G:474:ARG:NH2	1:G:474:ARG:HG2	2.34	0.43
1:G:562:GLU:OE1	1:G:630:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:GLN:O	2:C:301:GLN:HG3	2.19	0.43
2:C:311:SER:C	2:C:313:TRP:N	2.76	0.43
1:A:613:TYR:CE1	1:A:620:ILE:HD13	2.53	0.43
2:F:374:ASP:OD2	2:F:377:ALA:N	2.49	0.43
2:B:361:TYR:HA	2:B:395:VAL:HG21	2.01	0.42
1:D:590:VAL:HG13	1:D:591:THR:N	2.34	0.42
2:E:307:ILE:HG22	2:E:389:GLY:O	2.19	0.42
2:F:311:SER:C	2:F:313:TRP:H	2.27	0.42
1:G:529:TYR:CE1	1:G:566:SER:HB2	2.54	0.42
2:I:311:SER:C	2:I:313:TRP:N	2.76	0.42
2:H:362:PHE:O	2:H:382:HIS:HE1	2.03	0.42
1:J:474:ARG:HE	1:J:474:ARG:HB2	1.60	0.42
1:A:667:LYS:HE3	1:A:667:LYS:HB3	1.85	0.42
2:E:351:VAL:O	2:E:355:ARG:HG3	2.20	0.42
1:D:493:ASP:HB2	1:D:510:ILE:CD1	2.50	0.42
1:D:562:GLU:OE2	1:D:630:LEU:HD13	2.18	0.42
2:F:319:ILE:HD12	2:F:343:TYR:CD2	2.55	0.42
1:G:646:LYS:HG2	1:J:558:ILE:HG12	2.01	0.42
2:K:313:TRP:CZ2	2:K:322:ILE:HG21	2.54	0.42
1:G:468:ARG:H	1:G:468:ARG:HD2	1.84	0.42
2:H:368:ARG:HA	2:H:378:LEU:CD1	2.50	0.42
1:J:461:ARG:HH11	1:J:461:ARG:CG	2.32	0.42
2:C:374:ASP:OD1	2:C:376:ALA:HB3	2.20	0.42
1:D:492:VAL:O	1:D:493:ASP:C	2.62	0.42
2:F:307:ILE:HD13	2:F:390:LEU:HD23	2.01	0.42
1:J:546:ILE:O	1:J:560:GLN:HA	2.20	0.42
1:A:470:ARG:H	1:A:470:ARG:HG2	1.50	0.42
1:A:562:GLU:HG2	1:A:630:LEU:CD1	2.49	0.42
1:D:667:LYS:HE2	1:D:667:LYS:HA	2.00	0.42
1:G:591:THR:CG2	2:H:369:ARG:O	2.68	0.42
2:C:381:LEU:HD12	2:C:381:LEU:O	2.20	0.42
2:F:303:HIS:CD2	2:F:303:HIS:N	2.87	0.42
1:G:536:ARG:CZ	1:G:616:ASP:O	2.68	0.42
1:A:468:ARG:HA	1:A:468:ARG:HD3	1.87	0.42
2:C:369:ARG:NH1	1:D:659:GLU:OE1	2.53	0.42
1:A:583:LEU:N	1:A:583:LEU:HD23	2.35	0.42
2:B:305:ILE:HG21	2:B:355:ARG:HD3	2.01	0.42
2:C:349:PHE:O	2:C:353:SER:HB2	2.19	0.42
1:D:575:PHE:O	1:D:578:SER:N	2.50	0.42
2:K:339:THR:CG2	4:K:510:HOH:O	2.68	0.42
2:L:334:ARG:O	2:L:334:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:PRO:HD2	1:A:589:PHE:CE2	2.55	0.41
1:A:659:GLU:CG	2:F:370:ASN:OD1	2.68	0.41
1:D:542:LEU:HD23	1:D:629:MET:HG2	2.02	0.41
1:D:559:ASP:OD2	1:D:650:PRO:HB3	2.20	0.41
1:G:537:LEU:HD13	1:G:538:GLY:N	2.35	0.41
1:D:536:ARG:NH2	1:D:540:ASP:OD1	2.54	0.41
1:D:667:LYS:HA	1:D:667:LYS:CE	2.49	0.41
1:J:475:ASP:OD1	1:J:476:THR:N	2.53	0.41
1:A:544:ILE:HG12	1:A:604:TYR:CD1	2.55	0.41
1:D:497:ARG:CZ	1:D:506:ARG:NH2	2.83	0.41
1:G:554:GLN:HB2	1:G:655:ILE:O	2.21	0.41
2:I:341:GLU:HG3	2:I:342:VAL:N	2.35	0.41
1:A:469:ASP:C	1:A:471:PHE:H	2.28	0.41
2:F:302:ALA:HB3	2:F:305:ILE:HG12	2.03	0.41
1:G:543:ARG:NH2	1:G:633:ILE:CD1	2.82	0.41
1:G:565:ILE:HG22	1:G:601:VAL:HG22	2.01	0.41
1:G:590:VAL:HG13	1:G:591:THR:HG22	2.02	0.41
1:J:551:VAL:HG11	1:J:660:LEU:HD13	2.02	0.41
2:B:327:LEU:CD2	2:B:380:ARG:HG2	2.50	0.41
1:D:536:ARG:HH22	1:D:617:GLY:N	2.18	0.41
2:K:344:MET:HG2	2:K:347:ARG:NH1	2.36	0.41
2:L:349:PHE:O	2:L:353:SER:HB2	2.21	0.41
2:L:381:LEU:HD12	2:L:381:LEU:C	2.44	0.41
2:B:354:TYR:CD2	2:B:354:TYR:C	2.98	0.41
1:D:560:GLN:HG2	1:D:648:PHE:CE2	2.56	0.41
1:G:531:GLU:C	1:G:532:LEU:HD12	2.45	0.41
1:A:638:VAL:CG1	2:C:345:ARG:HG2	2.51	0.41
1:D:479:TRP:HD1	1:D:521:ILE:CD1	2.31	0.41
1:J:536:ARG:HG3	1:J:536:ARG:HH11	1.83	0.41
2:K:339:THR:CG2	2:K:340:PRO:N	2.83	0.41
1:A:590:VAL:HG13	1:A:591:THR:N	2.36	0.41
1:D:477:LEU:CD2	1:D:477:LEU:C	2.94	0.41
1:D:536:ARG:HD3	1:D:536:ARG:N	2.35	0.41
2:F:307:ILE:CG2	2:F:308:PRO:N	2.83	0.41
1:J:630:LEU:HB3	1:J:631:PRO:HD2	2.02	0.41
1:A:529:TYR:C	1:A:531:GLU:N	2.79	0.41
1:A:542:LEU:HB3	1:A:629:MET:CE	2.49	0.41
2:F:319:ILE:HD12	2:F:343:TYR:CE2	2.55	0.41
1:G:532:LEU:O	1:G:533:ASN:HB2	2.20	0.41
1:G:659:GLU:OE1	2:L:369:ARG:NH1	2.54	0.41
2:H:347:ARG:HA	2:H:381:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:477:LEU:CD2	1:J:491:PHE:CZ	3.03	0.41
2:K:307:ILE:HD13	4:K:514:HOH:O	2.21	0.41
1:A:542:LEU:HG	1:A:629:MET:CE	2.50	0.41
2:B:306:VAL:HG12	2:B:394:GLN:OE1	2.21	0.41
1:D:455:GLU:N	4:D:707:HOH:O	2.52	0.41
2:E:320:HIS:ND1	2:E:322:ILE:HG13	2.35	0.41
1:J:564:ASP:N	2:L:374:ASP:OD1	2.53	0.41
2:B:329:GLU:CG	4:B:415:HOH:O	2.63	0.40
2:B:335:ILE:HD13	2:B:335:ILE:HA	1.96	0.40
2:F:341:GLU:CG	2:F:342:VAL:N	2.83	0.40
2:F:396:ASP:OD2	2:F:396:ASP:N	2.54	0.40
1:G:462:LEU:HD21	1:G:517:ILE:HG12	2.03	0.40
1:G:467:ASP:OD1	1:G:468:ARG:NH1	2.55	0.40
1:G:613:TYR:CE1	1:G:615:PHE:HA	2.56	0.40
2:K:324:VAL:HA	2:K:331:PHE:CE2	2.56	0.40
1:A:464:PHE:O	1:A:472:PHE:HA	2.22	0.40
1:G:477:LEU:HD12	1:G:477:LEU:O	2.21	0.40
1:G:570:ASN:O	1:G:572:PRO:HD3	2.22	0.40
2:I:314:PHE:CD2	2:I:390:LEU:HD13	2.56	0.40
1:D:481:LYS:HG3	1:D:521:ILE:CG2	2.51	0.40
2:E:306:VAL:O	2:E:306:VAL:CG2	2.70	0.40
2:F:345:ARG:HG2	2:F:345:ARG:HH11	1.85	0.40
1:G:507:GLU:O	1:G:507:GLU:HG2	2.20	0.40
1:G:537:LEU:HD22	1:G:537:LEU:HA	1.81	0.40
2:I:354:TYR:OH	2:I:394:GLN:HG3	2.21	0.40
1:J:462:LEU:O	1:J:474:ARG:HA	2.21	0.40
1:D:492:VAL:O	1:D:495:MET:N	2.55	0.40
2:H:311:SER:C	2:H:313:TRP:N	2.79	0.40
1:J:551:VAL:HG11	1:J:660:LEU:CD1	2.52	0.40
2:F:320:HIS:ND1	2:F:321:SER:N	2.69	0.40
1:J:626:ARG:HE	1:J:626:ARG:HB3	1.61	0.40
2:L:341:GLU:HG3	2:L:342:VAL:N	2.36	0.40

All (3) 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)
2:E:398:LYS:O	2:K:380:ARG:NH1[3_445]	2.06	0.14
2:B:380:ARG:NH1	2:H:398:LYS:O[3_444]	2.16	0.04
2:B:319:ILE:O	2:E:334:ARG:NH1[4_647]	2.19	0.01

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	205/227 (90%)	184 (90%)	20 (10%)	1 (0%)	24	36
1	D	211/227 (93%)	195 (92%)	15 (7%)	1 (0%)	24	36
1	G	206/227 (91%)	186 (90%)	20 (10%)	0	100	100
1	J	203/227 (89%)	186 (92%)	15 (7%)	2 (1%)	12	18
2	B	92/187 (49%)	91 (99%)	1 (1%)	0	100	100
2	C	95/187 (51%)	88 (93%)	7 (7%)	0	100	100
2	E	97/187 (52%)	92 (95%)	5 (5%)	0	100	100
2	F	93/187 (50%)	83 (89%)	10 (11%)	0	100	100
2	H	95/187 (51%)	90 (95%)	5 (5%)	0	100	100
2	I	93/187 (50%)	84 (90%)	9 (10%)	0	100	100
2	K	92/187 (49%)	89 (97%)	3 (3%)	0	100	100
2	L	93/187 (50%)	86 (92%)	6 (6%)	1 (1%)	11	16
All	All	1575/2404 (66%)	1454 (92%)	116 (7%)	5 (0%)	36	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	333	ASN
1	J	580	CYS
1	A	665	LYS
1	J	470	ARG
1	D	664	ASP

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	193/209 (92%)	175 (91%)	18 (9%)	8	12
1	D	196/209 (94%)	184 (94%)	12 (6%)	17	29
1	G	194/209 (93%)	173 (89%)	21 (11%)	6	8
1	J	191/209 (91%)	177 (93%)	14 (7%)	13	21
2	B	87/173 (50%)	78 (90%)	9 (10%)	7	9
2	C	90/173 (52%)	76 (84%)	14 (16%)	2	2
2	E	92/173 (53%)	85 (92%)	7 (8%)	12	20
2	F	88/173 (51%)	83 (94%)	5 (6%)	18	31
2	H	90/173 (52%)	82 (91%)	8 (9%)	9	14
2	I	88/173 (51%)	80 (91%)	8 (9%)	9	13
2	K	87/173 (50%)	77 (88%)	10 (12%)	5	7
2	L	88/173 (51%)	80 (91%)	8 (9%)	9	13
All	All	1484/2220 (67%)	1350 (91%)	134 (9%)	9	13

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	ARG
1	A	470	ARG
1	A	471	PHE
1	A	496	LEU
1	A	497	ARG
1	A	530	ILE
1	A	540	ASP
1	A	544	ILE
1	A	596	SER
1	A	621	GLU
1	A	626	ARG
1	A	628	ARG
1	A	632	THR
1	A	647	ILE
1	A	652	LEU
1	A	653	LEU
1	A	655	ILE
1	A	667	LYS
2	B	304	GLU

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Mol	Chain	Res	Type
2	B	305	ILE
2	B	317	GLU
2	B	333	ASN
2	B	371	VAL
2	B	372	SER
2	B	387	LYS
2	B	394	GLN
2	B	395	VAL
2	C	303	HIS
2	C	309	SER
2	C	316	LEU
2	C	318	LYS
2	C	332	THR
2	C	342	VAL
2	C	344	MET
2	C	353	SER
2	C	365	THR
2	C	366	THR
2	C	381	LEU
2	C	383	LYS
2	C	391	ILE
2	C	396	ASP
1	D	463	GLU
1	D	477	LEU
1	D	545	ARG
1	D	558	ILE
1	D	596	SER
1	D	625	ILE
1	D	629	MET
1	D	636	ASP
1	D	645	SER
1	D	647	ILE
1	D	653	LEU
1	D	667	LYS
2	E	301	GLN
2	E	306	VAL
2	E	309	SER
2	E	337	SER
2	E	344	MET
2	E	347	ARG
2	E	372	SER
2	F	303	HIS

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Mol	Chain	Res	Type
2	F	304	GLU
2	F	307	ILE
2	F	332	THR
2	F	394	GLN
1	G	461	ARG
1	G	467	ASP
1	G	474	ARG
1	G	477	LEU
1	G	478	LEU
1	G	501	PHE
1	G	508	GLN
1	G	510	ILE
1	G	537	LEU
1	G	543	ARG
1	G	562	GLU
1	G	568	SER
1	G	569	ASP
1	G	591	THR
1	G	603	MET
1	G	645	SER
1	G	646	LYS
1	G	647	ILE
1	G	653	LEU
1	G	667	LYS
1	G	668	ASP
2	H	309	SER
2	H	329	GLU
2	H	333	ASN
2	H	335	ILE
2	H	342	VAL
2	H	360	GLU
2	H	372	SER
2	H	374	ASP
2	I	303	HIS
2	I	305	ILE
2	I	309	SER
2	I	319	ILE
2	I	327	LEU
2	I	335	ILE
2	I	342	VAL
2	I	347	ARG
1	J	455	GLU

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Mol	Chain	Res	Type
1	J	465	ASP
1	J	467	ASP
1	J	468	ARG
1	J	511	ASP
1	J	522	GLN
1	J	581	GLN
1	J	584	GLU
1	J	585	LEU
1	J	590	VAL
1	J	591	THR
1	J	620	ILE
1	J	624	ASP
1	J	662	ARG
2	K	305	ILE
2	K	327	LEU
2	K	334	ARG
2	K	335	ILE
2	K	339	THR
2	K	344	MET
2	K	347	ARG
2	K	359	ASN
2	K	368	ARG
2	K	371	VAL
2	L	309	SER
2	L	326	SER
2	L	327	LEU
2	L	344	MET
2	L	359	ASN
2	L	364	VAL
2	L	387	LYS
2	L	394	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	GLN
1	A	560	GLN
2	B	370	ASN
1	D	509	HIS
1	D	614	ASN
2	E	301	GLN
1	G	466	GLN

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Mol	Chain	Res	Type
1	G	509	HIS
1	G	525	GLN
1	G	651	ASN
1	G	654	GLN
2	H	382	HIS
2	I	315	ASN
1	J	456	GLN
1	J	560	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	L	401	-	5,5,5	0.41	0	5,5,5	0.44	0
3	GOL	F	401	-	5,5,5	0.52	0	5,5,5	0.39	0
3	GOL	K	401	-	5,5,5	0.47	0	5,5,5	0.13	0
3	GOL	E	401	-	5,5,5	0.46	0	5,5,5	0.37	0
3	GOL	L	402	-	5,5,5	0.50	0	5,5,5	0.26	0
3	GOL	E	404	-	5,5,5	0.38	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	H	401	-	5,5,5	0.23	0	5,5,5	0.83	0
3	GOL	E	402	-	5,5,5	0.71	0	5,5,5	0.78	0
3	GOL	E	403	-	5,5,5	0.52	0	5,5,5	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	L	401	-	-	3/4/4/4	-
3	GOL	F	401	-	-	4/4/4/4	-
3	GOL	K	401	-	-	4/4/4/4	-
3	GOL	E	401	-	-	4/4/4/4	-
3	GOL	L	402	-	-	2/4/4/4	-
3	GOL	E	404	-	-	2/4/4/4	-
3	GOL	H	401	-	-	1/4/4/4	-
3	GOL	E	402	-	-	1/4/4/4	-
3	GOL	E	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	404	GOL	C1-C2-C3-O3
3	F	401	GOL	O1-C1-C2-O2
3	F	401	GOL	O1-C1-C2-C3
3	F	401	GOL	C1-C2-C3-O3
3	K	401	GOL	O1-C1-C2-O2
3	K	401	GOL	O1-C1-C2-C3
3	L	401	GOL	O1-C1-C2-C3
3	L	402	GOL	O1-C1-C2-O2
3	E	403	GOL	O2-C2-C3-O3
3	E	401	GOL	O1-C1-C2-C3
3	E	401	GOL	C1-C2-C3-O3
3	E	402	GOL	C1-C2-C3-O3
3	E	403	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	H	401	GOL	C1-C2-C3-O3
3	K	401	GOL	C1-C2-C3-O3
3	L	402	GOL	O1-C1-C2-C3
3	E	404	GOL	O2-C2-C3-O3
3	K	401	GOL	O2-C2-C3-O3
3	L	401	GOL	O1-C1-C2-O2
3	E	401	GOL	O2-C2-C3-O3
3	F	401	GOL	O2-C2-C3-O3
3	L	401	GOL	O2-C2-C3-O3
3	E	401	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	401	GOL	2	0
3	E	401	GOL	2	0
3	H	401	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	209/227 (92%)	-1.09	0 100 100	29, 45, 81, 94	0
1	D	213/227 (93%)	-1.14	1 (0%) 87 85	27, 46, 66, 78	0
1	G	210/227 (92%)	-1.10	0 100 100	28, 44, 74, 88	0
1	J	207/227 (91%)	-1.14	0 100 100	30, 45, 74, 94	0
2	B	94/187 (50%)	-1.23	0 100 100	26, 34, 52, 73	0
2	C	97/187 (51%)	-1.10	0 100 100	33, 42, 62, 85	0
2	E	99/187 (52%)	-1.17	0 100 100	26, 34, 62, 79	0
2	F	95/187 (50%)	-1.21	0 100 100	31, 41, 58, 73	0
2	H	97/187 (51%)	-1.21	0 100 100	26, 33, 50, 64	0
2	I	95/187 (50%)	-1.25	0 100 100	29, 40, 60, 79	0
2	K	94/187 (50%)	-1.22	0 100 100	30, 37, 59, 65	0
2	L	95/187 (50%)	-1.23	0 100 100	30, 41, 56, 61	0
All	All	1605/2404 (66%)	-1.16	1 (0%) 92 91	26, 41, 71, 94	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	667	LYS	2.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	E	401	6/6	0.96	0.07	43,53,63,63	0
3	GOL	H	401	6/6	0.97	0.06	46,59,71,71	0
3	GOL	E	404	6/6	0.98	0.05	43,52,62,69	0
3	GOL	E	403	6/6	0.98	0.05	33,52,60,63	0
3	GOL	K	401	6/6	0.98	0.08	51,62,70,70	0
3	GOL	L	401	6/6	0.98	0.05	50,60,64,65	0
3	GOL	L	402	6/6	0.98	0.05	47,57,62,64	0
3	GOL	E	402	6/6	0.99	0.04	28,36,41,48	0
3	GOL	F	401	6/6	0.99	0.06	29,48,59,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.