



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:53 AM UTC

PDB ID : 2XWJ / pdb_00002xwj
Title : Crystal Structure of Complement C3b in Complex with Factor B
Authors : Forneris, F.; Ricklin, D.; Wu, J.; Tzekou, A.; Wallace, R.S.; Lambris, J.D.; Gros, P.
Deposited on : 2010-11-04
Resolution : 4.00 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

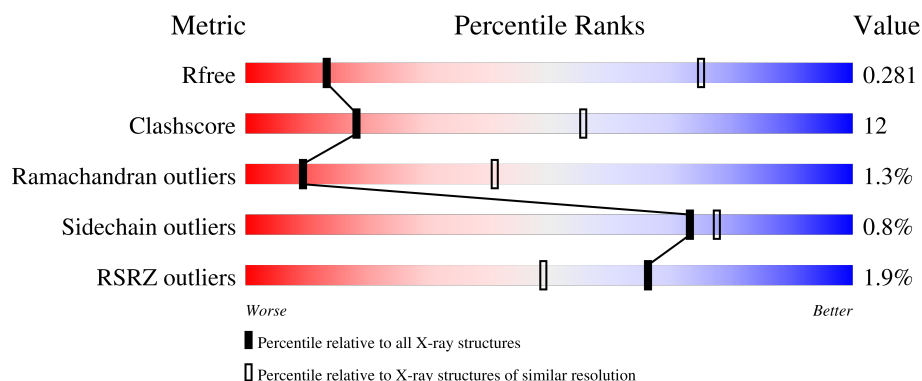
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	645	2% 71% 27% ..
1	C	645	3% 71% 27% .
1	E	645	5% 71% 28% .
1	G	645	% 71% 27% ..
2	B	915	2% 72% 26% ..

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Mol	Chain	Length	Quality of chain
2	D	915	3% 71% 27% ..
2	F	915	2% 73% 25% ..
2	H	915	2% 73% 24% ..
3	I	741	71% 25% .
3	J	741	2% 68% 26% ..
3	K	741	69% 25% ..
3	L	741	72% 23% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 71260 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	C	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	E	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	G	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			

- Molecule 2 is a protein called COMPLEMENT C3 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	D	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	F	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	H	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	engineered mutation	UNP P01024
D	991	GLU	GLN	engineered mutation	UNP P01024
F	991	GLU	GLN	engineered mutation	UNP P01024
H	991	GLU	GLN	engineered mutation	UNP P01024

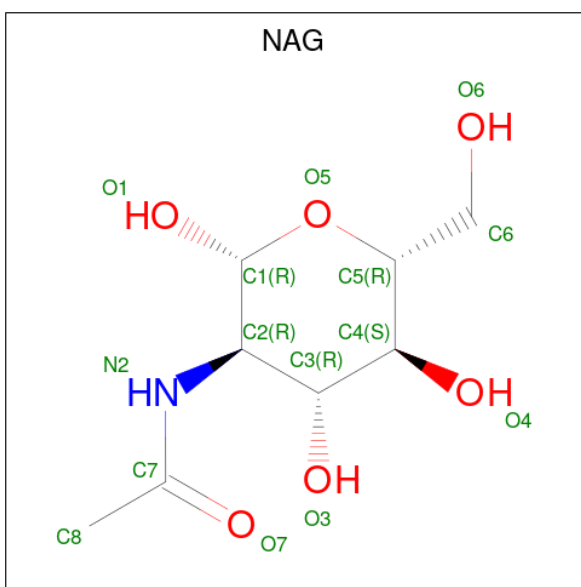
- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	712	Total	C	N	O	S	0	0	0
			5593	3514	970	1076	33			
3	J	713	Total	C	N	O	S	0	0	0
			5596	3514	971	1078	33			
3	K	713	Total	C	N	O	S	0	0	0
			5603	3519	971	1080	33			
3	L	711	Total	C	N	O	S	0	0	0
			5588	3511	969	1075	33			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	740	ALA	-	expression tag	UNP P00751
I	741	ALA	-	expression tag	UNP P00751
I	254	GLY	ASP	engineered mutation	UNP P00751
I	260	ASP	ASN	engineered mutation	UNP P00751
J	740	ALA	-	expression tag	UNP P00751
J	741	ALA	-	expression tag	UNP P00751
J	254	GLY	ASP	engineered mutation	UNP P00751
J	260	ASP	ASN	engineered mutation	UNP P00751
K	740	ALA	-	expression tag	UNP P00751
K	741	ALA	-	expression tag	UNP P00751
K	254	GLY	ASP	engineered mutation	UNP P00751
K	260	ASP	ASN	engineered mutation	UNP P00751
L	740	ALA	-	expression tag	UNP P00751
L	741	ALA	-	expression tag	UNP P00751
L	254	GLY	ASP	engineered mutation	UNP P00751
L	260	ASP	ASN	engineered mutation	UNP P00751

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Ni	0	0
			1	1		
5	J	1	Total	Ni	0	0
			1	1		
5	K	1	Total	Ni	0	0
			1	1		
5	L	1	Total	Ni	0	0
			1	1		

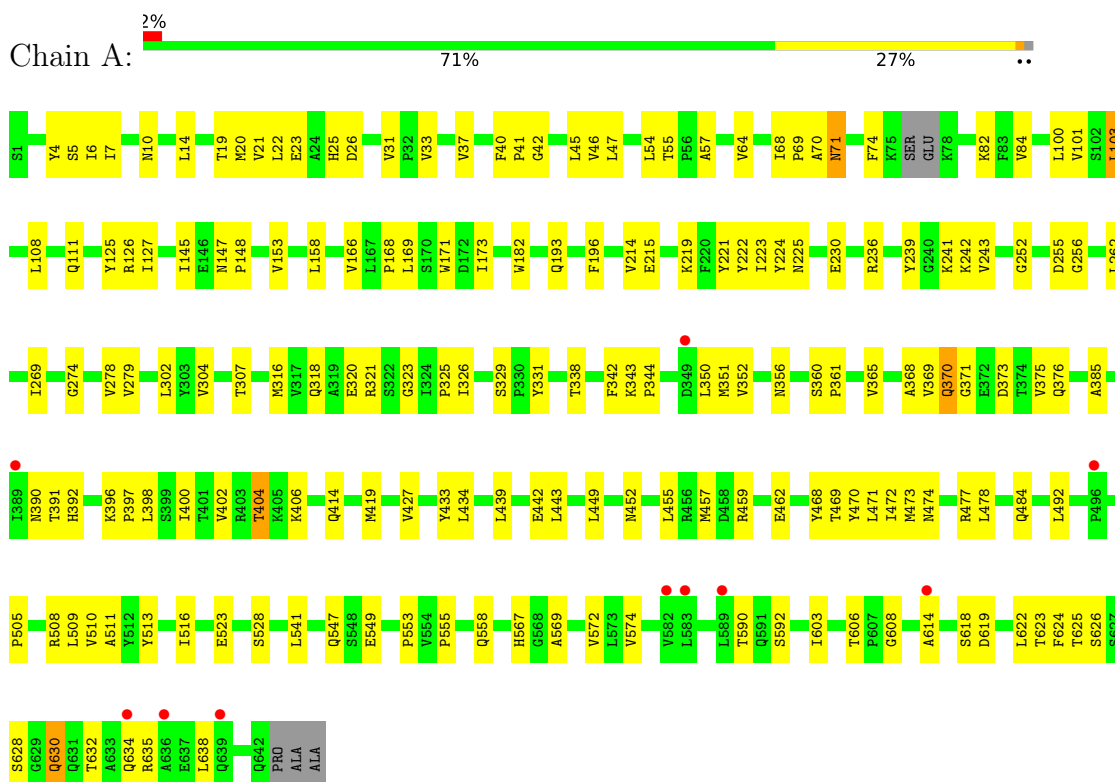
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total 2	O 2	0	0
6	J	2	Total 2	O 2	0	0
6	K	1	Total 1	O 1	0	0
6	K	1	Total 1	O 1	0	0
6	L	2	Total 2	O 2	0	0

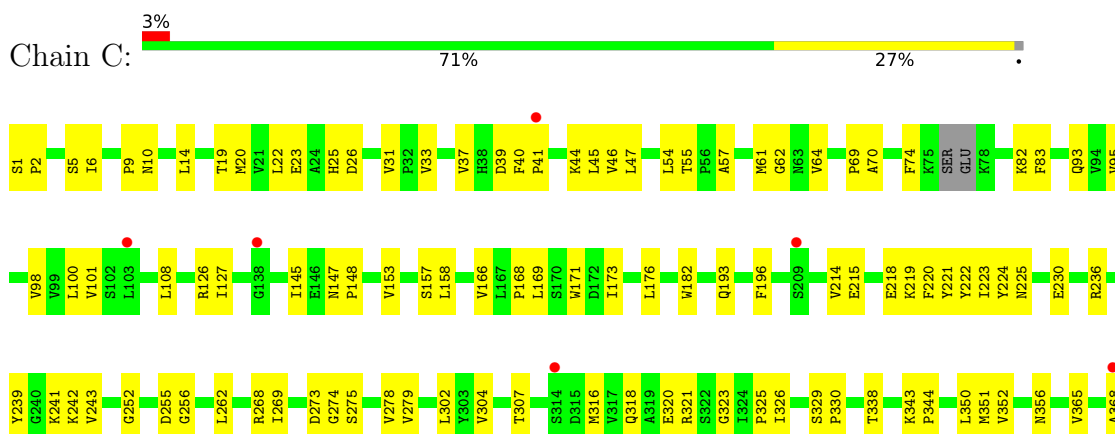
3 Residue-property plots [i](#)

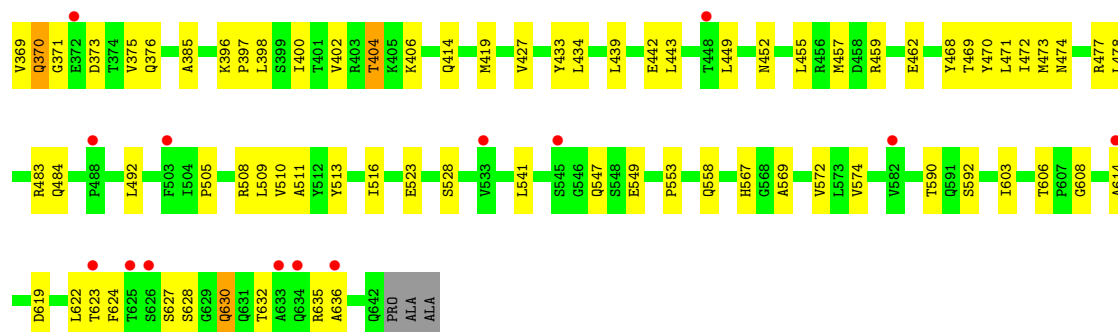
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: COMPLEMENT C3 BETA CHAIN

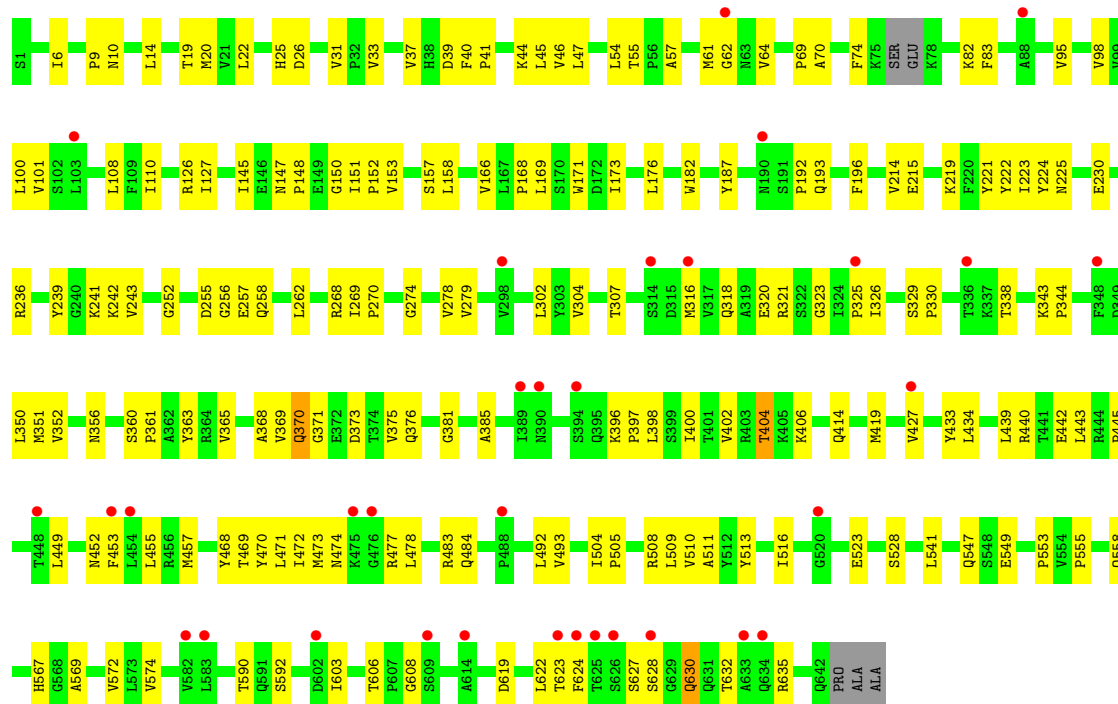


• Molecule 1: COMPLEMENT C3 BETA CHAIN

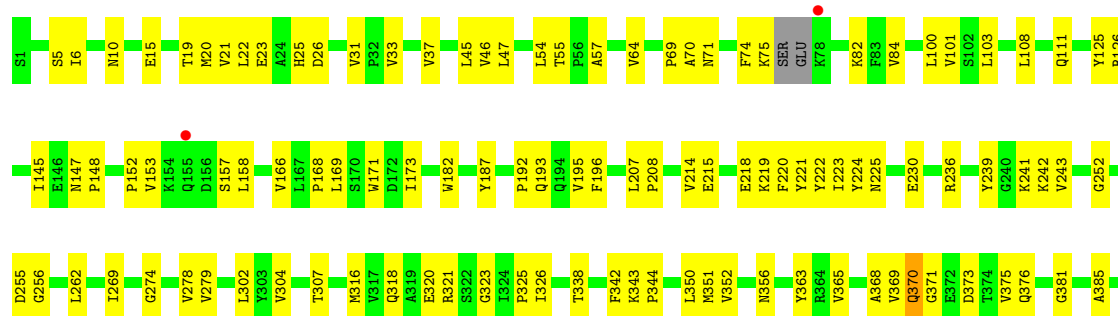


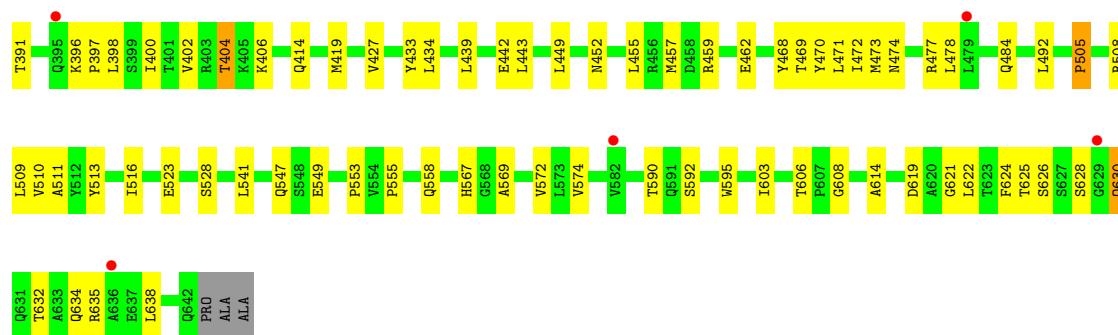


• Molecule 1: COMPLEMENT C3 BETA CHAIN

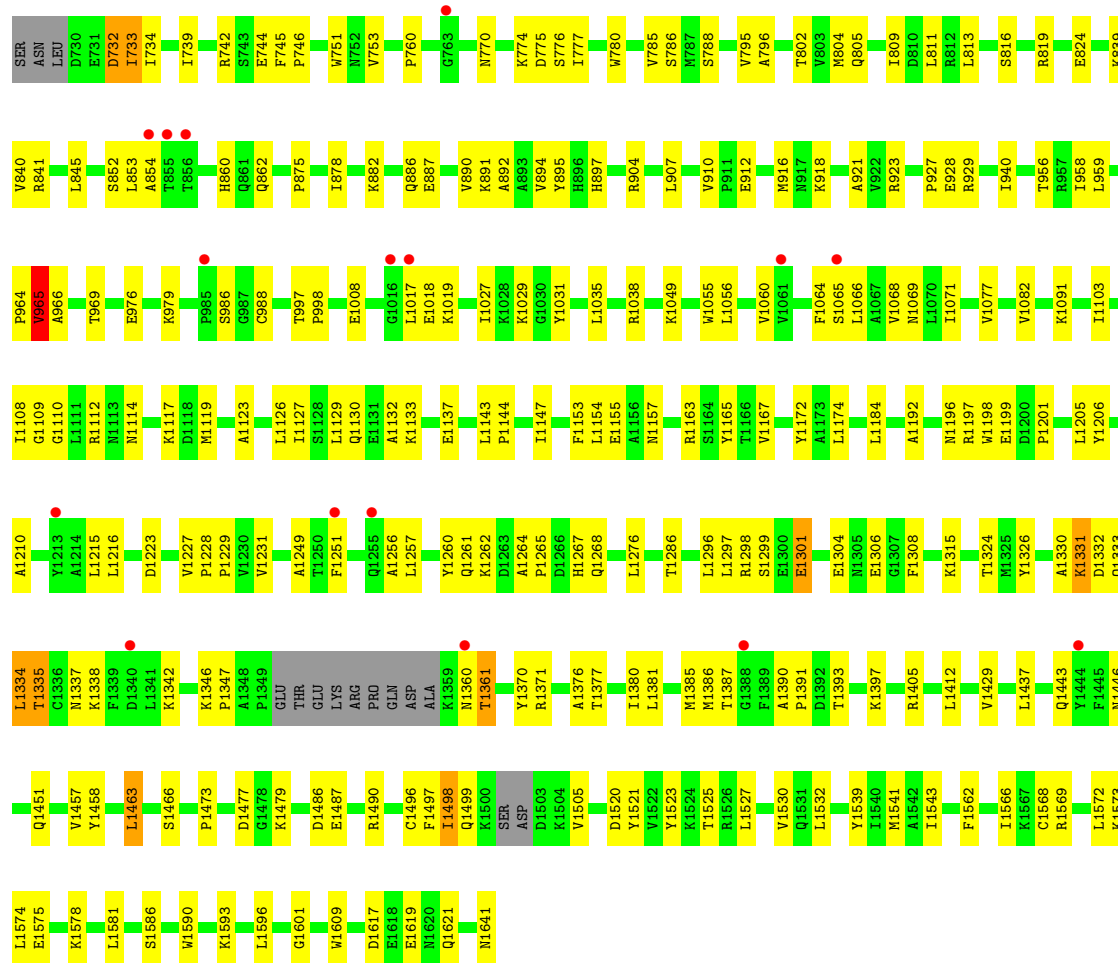


• Molecule 1: COMPLEMENT C3 BETA CHAIN

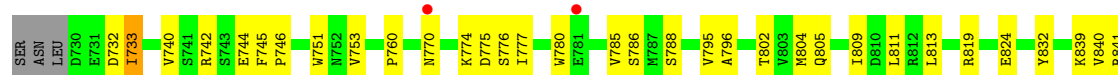


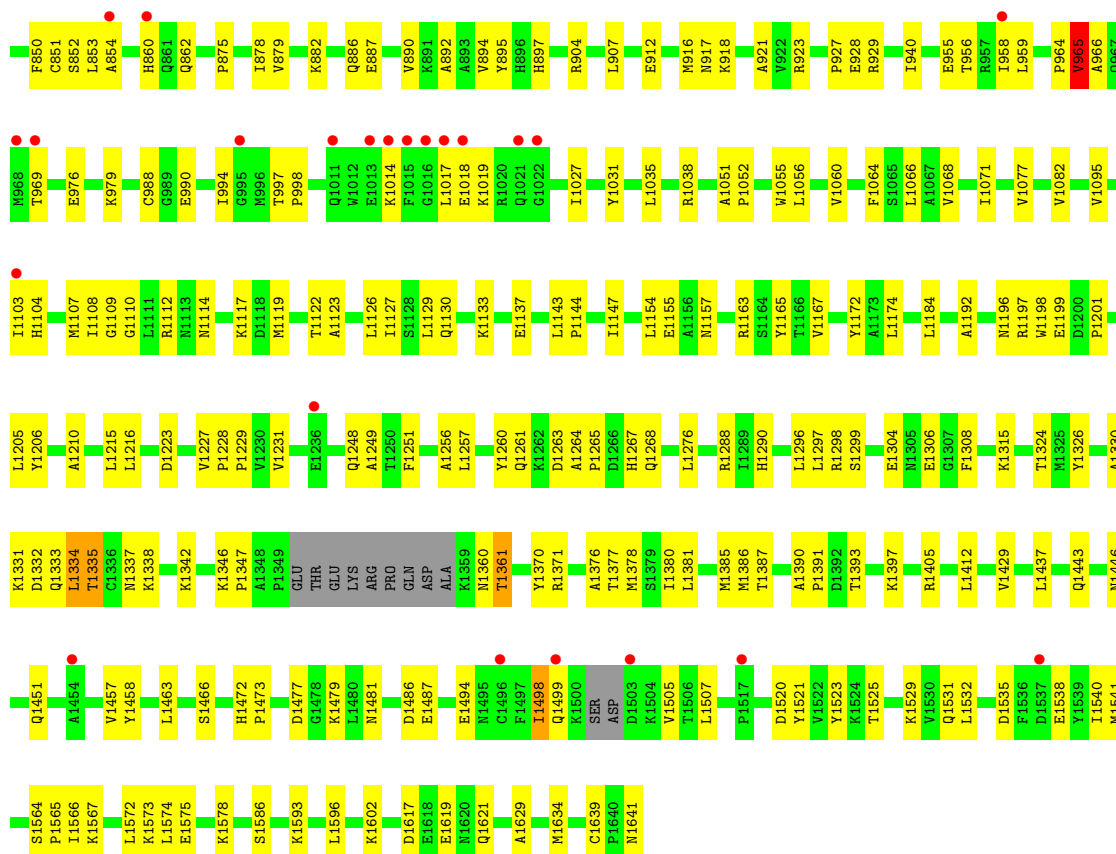


● Molecule 2: COMPLEMENT C3 ALPHA CHAIN

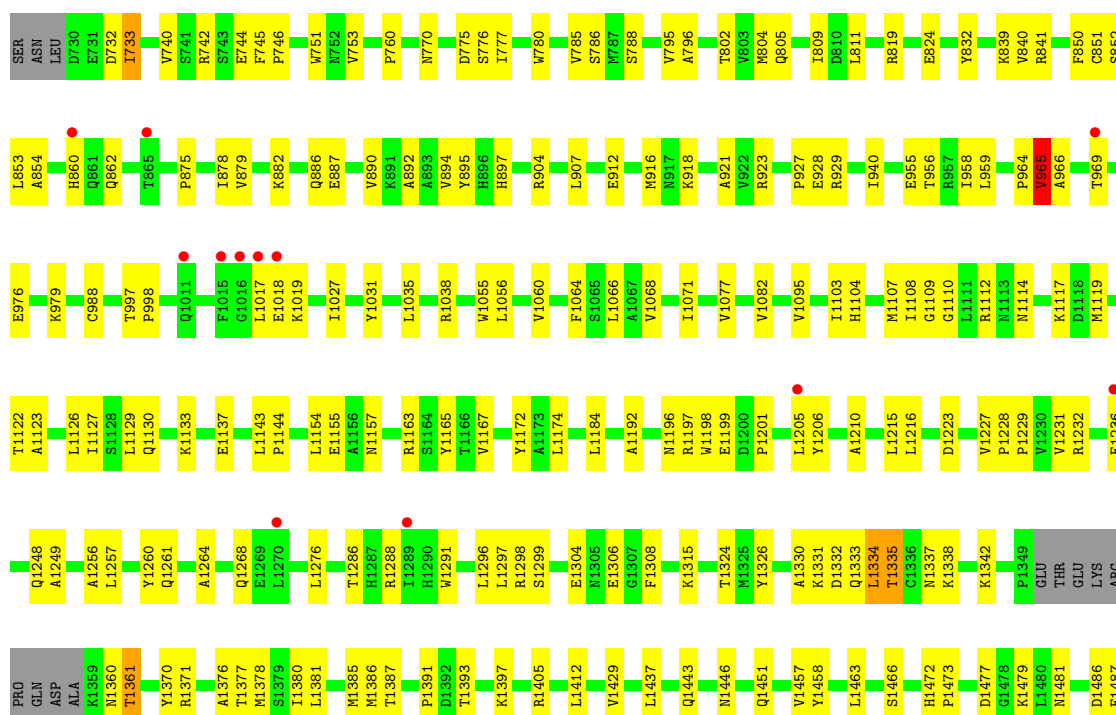


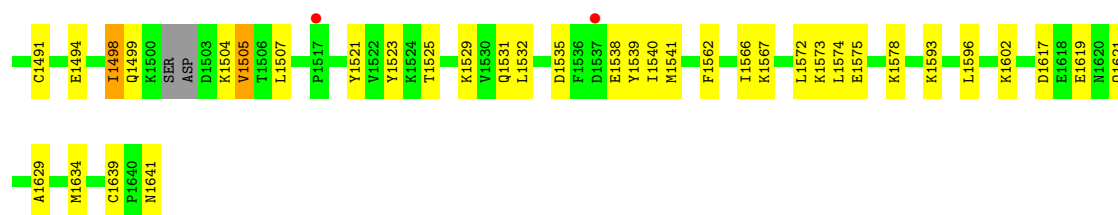
● Molecule 2: COMPLEMENT C3 ALPHA CHAIN



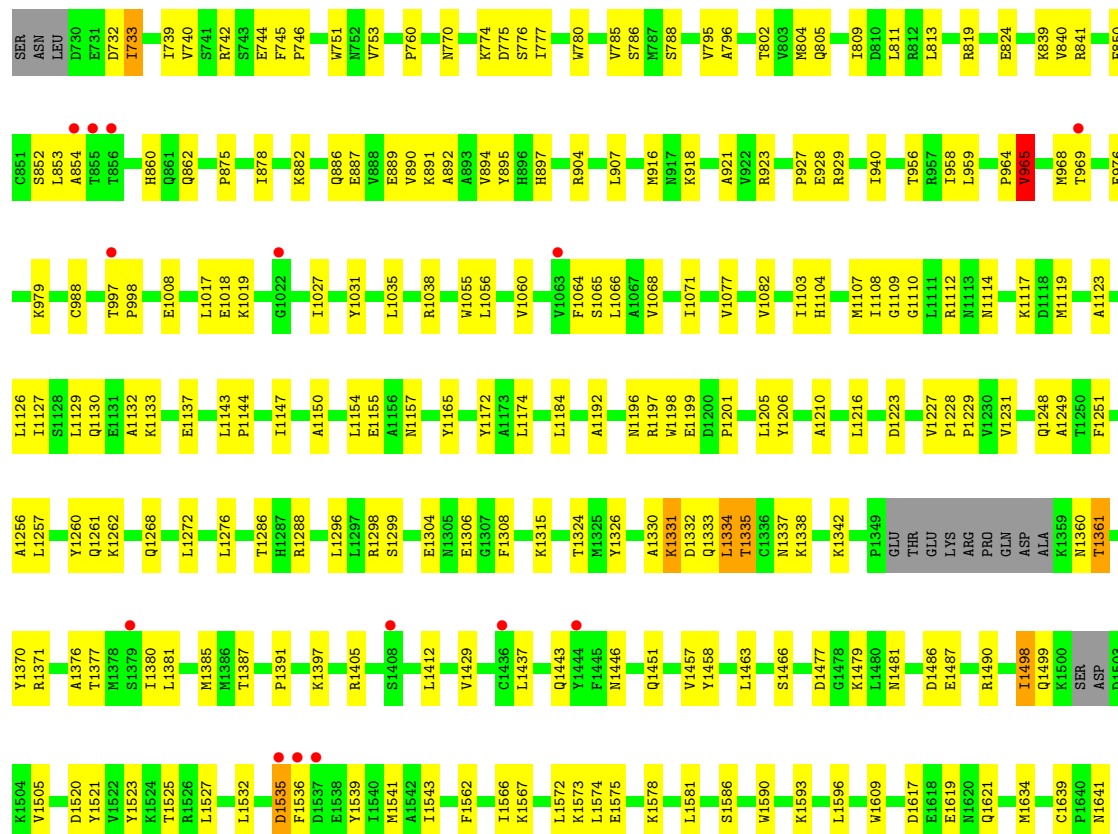


• Molecule 2: COMPLEMENT C3 ALPHA CHAIN

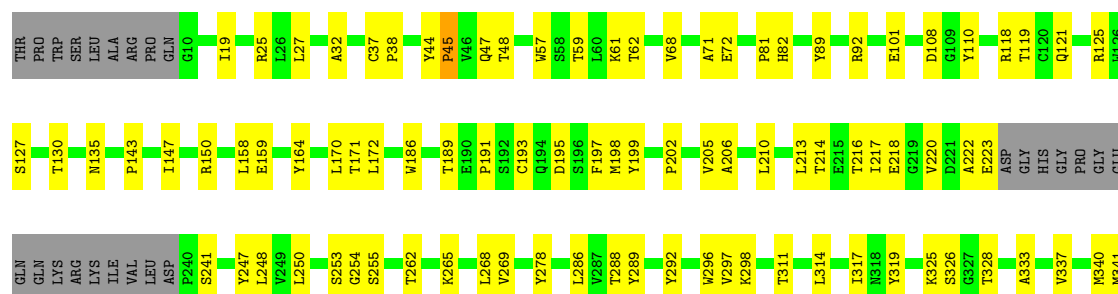




• Molecule 2: COMPLEMENT C3 ALPHA CHAIN

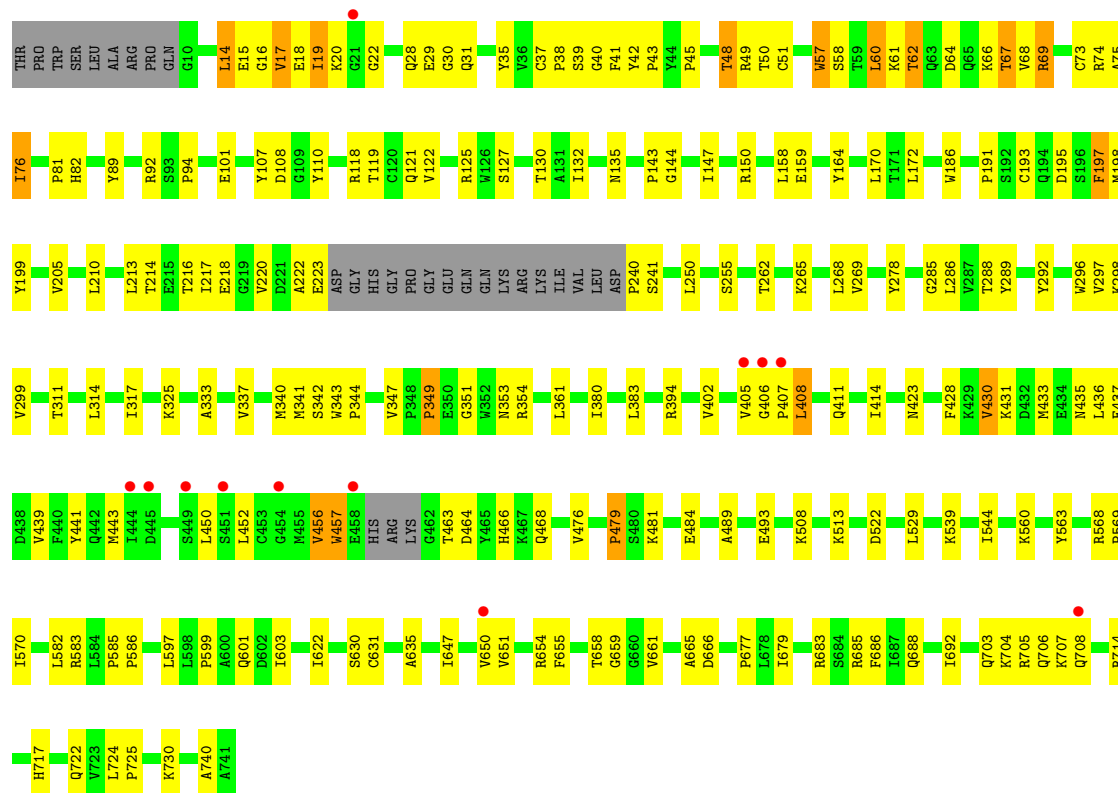


• Molecule 3: COMPLEMENT FACTOR B

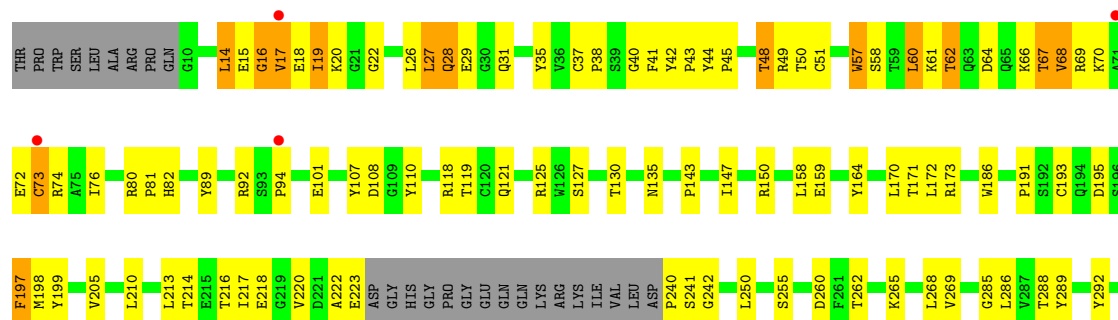


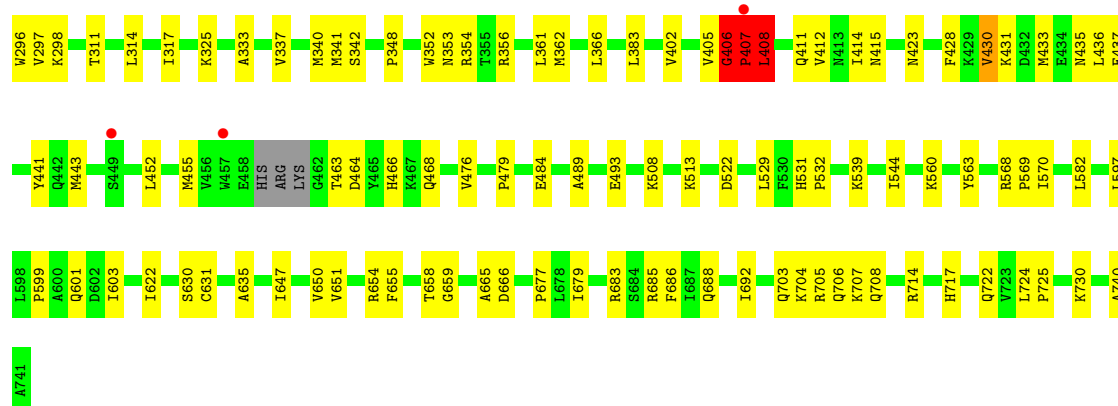


• Molecule 3: COMPLEMENT FACTOR B

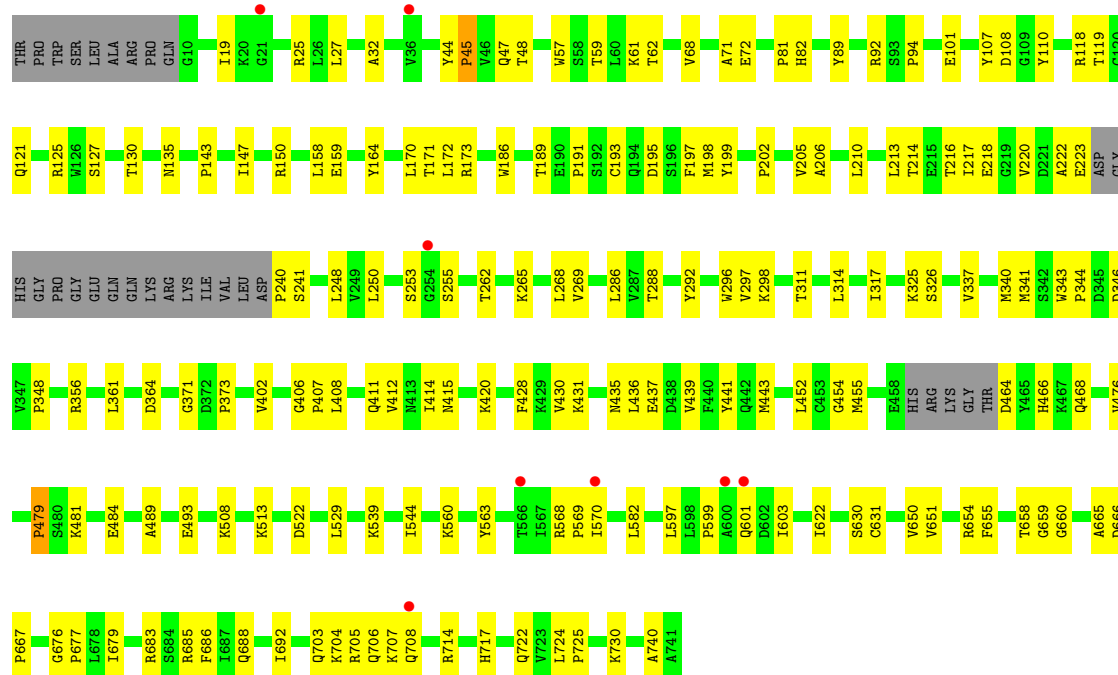
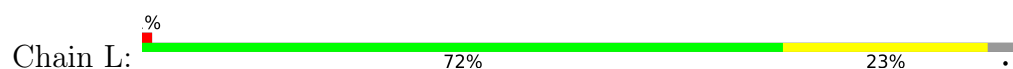


• Molecule 3: COMPLEMENT FACTOR B





• Molecule 3: COMPLEMENT FACTOR B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	262.16Å 297.87Å 341.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.76 – 4.00 72.76 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (72.76-4.00) 93.2 (72.76-4.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 4.01Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.228 , 0.281 0.229 , 0.281	Depositor DCC
R_{free} test set	5251 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtrriage
Anisotropy	0.640	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 116.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	71260	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.10 % 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 2.4810e-04. 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, 0.333 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: NI, NAG

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	0.23	0/5092	0.70	2/6917 (0.0%)
1	C	0.23	0/5092	0.68	0/6917
1	E	0.23	0/5092	0.68	0/6917
1	G	0.23	0/5092	0.69	0/6917
2	B	0.24	0/7340	0.67	0/9936
2	D	0.25	0/7340	0.67	0/9936
2	F	0.24	0/7340	0.67	0/9936
2	H	0.24	0/7340	0.66	0/9936
3	I	0.24	0/5717	0.68	2/7739 (0.0%)
3	J	0.24	0/5720	0.70	1/7743 (0.0%)
3	K	0.24	0/5727	0.70	4/7752 (0.1%)
3	L	0.23	0/5712	0.68	0/7732
All	All	0.24	0/72604	0.68	9/98378 (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
3	J	0	1
3	K	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	406	GLY	CA-C-N	5.82	127.12	119.84
3	K	406	GLY	C-N-CA	5.82	127.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ILE	CA-C-N	5.68	125.67	120.21
1	A	68	ILE	C-N-CA	5.68	125.67	120.21
3	I	348	PRO	CA-C-N	5.47	125.67	120.31
3	I	348	PRO	C-N-CA	5.47	125.67	120.31
3	K	16	GLY	N-CA-C	-5.24	108.77	115.42
3	K	408	LEU	N-CA-C	-5.17	99.78	110.80
3	J	16	GLY	N-CA-C	-5.08	108.97	115.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	407	PRO	Peptide
3	K	407	PRO	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	4992	0	5056	140	0
1	C	4992	0	5056	139	0
1	E	4992	0	5056	143	0
1	G	4992	0	5056	129	0
2	B	7197	0	7124	181	0
2	D	7197	0	7124	186	0
2	F	7197	0	7123	177	0
2	H	7197	0	7123	171	0
3	I	5593	0	5438	127	0
3	J	5596	0	5437	150	0
3	K	5603	0	5450	168	0
3	L	5588	0	5436	114	0
4	B	14	0	13	0	0
4	D	14	0	13	1	0
4	F	14	0	13	0	0
4	H	14	0	13	0	0
4	I	14	0	13	0	0
4	J	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	14	0	13	6	0
4	L	14	0	13	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
All	All	71260	0	70583	1712	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1712) 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)
3:K:352:TRP:HZ2	4:K:1353:NAG:H82	1.05	1.19
2:F:964:PRO:HA	2:F:965:VAL:HB	1.28	1.15
2:D:964:PRO:HA	2:D:965:VAL:HB	1.27	1.13
2:H:964:PRO:HA	2:H:965:VAL:HB	1.26	1.13
1:G:69:PRO:HA	1:G:70:ALA:HB3	1.32	1.11
2:B:964:PRO:HA	2:B:965:VAL:HB	1.30	1.09
1:E:69:PRO:HA	1:E:70:ALA:HB3	1.34	1.09
1:C:69:PRO:HA	1:C:70:ALA:HB3	1.34	1.06
2:B:1029:LYS:HE3	1:E:258:GLN:HB2	1.43	1.00
3:J:29:GLU:H	3:J:30:GLY:HA2	1.24	1.00
3:K:352:TRP:CZ2	4:K:1353:NAG:H82	1.96	0.99
2:H:819:ARG:HH12	2:H:1487:GLU:HB3	1.27	0.97
1:C:628:SER:HB2	1:C:630:GLN:HE22	1.32	0.94
1:A:628:SER:HB2	1:A:630:GLN:HE22	1.34	0.92
1:E:628:SER:HB2	1:E:630:GLN:HE22	1.33	0.91
1:G:628:SER:HB2	1:G:630:GLN:HE22	1.33	0.91
2:H:964:PRO:HA	2:H:965:VAL:CB	2.03	0.88
3:J:60:LEU:H	3:J:60:LEU:HD23	1.35	0.88
3:K:60:LEU:HD23	3:K:60:LEU:H	1.38	0.88
2:D:964:PRO:HA	2:D:965:VAL:CB	2.03	0.87
2:F:964:PRO:HA	2:F:965:VAL:CB	2.04	0.87
3:K:405:VAL:HG21	3:K:436:LEU:HD22	1.53	0.87
2:D:1017:LEU:HD12	2:D:1018:GLU:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LYS:HD2	1:G:103:LEU:HD11	1.55	0.87
2:B:1049:LYS:HD2	1:E:150:GLY:HA3	1.53	0.87
3:J:405:VAL:HG21	3:J:436:LEU:HD22	1.55	0.87
2:B:733:ILE:HD11	2:B:841:ARG:HH21	1.39	0.85
3:I:345:ASP:HA	3:I:346:ASP:C	2.00	0.85
2:B:819:ARG:HH12	2:B:1487:GLU:HB3	1.40	0.84
1:G:100:LEU:HD21	1:G:638:LEU:HD23	1.59	0.84
2:H:733:ILE:HD11	2:H:841:ARG:HH21	1.41	0.84
2:B:964:PRO:HA	2:B:965:VAL:CB	2.05	0.83
2:H:964:PRO:CA	2:H:965:VAL:HB	2.08	0.83
3:K:45:PRO:HG2	3:K:68:VAL:HG21	1.60	0.82
3:K:49:ARG:HH21	3:K:60:LEU:HB3	1.44	0.82
3:J:49:ARG:HH21	3:J:60:LEU:HB3	1.45	0.81
2:D:964:PRO:CA	2:D:965:VAL:HB	2.09	0.81
1:C:268:ARG:HB2	2:D:1378:MET:HE1	1.61	0.81
2:B:1091:LYS:HZ2	2:F:1232:ARG:HH22	1.29	0.81
2:D:733:ILE:HD11	2:D:841:ARG:HH21	1.44	0.80
2:F:733:ILE:HG22	2:F:895:TYR:HA	1.62	0.80
2:F:1017:LEU:HD12	2:F:1018:GLU:H	1.44	0.80
3:I:222:ALA:HA	3:I:223:GLU:C	2.08	0.79
2:B:964:PRO:CA	2:B:965:VAL:HB	2.11	0.78
2:D:965:VAL:HG13	2:D:1268:GLN:HG2	1.65	0.78
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.46	0.78
2:B:965:VAL:HG13	2:B:1268:GLN:HG2	1.65	0.78
3:K:489:ALA:HB2	3:K:677:PRO:HG3	1.66	0.78
2:H:965:VAL:HG13	2:H:1268:GLN:HG2	1.64	0.78
3:L:489:ALA:HB2	3:L:677:PRO:HG3	1.65	0.78
2:F:964:PRO:CA	2:F:965:VAL:HB	2.10	0.78
2:H:1387:THR:HG22	2:H:1451:GLN:H	1.47	0.78
2:F:965:VAL:HG13	2:F:1268:GLN:HG2	1.64	0.77
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.47	0.77
2:F:1387:THR:HG22	2:F:1451:GLN:H	1.47	0.77
3:I:489:ALA:HB2	3:I:677:PRO:HG3	1.65	0.77
1:E:69:PRO:HA	1:E:70:ALA:CB	2.15	0.76
3:J:489:ALA:HB2	3:J:677:PRO:HG3	1.66	0.76
3:J:222:ALA:HA	3:J:223:GLU:C	2.11	0.76
3:L:222:ALA:HA	3:L:223:GLU:C	2.11	0.76
3:K:262:THR:HA	3:K:265:LYS:HE2	1.68	0.75
1:A:10:ASN:HB2	1:A:635:ARG:HH11	1.48	0.75
2:H:733:ILE:HG22	2:H:895:TYR:HA	1.67	0.75
3:K:222:ALA:HA	3:K:223:GLU:C	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1091:LYS:NZ	2:F:1232:ARG:HH22	1.86	0.74
3:K:19:ILE:HD11	3:K:73:CYS:HB2	1.68	0.74
1:E:268:ARG:HB2	2:F:1378:MET:HE1	1.68	0.74
2:F:733:ILE:HD11	2:F:841:ARG:HH21	1.51	0.74
2:H:819:ARG:NH1	2:H:1487:GLU:HB3	2.02	0.74
2:B:1532:LEU:HD23	2:B:1532:LEU:H	1.51	0.74
3:I:262:THR:HA	3:I:265:LYS:HE2	1.70	0.74
3:L:262:THR:HA	3:L:265:LYS:HE2	1.69	0.74
2:D:733:ILE:HG22	2:D:895:TYR:HA	1.69	0.74
3:I:343:TRP:HB2	3:I:347:VAL:HG12	1.68	0.74
2:B:1049:LYS:CD	1:E:150:GLY:HA3	2.19	0.73
3:J:539:LYS:HB3	3:J:544:ILE:HB	1.71	0.73
1:C:61:MET:SD	1:C:483:ARG:HG2	2.29	0.73
3:J:262:THR:HA	3:J:265:LYS:HE2	1.69	0.72
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.70	0.72
3:J:29:GLU:N	3:J:30:GLY:HA2	1.99	0.72
3:I:430:VAL:HG21	3:I:436:LEU:HB2	1.72	0.72
3:I:539:LYS:HB3	3:I:544:ILE:HB	1.71	0.72
3:K:539:LYS:HB3	3:K:544:ILE:HB	1.71	0.72
3:L:539:LYS:HB3	3:L:544:ILE:HB	1.70	0.72
1:A:71:ASN:HD22	1:A:74:PHE:HE1	1.38	0.72
1:C:19:THR:HB	1:C:478:LEU:HB2	1.70	0.72
2:D:1641:ASN:HB3	3:J:255:SER:HB3	1.72	0.72
1:G:558:GLN:HB3	2:H:770:ASN:HD21	1.55	0.72
1:C:40:PHE:CD1	1:C:41:PRO:HA	2.24	0.71
1:C:558:GLN:HB3	2:D:770:ASN:HD21	1.55	0.71
3:L:430:VAL:HG21	3:L:436:LEU:HB2	1.72	0.71
3:K:195:ASP:HB2	3:K:198:MET:HE3	1.73	0.71
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	1.73	0.71
1:C:69:PRO:HA	1:C:70:ALA:CB	2.15	0.71
1:E:40:PHE:CD1	1:E:41:PRO:HA	2.25	0.71
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.55	0.70
1:E:558:GLN:HB3	2:F:770:ASN:HD21	1.55	0.70
1:G:634:GLN:CD	2:H:1017:LEU:HD23	2.17	0.70
3:K:40:GLY:HA2	3:K:76:ILE:HD12	1.71	0.70
1:C:153:VAL:HG12	2:D:1297:LEU:HD12	1.74	0.70
3:I:195:ASP:HB2	3:I:198:MET:HE3	1.74	0.70
1:A:634:GLN:OE1	2:B:1017:LEU:HD11	1.91	0.70
2:B:733:ILE:HG22	2:B:895:TYR:HA	1.73	0.70
2:H:1017:LEU:HD12	2:H:1018:GLU:H	1.55	0.69
3:L:195:ASP:HB2	3:L:198:MET:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:452:ASN:HB3	1:G:492:LEU:HD11	1.74	0.69
1:E:452:ASN:HB3	1:E:492:LEU:HD11	1.74	0.69
3:K:48:THR:HB	3:K:408:LEU:HD21	1.73	0.69
3:K:366:LEU:HD11	3:K:408:LEU:HB3	1.75	0.69
1:A:5:SER:HA	1:A:626:SER:HA	1.74	0.69
1:C:452:ASN:HB3	1:C:492:LEU:HD11	1.74	0.69
1:A:70:ALA:N	1:A:71:ASN:HB2	2.06	0.69
3:J:29:GLU:H	3:J:30:GLY:CA	2.01	0.69
3:K:44:TYR:CD2	3:K:72:GLU:HB2	2.28	0.69
1:A:10:ASN:CB	1:A:635:ARG:HH11	2.05	0.69
1:A:392:HIS:HE1	1:C:275:SER:OG	1.76	0.69
3:K:222:ALA:N	3:K:223:GLU:HB2	2.07	0.68
3:K:61:LYS:HG2	3:K:67:THR:HA	1.75	0.68
2:B:742:ARG:HH12	2:B:777:ILE:HG13	1.58	0.68
1:E:158:LEU:HD21	1:E:169:LEU:HD21	1.74	0.68
1:A:158:LEU:HD21	1:A:169:LEU:HD21	1.75	0.68
1:C:158:LEU:HD21	1:C:169:LEU:HD21	1.74	0.68
2:D:840:VAL:HG22	2:D:894:VAL:HG12	1.74	0.68
1:G:158:LEU:HD21	1:G:169:LEU:HD21	1.74	0.68
3:J:17:VAL:HB	3:J:18:GLU:OE1	1.92	0.68
3:K:50:THR:O	3:K:57:TRP:HB2	1.94	0.68
1:A:452:ASN:HB3	1:A:492:LEU:HD11	1.75	0.68
2:B:1017:LEU:HD12	2:B:1018:GLU:H	1.58	0.68
1:G:69:PRO:HA	1:G:70:ALA:CB	2.13	0.68
2:F:1331:LYS:HA	2:F:1332:ASP:HB2	1.76	0.68
3:J:195:ASP:HB2	3:J:198:MET:HE3	1.74	0.68
1:E:168:PRO:HB3	3:K:108:ASP:HB3	1.76	0.68
2:H:1082:VAL:HG13	2:H:1129:LEU:HD22	1.75	0.68
2:B:840:VAL:HG22	2:B:894:VAL:HG12	1.76	0.67
2:F:840:VAL:HG22	2:F:894:VAL:HG12	1.75	0.67
2:D:785:VAL:HG22	2:D:795:VAL:HG12	1.77	0.67
3:J:61:LYS:HG2	3:J:67:THR:HA	1.77	0.67
3:J:430:VAL:HG11	3:J:436:LEU:HD13	1.77	0.67
2:H:840:VAL:HG22	2:H:894:VAL:HG12	1.76	0.67
2:B:785:VAL:HG22	2:B:795:VAL:HG12	1.77	0.67
3:J:222:ALA:N	3:J:223:GLU:HB2	2.10	0.67
3:K:67:THR:HB	3:K:69:ARG:CZ	2.24	0.67
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.77	0.66
1:C:95:VAL:HG22	1:C:627:SER:HB3	1.77	0.66
3:J:50:THR:O	3:J:57:TRP:HB2	1.96	0.66
2:B:916:MET:HA	2:B:916:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:785:VAL:HG22	2:F:795:VAL:HG12	1.76	0.66
3:J:437:GLU:HB3	3:J:441:TYR:HE2	1.61	0.66
3:K:430:VAL:HG11	3:K:436:LEU:HD13	1.77	0.66
1:G:157:SER:HB3	3:L:630:SER:OG	1.95	0.66
1:A:606:THR:HB	1:A:619:ASP:HB3	1.79	0.65
3:K:45:PRO:CG	3:K:68:VAL:HG21	2.27	0.65
3:K:61:LYS:HA	3:K:68:VAL:H	1.61	0.65
3:K:66:LYS:HD3	3:K:69:ARG:HH12	1.61	0.65
3:L:222:ALA:N	3:L:223:GLU:HB2	2.10	0.65
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.15	0.65
3:I:481:LYS:HD2	3:I:483:HIS:HD2	1.61	0.65
2:H:785:VAL:HG22	2:H:795:VAL:HG12	1.78	0.65
2:B:1566:ILE:H	2:B:1566:ILE:HD12	1.61	0.65
1:C:45:LEU:HB2	1:C:46:VAL:HB	1.78	0.65
2:H:860:HIS:CE1	2:H:862:GLN:HE22	2.15	0.65
1:G:6:ILE:HD13	1:G:22:LEU:HD23	1.78	0.65
1:G:606:THR:HG22	1:G:608:GLY:H	1.62	0.65
3:J:508:LYS:HE2	3:J:508:LYS:HA	1.79	0.65
2:D:1276:LEU:HD23	2:D:1276:LEU:H	1.62	0.64
3:I:298:LYS:HA	3:I:340:MET:HE3	1.79	0.64
1:A:14:LEU:HD11	1:A:103:LEU:HD13	1.79	0.64
1:A:606:THR:HG22	1:A:608:GLY:H	1.63	0.64
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.16	0.64
1:E:55:THR:HG22	1:E:57:ALA:H	1.63	0.64
1:A:351:MET:HE2	1:A:351:MET:HA	1.80	0.64
1:A:455:LEU:HD11	1:A:457:MET:HE3	1.80	0.64
1:C:268:ARG:HH11	2:D:1378:MET:HE3	1.62	0.64
3:L:508:LYS:HE2	3:L:508:LYS:HA	1.80	0.64
1:E:45:LEU:HB2	1:E:46:VAL:HB	1.78	0.64
1:E:455:LEU:HD11	1:E:457:MET:HE3	1.80	0.64
2:F:860:HIS:CE1	2:F:862:GLN:HE22	2.16	0.64
1:G:55:THR:HG22	1:G:57:ALA:H	1.62	0.64
3:I:481:LYS:HD2	3:I:483:HIS:CD2	2.31	0.64
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.80	0.64
1:E:606:THR:HB	1:E:619:ASP:HB3	1.79	0.64
3:J:343:TRP:CD1	3:J:347:VAL:H	2.15	0.64
1:A:55:THR:HG22	1:A:57:ALA:H	1.63	0.64
2:B:1049:LYS:HD2	1:E:150:GLY:CA	2.24	0.64
1:G:606:THR:HB	1:G:619:ASP:HB3	1.79	0.64
1:G:634:GLN:OE1	2:H:1017:LEU:HB3	1.98	0.64
1:C:55:THR:HG22	1:C:57:ALA:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:THR:HG22	1:C:608:GLY:H	1.63	0.63
1:G:6:ILE:HG22	1:G:625:THR:O	1.98	0.63
3:J:40:GLY:HA2	3:J:76:ILE:HD12	1.79	0.63
3:K:437:GLU:HB3	3:K:441:TYR:HE2	1.62	0.63
1:C:45:LEU:HD23	1:C:45:LEU:H	1.64	0.63
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.80	0.63
1:E:350:LEU:HD21	1:E:400:ILE:HG21	1.80	0.63
2:F:1288:ARG:NH1	3:K:665:ALA:HB1	2.12	0.63
3:I:508:LYS:HE2	3:I:508:LYS:HA	1.79	0.63
1:E:351:MET:HE2	1:E:351:MET:HA	1.80	0.63
1:E:606:THR:HG22	1:E:608:GLY:H	1.62	0.63
2:B:1276:LEU:HD23	2:B:1276:LEU:H	1.63	0.63
1:C:455:LEU:HD11	1:C:457:MET:HE3	1.81	0.63
1:C:606:THR:HB	1:C:619:ASP:HB3	1.79	0.63
1:E:45:LEU:HD23	1:E:45:LEU:H	1.64	0.63
2:F:1276:LEU:HD23	2:F:1276:LEU:H	1.62	0.63
3:K:508:LYS:HE2	3:K:508:LYS:HA	1.79	0.63
1:G:350:LEU:HD21	1:G:400:ILE:HG21	1.79	0.63
2:B:1029:LYS:HE3	1:E:258:GLN:CB	2.23	0.63
2:H:1276:LEU:HD23	2:H:1276:LEU:H	1.63	0.63
3:K:298:LYS:HA	3:K:340:MET:HE3	1.80	0.63
2:F:1566:ILE:H	2:F:1566:ILE:HD12	1.64	0.63
2:B:1641:ASN:HB3	3:I:255:SER:HB3	1.81	0.63
2:F:1126:LEU:HG	2:F:1130:GLN:HE21	1.64	0.63
2:D:1566:ILE:HD12	2:D:1566:ILE:H	1.64	0.63
1:E:268:ARG:HH11	2:F:1378:MET:HE3	1.64	0.63
3:J:347:VAL:O	3:J:349:PRO:HD3	1.99	0.63
3:K:476:VAL:HB	3:K:484:GLU:HB3	1.81	0.63
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.80	0.62
1:A:478:LEU:HD21	1:A:622:LEU:HD21	1.79	0.62
2:F:1641:ASN:HB3	3:K:255:SER:HB3	1.81	0.62
2:F:819:ARG:HH12	2:F:1487:GLU:HB3	1.65	0.62
1:C:590:THR:HG22	1:C:592:SER:H	1.64	0.62
2:F:1333:GLN:HA	2:F:1334:LEU:HB3	1.82	0.62
1:G:351:MET:HE2	1:G:351:MET:HA	1.80	0.62
2:H:1481:ASN:HD22	2:H:1567:LYS:HE3	1.65	0.62
3:K:44:TYR:HD2	3:K:72:GLU:HB2	1.62	0.62
1:G:45:LEU:HD23	1:G:45:LEU:H	1.65	0.62
1:G:455:LEU:HD11	1:G:457:MET:HE3	1.80	0.62
2:H:1566:ILE:H	2:H:1566:ILE:HD12	1.65	0.62
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:751:TRP:HB3	3:K:107:TYR:CD1	2.35	0.62
1:G:45:LEU:HB2	1:G:46:VAL:HB	1.81	0.62
2:B:1532:LEU:HD12	2:B:1569:ARG:HH11	1.65	0.62
2:H:1126:LEU:HG	2:H:1130:GLN:HE21	1.65	0.62
2:B:1109:GLY:HA2	2:B:1205:LEU:HD21	1.82	0.62
2:B:1286:THR:HG22	3:I:665:ALA:HB3	1.82	0.62
1:G:590:THR:HG22	1:G:592:SER:H	1.65	0.62
2:D:1109:GLY:HA2	2:D:1205:LEU:HD21	1.82	0.61
1:E:478:LEU:HD21	1:E:622:LEU:HD21	1.81	0.61
2:F:916:MET:HE2	2:F:916:MET:HA	1.81	0.61
3:L:455:MET:HB2	3:L:568:ARG:HD3	1.81	0.61
1:A:74:PHE:C	1:A:82:LYS:HZ3	2.08	0.61
2:D:916:MET:HE2	2:D:916:MET:HA	1.80	0.61
3:K:48:THR:CB	3:K:408:LEU:HD21	2.29	0.61
2:H:1333:GLN:HA	2:H:1334:LEU:HB3	1.83	0.61
1:A:45:LEU:HD23	1:A:45:LEU:H	1.65	0.61
1:A:590:THR:HG22	1:A:592:SER:H	1.65	0.61
1:A:242:LYS:HB3	1:A:274:GLY:HA3	1.83	0.61
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.82	0.61
1:G:478:LEU:HD21	1:G:622:LEU:HD21	1.81	0.61
1:A:45:LEU:HB2	1:A:46:VAL:HB	1.81	0.61
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.65	0.61
1:E:590:THR:HG22	1:E:592:SER:H	1.64	0.61
3:K:352:TRP:HZ2	4:K:1353:NAG:C8	1.97	0.61
2:D:1333:GLN:HA	2:D:1334:LEU:HB3	1.82	0.61
1:E:61:MET:SD	1:E:483:ARG:HG2	2.40	0.61
1:G:242:LYS:HB3	1:G:274:GLY:HA3	1.83	0.61
3:J:45:PRO:HG2	3:J:68:VAL:HG21	1.83	0.61
3:K:35:TYR:HB2	3:K:43:PRO:HB3	1.83	0.61
3:K:44:TYR:HB3	3:K:73:CYS:HA	1.83	0.61
1:C:351:MET:HE2	1:C:351:MET:HA	1.80	0.61
2:D:742:ARG:HH12	2:D:777:ILE:HG13	1.66	0.61
3:L:298:LYS:HA	3:L:340:MET:HE3	1.83	0.60
1:E:242:LYS:HB3	1:E:274:GLY:HA3	1.83	0.60
3:K:27:LEU:O	3:K:28:GLN:HG2	2.01	0.60
1:C:242:LYS:HB3	1:C:274:GLY:HA3	1.81	0.60
2:F:1494:GLU:HB2	2:F:1602:LYS:HD3	1.83	0.60
2:F:1333:GLN:HA	2:F:1334:LEU:CB	2.31	0.60
2:H:921:ALA:HB1	2:H:923:ARG:HE	1.66	0.60
3:J:48:THR:HG21	3:J:408:LEU:HD11	1.84	0.60
3:J:298:LYS:HA	3:J:340:MET:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.83	0.60
2:D:921:ALA:HB1	2:D:923:ARG:HE	1.67	0.60
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.83	0.60
1:G:71:ASN:HD22	1:G:74:PHE:HE1	1.50	0.60
3:I:476:VAL:HB	3:I:484:GLU:HB3	1.84	0.60
3:J:14:LEU:HG	3:J:17:VAL:HG12	1.84	0.60
2:B:921:ALA:HB1	2:B:923:ARG:HE	1.67	0.60
1:C:307:THR:HG21	1:C:316:MET:HE3	1.83	0.60
2:H:1109:GLY:HA2	2:H:1205:LEU:HD21	1.83	0.60
2:H:1641:ASN:HB3	3:L:255:SER:HB3	1.83	0.60
2:F:1338:LYS:HA	2:F:1371:ARG:HB2	1.84	0.60
1:E:74:PHE:C	1:E:82:LYS:HZ3	2.10	0.60
2:F:921:ALA:HB1	2:F:923:ARG:HE	1.67	0.60
2:F:1109:GLY:HA2	2:F:1205:LEU:HD21	1.83	0.60
3:J:62:THR:HG23	3:J:68:VAL:HG21	1.84	0.60
1:A:126:ARG:HG2	1:A:168:PRO:HA	1.84	0.59
2:D:1333:GLN:HA	2:D:1334:LEU:CB	2.31	0.59
1:G:307:THR:HG21	1:G:316:MET:HE3	1.84	0.59
3:K:17:VAL:HB	3:K:18:GLU:OE1	2.03	0.59
2:H:1338:LYS:HA	2:H:1371:ARG:HB2	1.83	0.59
1:A:307:THR:HG21	1:A:316:MET:HE3	1.84	0.59
1:A:400:ILE:HD13	1:A:419:MET:HE3	1.84	0.59
1:E:473:MET:HB2	1:E:508:ARG:HB2	1.85	0.59
1:A:42:GLY:HA2	2:B:1069:ASN:HB3	1.84	0.59
2:B:1333:GLN:HA	2:B:1334:LEU:CB	2.32	0.59
1:G:400:ILE:HD13	1:G:419:MET:HE3	1.85	0.59
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.85	0.59
2:B:1333:GLN:HA	2:B:1334:LEU:HB3	1.83	0.59
2:H:1331:LYS:HA	2:H:1332:ASP:C	2.26	0.59
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.84	0.59
2:H:916:MET:HE2	2:H:916:MET:HA	1.84	0.59
3:K:48:THR:HG21	3:K:408:LEU:HD11	1.84	0.59
3:K:66:LYS:O	3:K:67:THR:C	2.45	0.59
1:E:269:ILE:HD13	1:E:278:VAL:HB	1.84	0.59
3:J:61:LYS:HA	3:J:68:VAL:H	1.67	0.59
3:K:14:LEU:HG	3:K:17:VAL:HG12	1.84	0.59
2:B:1385:MET:HE2	2:B:1385:MET:HA	1.84	0.59
3:I:222:ALA:N	3:I:223:GLU:HB2	2.18	0.59
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.85	0.59
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.85	0.59
2:D:1525:THR:HB	2:D:1541:MET:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:LEU:HD21	1:E:449:LEU:HD13	1.85	0.59
1:G:470:TYR:HB2	1:G:509:LEU:HD21	1.85	0.59
2:H:1333:GLN:HA	2:H:1334:LEU:CB	2.31	0.59
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.85	0.59
3:J:476:VAL:HB	3:J:484:GLU:HB3	1.83	0.59
3:J:603:ILE:HB	3:J:622:ILE:HB	1.83	0.59
2:B:819:ARG:NH1	2:B:1487:GLU:HB3	2.14	0.58
1:C:269:ILE:HD13	1:C:278:VAL:HB	1.84	0.58
2:D:1205:LEU:HD12	2:D:1249:ALA:HB2	1.85	0.58
1:E:572:VAL:HG12	2:F:753:VAL:HG22	1.85	0.58
1:G:473:MET:HB2	1:G:508:ARG:HB2	1.84	0.58
3:J:35:TYR:HB2	3:J:43:PRO:HB3	1.84	0.58
1:C:40:PHE:CD2	1:C:83:PHE:HB2	2.38	0.58
1:E:307:THR:HG21	1:E:316:MET:HE3	1.83	0.58
1:A:7:ILE:HA	1:A:623:THR:O	2.03	0.58
1:C:470:TYR:HB2	1:C:509:LEU:HD21	1.86	0.58
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.85	0.58
1:G:269:ILE:HD13	1:G:278:VAL:HB	1.84	0.58
3:K:405:VAL:HG11	3:K:433:MET:HE2	1.85	0.58
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.86	0.58
1:C:222:TYR:HE2	1:C:224:TYR:HB2	1.69	0.58
1:E:19:THR:HB	1:E:478:LEU:HB2	1.83	0.58
3:L:603:ILE:HB	3:L:622:ILE:HB	1.85	0.58
1:A:6:ILE:HD11	1:A:20:MET:HG2	1.86	0.58
2:D:1529:LYS:HB3	2:D:1540:ILE:HD12	1.86	0.58
1:E:470:TYR:HB2	1:E:509:LEU:HD21	1.85	0.58
2:F:1205:LEU:HD12	2:F:1249:ALA:HB2	1.85	0.58
1:E:400:ILE:HD13	1:E:419:MET:HE3	1.86	0.58
1:G:126:ARG:HG2	1:G:168:PRO:HA	1.86	0.58
1:G:222:TYR:HE2	1:G:224:TYR:HB2	1.69	0.58
1:C:9:PRO:HA	1:C:622:LEU:HD23	1.84	0.58
3:L:346:ASP:O	3:L:348:PRO:HD3	2.04	0.58
1:E:252:GLY:HA2	1:E:262:LEU:HG	1.85	0.58
3:I:603:ILE:HB	3:I:622:ILE:HB	1.86	0.58
1:C:126:ARG:HG2	1:C:168:PRO:HA	1.85	0.58
2:H:1143:LEU:HB3	2:H:1144:PRO:HD3	1.86	0.58
2:H:1385:MET:HA	2:H:1385:MET:HE2	1.85	0.58
1:A:269:ILE:HD13	1:A:278:VAL:HB	1.85	0.57
1:C:400:ILE:HD13	1:C:419:MET:HE3	1.85	0.57
2:F:1143:LEU:HB3	2:F:1144:PRO:HD3	1.85	0.57
1:G:6:ILE:HD11	1:G:20:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:TYR:HE2	1:E:224:TYR:HB2	1.69	0.57
2:F:1521:TYR:HB2	2:F:1523:TYR:CE2	2.40	0.57
1:G:396:LYS:HD2	1:G:397:PRO:HD2	1.86	0.57
2:B:1205:LEU:HD12	2:B:1249:ALA:HB2	1.85	0.57
1:E:6:ILE:HD13	1:E:22:LEU:HD23	1.87	0.57
2:H:1205:LEU:HD12	2:H:1249:ALA:HB2	1.85	0.57
1:E:40:PHE:CD2	1:E:83:PHE:HB2	2.39	0.57
1:G:252:GLY:HA2	1:G:262:LEU:HG	1.86	0.57
3:K:15:GLU:C	3:K:17:VAL:H	2.13	0.57
3:K:31:GLN:HA	3:K:51:CYS:HB3	1.87	0.57
1:A:443:LEU:HD21	1:A:449:LEU:HD13	1.86	0.57
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.40	0.57
2:D:742:ARG:NH1	2:D:777:ILE:HG13	2.19	0.57
2:D:1385:MET:HE2	2:D:1385:MET:HA	1.85	0.57
2:F:1385:MET:HE2	2:F:1385:MET:HA	1.85	0.57
1:G:572:VAL:HG12	2:H:753:VAL:HG22	1.85	0.57
2:F:851:CYS:HB2	2:F:1491:CYS:HB2	1.79	0.57
1:A:69:PRO:HB2	1:A:71:ASN:CG	2.30	0.57
1:C:443:LEU:HD21	1:C:449:LEU:HD13	1.85	0.57
1:E:222:TYR:CE2	1:E:224:TYR:HB2	2.40	0.57
3:J:19:ILE:HD11	3:J:73:CYS:HB2	1.85	0.57
3:K:603:ILE:HB	3:K:622:ILE:HB	1.85	0.57
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.86	0.57
2:D:1575:GLU:HB2	2:D:1578:LYS:HD2	1.86	0.57
1:E:541:LEU:HG	2:F:796:ALA:HB2	1.87	0.57
2:F:742:ARG:HB3	2:F:775:ASP:HB3	1.85	0.57
3:I:347:VAL:HG13	3:I:349:PRO:N	2.19	0.57
2:F:1575:GLU:HB2	2:F:1578:LYS:HD2	1.87	0.57
2:H:1286:THR:HG22	3:L:665:ALA:HB3	1.87	0.57
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.41	0.56
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.40	0.56
2:B:1463:LEU:O	2:B:1463:LEU:HD12	2.05	0.56
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.87	0.56
2:H:1027:ILE:HG22	2:H:1071:ILE:HD13	1.86	0.56
1:A:470:TYR:HB2	1:A:509:LEU:HD21	1.86	0.56
1:C:396:LYS:HD2	1:C:397:PRO:HD2	1.87	0.56
1:G:108:LEU:HB2	1:G:196:PHE:CD1	2.41	0.56
1:G:443:LEU:HD21	1:G:449:LEU:HD13	1.86	0.56
3:I:654:ARG:HG3	3:I:722:GLN:HB3	1.88	0.56
1:A:396:LYS:HD2	1:A:397:PRO:HD2	1.86	0.56
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1529:LYS:HB3	2:F:1540:ILE:HD12	1.86	0.56
1:G:222:TYR:CE2	1:G:224:TYR:HB2	2.40	0.56
3:K:19:ILE:CD1	3:K:73:CYS:HB2	2.34	0.56
1:A:222:TYR:HE2	1:A:224:TYR:HB2	1.69	0.56
2:B:1575:GLU:HB2	2:B:1578:LYS:HD2	1.86	0.56
2:F:976:GLU:HA	2:F:979:LYS:HE3	1.88	0.56
3:L:202:PRO:HG3	3:L:435:ASN:HB3	1.87	0.56
1:A:6:ILE:HD11	1:A:20:MET:CG	2.36	0.56
2:B:1049:LYS:NZ	1:E:150:GLY:HA3	2.20	0.56
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.41	0.56
3:J:654:ARG:HG3	3:J:722:GLN:HB3	1.88	0.56
1:A:10:ASN:HB2	1:A:635:ARG:NH1	2.19	0.56
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.88	0.56
1:E:171:TRP:CZ3	1:E:173:ILE:HG12	2.41	0.56
2:B:804:MET:HG2	2:B:805:GLN:N	2.20	0.56
2:D:1331:LYS:HA	2:D:1332:ASP:C	2.30	0.56
1:E:126:ARG:HG2	1:E:168:PRO:HA	1.87	0.56
2:H:976:GLU:HA	2:H:979:LYS:HE3	1.88	0.56
3:J:411:GLN:HA	3:J:414:ILE:HG12	1.87	0.56
3:K:411:GLN:HA	3:K:414:ILE:HG12	1.87	0.56
2:D:1017:LEU:HD12	2:D:1018:GLU:N	2.16	0.56
2:F:1525:THR:HB	2:F:1541:MET:HB3	1.86	0.56
2:B:1521:TYR:HB2	2:B:1523:TYR:CE2	2.41	0.56
1:C:168:PRO:HB3	3:J:108:ASP:HB3	1.87	0.56
1:E:108:LEU:HB2	1:E:196:PHE:CD1	2.41	0.56
2:F:1027:ILE:HG22	2:F:1071:ILE:HD13	1.88	0.56
3:L:218:GLU:HB3	3:L:452:LEU:HD21	1.87	0.56
3:L:654:ARG:HG3	3:L:722:GLN:HB3	1.88	0.56
2:B:1335:THR:C	2:B:1337:ASN:H	2.15	0.56
2:F:1288:ARG:HH11	3:K:665:ALA:HB1	1.70	0.56
2:B:742:ARG:NH1	2:B:777:ILE:HG13	2.20	0.55
1:E:510:VAL:HG12	1:E:528:SER:HB3	1.87	0.55
2:F:1335:THR:C	2:F:1337:ASN:H	2.14	0.55
2:F:1360:ASN:O	2:F:1361:THR:HG22	2.07	0.55
3:J:15:GLU:C	3:J:17:VAL:H	2.12	0.55
3:K:81:PRO:HG3	3:K:147:ILE:HG23	1.89	0.55
1:C:171:TRP:CZ3	1:C:173:ILE:HG12	2.41	0.55
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.88	0.55
2:D:1360:ASN:O	2:D:1361:THR:HG22	2.07	0.55
1:E:157:SER:HB3	3:K:630:SER:OG	2.06	0.55
3:K:361:LEU:HD21	3:K:402:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.88	0.55
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	1.88	0.55
2:F:1192:ALA:HB2	2:F:1198:TRP:CE2	2.41	0.55
1:G:6:ILE:HD11	1:G:20:MET:CG	2.37	0.55
1:G:510:VAL:HG12	1:G:528:SER:HB3	1.88	0.55
2:H:1575:GLU:HB2	2:H:1578:LYS:HD2	1.88	0.55
3:J:49:ARG:HH12	3:J:57:TRP:CD1	2.24	0.55
3:J:60:LEU:H	3:J:60:LEU:CD2	2.15	0.55
3:L:205:VAL:HG13	3:L:428:PHE:CD1	2.40	0.55
1:A:10:ASN:HB3	1:A:635:ARG:CD	2.37	0.55
2:B:1110:GLY:HA2	2:B:1206:TYR:CD2	2.41	0.55
1:E:396:LYS:HD2	1:E:397:PRO:HD2	1.87	0.55
1:C:40:PHE:CE1	2:D:1017:LEU:HD13	2.42	0.55
1:C:541:LEU:HG	2:D:796:ALA:HB2	1.88	0.55
1:A:6:ILE:HG22	1:A:625:THR:O	2.07	0.55
1:C:74:PHE:C	1:C:82:LYS:HZ3	2.14	0.55
2:D:976:GLU:HA	2:D:979:LYS:HE3	1.87	0.55
2:H:739:ILE:HB	2:H:891:LYS:HD3	1.89	0.55
1:A:103:LEU:HD22	1:A:103:LEU:H	1.71	0.55
1:A:541:LEU:HG	2:B:796:ALA:HB2	1.89	0.55
2:D:1335:THR:C	2:D:1337:ASN:H	2.15	0.55
2:F:1082:VAL:HG13	2:F:1129:LEU:HD22	1.87	0.55
3:I:455:MET:HB2	3:I:568:ARG:HD3	1.87	0.55
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.89	0.55
1:A:171:TRP:CZ3	1:A:173:ILE:HG12	2.42	0.55
2:B:976:GLU:HA	2:B:979:LYS:HE3	1.87	0.55
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.41	0.55
1:G:171:TRP:CZ3	1:G:173:ILE:HG12	2.42	0.55
1:G:214:VAL:HG23	1:G:321:ARG:HB2	1.88	0.55
2:D:744:GLU:C	2:D:746:PRO:HD3	2.32	0.55
2:D:1288:ARG:HH11	3:J:665:ALA:HB1	1.71	0.55
2:D:1521:TYR:HB2	2:D:1523:TYR:CE2	2.41	0.55
1:E:147:ASN:HB2	1:E:148:PRO:HD2	1.89	0.55
2:H:1360:ASN:O	2:H:1361:THR:HG22	2.07	0.55
2:F:1110:GLY:HA2	2:F:1206:TYR:CD2	2.42	0.55
2:H:1330:ALA:O	2:H:1331:LYS:C	2.50	0.55
2:H:1521:TYR:HB2	2:H:1523:TYR:CE2	2.42	0.55
2:H:1641:ASN:OXT	3:L:253:SER:HB2	2.07	0.55
3:I:631:CYS:SG	3:I:714:ARG:HD2	2.47	0.55
3:K:49:ARG:HH12	3:K:57:TRP:CD1	2.24	0.55
1:A:365:VAL:HA	1:A:406:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1027:ILE:HG22	2:D:1071:ILE:HD13	1.89	0.54
2:F:1381:LEU:HD23	2:F:1457:VAL:HG12	1.89	0.54
2:H:1192:ALA:HB2	2:H:1198:TRP:CE2	2.42	0.54
3:J:599:PRO:HB2	3:J:601:GLN:HG2	1.89	0.54
3:K:170:LEU:HD23	3:K:193:CYS:HB3	1.89	0.54
1:A:103:LEU:H	1:A:103:LEU:CD2	2.20	0.54
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.89	0.54
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.87	0.54
2:D:1331:LYS:HA	2:D:1332:ASP:HB2	1.89	0.54
3:J:66:LYS:O	3:J:67:THR:C	2.50	0.54
3:K:654:ARG:HG3	3:K:722:GLN:HB3	1.88	0.54
2:H:997:THR:N	2:H:998:PRO:HD2	2.23	0.54
3:J:62:THR:HB	3:J:64:ASP:H	1.72	0.54
3:L:81:PRO:HG3	3:L:147:ILE:HG23	1.89	0.54
1:C:69:PRO:CA	1:C:70:ALA:HB3	2.24	0.54
2:D:1381:LEU:HD23	2:D:1457:VAL:HG12	1.89	0.54
1:G:365:VAL:HA	1:G:406:LYS:HE2	1.90	0.54
3:I:81:PRO:HG3	3:I:147:ILE:HG23	1.89	0.54
2:B:744:GLU:C	2:B:746:PRO:HD3	2.33	0.54
2:D:850:PHE:HZ	2:D:907:LEU:HD21	1.73	0.54
1:E:214:VAL:HG23	1:E:321:ARG:HB2	1.89	0.54
3:I:47:GLN:HG3	3:I:48:THR:HG23	1.89	0.54
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.43	0.54
1:C:365:VAL:HA	1:C:406:LYS:HE2	1.90	0.54
2:F:732:ASP:O	2:F:733:ILE:HG12	2.07	0.54
1:G:147:ASN:HB2	1:G:148:PRO:HD2	1.89	0.54
3:K:42:TYR:CZ	3:K:74:ARG:HB2	2.43	0.54
1:G:541:LEU:HG	2:H:796:ALA:HB2	1.90	0.54
2:H:1335:THR:C	2:H:1337:ASN:H	2.14	0.54
3:J:423:ASN:HD22	3:J:683:ARG:HH12	1.55	0.54
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.89	0.54
2:B:1381:LEU:HD23	2:B:1457:VAL:HG12	1.89	0.54
2:H:1110:GLY:HA2	2:H:1206:TYR:CD2	2.42	0.54
3:K:292:TYR:HE2	3:K:325:LYS:HD3	1.73	0.54
2:F:1498:ILE:HG22	2:F:1499:GLN:HG2	1.89	0.54
3:I:202:PRO:HG3	3:I:435:ASN:HB3	1.89	0.54
3:L:286:LEU:H	3:L:297:VAL:HB	1.73	0.54
1:C:603:ILE:HB	1:C:635:ARG:HH12	1.73	0.53
2:D:1110:GLY:HA2	2:D:1206:TYR:CD2	2.43	0.53
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.09	0.53
1:E:603:ILE:HB	1:E:635:ARG:HH12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1381:LEU:HD23	2:H:1457:VAL:HG12	1.89	0.53
1:C:369:VAL:HG22	1:C:402:VAL:HG22	1.90	0.53
1:G:510:VAL:HG21	1:G:622:LEU:HD12	1.90	0.53
1:A:10:ASN:HB3	1:A:635:ARG:HD3	1.89	0.53
1:C:230:GLU:HG2	1:C:279:VAL:HG22	1.91	0.53
3:I:286:LEU:H	3:I:297:VAL:HB	1.73	0.53
3:J:437:GLU:HB3	3:J:441:TYR:CE2	2.42	0.53
2:B:997:THR:N	2:B:998:PRO:HD2	2.23	0.53
2:D:997:THR:N	2:D:998:PRO:HD2	2.23	0.53
3:I:570:ILE:HD13	3:I:688:GLN:HB2	1.90	0.53
3:I:599:PRO:HB2	3:I:601:GLN:HG2	1.89	0.53
3:K:62:THR:HB	3:K:64:ASP:H	1.73	0.53
1:G:5:SER:HA	1:G:626:SER:HA	1.90	0.53
2:H:1038:ARG:NH1	2:H:1077:VAL:HG22	2.23	0.53
3:J:170:LEU:HD23	3:J:193:CYS:HB3	1.91	0.53
3:J:361:LEU:HD21	3:J:402:VAL:HG22	1.91	0.53
3:L:47:GLN:HG3	3:L:48:THR:HG23	1.89	0.53
3:L:599:PRO:HB2	3:L:601:GLN:HG2	1.89	0.53
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.08	0.53
2:F:744:GLU:C	2:F:746:PRO:HD3	2.32	0.53
2:F:997:THR:N	2:F:998:PRO:HD2	2.23	0.53
2:F:1481:ASN:HD22	2:F:1567:LYS:HE3	1.73	0.53
3:L:407:PRO:HB2	3:L:408:LEU:HD22	1.90	0.53
2:B:966:ALA:HA	2:B:1267:HIS:HB3	1.90	0.53
2:B:1490:ARG:HD2	2:B:1590:TRP:CZ3	2.43	0.53
2:D:1288:ARG:NH1	3:J:665:ALA:HB1	2.24	0.53
3:K:437:GLU:HB3	3:K:441:TYR:CE2	2.43	0.53
2:B:1331:LYS:HA	2:B:1332:ASP:C	2.33	0.53
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.24	0.53
2:F:1385:MET:HG3	2:F:1391:PRO:HD3	1.91	0.53
1:A:230:GLU:HG2	1:A:279:VAL:HG22	1.91	0.53
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.91	0.53
1:G:84:VAL:HG13	1:G:101:VAL:HG21	1.90	0.53
1:G:230:GLU:HG2	1:G:279:VAL:HG22	1.91	0.53
1:G:472:ILE:HD13	1:G:509:LEU:HD23	1.91	0.53
2:H:744:GLU:C	2:H:746:PRO:HD3	2.33	0.53
3:J:81:PRO:HG3	3:J:147:ILE:HG23	1.90	0.53
1:E:365:VAL:HA	1:E:406:LYS:HE2	1.90	0.53
1:E:510:VAL:HG21	1:E:622:LEU:HD12	1.91	0.53
3:I:218:GLU:HB3	3:I:452:LEU:HD21	1.91	0.53
3:L:570:ILE:HD13	3:L:688:GLN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1360:ASN:O	2:B:1361:THR:HG22	2.08	0.52
2:H:804:MET:HG2	2:H:805:GLN:N	2.24	0.52
3:I:407:PRO:HB2	3:I:408:LEU:HD22	1.90	0.52
3:L:631:CYS:SG	3:L:714:ARG:HD2	2.49	0.52
3:K:430:VAL:HG21	3:K:436:LEU:HB2	1.92	0.52
2:D:1338:LYS:HD2	2:D:1338:LYS:N	2.25	0.52
2:F:1038:ARG:NH1	2:F:1077:VAL:HG22	2.23	0.52
3:K:631:CYS:SG	3:K:714:ARG:HD2	2.49	0.52
3:L:170:LEU:HD23	3:L:193:CYS:HB3	1.90	0.52
1:E:9:PRO:HA	1:E:622:LEU:HD23	1.92	0.52
1:E:230:GLU:HG2	1:E:279:VAL:HG22	1.91	0.52
1:E:472:ILE:HD13	1:E:509:LEU:HD23	1.92	0.52
2:F:907:LEU:HD23	2:F:907:LEU:H	1.74	0.52
2:H:1385:MET:HG3	2:H:1391:PRO:HD3	1.92	0.52
2:F:1172:TYR:CE1	2:F:1216:LEU:HB3	2.44	0.52
2:H:1387:THR:CG2	2:H:1451:GLN:H	2.21	0.52
1:A:369:VAL:HG22	1:A:402:VAL:HG22	1.91	0.52
2:D:1385:MET:HG3	2:D:1391:PRO:HD3	1.91	0.52
2:F:1123:ALA:O	2:F:1127:ILE:HG13	2.09	0.52
2:H:732:ASP:O	2:H:733:ILE:HG12	2.10	0.52
3:I:170:LEU:HD23	3:I:193:CYS:HB3	1.91	0.52
3:J:631:CYS:SG	3:J:714:ARG:HD2	2.49	0.52
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.25	0.52
2:B:1338:LYS:N	2:B:1338:LYS:HD2	2.25	0.52
3:J:37:CYS:HB3	3:J:41:PHE:HB2	1.92	0.52
3:K:570:ILE:HD13	3:K:688:GLN:HB2	1.91	0.52
1:E:223:ILE:H	1:E:223:ILE:HD12	1.75	0.52
2:F:1617:ASP:O	2:F:1621:GLN:HG3	2.09	0.52
1:G:369:VAL:HG22	1:G:402:VAL:HG22	1.91	0.52
2:H:1338:LYS:N	2:H:1338:LYS:HD2	2.25	0.52
3:L:659:GLY:HA2	3:L:666:ASP:HB2	1.92	0.52
1:A:510:VAL:HG21	1:A:622:LEU:HD12	1.92	0.52
2:B:1385:MET:HG3	2:B:1391:PRO:HD3	1.91	0.52
1:C:636:ALA:HB1	2:D:1014:LYS:HZ1	1.74	0.52
1:E:22:LEU:HD13	1:E:33:VAL:HG11	1.91	0.52
1:E:434:LEU:HB2	1:E:513:TYR:HE2	1.75	0.52
1:G:603:ILE:HB	1:G:635:ARG:HH12	1.74	0.52
3:I:205:VAL:HG13	3:I:428:PHE:CD1	2.45	0.52
3:I:268:LEU:HB2	3:I:314:LEU:HD21	1.92	0.52
3:K:67:THR:HB	3:K:69:ARG:NE	2.25	0.52
3:K:67:THR:O	3:K:69:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:599:PRO:HB2	3:K:601:GLN:HG2	1.90	0.52
1:A:223:ILE:H	1:A:223:ILE:HD12	1.76	0.51
2:B:1330:ALA:O	2:B:1331:LYS:C	2.53	0.51
2:D:1104:HIS:O	2:D:1107:MET:HG2	2.09	0.51
3:I:345:ASP:CA	3:I:346:ASP:C	2.81	0.51
3:K:268:LEU:HB2	3:K:314:LEU:HD21	1.92	0.51
1:C:22:LEU:HD13	1:C:33:VAL:HG11	1.91	0.51
2:F:1338:LYS:HD2	2:F:1338:LYS:N	2.25	0.51
3:J:570:ILE:HD13	3:J:688:GLN:HB2	1.92	0.51
3:K:220:VAL:HG22	3:K:356:ARG:HD3	1.92	0.51
2:B:1463:LEU:HD12	2:B:1463:LEU:C	2.35	0.51
1:C:370:GLN:HA	1:C:370:GLN:HE21	1.76	0.51
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.91	0.51
1:C:510:VAL:HG21	1:C:622:LEU:HD12	1.91	0.51
2:D:751:TRP:HB3	3:J:107:TYR:CD1	2.46	0.51
3:I:454:GLY:H	3:I:570:ILE:HA	1.76	0.51
3:K:60:LEU:HD23	3:K:60:LEU:N	2.16	0.51
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.45	0.51
2:H:740:VAL:HG21	3:L:94:PRO:HB3	1.91	0.51
3:J:60:LEU:HD23	3:J:60:LEU:N	2.14	0.51
2:D:1197:ARG:HE	2:D:1199:GLU:CD	2.19	0.51
2:H:889:GLU:HB2	2:H:904:ARG:HG3	1.92	0.51
2:H:1104:HIS:O	2:H:1107:MET:HG2	2.10	0.51
3:K:37:CYS:HB3	3:K:41:PHE:HB2	1.92	0.51
1:A:103:LEU:HD22	1:A:103:LEU:N	2.26	0.51
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.92	0.51
2:F:1331:LYS:HA	2:F:1332:ASP:C	2.36	0.51
3:L:213:LEU:O	3:L:217:ILE:HG13	2.11	0.51
3:L:268:LEU:HB2	3:L:314:LEU:HD21	1.92	0.51
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.75	0.51
2:B:1301:GLU:H	2:B:1301:GLU:CD	2.19	0.51
2:D:804:MET:HG2	2:D:805:GLN:N	2.25	0.51
2:H:887:GLU:OE2	2:H:904:ARG:HD2	2.11	0.51
3:J:268:LEU:HB2	3:J:314:LEU:HD21	1.92	0.51
1:C:223:ILE:HD12	1:C:223:ILE:H	1.76	0.51
2:F:1197:ARG:HE	2:F:1199:GLU:CD	2.19	0.51
1:G:69:PRO:CA	1:G:70:ALA:HB3	2.22	0.51
1:G:223:ILE:H	1:G:223:ILE:HD12	1.75	0.51
1:G:368:ALA:HB2	1:G:376:GLN:HG2	1.93	0.51
2:H:968:MET:O	2:H:969:THR:HB	2.10	0.51
2:H:1617:ASP:O	2:H:1621:GLN:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:143:PRO:HG3	3:J:186:TRP:CE2	2.45	0.51
3:J:292:TYR:HE2	3:J:325:LYS:HD3	1.75	0.51
3:J:405:VAL:HG11	3:J:433:MET:HE2	1.91	0.51
3:J:659:GLY:HA2	3:J:666:ASP:HB2	1.93	0.51
3:K:62:THR:N	3:K:68:VAL:HG23	2.26	0.51
3:L:206:ALA:HB2	3:L:439:VAL:HG13	1.93	0.51
1:E:404:THR:HG23	1:E:414:GLN:HB3	1.93	0.51
3:I:650:VAL:HG23	3:I:651:VAL:HG23	1.93	0.51
3:K:650:VAL:HG23	3:K:651:VAL:HG23	1.93	0.51
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.93	0.50
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.92	0.50
1:C:166:VAL:O	1:C:168:PRO:HD3	2.12	0.50
1:E:368:ALA:HB2	1:E:376:GLN:HG2	1.93	0.50
1:E:370:GLN:HA	1:E:370:GLN:HE21	1.76	0.50
3:I:659:GLY:HA2	3:I:666:ASP:HB2	1.92	0.50
3:K:213:LEU:O	3:K:217:ILE:HG13	2.11	0.50
3:L:143:PRO:HG3	3:L:186:TRP:CE2	2.46	0.50
1:C:221:TYR:HD2	1:C:326:ILE:HG23	1.76	0.50
2:H:1527:LEU:HD23	2:H:1575:GLU:C	2.36	0.50
3:I:345:ASP:HA	3:I:346:ASP:O	2.10	0.50
3:J:650:VAL:HG23	3:J:651:VAL:HG23	1.93	0.50
2:B:887:GLU:OE2	2:B:904:ARG:HD2	2.11	0.50
2:B:1566:ILE:HD12	2:B:1566:ILE:N	2.24	0.50
1:C:338:THR:HG21	1:C:419:MET:HE1	1.93	0.50
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.11	0.50
3:I:143:PRO:HG3	3:I:186:TRP:CE2	2.46	0.50
3:K:205:VAL:HG13	3:K:428:PHE:CD1	2.47	0.50
1:C:40:PHE:CE1	2:D:1017:LEU:CD1	2.94	0.50
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.75	0.50
1:E:221:TYR:HD2	1:E:326:ILE:HG23	1.76	0.50
1:E:338:THR:HG21	1:E:419:MET:HE1	1.93	0.50
1:E:369:VAL:HG22	1:E:402:VAL:HG22	1.92	0.50
1:G:166:VAL:O	1:G:168:PRO:HD3	2.12	0.50
3:I:213:LEU:O	3:I:217:ILE:HG13	2.11	0.50
3:L:220:VAL:HG22	3:L:356:ARG:HD3	1.93	0.50
1:A:390:ASN:ND2	1:C:273:ASP:OD2	2.45	0.50
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.47	0.50
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.93	0.50
2:D:1498:ILE:HG22	2:D:1499:GLN:HG2	1.91	0.50
1:G:434:LEU:HB2	1:G:513:TYR:HE2	1.77	0.50
2:H:1498:ILE:HG22	2:H:1499:GLN:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:654:ARG:HG3	3:J:722:GLN:CB	2.42	0.50
3:K:143:PRO:HG3	3:K:186:TRP:CE2	2.46	0.50
3:L:19:ILE:HG13	3:L:71:ALA:C	2.37	0.50
1:C:368:ALA:HB2	1:C:376:GLN:HG2	1.94	0.50
1:C:404:THR:HG23	1:C:414:GLN:HB3	1.93	0.50
3:J:213:LEU:O	3:J:217:ILE:HG13	2.12	0.50
1:A:166:VAL:O	1:A:168:PRO:HD3	2.11	0.50
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.93	0.50
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.11	0.50
2:H:1172:TYR:CE1	2:H:1216:LEU:HB3	2.46	0.50
3:J:430:VAL:HG21	3:J:436:LEU:HB2	1.92	0.50
1:C:193:GLN:CD	1:C:193:GLN:H	2.20	0.50
2:F:809:ILE:HD11	2:F:892:ALA:HB3	1.94	0.50
2:F:1387:THR:CG2	2:F:1451:GLN:H	2.22	0.50
2:H:809:ILE:HD11	2:H:892:ALA:HB3	1.94	0.50
3:K:659:GLY:HA2	3:K:666:ASP:HB2	1.93	0.50
3:L:654:ARG:HG3	3:L:722:GLN:CB	2.42	0.50
1:E:404:THR:HG23	1:E:414:GLN:HE21	1.77	0.50
2:H:742:ARG:HB3	2:H:775:ASP:HB3	1.93	0.50
2:H:1197:ARG:HE	2:H:1199:GLU:CD	2.19	0.50
3:I:458:GLU:HA	3:I:459:HIS:CB	2.42	0.50
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.93	0.49
1:C:176:LEU:HD12	2:D:955:GLU:OE2	2.12	0.49
2:F:850:PHE:HZ	2:F:907:LEU:HD21	1.77	0.49
2:H:1123:ALA:O	2:H:1127:ILE:HG13	2.11	0.49
1:G:404:THR:HG23	1:G:414:GLN:HB3	1.94	0.49
3:K:60:LEU:H	3:K:60:LEU:CD2	2.18	0.49
1:E:37:VAL:HG12	1:E:47:LEU:HD12	1.94	0.49
3:L:650:VAL:HG23	3:L:651:VAL:HG23	1.93	0.49
1:E:176:LEU:HD12	2:F:955:GLU:OE2	2.13	0.49
2:F:804:MET:HG2	2:F:805:GLN:N	2.28	0.49
1:G:20:MET:HB3	1:G:64:VAL:HG23	1.95	0.49
1:G:221:TYR:HD2	1:G:326:ILE:HG23	1.77	0.49
2:H:751:TRP:CD1	3:L:108:ASP:HB2	2.48	0.49
3:I:411:GLN:HA	3:I:414:ILE:HG12	1.94	0.49
3:L:411:GLN:HA	3:L:414:ILE:HG12	1.93	0.49
1:A:370:GLN:HE21	1:A:370:GLN:HA	1.77	0.49
2:D:850:PHE:CZ	2:D:907:LEU:HD21	2.47	0.49
1:E:541:LEU:HD22	2:F:786:SER:HB3	1.93	0.49
2:H:1228:PRO:HB2	2:H:1229:PRO:HD3	1.94	0.49
3:I:164:TYR:CG	3:I:191:PRO:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:206:ALA:HB2	3:I:439:VAL:HG13	1.94	0.49
3:I:220:VAL:HG22	3:I:356:ARG:HD3	1.93	0.49
3:I:654:ARG:HG3	3:I:722:GLN:CB	2.42	0.49
1:A:193:GLN:CD	1:A:193:GLN:H	2.20	0.49
2:B:1498:ILE:HG22	2:B:1499:GLN:HG2	1.93	0.49
1:C:404:THR:HG23	1:C:414:GLN:HE21	1.77	0.49
2:D:819:ARG:HH12	2:D:1487:GLU:HB3	1.78	0.49
1:G:338:THR:HG21	1:G:419:MET:HE1	1.95	0.49
3:K:158:LEU:HG	3:K:159:GLU:HG3	1.95	0.49
3:K:269:VAL:HG13	3:K:311:THR:HG23	1.94	0.49
1:A:338:THR:HG21	1:A:419:MET:HE1	1.95	0.49
1:A:368:ALA:HB2	1:A:376:GLN:HG2	1.94	0.49
2:B:809:ILE:HD11	2:B:892:ALA:HB3	1.94	0.49
1:E:193:GLN:H	1:E:193:GLN:CD	2.20	0.49
3:I:337:VAL:HG12	3:I:341:MET:HE3	1.94	0.49
3:J:158:LEU:HG	3:J:159:GLU:HG3	1.94	0.49
3:J:342:SER:HA	3:J:383:LEU:HD21	1.95	0.49
1:A:37:VAL:HG12	1:A:47:LEU:HD12	1.95	0.49
2:B:1197:ARG:HE	2:B:1199:GLU:CD	2.21	0.49
1:C:98:VAL:HG21	2:D:1017:LEU:HD21	1.95	0.49
2:F:1228:PRO:HB2	2:F:1229:PRO:HD3	1.94	0.49
3:K:67:THR:HG22	3:K:69:ARG:HG3	1.93	0.49
3:L:158:LEU:HG	3:L:159:GLU:HG3	1.94	0.49
1:A:221:TYR:HD2	1:A:326:ILE:HG23	1.76	0.49
3:I:250:LEU:HB3	3:I:288:THR:HG22	1.95	0.49
3:J:60:LEU:HD12	3:J:69:ARG:O	2.13	0.49
2:B:1443:GLN:HE21	2:B:1446:ASN:HA	1.78	0.49
2:D:809:ILE:HD11	2:D:892:ALA:HB3	1.94	0.49
2:F:1017:LEU:C	2:F:1019:LYS:H	2.21	0.49
1:G:404:THR:HG23	1:G:414:GLN:HE21	1.78	0.49
2:H:894:VAL:HG23	2:H:897:HIS:HB2	1.95	0.49
3:J:41:PHE:HD1	3:J:75:ALA:HA	1.78	0.49
1:C:37:VAL:HG12	1:C:47:LEU:HD12	1.95	0.48
1:E:166:VAL:O	1:E:168:PRO:HD3	2.12	0.48
1:G:15:GLU:HG2	1:G:70:ALA:HB2	1.94	0.48
1:G:193:GLN:H	1:G:193:GLN:CD	2.21	0.48
1:G:370:GLN:HA	1:G:370:GLN:HE21	1.77	0.48
2:H:1017:LEU:C	2:H:1019:LYS:H	2.20	0.48
3:I:158:LEU:HG	3:I:159:GLU:HG3	1.95	0.48
3:J:57:TRP:O	3:J:58:SER:C	2.56	0.48
3:J:337:VAL:HG12	3:J:341:MET:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG12	2:B:1297:LEU:HD12	1.95	0.48
1:A:603:ILE:HB	1:A:635:ARG:HH12	1.78	0.48
2:F:1103:ILE:H	2:F:1103:ILE:HD12	1.78	0.48
2:H:1055:TRP:CZ2	2:H:1108:ILE:HA	2.48	0.48
2:H:1133:LYS:O	2:H:1137:GLU:HB2	2.14	0.48
3:J:62:THR:HG23	3:J:68:VAL:CG2	2.43	0.48
3:J:724:LEU:HB2	3:J:725:PRO:HD3	1.95	0.48
2:B:1103:ILE:H	2:B:1103:ILE:HD12	1.78	0.48
2:H:732:ASP:CG	2:H:733:ILE:H	2.21	0.48
3:K:654:ARG:HG3	3:K:722:GLN:CB	2.42	0.48
3:L:44:TYR:HB3	3:L:72:GLU:O	2.14	0.48
1:A:6:ILE:HD12	1:A:21:VAL:O	2.14	0.48
1:A:404:THR:HG23	1:A:414:GLN:HE21	1.78	0.48
2:B:1133:LYS:O	2:B:1137:GLU:HB2	2.14	0.48
2:D:1566:ILE:HD12	2:D:1566:ILE:N	2.27	0.48
1:E:369:VAL:HG12	1:E:371:GLY:H	1.78	0.48
2:F:1331:LYS:CA	2:F:1332:ASP:HB2	2.41	0.48
2:F:1531:GLN:HB2	2:F:1538:GLU:HB2	1.94	0.48
2:H:1443:GLN:HE21	2:H:1446:ASN:HA	1.79	0.48
2:B:739:ILE:HB	2:B:891:LYS:HD3	1.94	0.48
2:D:1114:ASN:HB2	2:D:1117:LYS:HB2	1.96	0.48
1:G:255:ASP:CG	1:G:256:GLY:H	2.22	0.48
1:G:541:LEU:HD22	2:H:786:SER:HB3	1.94	0.48
2:H:742:ARG:HH12	2:H:777:ILE:HG13	1.79	0.48
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.94	0.48
2:B:777:ILE:HG23	2:B:804:MET:HA	1.95	0.48
2:H:745:PHE:N	2:H:746:PRO:HD3	2.29	0.48
3:I:529:LEU:HD13	3:I:730:LYS:HD2	1.96	0.48
1:A:553:PRO:HD2	2:B:802:THR:O	2.14	0.48
1:C:10:ASN:HA	1:C:623:THR:HG23	1.96	0.48
1:C:369:VAL:HG12	1:C:371:GLY:H	1.78	0.48
1:G:6:ILE:HD12	1:G:21:VAL:O	2.14	0.48
2:H:777:ILE:HG23	2:H:804:MET:HA	1.95	0.48
2:H:1566:ILE:HD12	2:H:1566:ILE:N	2.28	0.48
3:I:44:TYR:HB3	3:I:72:GLU:O	2.14	0.48
3:J:218:GLU:HB3	3:J:452:LEU:HD21	1.94	0.48
3:J:269:VAL:HG13	3:J:311:THR:HG23	1.94	0.48
3:K:164:TYR:CG	3:K:191:PRO:HG2	2.49	0.48
3:K:353:ASN:HB3	4:K:1353:NAG:HN2	1.78	0.48
3:L:724:LEU:HB2	3:L:725:PRO:HD3	1.95	0.48
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1017:LEU:C	2:D:1019:LYS:H	2.22	0.48
1:E:553:PRO:HD2	2:F:802:THR:O	2.14	0.48
3:I:214:THR:O	3:I:218:GLU:HG3	2.13	0.48
3:I:724:LEU:HB2	3:I:725:PRO:HD3	1.95	0.48
3:J:19:ILE:HD12	3:J:20:LYS:N	2.29	0.48
3:L:214:THR:O	3:L:218:GLU:HG3	2.14	0.48
1:A:222:TYR:HB3	1:A:225:ASN:HB2	1.96	0.48
1:A:255:ASP:CG	1:A:256:GLY:H	2.21	0.48
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.49	0.48
2:D:1531:GLN:HB2	2:D:1538:GLU:HB2	1.96	0.48
1:E:222:TYR:HB3	1:E:225:ASN:HB2	1.96	0.48
2:F:1104:HIS:O	2:F:1107:MET:HG2	2.14	0.48
2:F:1304:GLU:HG2	2:F:1306:GLU:HG2	1.96	0.48
3:J:164:TYR:CG	3:J:191:PRO:HG2	2.49	0.48
1:C:255:ASP:CG	1:C:256:GLY:H	2.21	0.48
2:F:745:PHE:N	2:F:746:PRO:HD3	2.29	0.48
2:F:1443:GLN:HE21	2:F:1446:ASN:HA	1.79	0.48
3:I:292:TYR:HE2	3:I:325:LYS:HD3	1.78	0.48
3:J:35:TYR:CE2	3:J:49:ARG:HD2	2.48	0.48
3:J:214:THR:O	3:J:218:GLU:HG3	2.14	0.48
1:A:4:TYR:O	1:A:626:SER:HA	2.13	0.47
2:B:894:VAL:HG23	2:B:897:HIS:HB2	1.96	0.47
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	1.96	0.47
1:E:69:PRO:CA	1:E:70:ALA:HB3	2.23	0.47
2:F:777:ILE:HG23	2:F:804:MET:HA	1.96	0.47
2:F:1566:ILE:HD12	2:F:1566:ILE:N	2.28	0.47
2:H:1525:THR:HG22	2:H:1543:ILE:HA	1.95	0.47
3:J:82:HIS:CE1	3:J:150:ARG:HB2	2.49	0.47
2:B:1114:ASN:HB2	2:B:1117:LYS:HB2	1.95	0.47
1:C:398:LEU:HD22	1:C:400:ILE:HD11	1.97	0.47
1:G:369:VAL:HG12	1:G:371:GLY:H	1.78	0.47
1:G:516:ILE:N	1:G:516:ILE:HD12	2.29	0.47
2:H:813:LEU:HD23	2:H:907:LEU:HD13	1.96	0.47
3:J:354:ARG:HG2	4:J:1353:NAG:H82	1.96	0.47
1:A:236:ARG:HA	1:A:243:VAL:HG23	1.96	0.47
2:B:1017:LEU:C	2:B:1019:LYS:H	2.21	0.47
2:D:732:ASP:O	2:D:733:ILE:HG12	2.14	0.47
2:D:1304:GLU:HG2	2:D:1306:GLU:HG2	1.97	0.47
1:E:255:ASP:CG	1:E:256:GLY:H	2.22	0.47
1:E:516:ILE:HD12	1:E:516:ILE:N	2.29	0.47
2:F:852:SER:HB3	2:F:878:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1055:TRP:CZ2	2:F:1108:ILE:HA	2.49	0.47
1:G:222:TYR:HB3	1:G:225:ASN:HB2	1.96	0.47
3:I:210:LEU:HD11	3:I:443:MET:HG2	1.97	0.47
3:I:458:GLU:HA	3:I:459:HIS:C	2.38	0.47
3:L:164:TYR:CG	3:L:191:PRO:HG2	2.49	0.47
3:L:361:LEU:HD21	3:L:402:VAL:HG22	1.96	0.47
1:A:516:ILE:N	1:A:516:ILE:HD12	2.29	0.47
2:B:745:PHE:N	2:B:746:PRO:HD3	2.29	0.47
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.21	0.47
2:B:1530:VAL:HG12	2:B:1532:LEU:HD22	1.96	0.47
1:C:100:LEU:HD12	1:C:101:VAL:H	1.80	0.47
2:D:1443:GLN:HE21	2:D:1446:ASN:HA	1.79	0.47
3:I:19:ILE:HG13	3:I:71:ALA:C	2.39	0.47
3:K:352:TRP:CZ2	4:K:1353:NAG:C8	2.83	0.47
3:L:250:LEU:HB3	3:L:288:THR:HG22	1.95	0.47
3:L:513:LYS:HB3	3:L:522:ASP:HB3	1.97	0.47
1:C:239:TYR:HD1	2:D:804:MET:HE2	1.79	0.47
2:D:813:LEU:HD23	2:D:907:LEU:HB3	1.95	0.47
1:G:398:LEU:HD22	1:G:400:ILE:HD11	1.97	0.47
2:H:1114:ASN:HB2	2:H:1117:LYS:HB2	1.95	0.47
3:J:45:PRO:CG	3:J:68:VAL:HG21	2.45	0.47
3:K:214:THR:O	3:K:218:GLU:HG3	2.13	0.47
2:B:1304:GLU:HG2	2:B:1306:GLU:HG2	1.96	0.47
1:C:569:ALA:HB2	2:D:788:SER:HB2	1.97	0.47
2:D:907:LEU:HD23	2:D:907:LEU:H	1.80	0.47
2:D:1494:GLU:HB2	2:D:1602:LYS:HD3	1.97	0.47
2:D:1617:ASP:C	2:D:1619:GLU:H	2.23	0.47
1:G:239:TYR:HD1	2:H:804:MET:HE2	1.79	0.47
1:G:553:PRO:HD2	2:H:802:THR:O	2.15	0.47
3:I:248:LEU:HD22	3:I:268:LEU:HD22	1.97	0.47
3:I:361:LEU:HD21	3:I:402:VAL:HG22	1.95	0.47
3:I:706:GLN:C	3:I:708:GLN:H	2.23	0.47
3:J:706:GLN:C	3:J:708:GLN:H	2.23	0.47
3:L:705:ARG:O	3:L:707:LYS:HG3	2.15	0.47
1:C:222:TYR:HB3	1:C:225:ASN:HB2	1.96	0.47
1:C:516:ILE:HD12	1:C:516:ILE:N	2.29	0.47
2:D:1154:LEU:HB2	2:D:1174:LEU:HD21	1.97	0.47
2:F:894:VAL:HG23	2:F:897:HIS:HB2	1.95	0.47
2:F:1507:LEU:HD11	2:F:1629:ALA:HB3	1.96	0.47
1:G:236:ARG:HA	1:G:243:VAL:HG23	1.97	0.47
2:H:1066:LEU:HD23	2:H:1066:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:344:PRO:O	3:I:345:ASP:HB3	2.14	0.47
3:I:655:PHE:HA	3:I:717:HIS:O	2.14	0.47
3:I:705:ARG:O	3:I:707:LYS:HG3	2.15	0.47
3:J:240:PRO:HA	3:J:241:SER:HA	1.54	0.47
3:K:57:TRP:O	3:K:58:SER:C	2.57	0.47
3:K:724:LEU:HB2	3:K:725:PRO:HD3	1.95	0.47
3:L:292:TYR:HE2	3:L:325:LYS:HD3	1.80	0.47
1:A:223:ILE:HD12	1:A:223:ILE:N	2.30	0.47
1:C:31:VAL:HG13	1:C:54:LEU:HB2	1.96	0.47
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	1.97	0.47
2:D:1290:HIS:CE1	3:J:661:VAL:HG11	2.49	0.47
1:E:223:ILE:HD12	1:E:223:ILE:N	2.30	0.47
1:E:239:TYR:HD1	2:F:804:MET:HE2	1.80	0.47
1:E:443:LEU:HD11	1:E:449:LEU:HD22	1.97	0.47
3:K:423:ASN:HD22	3:K:683:ARG:HH12	1.63	0.47
1:E:236:ARG:HA	1:E:243:VAL:HG23	1.97	0.47
2:F:1114:ASN:HB2	2:F:1117:LYS:HB2	1.96	0.47
2:H:751:TRP:HB3	3:L:107:TYR:CD1	2.50	0.47
3:I:513:LYS:HB3	3:I:522:ASP:HB3	1.97	0.47
3:K:19:ILE:HD12	3:K:20:LYS:N	2.30	0.47
3:K:35:TYR:CE2	3:K:49:ARG:HD2	2.49	0.47
3:K:655:PHE:HA	3:K:717:HIS:O	2.15	0.47
3:L:189:THR:HG22	3:L:420:LYS:HB3	1.97	0.47
3:L:464:ASP:C	3:L:466:HIS:H	2.22	0.47
3:L:493:GLU:OE1	3:L:560:LYS:HE3	2.15	0.47
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.51	0.47
2:F:732:ASP:CG	2:F:733:ILE:H	2.22	0.47
2:F:851:CYS:HB3	2:F:879:VAL:HB	1.95	0.47
2:F:1133:LYS:O	2:F:1137:GLU:HB2	2.14	0.47
2:H:1008:GLU:OE1	2:H:1262:LYS:HD3	2.15	0.47
3:J:62:THR:N	3:J:68:VAL:HG23	2.30	0.47
3:J:513:LYS:HB3	3:J:522:ASP:HB3	1.97	0.47
3:K:27:LEU:C	3:K:28:GLN:HG2	2.40	0.47
3:K:250:LEU:HB3	3:K:288:THR:HG22	1.97	0.47
3:L:655:PHE:HA	3:L:717:HIS:O	2.15	0.47
2:H:751:TRP:NE1	3:L:108:ASP:HB2	2.30	0.46
3:I:493:GLU:OE1	3:I:560:LYS:HE3	2.15	0.46
3:K:82:HIS:CE1	3:K:150:ARG:HB2	2.50	0.46
3:K:705:ARG:O	3:K:707:LYS:HG3	2.15	0.46
1:A:25:HIS:HA	1:A:26:ASP:HA	1.52	0.46
1:A:45:LEU:HA	1:A:46:VAL:HA	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG12	1:A:371:GLY:H	1.79	0.46
1:C:236:ARG:HA	1:C:243:VAL:HG23	1.96	0.46
1:C:553:PRO:HD2	2:D:802:THR:O	2.15	0.46
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.97	0.46
1:E:398:LEU:HD22	1:E:400:ILE:HD11	1.96	0.46
2:H:882:LYS:HG3	2:H:886:GLN:NE2	2.31	0.46
2:H:1008:GLU:CD	2:H:1262:LYS:HD3	2.39	0.46
3:J:703:GLN:HG2	3:J:704:LYS:HG3	1.97	0.46
3:L:706:GLN:C	3:L:708:GLN:H	2.23	0.46
1:A:19:THR:HB	1:A:478:LEU:HB2	1.96	0.46
2:B:904:ARG:NH2	3:I:82:HIS:HB2	2.30	0.46
2:B:1527:LEU:HD23	2:B:1575:GLU:C	2.40	0.46
2:D:777:ILE:HG23	2:D:804:MET:HA	1.97	0.46
2:D:894:VAL:HG23	2:D:897:HIS:HB2	1.96	0.46
2:D:1133:LYS:O	2:D:1137:GLU:HB2	2.14	0.46
2:D:1333:GLN:HA	2:D:1334:LEU:C	2.40	0.46
2:D:1532:LEU:HD12	2:D:1532:LEU:N	2.30	0.46
2:F:854:ALA:HB2	2:F:860:HIS:HB3	1.98	0.46
3:J:89:TYR:CE2	3:J:92:ARG:HG2	2.51	0.46
3:J:118:ARG:NH1	3:J:130:THR:HA	2.31	0.46
3:J:205:VAL:HG13	3:J:428:PHE:CD1	2.51	0.46
3:K:68:VAL:C	3:K:70:LYS:N	2.72	0.46
3:K:342:SER:HA	3:K:383:LEU:HD21	1.97	0.46
2:B:912:GLU:HG3	2:B:1331:LYS:NZ	2.31	0.46
2:B:1008:GLU:OE1	2:B:1262:LYS:HD3	2.16	0.46
2:D:745:PHE:N	2:D:746:PRO:HD3	2.29	0.46
2:D:1103:ILE:H	2:D:1103:ILE:HD12	1.79	0.46
2:D:1572:LEU:HB3	2:D:1574:LEU:HG	1.98	0.46
1:E:474:ASN:O	1:E:477:ARG:HG2	2.16	0.46
2:F:1154:LEU:HB2	2:F:1174:LEU:HD21	1.97	0.46
1:G:148:PRO:HD3	1:G:182:TRP:CE2	2.50	0.46
2:H:852:SER:HB3	2:H:878:ILE:HG22	1.97	0.46
3:I:82:HIS:CE1	3:I:150:ARG:HB2	2.50	0.46
3:L:240:PRO:HA	3:L:241:SER:HA	1.53	0.46
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.50	0.46
1:C:45:LEU:HA	1:C:46:VAL:HA	1.67	0.46
2:D:740:VAL:HG21	3:J:94:PRO:HB3	1.95	0.46
2:D:852:SER:HB3	2:D:878:ILE:HG22	1.97	0.46
2:D:854:ALA:HB2	2:D:860:HIS:HB3	1.97	0.46
1:E:20:MET:HB3	1:E:64:VAL:HG23	1.97	0.46
1:E:40:PHE:CE1	2:F:1017:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1066:LEU:HD23	2:F:1066:LEU:O	2.14	0.46
2:H:904:ARG:NH2	3:L:82:HIS:HB2	2.30	0.46
3:J:210:LEU:HD11	3:J:443:MET:HG2	1.98	0.46
3:K:706:GLN:C	3:K:708:GLN:H	2.23	0.46
1:A:19:THR:HB	1:A:478:LEU:HD12	1.97	0.46
1:A:239:TYR:HD1	2:B:804:MET:HE2	1.79	0.46
1:A:398:LEU:HD22	1:A:400:ILE:HD11	1.97	0.46
2:B:1617:ASP:C	2:B:1619:GLU:H	2.24	0.46
1:C:148:PRO:HD3	1:C:182:TRP:CE2	2.51	0.46
1:E:100:LEU:HD12	1:E:101:VAL:H	1.81	0.46
1:E:569:ALA:HB2	2:F:788:SER:HB2	1.97	0.46
2:H:940:ILE:HD12	2:H:1308:PHE:CE2	2.51	0.46
2:H:1304:GLU:HG2	2:H:1306:GLU:HG2	1.97	0.46
3:J:31:GLN:HA	3:J:51:CYS:HB3	1.97	0.46
3:J:222:ALA:CA	3:J:223:GLU:C	2.87	0.46
3:K:67:THR:O	3:K:69:ARG:N	2.48	0.46
3:K:89:TYR:CE2	3:K:92:ARG:HG2	2.50	0.46
1:C:157:SER:HB3	3:J:630:SER:OG	2.16	0.46
1:C:316:MET:HE2	1:C:318:GLN:HE21	1.81	0.46
1:C:443:LEU:HD11	1:C:449:LEU:HD22	1.97	0.46
2:F:940:ILE:HD12	2:F:1308:PHE:CE2	2.51	0.46
1:G:37:VAL:HG12	1:G:47:LEU:HD12	1.97	0.46
2:H:1216:LEU:HD21	2:H:1256:ALA:HA	1.97	0.46
3:I:622:ILE:HA	3:I:658:THR:HG22	1.98	0.46
3:J:296:TRP:CE2	3:J:317:ILE:HG22	2.51	0.46
3:J:456:VAL:HG12	3:J:457:TRP:N	2.31	0.46
3:J:705:ARG:O	3:J:707:LYS:HG3	2.16	0.46
1:A:352:VAL:HB	1:A:385:ALA:HB3	1.98	0.46
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.16	0.46
1:C:215:GLU:HG2	1:C:321:ARG:HH22	1.81	0.46
1:C:352:VAL:HB	1:C:385:ALA:HB3	1.98	0.46
1:C:474:ASN:O	1:C:477:ARG:HG2	2.16	0.46
2:D:1066:LEU:O	2:D:1066:LEU:HD23	2.14	0.46
1:E:31:VAL:HG13	1:E:54:LEU:HB2	1.96	0.46
1:E:148:PRO:HD3	1:E:182:TRP:CE2	2.51	0.46
2:F:927:PRO:C	2:F:929:ARG:H	2.24	0.46
2:H:1572:LEU:HB3	2:H:1574:LEU:HG	1.98	0.46
2:H:1617:ASP:C	2:H:1619:GLU:H	2.23	0.46
3:K:513:LYS:HB3	3:K:522:ASP:HB3	1.97	0.46
3:L:82:HIS:CE1	3:L:150:ARG:HB2	2.50	0.46
3:L:337:VAL:HG12	3:L:341:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.98	0.46
1:A:624:PHE:H	1:A:632:THR:CG2	2.29	0.46
1:C:147:ASN:HA	1:C:182:TRP:CE3	2.51	0.46
1:C:223:ILE:HD12	1:C:223:ILE:N	2.30	0.46
1:E:45:LEU:HA	1:E:46:VAL:HA	1.67	0.46
1:G:474:ASN:O	1:G:477:ARG:HG2	2.15	0.46
2:H:1056:LEU:O	2:H:1060:VAL:HG23	2.16	0.46
2:H:1103:ILE:HD12	2:H:1103:ILE:H	1.81	0.46
2:H:1525:THR:HB	2:H:1541:MET:HB3	1.98	0.46
3:I:437:GLU:HB3	3:I:441:TYR:CE2	2.51	0.46
3:J:655:PHE:HA	3:J:717:HIS:O	2.15	0.46
3:K:529:LEU:HD13	3:K:730:LYS:HD2	1.97	0.46
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.98	0.46
1:A:69:PRO:HB3	1:A:70:ALA:C	2.41	0.46
1:A:147:ASN:HA	1:A:182:TRP:CE3	2.51	0.46
2:B:804:MET:HG2	2:B:805:GLN:H	1.80	0.46
2:B:1066:LEU:O	2:B:1066:LEU:HD23	2.16	0.46
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.98	0.46
2:D:804:MET:HG2	2:D:805:GLN:H	1.81	0.46
2:D:966:ALA:HA	2:D:1267:HIS:HB3	1.97	0.46
1:E:316:MET:HE2	1:E:318:GLN:HE21	1.81	0.46
2:F:1572:LEU:HB3	2:F:1574:LEU:HG	1.98	0.46
1:G:223:ILE:HD12	1:G:223:ILE:N	2.30	0.46
3:K:296:TRP:CE2	3:K:317:ILE:HG22	2.51	0.46
2:B:940:ILE:HD12	2:B:1308:PHE:CE2	2.51	0.45
1:C:83:PHE:CZ	1:C:100:LEU:HD13	2.51	0.45
2:D:882:LYS:HG3	2:D:886:GLN:NE2	2.30	0.45
1:E:427:VAL:HB	1:E:523:GLU:HG3	1.98	0.45
3:I:118:ARG:NH1	3:I:130:THR:HA	2.31	0.45
3:J:82:HIS:HE1	3:J:150:ARG:HB2	1.82	0.45
2:B:1103:ILE:HD12	2:B:1103:ILE:N	2.31	0.45
2:B:1155:GLU:HG3	2:B:1184:LEU:HD21	1.97	0.45
2:B:1572:LEU:HB3	2:B:1574:LEU:HG	1.97	0.45
1:C:23:GLU:HG2	1:C:483:ARG:HH21	1.81	0.45
2:F:1155:GLU:HG3	2:F:1184:LEU:HD21	1.99	0.45
2:F:1331:LYS:HA	2:F:1332:ASP:CB	2.39	0.45
1:G:10:ASN:ND2	1:G:621:GLY:HA2	2.30	0.45
3:I:89:TYR:CE2	3:I:92:ARG:HG2	2.51	0.45
3:I:431:LYS:HB3	3:I:435:ASN:HD22	1.81	0.45
3:J:529:LEU:HD13	3:J:730:LYS:HD2	1.97	0.45
3:K:679:ILE:HG21	3:K:686:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1153:PHE:HE1	2:F:1236:GLU:OE1	1.99	0.45
2:B:1520:ASP:HB2	2:B:1586:SER:HB3	1.97	0.45
2:H:854:ALA:HB2	2:H:860:HIS:HB3	1.98	0.45
2:H:1380:ILE:N	2:H:1380:ILE:HD12	2.32	0.45
3:K:62:THR:HG23	3:K:68:VAL:CG2	2.46	0.45
3:K:703:GLN:HG2	3:K:704:LYS:HG3	1.98	0.45
1:A:400:ILE:N	1:A:400:ILE:HD12	2.32	0.45
2:B:1296:LEU:HD23	2:B:1298:ARG:CZ	2.46	0.45
2:B:1525:THR:HB	2:B:1541:MET:HB3	1.98	0.45
1:C:25:HIS:HA	1:C:26:ASP:HA	1.55	0.45
2:F:882:LYS:HG3	2:F:886:GLN:NE2	2.31	0.45
1:G:147:ASN:HA	1:G:182:TRP:CE3	2.51	0.45
1:G:352:VAL:HB	1:G:385:ALA:HB3	1.99	0.45
1:G:427:VAL:HB	1:G:523:GLU:HG3	1.97	0.45
1:G:634:GLN:NE2	2:H:1017:LEU:HD23	2.31	0.45
2:H:839:LYS:HB3	2:H:895:TYR:HB2	1.99	0.45
2:H:1376:ALA:HB3	2:H:1429:VAL:HG23	1.99	0.45
3:K:241:SER:HA	3:K:242:GLY:HA3	1.73	0.45
3:L:89:TYR:CE2	3:L:92:ARG:HG2	2.52	0.45
2:B:882:LYS:HG3	2:B:886:GLN:NE2	2.31	0.45
2:D:918:LYS:HE3	2:D:1326:TYR:OH	2.16	0.45
2:F:887:GLU:OE2	2:F:904:ARG:HD2	2.15	0.45
2:F:1103:ILE:HD12	2:F:1103:ILE:N	2.31	0.45
3:J:493:GLU:OE1	3:J:560:LYS:HE3	2.16	0.45
2:B:1154:LEU:HB2	2:B:1174:LEU:HD21	1.99	0.45
2:D:940:ILE:HD12	2:D:1308:PHE:CE2	2.51	0.45
2:D:1315:LYS:HD2	2:D:1315:LYS:N	2.32	0.45
2:F:918:LYS:HE3	2:F:1326:TYR:OH	2.17	0.45
2:F:1617:ASP:C	2:F:1619:GLU:H	2.23	0.45
3:J:250:LEU:HB3	3:J:288:THR:HG22	1.99	0.45
3:L:431:LYS:HB3	3:L:435:ASN:HD22	1.82	0.45
2:B:839:LYS:HB3	2:B:895:TYR:HB2	1.99	0.45
2:D:1095:VAL:HG13	2:D:1122:THR:OG1	2.16	0.45
2:D:1463:LEU:O	2:D:1463:LEU:HD23	2.17	0.45
1:E:151:ILE:HG22	2:F:1297:LEU:HG	1.97	0.45
1:E:400:ILE:HD12	1:E:400:ILE:N	2.32	0.45
1:G:19:THR:HB	1:G:478:LEU:HB2	1.99	0.45
1:G:69:PRO:HB2	1:G:71:ASN:CG	2.42	0.45
1:G:569:ALA:HB2	2:H:788:SER:HB2	1.97	0.45
3:J:679:ILE:HG21	3:J:686:PHE:HB3	1.99	0.45
3:L:529:LEU:HD13	3:L:730:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:927:PRO:C	2:B:929:ARG:H	2.24	0.45
2:B:1065:SER:OG	2:B:1132:ALA:HB2	2.16	0.45
2:B:1301:GLU:CD	2:B:1301:GLU:N	2.74	0.45
2:D:1507:LEU:HD11	2:D:1629:ALA:HB3	1.99	0.45
1:E:95:VAL:HG22	1:E:627:SER:HB3	1.98	0.45
1:G:145:ILE:O	1:G:153:VAL:HG22	2.17	0.45
2:H:1223:ASP:O	2:H:1227:VAL:HG23	2.17	0.45
2:H:1337:ASN:HB3	2:H:1338:LYS:HD2	1.99	0.45
3:I:278:TYR:CD1	3:I:450:LEU:HD11	2.52	0.45
3:I:703:GLN:HG2	3:I:704:LYS:HG3	1.98	0.45
3:J:35:TYR:OH	3:J:49:ARG:HD2	2.17	0.45
3:L:622:ILE:HA	3:L:658:THR:HG22	1.99	0.45
2:B:733:ILE:HG13	2:B:734:ILE:N	2.31	0.45
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.97	0.45
2:B:1119:MET:HE1	2:B:1154:LEU:HA	1.99	0.45
1:C:39:ASP:OD2	1:C:44:LYS:HB3	2.17	0.45
2:D:1376:ALA:HB3	2:D:1429:VAL:HG23	1.99	0.45
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.22	0.45
1:E:147:ASN:HA	1:E:182:TRP:CE3	2.52	0.45
1:E:343:LYS:N	1:E:343:LYS:HD2	2.31	0.45
2:F:1017:LEU:HD12	2:F:1018:GLU:N	2.21	0.45
2:F:1532:LEU:HD12	2:F:1532:LEU:N	2.31	0.45
2:H:1458:TYR:HB3	2:H:1466:SER:HB3	1.99	0.45
2:H:1641:ASN:N	3:L:326:SER:O	2.50	0.45
3:I:347:VAL:HG13	3:I:349:PRO:CG	2.47	0.45
1:A:302:LEU:HG	1:A:326:ILE:HD11	1.99	0.45
2:B:1119:MET:SD	2:B:1157:ASN:HB2	2.57	0.45
2:B:1331:LYS:HA	2:B:1332:ASP:HB2	1.98	0.45
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.99	0.45
1:E:352:VAL:HB	1:E:385:ALA:HB3	2.00	0.45
1:G:400:ILE:HD12	1:G:400:ILE:N	2.32	0.45
2:H:927:PRO:C	2:H:929:ARG:H	2.24	0.45
2:H:1463:LEU:O	2:H:1463:LEU:HD23	2.17	0.45
3:J:110:TYR:CE1	3:J:135:ASN:HB3	2.52	0.45
3:K:218:GLU:HB3	3:K:452:LEU:HD21	1.99	0.45
3:K:240:PRO:HA	3:K:241:SER:HA	1.53	0.45
3:K:286:LEU:H	3:K:297:VAL:HB	1.82	0.45
3:K:493:GLU:OE1	3:K:560:LYS:HE3	2.16	0.45
2:B:1337:ASN:HB3	2:B:1338:LYS:HD2	2.00	0.44
2:D:851:CYS:HB3	2:D:879:VAL:HB	2.00	0.44
2:D:927:PRO:C	2:D:929:ARG:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1330:ALA:O	2:D:1331:LYS:C	2.60	0.44
2:D:1380:ILE:HD12	2:D:1380:ILE:N	2.32	0.44
1:E:268:ARG:HD3	2:F:1378:MET:CE	2.47	0.44
2:F:1296:LEU:HD23	2:F:1298:ARG:CZ	2.47	0.44
2:H:1103:ILE:HD12	2:H:1103:ILE:N	2.32	0.44
3:I:349:PRO:HD2	3:I:352:TRP:CD1	2.53	0.44
3:J:464:ASP:C	3:J:466:HIS:H	2.24	0.44
3:K:353:ASN:OD1	3:K:354:ARG:HG3	2.17	0.44
3:K:622:ILE:HA	3:K:658:THR:HG22	1.99	0.44
3:L:248:LEU:HD22	3:L:268:LEU:HD22	1.99	0.44
1:A:474:ASN:O	1:A:477:ARG:HG2	2.17	0.44
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.97	0.44
1:C:400:ILE:N	1:C:400:ILE:HD12	2.32	0.44
2:D:811:LEU:HD22	2:D:890:VAL:HG22	2.00	0.44
1:E:45:LEU:H	1:E:45:LEU:CD2	2.31	0.44
1:E:83:PHE:CZ	1:E:100:LEU:HD13	2.51	0.44
2:F:811:LEU:HD22	2:F:890:VAL:HG22	1.99	0.44
2:F:1315:LYS:HD2	2:F:1315:LYS:N	2.32	0.44
2:F:1337:ASN:HB3	2:F:1338:LYS:HD2	1.99	0.44
2:F:1380:ILE:N	2:F:1380:ILE:HD12	2.32	0.44
1:G:316:MET:HE2	1:G:318:GLN:HE21	1.81	0.44
3:K:110:TYR:CE1	3:K:135:ASN:HB3	2.52	0.44
3:L:437:GLU:HB3	3:L:441:TYR:CE2	2.51	0.44
3:L:679:ILE:HG21	3:L:686:PHE:HB3	2.00	0.44
3:L:703:GLN:HG2	3:L:704:LYS:HG3	1.98	0.44
1:A:5:SER:HA	1:A:625:THR:O	2.17	0.44
1:A:316:MET:HE2	1:A:318:GLN:HE21	1.81	0.44
1:A:343:LYS:HD2	1:A:343:LYS:N	2.32	0.44
2:B:918:LYS:HE3	2:B:1326:TYR:OH	2.16	0.44
2:B:1315:LYS:N	2:B:1315:LYS:HD2	2.33	0.44
1:C:145:ILE:O	1:C:153:VAL:HG22	2.18	0.44
1:C:343:LYS:HD2	1:C:343:LYS:N	2.32	0.44
1:E:624:PHE:H	1:E:632:THR:CG2	2.31	0.44
2:F:1216:LEU:HD21	2:F:1256:ALA:HA	1.98	0.44
1:G:343:LYS:N	1:G:343:LYS:HD2	2.32	0.44
2:H:751:TRP:HD1	3:L:108:ASP:H	1.66	0.44
2:H:918:LYS:HE3	2:H:1326:TYR:OH	2.17	0.44
3:K:35:TYR:OH	3:K:49:ARG:HD2	2.18	0.44
3:K:216:THR:O	3:K:220:VAL:HG23	2.18	0.44
3:K:406:GLY:O	3:K:408:LEU:N	2.49	0.44
3:K:568:ARG:HA	3:K:569:PRO:HD3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:118:ARG:NH1	3:L:130:THR:HA	2.33	0.44
1:A:5:SER:OG	1:A:23:GLU:HB2	2.18	0.44
2:B:1458:TYR:HB3	2:B:1466:SER:HB3	1.99	0.44
2:F:1463:LEU:O	2:F:1463:LEU:HD23	2.18	0.44
1:G:31:VAL:HG13	1:G:54:LEU:HB2	1.99	0.44
1:G:624:PHE:H	1:G:632:THR:CG2	2.30	0.44
3:I:347:VAL:HG13	3:I:349:PRO:CD	2.48	0.44
3:J:286:LEU:H	3:J:297:VAL:HB	1.82	0.44
3:L:364:ASP:HB3	3:L:406:GLY:HA3	2.00	0.44
1:A:145:ILE:O	1:A:153:VAL:HG22	2.17	0.44
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.99	0.44
2:B:956:THR:HG23	2:B:1324:THR:HG22	1.99	0.44
1:C:268:ARG:HD3	2:D:1378:MET:CE	2.48	0.44
1:C:323:GLY:O	1:C:325:PRO:HD3	2.18	0.44
2:D:1593:LYS:HE2	2:D:1596:LEU:HD11	2.00	0.44
1:E:39:ASP:OD2	1:E:44:LYS:HB3	2.18	0.44
1:E:40:PHE:CE1	2:F:1017:LEU:CD1	3.01	0.44
2:H:907:LEU:H	2:H:907:LEU:HD23	1.83	0.44
2:H:1119:MET:HE1	2:H:1154:LEU:HA	2.00	0.44
2:H:1315:LYS:N	2:H:1315:LYS:HD2	2.32	0.44
2:H:1405:ARG:HE	2:H:1437:LEU:HD23	1.82	0.44
3:I:45:PRO:HB3	3:I:62:THR:HG22	1.99	0.44
3:I:110:TYR:CE1	3:I:135:ASN:HB3	2.53	0.44
3:I:349:PRO:HG2	3:I:352:TRP:HB3	1.99	0.44
3:J:216:THR:O	3:J:220:VAL:HG23	2.18	0.44
3:K:76:ILE:HG12	3:K:197:PHE:CE1	2.52	0.44
3:K:705:ARG:HA	3:K:705:ARG:HD3	1.87	0.44
3:L:435:ASN:O	3:L:439:VAL:HG23	2.18	0.44
1:C:93:GLN:HE21	1:C:627:SER:HB2	1.82	0.44
2:D:1103:ILE:HD12	2:D:1103:ILE:N	2.32	0.44
1:E:147:ASN:HB2	1:E:148:PRO:CD	2.48	0.44
1:E:373:ASP:C	1:E:375:VAL:H	2.26	0.44
2:F:1286:THR:HG22	3:K:665:ALA:HB3	2.00	0.44
1:G:302:LEU:HG	1:G:326:ILE:HD11	2.00	0.44
3:I:342:SER:HA	3:I:383:LEU:HD21	2.00	0.44
2:D:1397:LYS:HZ2	2:D:1412:LEU:HD23	1.83	0.44
1:E:10:ASN:HA	1:E:623:THR:HG23	1.98	0.44
1:E:469:THR:O	1:E:511:ALA:HA	2.18	0.44
3:I:32:ALA:HA	3:I:57:TRP:HZ3	1.83	0.44
4:K:1353:NAG:H83	4:K:1353:NAG:O3	2.18	0.44
3:L:454:GLY:H	3:L:570:ILE:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:479:PRO:C	3:L:481:LYS:H	2.26	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.48	0.44
2:B:1539:TYR:HB2	2:B:1562:PHE:HB2	2.00	0.44
1:C:469:THR:O	1:C:511:ALA:HA	2.18	0.44
2:D:839:LYS:HB3	2:D:895:TYR:HB2	1.99	0.44
2:D:1331:LYS:CA	2:D:1332:ASP:HB2	2.48	0.44
2:F:1333:GLN:HA	2:F:1334:LEU:C	2.42	0.44
2:F:1481:ASN:ND2	2:F:1567:LYS:HE3	2.32	0.44
2:H:1055:TRP:HZ2	2:H:1248:GLN:HE21	1.66	0.44
3:I:371:GLY:O	3:I:373:PRO:HD3	2.18	0.44
3:K:19:ILE:HG23	3:K:22:GLY:C	2.42	0.44
3:K:118:ARG:NH1	3:K:130:THR:HA	2.33	0.44
3:L:343:TRP:HA	3:L:344:PRO:HD3	1.86	0.44
1:A:215:GLU:HG2	1:A:321:ARG:HH22	1.83	0.43
1:A:373:ASP:C	1:A:375:VAL:H	2.26	0.43
1:C:624:PHE:H	1:C:632:THR:CG2	2.31	0.43
2:D:1119:MET:SD	2:D:1157:ASN:HB2	2.58	0.43
2:D:1155:GLU:HG3	2:D:1184:LEU:HD21	1.99	0.43
1:E:145:ILE:O	1:E:153:VAL:HG22	2.17	0.43
2:F:850:PHE:CZ	2:F:907:LEU:HD21	2.52	0.43
1:G:147:ASN:HB2	1:G:148:PRO:CD	2.48	0.43
1:G:443:LEU:HD11	1:G:449:LEU:HD22	1.98	0.43
2:H:811:LEU:HD22	2:H:890:VAL:HG22	1.99	0.43
2:H:853:LEU:HB2	2:H:860:HIS:CD2	2.53	0.43
2:H:1064:PHE:O	2:H:1068:VAL:HG13	2.18	0.43
2:H:1463:LEU:HD23	2:H:1463:LEU:C	2.43	0.43
3:I:216:THR:O	3:I:220:VAL:HG23	2.18	0.43
3:I:478:ARG:HB2	3:I:482:GLY:HA3	2.00	0.43
3:J:622:ILE:HA	3:J:658:THR:HG22	2.00	0.43
3:K:222:ALA:CA	3:K:223:GLU:C	2.86	0.43
3:K:464:ASP:C	3:K:466:HIS:H	2.26	0.43
1:A:6:ILE:CG2	1:A:625:THR:HB	2.48	0.43
2:B:853:LEU:HB2	2:B:860:HIS:CD2	2.53	0.43
2:D:1337:ASN:HB3	2:D:1338:LYS:HD2	1.99	0.43
1:E:98:VAL:HG21	2:F:1017:LEU:HD21	2.00	0.43
2:F:839:LYS:HB3	2:F:895:TYR:HB2	2.00	0.43
1:G:15:GLU:CG	1:G:70:ALA:HB2	2.48	0.43
3:I:705:ARG:HA	3:I:705:ARG:HD3	1.87	0.43
1:C:14:LEU:HD22	1:C:69:PRO:O	2.18	0.43
1:C:373:ASP:C	1:C:375:VAL:H	2.26	0.43
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:958:ILE:O	2:F:1299:SER:HA	2.19	0.43
2:H:804:MET:HG2	2:H:805:GLN:H	1.82	0.43
2:H:958:ILE:O	2:H:1299:SER:HA	2.18	0.43
2:H:1165:TYR:HD1	2:H:1210:ALA:HB2	1.83	0.43
3:I:679:ILE:HG21	3:I:686:PHE:HB3	2.01	0.43
3:J:456:VAL:HG12	3:J:457:TRP:H	1.83	0.43
3:K:27:LEU:O	3:K:28:GLN:O	2.37	0.43
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.19	0.43
2:B:854:ALA:HB2	2:B:860:HIS:HB3	1.98	0.43
2:B:1376:ALA:HB3	2:B:1429:VAL:HG23	1.99	0.43
2:B:1380:ILE:HD12	2:B:1380:ILE:N	2.32	0.43
2:B:1641:ASN:N	3:I:326:SER:O	2.51	0.43
2:F:824:GLU:OE2	2:F:875:PRO:HB3	2.18	0.43
2:F:1056:LEU:O	2:F:1060:VAL:HG23	2.18	0.43
1:G:469:THR:O	1:G:511:ALA:HA	2.17	0.43
3:I:172:LEU:HD11	3:I:191:PRO:HB3	2.00	0.43
3:I:328:THR:CG2	3:I:367:HIS:HA	2.49	0.43
3:J:29:GLU:N	3:J:30:GLY:CA	2.70	0.43
3:J:285:GLY:HA3	3:J:340:MET:HE1	2.00	0.43
3:L:110:TYR:CE1	3:L:135:ASN:HB3	2.52	0.43
3:L:121:GLN:HE21	3:L:127:SER:HB3	1.84	0.43
1:A:344:PRO:HD2	1:A:433:TYR:CE1	2.54	0.43
2:B:751:TRP:CD1	3:I:108:ASP:HB2	2.54	0.43
2:B:811:LEU:HD22	2:B:890:VAL:HG22	1.99	0.43
2:B:1496:CYS:HB3	2:B:1568:CYS:HB3	1.80	0.43
1:C:439:LEU:H	1:C:439:LEU:HD12	1.83	0.43
2:D:927:PRO:O	2:D:928:GLU:HB2	2.19	0.43
2:D:1119:MET:HE1	2:D:1154:LEU:HA	1.99	0.43
2:D:1463:LEU:HD23	2:D:1463:LEU:C	2.43	0.43
1:E:40:PHE:HD2	1:E:83:PHE:HB2	1.83	0.43
2:F:1458:TYR:HB3	2:F:1466:SER:HB3	1.99	0.43
3:K:220:VAL:O	3:K:222:ALA:N	2.50	0.43
3:L:45:PRO:HB3	3:L:62:THR:HG22	1.99	0.43
1:A:100:LEU:HD21	1:A:638:LEU:HA	1.99	0.43
2:B:1064:PHE:O	2:B:1068:VAL:HG13	2.18	0.43
2:B:1332:ASP:HB3	2:B:1333:GLN:H	1.68	0.43
1:C:241:LYS:HG3	2:D:832:TYR:CE1	2.54	0.43
1:C:344:PRO:HD2	1:C:433:TYR:CE1	2.54	0.43
1:E:302:LEU:HG	1:E:326:ILE:HD11	2.01	0.43
2:F:1031:TYR:O	2:F:1035:LEU:HG	2.19	0.43
2:F:1108:ILE:HD11	2:F:1112:ARG:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1463:LEU:HD23	2:F:1463:LEU:C	2.44	0.43
2:F:1634:MET:HE1	2:F:1639:CYS:SG	2.59	0.43
1:G:373:ASP:C	1:G:375:VAL:H	2.26	0.43
2:H:1257:LEU:O	2:H:1261:GLN:HG2	2.19	0.43
2:H:1520:ASP:HB2	2:H:1586:SER:HB3	1.99	0.43
3:I:344:PRO:HB2	3:I:346:ASP:HB2	2.01	0.43
2:B:1260:TYR:O	2:B:1264:ALA:HB2	2.19	0.43
1:C:23:GLU:CG	1:C:483:ARG:HH21	2.31	0.43
1:C:628:SER:HB2	1:C:630:GLN:NE2	2.16	0.43
1:E:215:GLU:HG2	1:E:321:ARG:HH22	1.83	0.43
1:E:439:LEU:H	1:E:439:LEU:HD12	1.83	0.43
1:G:344:PRO:HD2	1:G:433:TYR:CE1	2.54	0.43
2:H:824:GLU:OE2	2:H:875:PRO:HB3	2.18	0.43
2:H:1593:LYS:HE2	2:H:1596:LEU:HD11	2.01	0.43
3:K:28:GLN:O	3:K:29:GLU:HB2	2.18	0.43
3:K:407:PRO:O	3:K:408:LEU:HD22	2.19	0.43
1:A:469:THR:O	1:A:511:ALA:HA	2.19	0.43
2:B:1031:TYR:O	2:B:1035:LEU:HG	2.19	0.43
1:C:219:LYS:NZ	1:C:356:ASN:HD22	2.17	0.43
2:D:1520:ASP:HB2	2:D:1586:SER:HB3	2.01	0.43
1:E:25:HIS:HA	1:E:26:ASP:HA	1.55	0.43
2:F:1223:ASP:O	2:F:1227:VAL:HG23	2.19	0.43
3:K:82:HIS:HE1	3:K:150:ARG:HB2	1.82	0.43
3:K:172:LEU:HD11	3:K:191:PRO:HB3	2.01	0.43
2:B:1215:LEU:HD23	2:B:1256:ALA:HB1	2.00	0.43
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.19	0.43
2:B:1497:PHE:HA	2:B:1601:GLY:O	2.18	0.43
2:F:1064:PHE:O	2:F:1068:VAL:HG13	2.19	0.43
1:G:25:HIS:HA	1:G:26:ASP:HA	1.52	0.43
2:H:904:ARG:HH22	3:L:82:HIS:HB2	1.83	0.43
2:H:956:THR:HG23	2:H:1324:THR:HG22	2.00	0.43
3:I:347:VAL:HA	3:I:348:PRO:O	2.18	0.43
3:J:278:TYR:CD1	3:J:450:LEU:HD11	2.54	0.43
2:B:746:PRO:HG2	2:B:774:LYS:HE3	2.01	0.43
2:B:927:PRO:O	2:B:928:GLU:HB2	2.19	0.43
2:F:966:ALA:HB2	2:F:1291:TRP:CH2	2.54	0.43
2:F:1405:ARG:HE	2:F:1437:LEU:HD23	1.84	0.43
3:K:250:LEU:HD12	3:K:362:MET:HB2	2.00	0.43
3:L:25:ARG:CZ	3:L:27:LEU:HD21	2.49	0.43
3:L:101:GLU:HG2	3:L:119:THR:OG1	2.19	0.43
3:L:216:THR:O	3:L:220:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HD2	1:A:103:LEU:HD21	2.01	0.42
2:B:1110:GLY:HA3	2:B:1165:TYR:CZ	2.54	0.42
2:D:1231:VAL:HG21	2:D:1260:TYR:CE1	2.54	0.42
2:D:1264:ALA:HA	2:D:1265:PRO:HD3	1.89	0.42
2:D:1458:TYR:HB3	2:D:1466:SER:HB3	2.00	0.42
2:H:1227:VAL:HB	2:H:1228:PRO:HD3	2.01	0.42
3:I:121:GLN:HE21	3:I:127:SER:HB3	1.84	0.42
3:I:582:LEU:HD21	3:I:597:LEU:HD21	2.01	0.42
3:J:69:ARG:H	3:J:69:ARG:HD2	1.84	0.42
3:L:705:ARG:HA	3:L:705:ARG:HD3	1.87	0.42
1:A:470:TYR:C	1:A:471:LEU:HD12	2.44	0.42
2:B:816:SER:HB2	2:B:910:VAL:HG23	2.00	0.42
2:F:956:THR:HG23	2:F:1324:THR:HG22	2.00	0.42
3:I:364:ASP:HB3	3:I:406:GLY:HA3	2.01	0.42
3:I:435:ASN:O	3:I:439:VAL:HG23	2.18	0.42
3:J:76:ILE:HG12	3:J:197:PHE:CE1	2.54	0.42
3:L:171:THR:HG23	3:L:412:VAL:HG22	2.01	0.42
3:L:210:LEU:HD11	3:L:443:MET:HG2	2.01	0.42
3:L:371:GLY:O	3:L:373:PRO:HD3	2.18	0.42
1:C:147:ASN:HB2	1:C:148:PRO:CD	2.49	0.42
2:D:958:ILE:O	2:D:1299:SER:HA	2.20	0.42
2:D:1257:LEU:O	2:D:1261:GLN:HG2	2.19	0.42
2:D:1405:ARG:HE	2:D:1437:LEU:HD23	1.84	0.42
1:E:323:GLY:O	1:E:325:PRO:HD3	2.18	0.42
3:I:189:THR:HG22	3:I:420:LYS:HB3	2.01	0.42
3:I:269:VAL:HG13	3:I:311:THR:HG23	2.02	0.42
3:I:692:ILE:HG12	3:I:717:HIS:CE1	2.54	0.42
3:J:19:ILE:HG23	3:J:22:GLY:C	2.43	0.42
3:J:41:PHE:HB3	3:J:74:ARG:O	2.19	0.42
3:K:692:ILE:HG12	3:K:717:HIS:CE1	2.54	0.42
3:L:437:GLU:HB3	3:L:441:TYR:HE2	1.84	0.42
1:A:241:LYS:HE2	2:B:804:MET:HE1	2.00	0.42
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.34	0.42
2:B:1108:ILE:HD11	2:B:1112:ARG:HA	2.01	0.42
2:B:1397:LYS:NZ	2:B:1412:LEU:HD23	2.34	0.42
2:D:1031:TYR:O	2:D:1035:LEU:HG	2.19	0.42
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.18	0.42
2:D:1064:PHE:O	2:D:1068:VAL:HG13	2.19	0.42
2:D:1107:MET:O	2:D:1248:GLN:HG2	2.19	0.42
2:D:1397:LYS:NZ	2:D:1412:LEU:HD23	2.34	0.42
1:E:344:PRO:HD2	1:E:433:TYR:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1119:MET:HE1	2:F:1154:LEU:HA	1.99	0.42
2:F:1119:MET:SD	2:F:1157:ASN:HB2	2.58	0.42
1:G:45:LEU:HA	1:G:46:VAL:HA	1.67	0.42
2:H:1119:MET:SD	2:H:1157:ASN:HB2	2.59	0.42
2:H:1296:LEU:HD23	2:H:1298:ARG:CZ	2.50	0.42
3:I:82:HIS:HE1	3:I:150:ARG:HB2	1.83	0.42
3:J:172:LEU:HD11	3:J:191:PRO:HB3	2.01	0.42
3:J:343:TRP:HA	3:J:344:PRO:HD3	1.90	0.42
3:K:80:ARG:HA	3:K:81:PRO:HD3	1.92	0.42
3:K:289:TYR:CG	3:K:333:ALA:HB2	2.54	0.42
3:L:172:LEU:HD11	3:L:191:PRO:HB3	2.01	0.42
3:L:683:ARG:O	3:L:685:ARG:HG2	2.20	0.42
2:B:1390:ALA:HA	2:B:1391:PRO:HD3	1.93	0.42
1:C:40:PHE:HD2	1:C:83:PHE:HB2	1.82	0.42
2:F:927:PRO:O	2:F:928:GLU:HB2	2.19	0.42
2:F:1231:VAL:HG21	2:F:1260:TYR:CE1	2.54	0.42
2:F:1593:LYS:HE2	2:F:1596:LEU:HD11	2.01	0.42
1:G:470:TYR:C	1:G:471:LEU:HD12	2.45	0.42
2:H:1154:LEU:HB2	2:H:1174:LEU:HD21	2.00	0.42
3:J:69:ARG:CD	3:J:69:ARG:N	2.82	0.42
3:J:341:MET:SD	3:J:380:ILE:HG23	2.59	0.42
3:L:476:VAL:HB	3:L:484:GLU:HB3	2.00	0.42
2:B:1477:ASP:OD1	2:B:1479:LYS:HD3	2.19	0.42
1:C:302:LEU:HG	1:C:326:ILE:HD11	2.01	0.42
2:D:956:THR:HG23	2:D:1324:THR:HG22	2.00	0.42
2:F:853:LEU:HB2	2:F:860:HIS:CD2	2.54	0.42
2:F:1227:VAL:HB	2:F:1228:PRO:HD3	2.02	0.42
2:F:1376:ALA:HB3	2:F:1429:VAL:HG23	2.01	0.42
1:G:5:SER:OG	1:G:23:GLU:HB2	2.19	0.42
2:H:1477:ASP:OD1	2:H:1479:LYS:HD3	2.19	0.42
3:J:353:ASN:HB2	3:J:394:ARG:NH1	2.35	0.42
3:J:582:LEU:HD21	3:J:597:LEU:HD21	2.01	0.42
3:K:692:ILE:HA	3:K:717:HIS:ND1	2.35	0.42
3:L:32:ALA:HA	3:L:57:TRP:HZ3	1.83	0.42
1:C:39:ASP:CG	1:C:44:LYS:HB3	2.45	0.42
2:D:853:LEU:HB2	2:D:860:HIS:CD2	2.54	0.42
2:D:1227:VAL:HB	2:D:1228:PRO:HD3	2.01	0.42
1:E:152:PRO:O	2:F:1296:LEU:HD12	2.20	0.42
2:F:966:ALA:HB2	2:F:1291:TRP:CZ3	2.55	0.42
2:F:1165:TYR:HD1	2:F:1210:ALA:HB2	1.84	0.42
2:F:1330:ALA:O	2:F:1331:LYS:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:323:GLY:O	1:G:325:PRO:HD3	2.19	0.42
2:H:776:SER:HB2	2:H:780:TRP:CZ2	2.55	0.42
3:I:171:THR:HG23	3:I:412:VAL:HG22	2.02	0.42
3:J:101:GLU:HG2	3:J:119:THR:OG1	2.20	0.42
3:L:82:HIS:HE1	3:L:150:ARG:HB2	1.82	0.42
3:L:269:VAL:HG13	3:L:311:THR:HG23	2.01	0.42
3:L:296:TRP:CE2	3:L:317:ILE:HG22	2.55	0.42
1:A:10:ASN:ND2	1:A:618:SER:O	2.50	0.42
2:D:1143:LEU:O	2:D:1147:ILE:HG13	2.19	0.42
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.19	0.42
1:E:268:ARG:HH11	2:F:1378:MET:CE	2.31	0.42
1:E:329:SER:HA	1:E:330:PRO:HD3	1.87	0.42
1:G:215:GLU:HG2	1:G:321:ARG:HH22	1.83	0.42
1:G:241:LYS:HE2	2:H:804:MET:HE1	2.01	0.42
1:G:439:LEU:HD12	1:G:439:LEU:H	1.84	0.42
2:H:1539:TYR:HB2	2:H:1562:PHE:HB2	2.01	0.42
3:I:125:ARG:HE	3:I:198:MET:HB3	1.85	0.42
3:J:431:LYS:HB3	3:J:435:ASN:HD22	1.84	0.42
3:J:692:ILE:HG12	3:J:717:HIS:CE1	2.55	0.42
3:L:692:ILE:HG12	3:L:717:HIS:CE1	2.55	0.42
1:A:323:GLY:O	1:A:325:PRO:HD3	2.19	0.42
2:B:732:ASP:O	2:B:733:ILE:HG12	2.20	0.42
2:B:1257:LEU:O	2:B:1261:GLN:HG2	2.19	0.42
1:C:45:LEU:H	1:C:45:LEU:CD2	2.30	0.42
2:D:904:ARG:NH2	3:J:82:HIS:HB2	2.34	0.42
1:E:39:ASP:CG	1:E:44:LYS:HB3	2.45	0.42
1:E:110:ILE:HG12	1:E:127:ILE:HG13	2.02	0.42
2:F:1393:THR:O	2:F:1397:LYS:HD3	2.19	0.42
2:H:997:THR:CG2	2:H:1251:PHE:HB2	2.50	0.42
3:I:431:LYS:HB3	3:I:435:ASN:ND2	2.35	0.42
3:J:299:VAL:HG13	3:J:340:MET:HE2	2.02	0.42
3:J:692:ILE:HA	3:J:717:HIS:ND1	2.35	0.42
3:K:57:TRP:CD1	3:K:57:TRP:H	2.38	0.42
3:K:61:LYS:HG2	3:K:67:THR:HG23	2.02	0.42
3:K:298:LYS:HZ2	3:K:340:MET:HA	1.85	0.42
3:K:408:LEU:HA	3:K:408:LEU:HD13	1.75	0.42
1:A:439:LEU:H	1:A:439:LEU:HD12	1.84	0.42
1:C:22:LEU:HB2	1:C:62:GLY:HA3	2.02	0.42
2:D:1133:LYS:HA	2:D:1143:LEU:HD21	2.02	0.42
2:D:1165:TYR:HD1	2:D:1210:ALA:HB2	1.84	0.42
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:SER:HA	1:E:361:PRO:HD3	1.95	0.42
3:I:25:ARG:CZ	3:I:27:LEU:HD21	2.49	0.42
3:I:296:TRP:CE2	3:I:317:ILE:HG22	2.54	0.42
3:K:19:ILE:HD11	3:K:73:CYS:CB	2.44	0.42
3:K:171:THR:HG23	3:K:412:VAL:HG22	2.02	0.42
3:K:563:TYR:CE1	3:K:569:PRO:HD3	2.55	0.42
2:B:1008:GLU:CD	2:B:1262:LYS:HD3	2.45	0.41
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.60	0.41
1:C:241:LYS:HE2	2:D:804:MET:HE1	2.01	0.41
2:D:1331:LYS:HA	2:D:1332:ASP:CB	2.50	0.41
1:G:630:GLN:NE2	1:G:630:GLN:H	2.18	0.41
2:H:1331:LYS:CA	2:H:1332:ASP:HB2	2.50	0.41
2:H:1333:GLN:HA	2:H:1334:LEU:C	2.45	0.41
3:J:705:ARG:HD3	3:J:705:ARG:HA	1.86	0.41
3:K:44:TYR:HB3	3:K:73:CYS:CA	2.49	0.41
3:K:62:THR:HG23	3:K:68:VAL:HG21	2.02	0.41
3:K:683:ARG:O	3:K:685:ARG:HG2	2.20	0.41
3:L:45:PRO:HG3	3:L:68:VAL:HG21	2.02	0.41
3:L:582:LEU:HD21	3:L:597:LEU:HD21	2.01	0.41
1:A:342:PHE:CD2	1:A:391:THR:HG21	2.55	0.41
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.02	0.41
2:B:1405:ARG:HE	2:B:1437:LEU:HD23	1.83	0.41
1:C:1:SER:HA	1:C:2:PRO:HD3	1.93	0.41
2:D:1370:TYR:CD1	2:D:1376:ALA:HB2	2.55	0.41
1:G:304:VAL:O	1:G:320:GLU:HA	2.21	0.41
2:H:1331:LYS:HA	2:H:1332:ASP:HB2	2.02	0.41
3:I:59:THR:HG23	3:I:61:LYS:HG2	2.02	0.41
3:I:683:ARG:O	3:I:685:ARG:HG2	2.20	0.41
3:J:568:ARG:HA	3:J:569:PRO:HD3	1.88	0.41
3:K:42:TYR:CE1	3:K:74:ARG:HB2	2.55	0.41
3:L:218:GLU:HB3	3:L:452:LEU:CD2	2.50	0.41
1:A:304:VAL:O	1:A:320:GLU:HA	2.20	0.41
2:B:813:LEU:HD23	2:B:907:LEU:HD13	2.01	0.41
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.85	0.41
2:B:1231:VAL:HG21	2:B:1260:TYR:CE1	2.56	0.41
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.20	0.41
2:B:1581:LEU:HB2	2:B:1609:TRP:HE3	1.85	0.41
1:C:268:ARG:HH11	2:D:1378:MET:CE	2.32	0.41
2:D:746:PRO:HG2	2:D:774:LYS:HE3	2.02	0.41
2:D:1215:LEU:HD23	2:D:1256:ALA:HB1	2.01	0.41
2:D:1477:ASP:OD1	2:D:1479:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:PHE:CD2	1:E:100:LEU:HA	2.55	0.41
1:E:241:LYS:HE2	2:F:804:MET:HE1	2.02	0.41
2:F:1370:TYR:CD1	2:F:1376:ALA:HB2	2.55	0.41
2:F:1386:MET:SD	2:F:1473:PRO:HD3	2.60	0.41
2:F:1477:ASP:OD1	2:F:1479:LYS:HD3	2.20	0.41
1:G:219:LYS:NZ	1:G:356:ASN:HD22	2.18	0.41
1:G:567:HIS:ND1	2:H:760:PRO:HG3	2.34	0.41
2:H:1155:GLU:HG3	2:H:1184:LEU:HD21	2.01	0.41
3:I:101:GLU:HG2	3:I:119:THR:OG1	2.20	0.41
3:J:69:ARG:H	3:J:69:ARG:CD	2.32	0.41
3:J:121:GLN:HE21	3:J:127:SER:HB3	1.85	0.41
3:J:289:TYR:CG	3:J:333:ALA:HB2	2.55	0.41
2:B:958:ILE:O	2:B:1299:SER:HA	2.19	0.41
1:C:470:TYR:C	1:C:471:LEU:HD12	2.46	0.41
2:D:813:LEU:HD23	2:D:907:LEU:HD13	2.02	0.41
2:D:1263:ASP:O	2:D:1265:PRO:HD3	2.20	0.41
2:D:1481:ASN:HD22	2:D:1567:LYS:HE3	1.85	0.41
2:F:1257:LEU:O	2:F:1261:GLN:HG2	2.20	0.41
3:I:347:VAL:HG13	3:I:349:PRO:HG3	2.02	0.41
3:J:479:PRO:C	3:J:481:LYS:H	2.28	0.41
3:K:216:THR:O	3:K:216:THR:HG22	2.20	0.41
3:K:337:VAL:HG12	3:K:341:MET:HE3	2.02	0.41
3:K:431:LYS:HB3	3:K:435:ASN:HD22	1.85	0.41
3:K:531:HIS:HA	3:K:532:PRO:HD3	1.93	0.41
3:L:173:ARG:HA	3:L:415:ASN:ND2	2.35	0.41
3:L:431:LYS:HB3	3:L:435:ASN:ND2	2.36	0.41
3:L:666:ASP:HA	3:L:667:PRO:HD3	1.93	0.41
1:A:459:ARG:HA	1:A:462:GLU:CG	2.51	0.41
1:A:614:ALA:HB1	1:A:632:THR:HA	2.02	0.41
1:C:304:VAL:O	1:C:320:GLU:HA	2.21	0.41
1:C:468:TYR:HB2	1:C:484:GLN:HB3	2.02	0.41
1:E:22:LEU:HB2	1:E:62:GLY:HA3	2.03	0.41
1:E:219:LYS:NZ	1:E:356:ASN:HD22	2.18	0.41
1:E:440:ARG:HA	1:E:440:ARG:HD2	1.92	0.41
2:F:1095:VAL:HG13	2:F:1122:THR:OG1	2.20	0.41
2:F:1163:ARG:O	2:F:1167:VAL:HG23	2.20	0.41
1:G:75:LYS:C	1:G:82:LYS:HZ1	2.29	0.41
2:H:1231:VAL:HG21	2:H:1260:TYR:CE1	2.55	0.41
3:J:585:PRO:HA	3:J:586:PRO:HD3	1.95	0.41
3:J:635:ALA:HB3	3:J:647:ILE:HD11	2.02	0.41
3:J:706:GLN:O	3:J:707:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:101:GLU:HG2	3:K:119:THR:OG1	2.20	0.41
3:L:59:THR:HG23	3:L:61:LYS:HG2	2.02	0.41
1:A:360:SER:HA	1:A:361:PRO:HD3	1.95	0.41
2:B:1360:ASN:O	2:B:1361:THR:O	2.38	0.41
2:B:1593:LYS:HE2	2:B:1596:LEU:HD11	2.01	0.41
2:D:1110:GLY:HA3	2:D:1165:TYR:CZ	2.55	0.41
2:D:1338:LYS:HD2	2:D:1338:LYS:H	1.86	0.41
2:D:1390:ALA:HA	2:D:1391:PRO:HD3	1.93	0.41
1:E:14:LEU:HD22	1:E:69:PRO:O	2.20	0.41
1:E:304:VAL:O	1:E:320:GLU:HA	2.21	0.41
2:H:927:PRO:O	2:H:928:GLU:HB2	2.19	0.41
2:H:1370:TYR:CD1	2:H:1376:ALA:HB2	2.55	0.41
3:J:351:GLY:HA2	3:J:354:ARG:HE	1.85	0.41
3:J:597:LEU:C	3:J:599:PRO:HD3	2.46	0.41
3:K:125:ARG:HE	3:K:198:MET:HB3	1.85	0.41
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.55	0.41
2:D:912:GLU:HG3	2:D:1331:LYS:NZ	2.35	0.41
2:D:997:THR:CG2	2:D:1251:PHE:HB2	2.50	0.41
2:D:1051:ALA:HA	2:D:1052:PRO:HD3	1.96	0.41
2:D:1108:ILE:HD11	2:D:1112:ARG:HA	2.01	0.41
2:F:1539:TYR:HB2	2:F:1562:PHE:HB2	2.02	0.41
1:G:218:GLU:C	1:G:220:PHE:H	2.29	0.41
2:H:1397:LYS:NZ	2:H:1412:LEU:HD23	2.35	0.41
3:I:247:TYR:OH	3:I:357:HIS:HD2	2.03	0.41
3:I:437:GLU:HB3	3:I:441:TYR:HE2	1.84	0.41
3:J:216:THR:O	3:J:216:THR:HG22	2.21	0.41
3:K:121:GLN:HE21	3:K:127:SER:HB3	1.85	0.41
3:L:597:LEU:C	3:L:599:PRO:HD3	2.46	0.41
1:A:7:ILE:HG22	1:A:622:LEU:HD22	2.03	0.41
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.21	0.41
1:C:567:HIS:ND1	2:D:760:PRO:HG3	2.34	0.41
2:D:1564:SER:HA	2:D:1565:PRO:HD3	1.97	0.41
1:E:567:HIS:ND1	2:F:760:PRO:HG3	2.35	0.41
1:G:207:LEU:HA	1:G:208:PRO:HD3	1.96	0.41
1:G:342:PHE:CD2	1:G:391:THR:HG21	2.55	0.41
2:H:850:PHE:HZ	2:H:907:LEU:HD21	1.85	0.41
2:H:1126:LEU:HD13	2:H:1150:ALA:HB3	2.03	0.41
2:H:1133:LYS:HA	2:H:1143:LEU:HD21	2.03	0.41
2:H:1143:LEU:O	2:H:1147:ILE:HG13	2.20	0.41
2:H:1535:ASP:CG	2:H:1536:PHE:H	2.28	0.41
2:H:1581:LEU:HB2	2:H:1609:TRP:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:568:ARG:HG3	3:I:569:PRO:HD2	2.03	0.41
3:I:597:LEU:C	3:I:599:PRO:HD3	2.46	0.41
3:I:706:GLN:O	3:I:707:LYS:HB2	2.20	0.41
3:J:42:TYR:HA	3:J:43:PRO:HD3	1.97	0.41
3:K:463:THR:HB	3:K:466:HIS:CE1	2.55	0.41
3:L:216:THR:O	3:L:216:THR:HG22	2.21	0.41
2:B:1143:LEU:O	2:B:1147:ILE:HG13	2.20	0.41
2:B:1331:LYS:CA	2:B:1332:ASP:HB2	2.51	0.41
2:B:1641:ASN:OXT	3:I:253:SER:HB2	2.21	0.41
1:C:126:ARG:C	1:C:127:ILE:HD12	2.46	0.41
1:C:329:SER:HA	1:C:330:PRO:HD3	1.87	0.41
1:C:630:GLN:NE2	1:C:630:GLN:H	2.19	0.41
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.56	0.41
1:E:151:ILE:CG2	2:F:1297:LEU:HG	2.50	0.41
1:E:453:PHE:HB2	1:E:493:VAL:HG22	2.03	0.41
1:E:468:TYR:HB2	1:E:484:GLN:HB3	2.03	0.41
1:E:470:TYR:C	1:E:471:LEU:HD12	2.45	0.41
2:F:776:SER:HB2	2:F:780:TRP:CZ2	2.56	0.41
2:F:1260:TYR:O	2:F:1264:ALA:HB2	2.21	0.41
1:G:103:LEU:H	1:G:103:LEU:HD22	1.86	0.41
1:G:152:PRO:O	2:H:1296:LEU:HD12	2.20	0.41
1:G:187:TYR:CD1	1:G:192:PRO:HA	2.56	0.41
1:G:459:ARG:HA	1:G:462:GLU:CG	2.51	0.41
1:G:468:TYR:HB2	1:G:484:GLN:HB3	2.03	0.41
2:H:1490:ARG:HD2	2:H:1590:TRP:CZ3	2.56	0.41
2:H:1532:LEU:N	2:H:1532:LEU:HD12	2.35	0.41
3:J:563:TYR:CE1	3:J:569:PRO:HD3	2.55	0.41
3:K:16:GLY:O	3:K:17:VAL:C	2.64	0.41
3:K:463:THR:HB	3:K:466:HIS:ND1	2.36	0.41
3:K:582:LEU:HD21	3:K:597:LEU:HD21	2.02	0.41
3:K:597:LEU:C	3:K:599:PRO:HD3	2.45	0.41
1:A:219:LYS:NZ	1:A:356:ASN:HD22	2.18	0.41
2:B:813:LEU:HD23	2:B:907:LEU:HD22	2.03	0.41
2:B:997:THR:CG2	2:B:1251:PHE:HB2	2.51	0.41
2:B:1346:LYS:HA	2:B:1347:PRO:HD3	1.95	0.41
1:C:459:ARG:HA	1:C:462:GLU:CG	2.51	0.41
1:C:614:ALA:HB1	1:C:632:THR:HA	2.03	0.41
2:D:1163:ARG:O	2:D:1167:VAL:HG23	2.21	0.41
2:D:1260:TYR:O	2:D:1264:ALA:HB2	2.21	0.41
2:F:1110:GLY:HA3	2:F:1165:TYR:CZ	2.56	0.41
2:F:1397:LYS:NZ	2:F:1412:LEU:HD23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1641:ASN:OXT	3:K:255:SER:HB3	2.21	0.41
2:H:746:PRO:HG2	2:H:774:LYS:HE3	2.02	0.41
3:I:254:GLY:HA2	3:I:319:TYR:OH	2.21	0.41
3:I:289:TYR:CG	3:I:333:ALA:HB2	2.56	0.41
3:J:463:THR:HB	3:J:466:HIS:CE1	2.56	0.41
3:K:285:GLY:HA3	3:K:340:MET:HE1	2.03	0.41
1:A:630:GLN:NE2	1:A:630:GLN:H	2.19	0.40
1:C:5:SER:OG	1:C:23:GLU:HB2	2.21	0.40
1:C:218:GLU:C	1:C:220:PHE:H	2.29	0.40
1:E:241:LYS:HG3	2:F:832:TYR:CE1	2.57	0.40
2:F:1472:HIS:HA	2:F:1473:PRO:HD3	1.99	0.40
2:H:1272:LEU:O	2:H:1288:ARG:HA	2.21	0.40
2:H:1332:ASP:HB3	2:H:1333:GLN:H	1.69	0.40
3:I:45:PRO:HG3	3:I:68:VAL:HG21	2.03	0.40
3:I:692:ILE:HA	3:I:717:HIS:ND1	2.35	0.40
3:J:423:ASN:ND2	3:J:583:ARG:HB2	2.36	0.40
3:J:683:ARG:O	3:J:685:ARG:HG2	2.21	0.40
3:L:408:LEU:HD22	3:L:408:LEU:N	2.37	0.40
3:L:563:TYR:CE1	3:L:569:PRO:HD3	2.55	0.40
3:L:706:GLN:O	3:L:707:LYS:HB2	2.21	0.40
1:A:111:GLN:O	1:A:125:TYR:HA	2.22	0.40
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.21	0.40
2:D:990:GLU:O	2:D:994:ILE:HG13	2.22	0.40
2:D:1296:LEU:HD23	2:D:1298:ARG:CZ	2.51	0.40
2:D:1386:MET:SD	2:D:1473:PRO:HD3	2.61	0.40
2:D:1472:HIS:HA	2:D:1473:PRO:HD3	1.98	0.40
2:F:912:GLU:HG3	2:F:1331:LYS:NZ	2.36	0.40
2:F:1215:LEU:HD23	2:F:1256:ALA:HB1	2.02	0.40
2:F:1231:VAL:HG21	2:F:1260:TYR:CD1	2.56	0.40
1:G:363:TYR:HD1	1:G:381:GLY:HA2	1.87	0.40
1:G:614:ALA:HB1	1:G:632:THR:HA	2.03	0.40
2:H:839:LYS:O	2:H:895:TYR:HD1	2.04	0.40
2:H:1031:TYR:O	2:H:1035:LEU:HG	2.20	0.40
2:H:1065:SER:OG	2:H:1132:ALA:HB2	2.21	0.40
2:H:1108:ILE:HD11	2:H:1112:ARG:HA	2.02	0.40
3:I:265:LYS:O	3:I:269:VAL:HG23	2.21	0.40
3:J:39:SER:OG	3:J:122:VAL:HG21	2.21	0.40
3:J:68:VAL:HG12	3:J:69:ARG:N	2.34	0.40
3:J:125:ARG:HE	3:J:198:MET:HB3	1.86	0.40
3:L:265:LYS:O	3:L:269:VAL:HG23	2.22	0.40
1:A:40:PHE:CD1	1:A:41:PRO:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.56	0.40
2:D:917:ASN:HD22	4:D:1917:NAG:C7	2.28	0.40
2:D:1055:TRP:HZ2	2:D:1248:GLN:HE21	1.69	0.40
2:D:1346:LYS:HA	2:D:1347:PRO:HD3	1.95	0.40
1:E:445:PRO:HG2	1:E:504:ILE:HD11	2.04	0.40
2:F:1504:LYS:O	2:F:1505:VAL:C	2.64	0.40
1:G:22:LEU:HD13	1:G:33:VAL:HG11	2.02	0.40
1:G:100:LEU:HD12	1:G:101:VAL:H	1.86	0.40
3:I:341:MET:SD	3:I:380:ILE:HG23	2.61	0.40
3:K:452:LEU:HB3	3:K:455:MET:HG3	2.03	0.40
1:A:22:LEU:HD13	1:A:33:VAL:HG11	2.03	0.40
1:C:83:PHE:CD2	1:C:100:LEU:HA	2.56	0.40
2:D:1634:MET:HE1	2:D:1639:CYS:SG	2.60	0.40
1:E:187:TYR:CD1	1:E:192:PRO:HA	2.57	0.40
2:F:804:MET:HG2	2:F:805:GLN:H	1.87	0.40
2:F:1055:TRP:HZ2	2:F:1248:GLN:HE21	1.70	0.40
1:G:111:GLN:O	1:G:125:TYR:HA	2.21	0.40
1:G:505:PRO:HG3	1:G:595:TRP:CE3	2.55	0.40
2:H:1634:MET:HE1	2:H:1639:CYS:SG	2.62	0.40
3:I:216:THR:O	3:I:216:THR:HG22	2.21	0.40
3:I:343:TRP:CB	3:I:347:VAL:HG12	2.45	0.40
3:I:347:VAL:HA	3:I:348:PRO:C	2.46	0.40
3:K:173:ARG:HA	3:K:415:ASN:ND2	2.35	0.40
3:K:635:ALA:HB3	3:K:647:ILE:HD11	2.03	0.40
3:K:706:GLN:O	3:K:707:LYS:HB2	2.21	0.40
3:L:125:ARG:HE	3:L:198:MET:HB3	1.85	0.40
3:L:676:GLY:HA2	3:L:677:PRO:HD3	1.84	0.40
1:A:100:LEU:HD12	1:A:101:VAL:H	1.86	0.40
1:A:126:ARG:C	1:A:127:ILE:HD12	2.47	0.40
1:A:329:SER:C	1:A:331:TYR:H	2.30	0.40
1:A:468:TYR:HB2	1:A:484:GLN:HB3	2.02	0.40
2:B:845:LEU:N	2:B:845:LEU:HD12	2.37	0.40
2:B:986:SER:HB2	1:E:257:GLU:CG	2.52	0.40
1:E:126:ARG:C	1:E:127:ILE:HD12	2.47	0.40
1:E:269:ILE:HA	1:E:270:PRO:HD3	1.92	0.40
1:E:363:TYR:HD1	1:E:381:GLY:HA2	1.87	0.40
2:F:740:VAL:HG21	3:K:94:PRO:HB3	2.03	0.40
1:G:187:TYR:HB3	1:G:195:VAL:HA	2.04	0.40
2:H:742:ARG:NH1	2:H:777:ILE:HG13	2.36	0.40
3:I:37:CYS:HA	3:I:38:PRO:HD3	1.95	0.40
3:I:563:TYR:CE1	3:I:569:PRO:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:641:TYR:HA	3:I:644:VAL:HG23	2.04	0.40
3:J:132:ILE:HG12	3:J:144:GLY:HA3	2.03	0.40
3:J:435:ASN:O	3:J:439:VAL:HG23	2.22	0.40
3:K:57:TRP:CD1	3:K:57:TRP:N	2.89	0.40
3:K:210:LEU:HD11	3:K:443:MET:HG2	2.04	0.40
3:K:260:ASP:O	3:K:433:MET:HE3	2.22	0.40
3:L:568:ARG:HG3	3:L:569:PRO:HD2	2.04	0.40
3:L:660:GLY:HA3	3:L:714:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

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	636/645 (99%)	574 (90%)	56 (9%)	6 (1%)	14	48
1	C	636/645 (99%)	575 (90%)	57 (9%)	4 (1%)	21	57
1	E	636/645 (99%)	573 (90%)	58 (9%)	5 (1%)	16	52
1	G	636/645 (99%)	578 (91%)	53 (8%)	5 (1%)	16	52
2	B	895/915 (98%)	785 (88%)	95 (11%)	15 (2%)	7	36
2	D	895/915 (98%)	787 (88%)	95 (11%)	13 (2%)	8	38
2	F	895/915 (98%)	785 (88%)	97 (11%)	13 (2%)	8	38
2	H	895/915 (98%)	790 (88%)	92 (10%)	13 (2%)	8	38
3	I	706/741 (95%)	636 (90%)	62 (9%)	8 (1%)	11	44
3	J	707/741 (95%)	630 (89%)	65 (9%)	12 (2%)	7	36
3	K	707/741 (95%)	627 (89%)	67 (10%)	13 (2%)	6	34
3	L	705/741 (95%)	641 (91%)	59 (8%)	5 (1%)	18	54
All	All	8949/9204 (97%)	7981 (89%)	856 (10%)	112 (1%)	9	41

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	733	ILE
2	B	965	VAL
2	B	1361	THR
2	D	733	ILE
2	D	965	VAL
2	D	969	THR
2	D	1361	THR
2	D	1498	ILE
2	F	733	ILE
2	F	965	VAL
2	F	1361	THR
2	F	1498	ILE
2	H	733	ILE
2	H	965	VAL
2	H	1361	THR
3	I	348	PRO
3	J	17	VAL
3	J	28	GLN
3	J	38	PRO
3	K	17	VAL
3	K	28	GLN
3	K	38	PRO
3	K	407	PRO
1	A	574	VAL
2	B	1335	THR
2	B	1377	THR
2	B	1498	ILE
2	B	1505	VAL
1	C	574	VAL
2	D	1335	THR
2	D	1377	THR
2	D	1505	VAL
1	E	574	VAL
2	F	1335	THR
2	F	1377	THR
1	G	574	VAL
2	H	1335	THR
2	H	1377	THR
2	H	1498	ILE
2	H	1505	VAL
3	I	197	PHE
3	I	199	TYR

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Mol	Chain	Res	Type
3	J	67	THR
3	J	197	PHE
3	J	199	TYR
3	J	349	PRO
3	J	457	TRP
3	K	67	THR
3	K	197	PHE
3	K	199	TYR
3	L	197	PHE
3	L	199	TYR
1	A	71	ASN
1	A	549	GLU
2	B	732	ASP
2	B	969	THR
1	C	549	GLU
1	E	549	GLU
2	F	1505	VAL
1	G	549	GLU
2	H	1331	LYS
2	H	1535	ASP
3	I	740	ALA
3	J	740	ALA
3	K	740	ALA
3	L	740	ALA
1	A	505	PRO
2	B	1196	ASN
2	B	1331	LYS
1	C	505	PRO
2	D	1196	ASN
1	E	505	PRO
2	F	1196	ASN
2	F	1535	ASP
1	G	505	PRO
2	H	1196	ASN
3	J	456	VAL
3	K	73	CYS
3	K	406	GLY
1	A	442	GLU
2	B	988	CYS
2	B	1265	PRO
2	B	1486	ASP
1	C	442	GLU

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Mol	Chain	Res	Type
2	D	988	CYS
2	D	1535	ASP
1	E	442	GLU
2	F	969	THR
2	F	988	CYS
1	G	442	GLU
2	H	988	CYS
2	H	1486	ASP
3	I	241	SER
3	I	481	LYS
3	K	348	PRO
3	K	479	PRO
2	D	1486	ASP
2	F	1486	ASP
3	I	345	ASP
3	J	406	GLY
3	J	479	PRO
3	K	68	VAL
2	B	1201	PRO
2	D	1201	PRO
2	F	1201	PRO
2	H	1201	PRO
3	L	479	PRO
1	A	555	PRO
1	E	555	PRO
1	G	555	PRO
3	I	45	PRO
3	L	45	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	564/567 (100%)	559 (99%)	5 (1%)	70	76
1	C	564/567 (100%)	560 (99%)	4 (1%)	76	79
1	E	564/567 (100%)	560 (99%)	4 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	564/567 (100%)	560 (99%)	4 (1%)	76	79
2	B	797/810 (98%)	790 (99%)	7 (1%)	70	76
2	D	797/810 (98%)	792 (99%)	5 (1%)	78	81
2	F	797/810 (98%)	792 (99%)	5 (1%)	78	81
2	H	797/810 (98%)	792 (99%)	5 (1%)	78	81
3	I	616/643 (96%)	614 (100%)	2 (0%)	86	85
3	J	616/643 (96%)	605 (98%)	11 (2%)	51	68
3	K	618/643 (96%)	607 (98%)	11 (2%)	51	68
3	L	616/643 (96%)	615 (100%)	1 (0%)	87	87
All	All	7910/8080 (98%)	7846 (99%)	64 (1%)	73	77

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	370	GLN
1	A	404	THR
1	A	547	GLN
1	A	630	GLN
2	B	959	LEU
2	B	965	VAL
2	B	1301	GLU
2	B	1334	LEU
2	B	1342	LYS
2	B	1463	LEU
2	B	1573	LYS
1	C	370	GLN
1	C	404	THR
1	C	547	GLN
1	C	630	GLN
2	D	959	LEU
2	D	965	VAL
2	D	1334	LEU
2	D	1342	LYS
2	D	1573	LYS
1	E	370	GLN
1	E	404	THR
1	E	547	GLN
1	E	630	GLN

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Mol	Chain	Res	Type
2	F	959	LEU
2	F	965	VAL
2	F	1334	LEU
2	F	1342	LYS
2	F	1573	LYS
1	G	370	GLN
1	G	404	THR
1	G	547	GLN
1	G	630	GLN
2	H	959	LEU
2	H	965	VAL
2	H	1334	LEU
2	H	1342	LYS
2	H	1573	LYS
3	I	347	VAL
3	I	481	LYS
3	J	14	LEU
3	J	19	ILE
3	J	48	THR
3	J	57	TRP
3	J	60	LEU
3	J	62	THR
3	J	69	ARG
3	J	76	ILE
3	J	408	LEU
3	J	430	VAL
3	J	468	GLN
3	K	14	LEU
3	K	19	ILE
3	K	26	LEU
3	K	27	LEU
3	K	48	THR
3	K	57	TRP
3	K	60	LEU
3	K	62	THR
3	K	408	LEU
3	K	430	VAL
3	K	468	GLN
3	L	468	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	38	HIS
1	A	59	ASN
1	A	71	ASN
1	A	87	GLN
1	A	104	GLN
1	A	111	GLN
1	A	258	GLN
1	A	318	GLN
1	A	356	ASN
1	A	370	GLN
1	A	392	HIS
1	A	414	GLN
1	A	490	GLN
1	A	552	GLN
1	A	558	GLN
1	A	630	GLN
2	B	770	ASN
2	B	835	ASN
2	B	860	HIS
2	B	862	GLN
2	B	961	GLN
2	B	1090	GLN
2	B	1130	GLN
2	B	1237	GLN
2	B	1255	GLN
2	B	1268	GLN
2	B	1443	GLN
2	B	1534	ASN
2	B	1545	GLN
1	C	38	HIS
1	C	59	ASN
1	C	87	GLN
1	C	93	GLN
1	C	104	GLN
1	C	111	GLN
1	C	132	HIS
1	C	258	GLN
1	C	318	GLN
1	C	356	ASN
1	C	370	GLN
1	C	414	GLN
1	C	490	GLN

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Mol	Chain	Res	Type
1	C	552	GLN
1	C	558	GLN
1	C	630	GLN
2	D	752	ASN
2	D	770	ASN
2	D	835	ASN
2	D	860	HIS
2	D	862	GLN
2	D	961	GLN
2	D	1090	GLN
2	D	1130	GLN
2	D	1237	GLN
2	D	1268	GLN
2	D	1443	GLN
2	D	1481	ASN
2	D	1545	GLN
1	E	38	HIS
1	E	59	ASN
1	E	104	GLN
1	E	111	GLN
1	E	132	HIS
1	E	258	GLN
1	E	311	HIS
1	E	318	GLN
1	E	356	ASN
1	E	370	GLN
1	E	414	GLN
1	E	490	GLN
1	E	552	GLN
1	E	558	GLN
1	E	630	GLN
2	F	752	ASN
2	F	770	ASN
2	F	835	ASN
2	F	860	HIS
2	F	862	GLN
2	F	961	GLN
2	F	1090	GLN
2	F	1130	GLN
2	F	1237	GLN
2	F	1268	GLN
2	F	1290	HIS

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Mol	Chain	Res	Type
2	F	1443	GLN
2	F	1481	ASN
2	F	1545	GLN
1	G	38	HIS
1	G	59	ASN
1	G	71	ASN
1	G	87	GLN
1	G	104	GLN
1	G	111	GLN
1	G	318	GLN
1	G	356	ASN
1	G	370	GLN
1	G	414	GLN
1	G	490	GLN
1	G	552	GLN
1	G	558	GLN
1	G	630	GLN
2	H	770	ASN
2	H	835	ASN
2	H	860	HIS
2	H	862	GLN
2	H	961	GLN
2	H	1090	GLN
2	H	1130	GLN
2	H	1237	GLN
2	H	1268	GLN
2	H	1443	GLN
2	H	1481	ASN
2	H	1545	GLN
3	I	82	HIS
3	I	97	ASN
3	I	121	GLN
3	I	194	GLN
3	I	357	HIS
3	I	367	HIS
3	I	415	ASN
3	I	435	ASN
3	I	448	GLN
3	I	483	HIS
3	I	591	GLN
3	J	77	HIS
3	J	97	ASN

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Mol	Chain	Res	Type
3	J	121	GLN
3	J	194	GLN
3	J	357	HIS
3	J	415	ASN
3	J	448	GLN
3	J	591	GLN
3	J	708	GLN
3	K	82	HIS
3	K	121	GLN
3	K	194	GLN
3	K	357	HIS
3	K	415	ASN
3	K	435	ASN
3	K	448	GLN
3	K	591	GLN
3	K	708	GLN
3	L	77	HIS
3	L	121	GLN
3	L	194	GLN
3	L	357	HIS
3	L	367	HIS
3	L	415	ASN
3	L	435	ASN
3	L	448	GLN
3	L	468	GLN
3	L	591	GLN
3	L	708	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	L	1353	3	14,14,15	0.53	0	17,19,21	0.58	0
4	NAG	K	1353	3	14,14,15	0.57	0	17,19,21	2.08	3 (17%)
4	NAG	B	1917	2	14,14,15	0.49	0	17,19,21	1.06	1 (5%)
4	NAG	D	1917	2	14,14,15	0.49	0	17,19,21	1.19	1 (5%)
4	NAG	I	1353	3	14,14,15	0.41	0	17,19,21	1.29	1 (5%)
4	NAG	J	1353	3	14,14,15	0.52	0	17,19,21	0.60	0
4	NAG	H	1917	2	14,14,15	0.49	0	17,19,21	1.16	2 (11%)
4	NAG	F	1917	2	14,14,15	0.50	0	17,19,21	0.82	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
4	NAG	L	1353	3	-	0/6/23/26	0/1/1/1
4	NAG	K	1353	3	-	2/6/23/26	0/1/1/1
4	NAG	B	1917	2	-	3/6/23/26	0/1/1/1
4	NAG	D	1917	2	-	2/6/23/26	0/1/1/1
4	NAG	I	1353	3	-	3/6/23/26	0/1/1/1
4	NAG	J	1353	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1917	2	-	1/6/23/26	0/1/1/1
4	NAG	F	1917	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1353	NAG	C2-N2-C7	-6.49	114.20	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1353	NAG	C1-O5-C5	4.39	118.08	112.19
4	D	1917	NAG	C2-N2-C7	-3.84	117.75	122.90
4	K	1353	NAG	C1-C2-N2	3.69	116.25	110.43
4	K	1353	NAG	O5-C1-C2	-3.63	105.67	111.29
4	H	1917	NAG	C1-O5-C5	2.84	116.00	112.19
4	B	1917	NAG	C1-O5-C5	2.55	115.60	112.19
4	H	1917	NAG	O5-C1-C2	2.11	114.55	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1353	NAG	C8-C7-N2-C2
4	K	1353	NAG	O7-C7-N2-C2
4	D	1917	NAG	C8-C7-N2-C2
4	D	1917	NAG	O7-C7-N2-C2
4	I	1353	NAG	C8-C7-N2-C2
4	I	1353	NAG	O7-C7-N2-C2
4	I	1353	NAG	O5-C5-C6-O6
4	B	1917	NAG	C8-C7-N2-C2
4	H	1917	NAG	C4-C5-C6-O6
4	B	1917	NAG	O7-C7-N2-C2
4	B	1917	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1353	NAG	6	0
4	D	1917	NAG	1	0
4	J	1353	NAG	1	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	640/645 (99%)	0.43	10 (1%) 70 52	68, 145, 225, 312	0
1	C	640/645 (99%)	0.53	20 (3%) 51 37	64, 139, 220, 312	0
1	E	640/645 (99%)	0.57	33 (5%) 33 27	69, 140, 221, 313	0
1	G	640/645 (99%)	0.32	7 (1%) 78 60	69, 146, 224, 313	0
2	B	901/915 (98%)	0.25	16 (1%) 67 50	48, 112, 181, 342	0
2	D	901/915 (98%)	0.32	25 (2%) 55 40	44, 110, 191, 351	0
2	F	901/915 (98%)	0.26	14 (1%) 70 52	52, 112, 189, 337	0
2	H	901/915 (98%)	0.24	14 (1%) 70 52	47, 112, 183, 341	0
3	I	712/741 (96%)	0.13	1 (0%) 92 87	46, 113, 180, 276	0
3	J	713/741 (96%)	0.21	12 (1%) 69 51	42, 110, 197, 343	0
3	K	713/741 (96%)	0.18	7 (0%) 79 61	43, 112, 201, 357	0
3	L	711/741 (95%)	0.15	8 (1%) 78 60	45, 112, 181, 276	0
All	All	9013/9204 (97%)	0.29	167 (1%) 66 49	42, 119, 202, 357	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1537	ASP	5.4
2	B	1065	SER	4.4
2	D	1015	PHE	4.2
3	K	71	ALA	4.0
1	A	636	ALA	3.9
3	J	407	PRO	3.9
3	K	457	TRP	3.8
1	E	626	SER	3.8
1	E	453	PHE	3.7
2	F	1016	GLY	3.6
2	B	1388	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	969	THR	3.5
1	E	389	ILE	3.5
2	F	1015	PHE	3.4
2	D	1016	GLY	3.4
2	B	1061	VAL	3.3
3	J	21	GLY	3.3
2	F	969	THR	3.3
1	E	625	THR	3.2
3	L	601	GLN	3.2
1	C	626	SER	3.2
3	J	445	ASP	3.1
3	K	73	CYS	3.1
1	E	633	ALA	3.1
1	E	325	PRO	3.1
1	G	78	LYS	3.0
2	F	1017	LEU	3.0
2	F	1289	ILE	3.0
1	C	634	GLN	2.9
2	D	1017	LEU	2.9
2	F	1236	GLU	2.9
3	L	600	ALA	2.9
1	C	368	ALA	2.9
3	J	708	GLN	2.9
1	C	503	PHE	2.8
1	E	103	LEU	2.8
2	H	997	THR	2.8
2	H	1536	PHE	2.8
2	D	1018	GLU	2.8
3	K	449	SER	2.8
3	J	406	GLY	2.7
1	G	636	ALA	2.7
2	B	855	THR	2.7
3	K	407	PRO	2.7
1	E	62	GLY	2.7
1	C	636	ALA	2.7
2	D	1517	PRO	2.7
2	H	1063	VAL	2.7
3	L	254	GLY	2.7
2	H	855	THR	2.7
1	E	624	PHE	2.7
1	E	583	LEU	2.7
1	C	623	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	609	SER	2.6
2	B	1251	PHE	2.6
1	E	623	THR	2.6
1	C	488	PRO	2.6
1	E	488	PRO	2.6
1	A	589	LEU	2.6
1	G	479	LEU	2.5
2	H	1436	CYS	2.5
2	F	860	HIS	2.5
1	E	602	ASP	2.5
1	E	448	THR	2.5
1	C	372	GLU	2.5
2	H	856	THR	2.5
2	H	1379	SER	2.5
2	D	1236	GLU	2.5
2	F	1011	GLN	2.5
1	E	190	ASN	2.5
2	H	1022	GLY	2.5
3	L	566	THR	2.5
1	A	349	ASP	2.5
1	C	533	VAL	2.5
2	D	968	MET	2.5
3	L	708	GLN	2.5
3	L	36	VAL	2.4
1	E	316	MET	2.4
1	E	475	LYS	2.4
1	E	427	VAL	2.4
2	H	1535	ASP	2.4
2	D	1454	ALA	2.4
2	B	1017	LEU	2.4
2	H	1444	TYR	2.4
3	J	449	SER	2.4
3	K	94	PRO	2.4
1	E	520	GLY	2.4
2	B	1016	GLY	2.4
2	B	1340	ASP	2.4
1	A	583	LEU	2.4
2	B	1444	TYR	2.4
1	E	634	GLN	2.4
3	L	21	GLY	2.4
2	B	1213	TYR	2.4
2	B	1360	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	614	ALA	2.3
1	E	390	ASN	2.3
2	D	770	ASN	2.3
2	F	1205	LEU	2.3
1	C	209	SER	2.3
2	D	1503	ASP	2.3
2	F	1537	ASP	2.3
1	E	454	LEU	2.3
2	D	1103	ILE	2.3
2	D	854	ALA	2.3
2	F	1018	GLU	2.3
2	B	854	ALA	2.3
2	D	860	HIS	2.3
3	K	17	VAL	2.3
1	E	348	PHE	2.3
1	E	476	GLY	2.2
2	B	763	GLY	2.2
1	E	298	VAL	2.2
2	D	781	GLU	2.2
1	A	496	PRO	2.2
2	D	1537	ASP	2.2
1	A	389	ILE	2.2
1	A	582	VAL	2.2
1	E	582	VAL	2.2
2	D	1499	GLN	2.2
1	C	614	ALA	2.2
2	F	865	THR	2.2
1	E	314	SER	2.2
1	C	103	LEU	2.2
2	D	1022	GLY	2.2
2	H	854	ALA	2.2
2	D	1014	LYS	2.2
1	C	633	ALA	2.2
1	A	634	GLN	2.2
1	A	639	GLN	2.2
1	G	582	VAL	2.2
3	J	454	GLY	2.1
2	B	985	PRO	2.1
2	F	1270	LEU	2.1
3	J	451	SER	2.1
2	D	1013	GLU	2.1
2	B	856	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	545	SER	2.1
1	E	628	SER	2.1
2	D	1011	GLN	2.1
2	D	1021	GLN	2.1
1	E	88	ALA	2.1
3	I	454	GLY	2.1
3	L	570	ILE	2.1
1	C	582	VAL	2.1
3	J	650	VAL	2.1
1	C	138	GLY	2.1
1	G	629	GLY	2.1
1	G	395	GLN	2.1
2	H	1408	SER	2.1
1	C	625	THR	2.1
1	E	336	THR	2.1
2	B	1255	GLN	2.0
3	J	458	GLU	2.0
1	E	394	SER	2.0
3	J	444	ILE	2.0
2	D	995	GLY	2.0
1	G	155	GLN	2.0
3	J	405	VAL	2.0
1	C	314	SER	2.0
2	D	958	ILE	2.0
1	A	614	ALA	2.0
1	C	41	PRO	2.0
2	F	1517	PRO	2.0
1	C	448	THR	2.0
2	H	969	THR	2.0
2	D	1496	CYS	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](#)

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($\text{\AA}^2$)	Q<0.9
4	NAG	B	1917	14/15	0.58	0.15	142,178,199,206	0
4	NAG	L	1353	14/15	0.62	0.15	105,162,190,209	0
4	NAG	K	1353	14/15	0.64	0.19	124,166,186,214	0
4	NAG	D	1917	14/15	0.65	0.17	103,150,180,210	0
4	NAG	F	1917	14/15	0.72	0.20	155,176,239,261	0
4	NAG	I	1353	14/15	0.72	0.13	111,169,185,187	0
4	NAG	H	1917	14/15	0.78	0.15	95,176,221,230	0
4	NAG	J	1353	14/15	0.80	0.11	107,156,170,179	0
5	NI	I	1742	1/1	0.99	0.14	209,209,209,209	0
5	NI	J	1742	1/1	1.00	0.03	62,62,62,62	0
5	NI	K	1742	1/1	1.00	0.08	102,102,102,102	0
5	NI	L	1742	1/1	1.00	0.04	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.