



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:00 PM UTC

PDB ID : 5TBZ / pdb_00005tbz
Title : E. Coli RNA Polymerase complexed with NusG
Authors : Liu, B.; Steitz, T.A.
Deposited on : 2016-09-13
Resolution : 7.00 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:

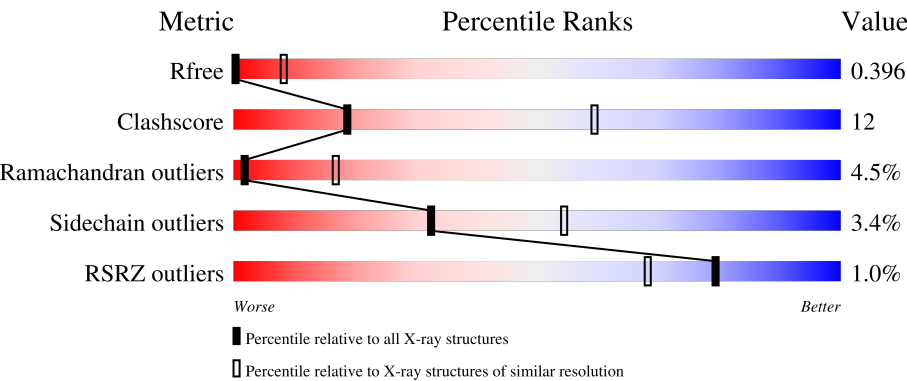
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1167 (10.00-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	242	% 73% 17% • 7%
1	B	242	2% 69% 18% • 11%
1	F	242	2% 71% 19% • 7%
1	G	242	4% 70% 17% • 11%
2	C	1342	% 75% 21% ••

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Mol	Chain	Length	Quality of chain
2	H	1342	74% 22% 2% 2%
3	D	1407	62% 25% 5% 7%
3	I	1407	64% 24% 7%
4	J	181	60% 19% 1% 19%
4	K	181	56% 22% 2% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50147 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	B	215	Total	C	N	O	S	0	0	0
			1657	1034	291	326	6			
1	F	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	G	216	Total	C	N	O	S	0	0	0
			1667	1040	294	327	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP P0A7Z6
A	-5	HIS	-	expression tag	UNP P0A7Z6
A	-4	HIS	-	expression tag	UNP P0A7Z6
A	-3	HIS	-	expression tag	UNP P0A7Z6
A	-2	HIS	-	expression tag	UNP P0A7Z6
A	-1	HIS	-	expression tag	UNP P0A7Z6
A	0	HIS	-	expression tag	UNP P0A7Z6
B	-6	ALA	-	expression tag	UNP P0A7Z6
B	-5	HIS	-	expression tag	UNP P0A7Z6
B	-4	HIS	-	expression tag	UNP P0A7Z6
B	-3	HIS	-	expression tag	UNP P0A7Z6
B	-2	HIS	-	expression tag	UNP P0A7Z6
B	-1	HIS	-	expression tag	UNP P0A7Z6
B	0	HIS	-	expression tag	UNP P0A7Z6
F	-6	ALA	-	expression tag	UNP P0A7Z6
F	-5	HIS	-	expression tag	UNP P0A7Z6
F	-4	HIS	-	expression tag	UNP P0A7Z6
F	-3	HIS	-	expression tag	UNP P0A7Z6
F	-2	HIS	-	expression tag	UNP P0A7Z6
F	-1	HIS	-	expression tag	UNP P0A7Z6
F	0	HIS	-	expression tag	UNP P0A7Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	ALA	-	expression tag	UNP P0A7Z6
G	-5	HIS	-	expression tag	UNP P0A7Z6
G	-4	HIS	-	expression tag	UNP P0A7Z6
G	-3	HIS	-	expression tag	UNP P0A7Z6
G	-2	HIS	-	expression tag	UNP P0A7Z6
G	-1	HIS	-	expression tag	UNP P0A7Z6
G	0	HIS	-	expression tag	UNP P0A7Z6

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

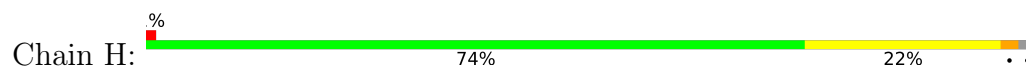
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			
2	H	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			

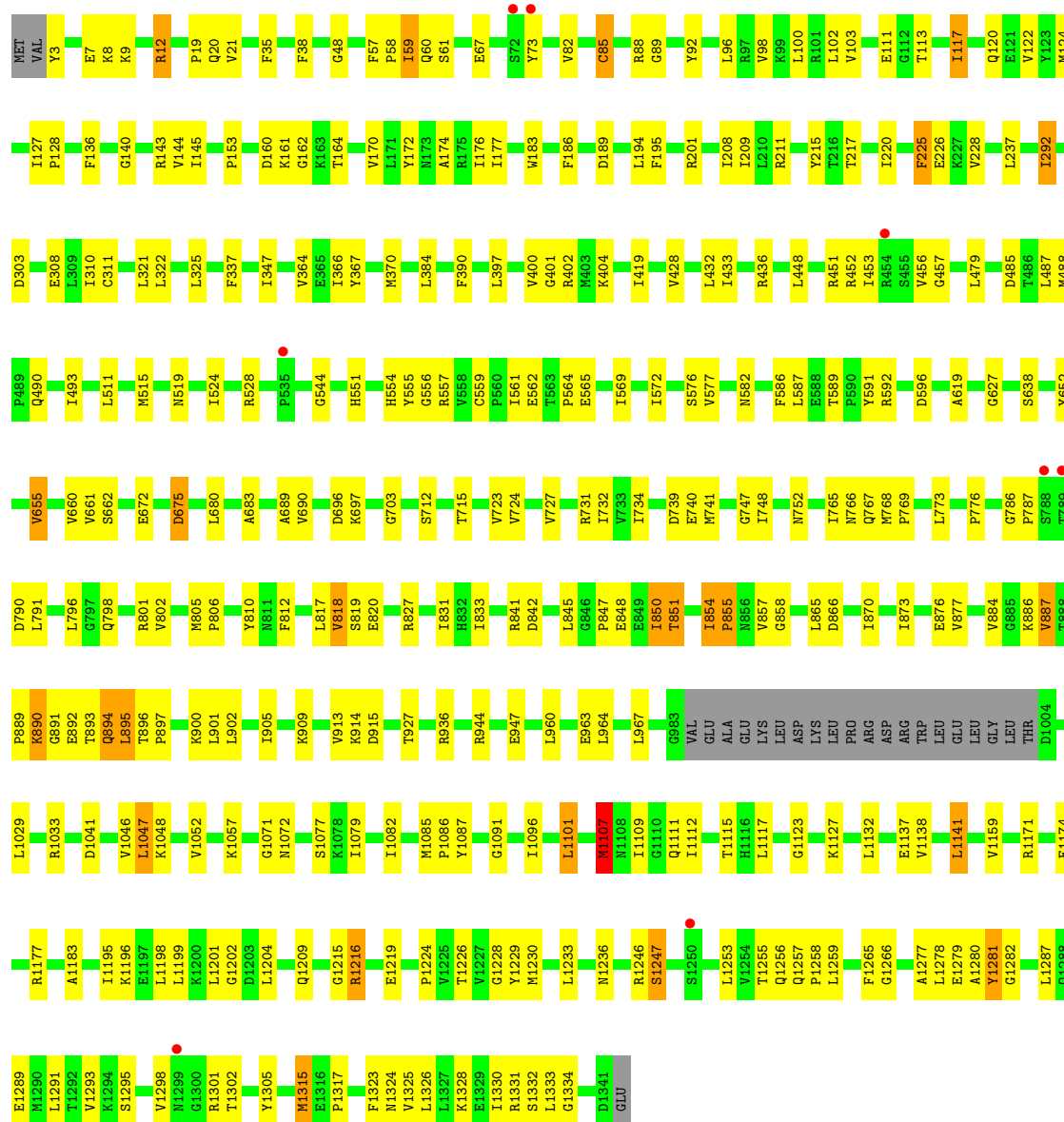
- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1302	Total	C	N	O	S	0	0	0
			10085	6326	1800	1911	48			
3	I	1306	Total	C	N	O	S	0	0	0
			10126	6353	1809	1916	48			

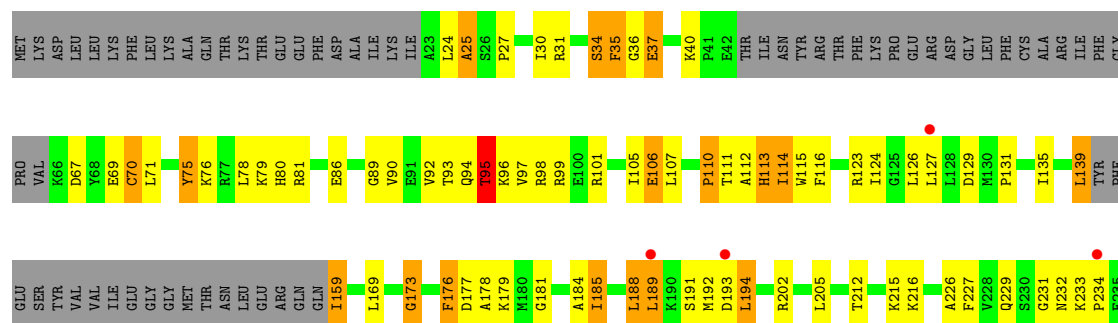
- Molecule 4 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			
4	K	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			





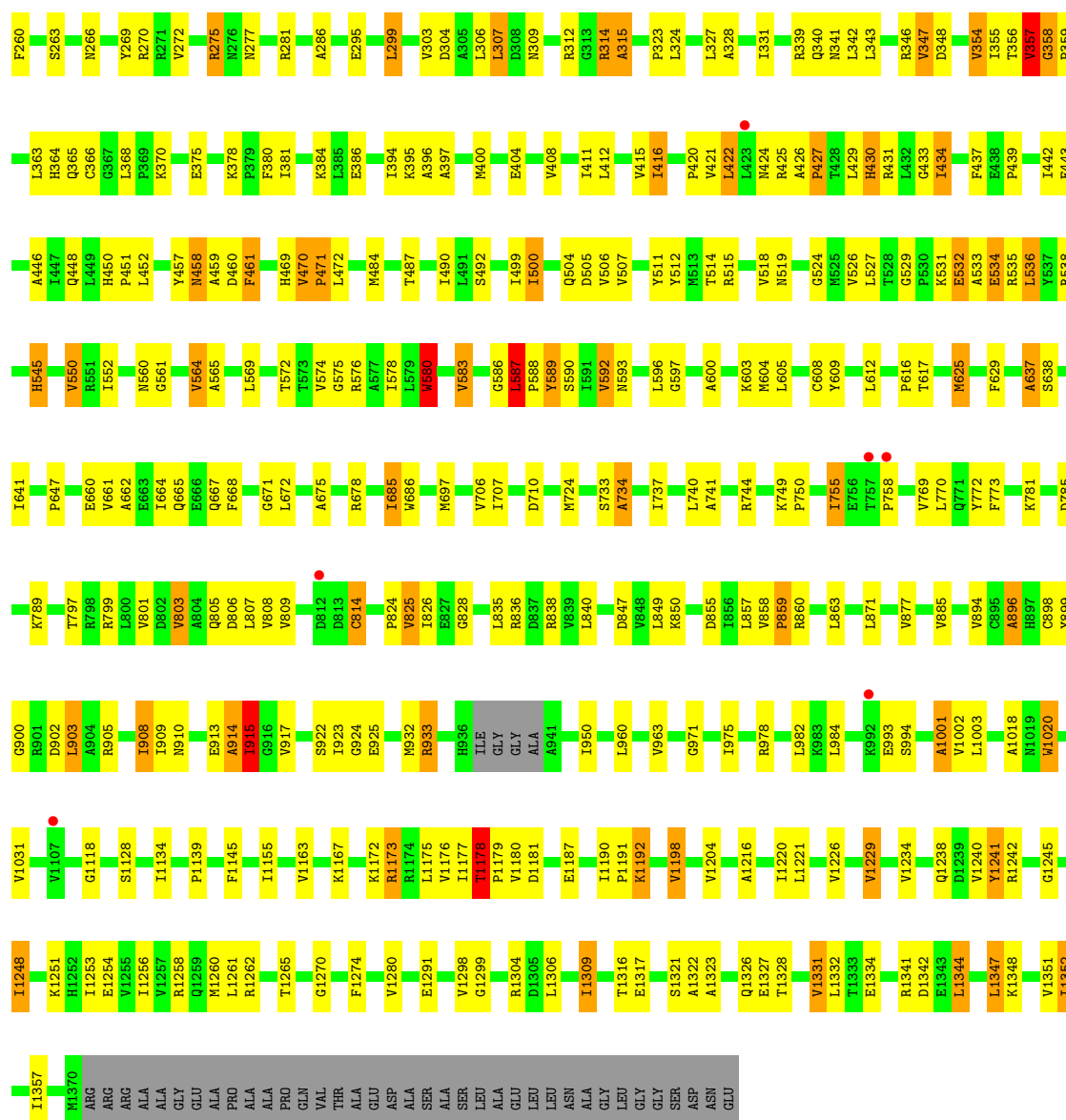
• Molecule 3: DNA-directed RNA polymerase subunit beta'





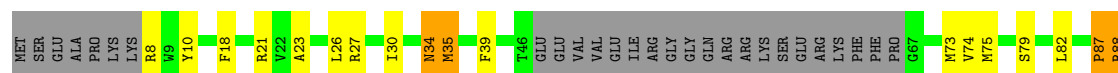
Device Type	Percentage
Smartphones	64%
Tablets	24%
Other devices	7%





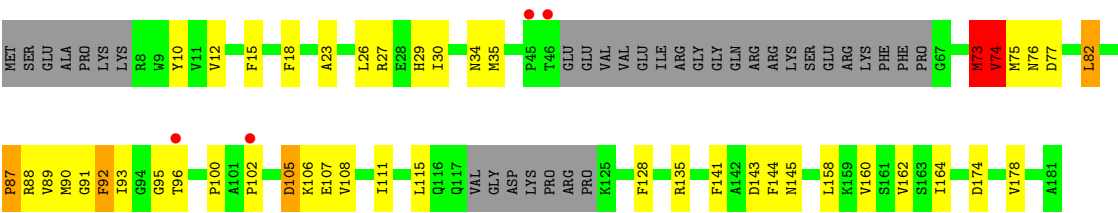
- Molecule 4: Transcription termination/antitermination protein NusG

Chain J: 60% 19% 19%



- Molecule 4: Transcription termination/antitermination protein NusG

Chain K: 2% 56% 22% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.16Å 313.78Å 162.79Å 90.00° 130.23° 90.00°	Depositor
Resolution (Å)	162.19 – 7.00 162.19 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (162.19-7.00) 93.1 (162.19-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.330 , 0.395 0.332 , 0.396	Depositor DCC
R_{free} test set	707 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	314.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 655.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.185 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	50147	wwPDB-VP
Average B, all atoms (Å ²)	330.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.70	0/1761	0.99	2/2387 (0.1%)
1	B	0.70	0/1676	0.98	3/2271 (0.1%)
1	F	0.70	0/1761	1.00	2/2387 (0.1%)
1	G	0.71	0/1687	0.97	3/2286 (0.1%)
2	C	0.61	0/10569	0.98	7/14258 (0.0%)
2	H	0.62	0/10569	0.98	6/14258 (0.0%)
3	D	0.66	0/10233	1.08	15/13816 (0.1%)
3	I	0.65	0/10277	1.07	11/13877 (0.1%)
4	J	0.73	0/1188	1.03	1/1603 (0.1%)
4	K	0.73	0/1188	1.08	4/1603 (0.2%)
All	All	0.65	0/50909	1.03	54/68746 (0.1%)

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
2	C	0	2
2	H	0	2
3	D	0	1
3	I	0	1
4	K	0	1
All	All	0	7

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	33	ARG	N-CA-C	9.19	122.27	111.71
1	A	33	ARG	N-CA-C	9.07	122.14	111.71
1	B	62	ASP	N-CA-C	9.04	121.14	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	ASP	N-CA-C	9.02	121.11	111.28
3	D	914	ALA	N-CA-C	8.51	120.18	111.07
3	I	914	ALA	N-CA-C	8.39	120.04	111.07
3	I	239	LEU	N-CA-C	8.36	123.05	109.59
4	K	92	PHE	N-CA-C	-8.12	103.50	113.41
4	K	73	MET	CA-C-N	7.16	134.87	121.97
4	K	73	MET	C-N-CA	7.16	134.87	121.97
3	D	34	SER	N-CA-C	6.78	119.99	107.99
3	I	896	ALA	N-CA-C	6.63	118.51	111.28
3	D	896	ALA	N-CA-C	6.55	118.42	111.28
2	H	773	LEU	N-CA-C	6.40	118.26	111.28
2	H	1107	MET	N-CA-C	6.30	118.69	108.41
3	I	733	SER	N-CA-C	6.20	116.03	107.73
2	C	1236	ASN	N-CA-C	6.18	117.82	111.14
1	G	193	GLU	N-CA-C	6.18	123.96	110.80
1	B	193	GLU	N-CA-C	6.12	123.84	110.80
2	C	1107	MET	N-CA-C	6.11	118.36	108.41
3	I	1001	ALA	N-CA-C	6.09	117.40	107.23
3	D	1001	ALA	N-CA-C	6.09	117.40	107.23
3	D	35	PHE	N-CA-C	6.07	120.53	113.18
4	K	74	VAL	N-CA-C	6.03	121.87	109.34
3	D	733	SER	N-CA-C	6.02	115.80	107.73
3	I	587	LEU	N-CA-C	5.80	122.64	109.81
2	H	1236	ASN	N-CA-C	5.71	117.31	111.14
3	D	587	LEU	N-CA-C	5.69	122.38	109.81
3	I	534	GLU	N-CA-C	5.67	117.14	111.07
3	D	1331	VAL	N-CA-C	5.63	117.14	111.00
2	H	59	ILE	N-CA-C	5.62	117.41	108.87
3	I	803	VAL	N-CA-C	-5.59	107.37	111.90
3	D	173	GLY	N-CA-C	5.56	126.36	113.18
2	H	1315	MET	N-CA-C	5.56	118.54	109.59
2	C	773	LEU	N-CA-C	5.51	117.28	111.28
4	J	34	ASN	N-CA-C	5.50	122.51	110.80
3	I	1331	VAL	N-CA-C	5.45	116.94	111.00
2	C	59	ILE	N-CA-C	5.40	117.08	108.87
3	D	1020	TRP	N-CA-C	5.40	117.39	109.24
3	D	534	GLU	N-CA-C	5.38	116.83	111.07
3	D	803	VAL	N-CA-C	-5.34	107.57	111.90
3	I	1020	TRP	N-CA-C	5.33	117.29	109.24
1	F	38	THR	N-CA-C	5.29	122.06	110.80
3	I	505	ASP	N-CA-C	5.20	119.10	112.34
1	A	38	THR	N-CA-C	5.20	121.86	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	25	ALA	N-CA-C	5.17	116.82	108.34
2	C	1315	MET	N-CA-C	5.16	118.22	109.76
2	C	82	VAL	N-CA-C	5.11	115.22	110.42
1	G	38	THR	N-CA-C	-5.09	104.14	110.41
3	D	675	ALA	N-CA-C	5.07	117.46	111.33
1	B	38	THR	N-CA-C	-5.06	104.19	110.41
2	C	772	SER	N-CA-C	5.03	116.42	110.19
2	H	82	VAL	N-CA-C	5.03	115.17	110.30
3	D	301	GLU	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	Peptide
2	C	855	PRO	Peptide
3	D	1178	THR	Peptide
2	H	57	PHE	Peptide
2	H	855	PRO	Peptide
3	I	1178	THR	Peptide
4	K	73	MET	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	1740	0	1767	40	0
1	B	1657	0	1686	38	0
1	F	1740	0	1767	38	0
1	G	1667	0	1693	35	0
2	C	10401	0	10414	224	0
2	H	10401	0	10414	237	0
3	D	10085	0	10303	379	2
3	I	10126	0	10341	319	0
4	J	1165	0	1145	28	0
4	K	1165	0	1145	32	0
All	All	50147	0	50675	1200	2

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 (1200) 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:I:1001:ALA:HA	3:I:1020:TRP:HE1	1.12	1.13
4:K:29:HIS:HB3	4:K:82:LEU:HG	1.35	1.06
3:D:226:ALA:HB1	3:D:227:PHE:HA	1.31	1.06
3:D:247:PRO:HB3	3:I:53:ARG:HH12	1.18	1.06
3:D:1001:ALA:HA	3:D:1020:TRP:HE1	1.12	1.06
3:D:247:PRO:HB3	3:I:53:ARG:NH1	1.74	1.03
3:D:885:VAL:HB	3:D:1258:ARG:HD3	1.40	1.02
2:C:12[A]:ARG:HG3	2:C:12[A]:ARG:HH11	1.20	1.02
3:I:885:VAL:HB	3:I:1258:ARG:HD3	1.40	1.02
3:D:272:VAL:HG22	3:D:306:LEU:CD1	1.90	1.02
3:D:1001:ALA:HA	3:D:1020:TRP:NE1	1.75	1.02
4:K:107:GLU:HG2	4:K:135:ARG:HG3	1.37	1.02
3:D:395:LYS:HZ3	2:H:905:ILE:HB	1.26	1.01
3:I:1001:ALA:HA	3:I:1020:TRP:NE1	1.75	1.01
3:D:272:VAL:HG22	3:D:306:LEU:HD11	1.42	1.00
3:I:65:VAL:HG23	3:I:71:LEU:HD22	1.44	1.00
2:C:697:LYS:HE2	2:C:790:ASP:HB3	1.44	0.99
2:H:697:LYS:HE2	2:H:790:ASP:HB3	1.45	0.98
3:D:535:ARG:HG2	3:D:538:ARG:NH1	1.80	0.96
3:I:535:ARG:HG2	3:I:538:ARG:NH1	1.80	0.96
3:D:34:SER:HB2	3:D:105:ILE:HG12	1.48	0.95
2:H:1334:GLY:HA3	3:I:113:HIS:HE1	1.32	0.94
2:H:619:ALA:HB3	3:I:769:VAL:HG21	1.47	0.93
3:D:113:HIS:NE2	3:D:239:LEU:HG	1.84	0.92
1:G:179:PRO:HA	1:G:209:GLY:HA3	1.52	0.91
2:H:805:MET:HE3	2:H:806:PRO:HD2	1.53	0.91
3:D:275:ARG:NH1	3:D:298:MET:O	2.04	0.91
2:H:226:GLU:HB2	2:H:337:PHE:CE2	2.07	0.90
3:I:420:PRO:HA	3:I:439:PRO:HD3	1.54	0.90
1:B:179:PRO:HA	1:B:209:GLY:HA3	1.53	0.88
3:D:420:PRO:HA	3:D:439:PRO:HD3	1.54	0.88
3:D:508:LEU:HD21	3:D:730:ALA:HB2	1.56	0.87
2:C:805:MET:HE3	2:C:806:PRO:HD2	1.56	0.86
4:K:75:MET:HE1	4:K:100:PRO:HG2	1.58	0.86
3:I:252:LEU:HD23	3:I:263:SER:HB3	1.57	0.85
3:D:123:ARG:CB	3:D:237:MET:HE1	2.08	0.84
3:D:808:VAL:HG13	3:D:914:ALA:HA	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:808:VAL:HG13	3:I:914:ALA:HA	1.58	0.84
2:H:1334:GLY:HA3	3:I:113:HIS:CE1	2.12	0.84
3:D:226:ALA:CB	3:D:227:PHE:HA	2.07	0.83
3:I:180:MET:HE3	3:I:184:ALA:HB2	1.60	0.83
2:H:887:VAL:HG13	2:H:909:LYS:HE2	1.60	0.83
3:D:275:ARG:NH1	3:D:302:ALA:H	1.77	0.82
4:K:87:PRO:HB2	4:K:88:ARG:HA	1.62	0.82
4:J:87:PRO:HB2	4:J:88:ARG:HA	1.61	0.81
1:G:61:ILE:HG12	1:G:142:MET:HE1	1.62	0.81
3:D:395:LYS:HE3	2:H:901:LEU:O	1.80	0.80
3:D:113:HIS:CD2	3:D:238:ILE:HA	2.17	0.80
3:D:252:LEU:HD13	3:D:260:PHE:HB3	1.63	0.79
3:D:252:LEU:HD23	3:D:263:SER:HB3	1.63	0.79
3:D:86:GLU:HB3	2:H:1253:LEU:CD2	2.13	0.79
1:A:45:ARG:HD3	1:B:38:THR:HG22	1.65	0.79
2:C:12[A]:ARG:HG3	2:C:12[A]:ARG:NH1	1.96	0.79
1:B:61:ILE:HG12	1:B:142:MET:HE1	1.63	0.79
2:C:619:ALA:HB3	3:D:769:VAL:HG21	1.62	0.79
3:D:1152:GLU:C	3:D:1194:ARG:HH22	1.91	0.79
1:F:61:ILE:HG12	1:F:142:MET:HE1	1.65	0.79
3:D:331:ILE:HG21	3:D:1332:LEU:CD1	2.13	0.78
3:D:169:LEU:HB3	3:D:176:PHE:CZ	2.18	0.77
3:D:139:LEU:HD13	3:D:185:ILE:HD11	1.65	0.77
1:A:61:ILE:HG12	1:A:142:MET:HE1	1.66	0.77
2:C:1332:SER:HA	3:D:243:PRO:HB2	1.66	0.77
1:A:45:ARG:HB2	1:B:38:THR:CG2	2.15	0.77
3:D:123:ARG:HB3	3:D:237:MET:HE1	1.66	0.76
3:D:34:SER:CB	3:D:105:ILE:HG12	2.15	0.76
3:D:506:VAL:HG22	3:D:629:PHE:CZ	2.20	0.76
3:I:849:LEU:HD22	3:I:877:VAL:HG11	1.66	0.75
3:D:327:LEU:O	3:D:331:ILE:HG13	1.86	0.75
2:H:855:PRO:HB3	2:H:914:LYS:HD3	1.69	0.75
3:I:506:VAL:HG22	3:I:629:PHE:CZ	2.20	0.75
3:D:86:GLU:HB3	2:H:1253:LEU:HD22	1.66	0.74
3:I:1226:VAL:HG22	3:I:1304:ARG:HH22	1.52	0.74
2:H:1330:ILE:HA	2:H:1333:LEU:HD12	1.68	0.74
2:C:1330:ILE:HA	2:C:1333:LEU:HD12	1.67	0.74
3:D:124:ILE:HG22	3:D:135:ILE:HD13	1.70	0.73
3:D:272:VAL:HG22	3:D:306:LEU:HD13	1.69	0.73
2:C:497:PRO:HB3	4:J:8:ARG:HD3	1.71	0.73
2:C:810:TYR:HA	3:D:357:VAL:HG11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:275:ARG:CZ	3:D:298:MET:O	2.36	0.73
3:D:664:ILE:HD11	3:D:685:ILE:HD12	1.71	0.72
4:K:107:GLU:CG	4:K:135:ARG:HG3	2.16	0.72
2:C:35:PHE:CZ	2:C:456:VAL:HB	2.25	0.72
3:D:81:ARG:HD3	2:H:890:LYS:HE3	1.70	0.72
3:D:275:ARG:HH12	3:D:302:ALA:H	1.37	0.72
2:H:35:PHE:CZ	2:H:456:VAL:HB	2.25	0.72
3:D:849:LEU:HD22	3:D:877:VAL:HG11	1.71	0.72
3:D:123:ARG:HH12	3:D:1333:THR:HB	1.55	0.71
3:D:647:PRO:HD3	3:D:697:MET:SD	2.31	0.71
2:C:801:ARG:HG3	2:C:1229:TYR:CE1	2.25	0.71
3:D:113:HIS:HD2	3:D:238:ILE:HA	1.56	0.71
3:I:664:ILE:HD11	3:I:685:ILE:HD12	1.70	0.71
2:C:889:PRO:C	3:I:78:LEU:HD12	2.16	0.71
3:D:123:ARG:HB2	3:D:237:MET:HE1	1.72	0.71
3:I:425:ARG:NH2	3:I:457:TYR:HB2	2.05	0.71
3:I:331:ILE:HB	3:I:1328:THR:OG1	1.91	0.71
2:H:801:ARG:HG3	2:H:1229:TYR:CE1	2.25	0.70
2:C:1295:SER:HA	2:C:1301:ARG:HH21	1.56	0.70
3:D:71:LEU:O	3:I:66:LYS:HA	1.91	0.70
1:F:45:ARG:NH2	1:G:37:HIS:HB3	2.05	0.70
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.72	0.70
2:C:1326:LEU:HG	3:D:341:ASN:ND2	2.05	0.70
2:C:559:CYS:SG	2:C:576:SER:HA	2.32	0.70
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.72	0.70
2:H:1209:GLN:HB3	2:H:1224:PRO:HB2	1.72	0.70
2:C:896:THR:HB	2:C:897:PRO:HD2	1.72	0.70
3:D:93:THR:HG22	2:H:890:LYS:HZ1	1.57	0.69
2:H:19:PRO:HB2	2:H:20:GLN:HG3	1.73	0.69
3:D:431:ARG:HH22	3:D:914:ALA:HB3	1.57	0.69
2:H:896:THR:HB	2:H:897:PRO:HD2	1.74	0.69
3:I:430:HIS:CE1	3:I:922:SER:HA	2.28	0.69
3:I:647:PRO:HD3	3:I:697:MET:SD	2.33	0.69
2:H:226:GLU:CB	2:H:337:PHE:CE2	2.75	0.69
3:I:114:ILE:HG12	3:I:304:ASP:HA	1.75	0.69
1:A:51:MET:HB3	1:A:179:PRO:HD2	1.74	0.69
2:H:559:CYS:SG	2:H:576:SER:HA	2.32	0.69
1:A:45:ARG:HD3	1:B:38:THR:CG2	2.23	0.69
3:I:431:ARG:HH22	3:I:914:ALA:HB3	1.58	0.69
3:D:71:LEU:HD21	3:I:51:PRO:HD3	1.75	0.68
2:H:1295:SER:HA	2:H:1301:ARG:HH21	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:HH22	3:D:581:MET:HG3	1.58	0.68
3:D:430:HIS:CE1	3:D:922:SER:HA	2.27	0.68
3:D:536:LEU:HD13	3:D:574:VAL:HG13	1.76	0.68
3:I:424:ASN:OD1	3:I:434:ILE:HA	1.93	0.68
3:D:424:ASN:OD1	3:D:434:ILE:HA	1.93	0.68
3:I:169:LEU:O	3:I:173:GLY:HA3	1.94	0.68
1:F:51:MET:HB3	1:F:179:PRO:HD2	1.76	0.68
2:H:226:GLU:HB2	2:H:337:PHE:HE2	1.58	0.68
4:K:87:PRO:HB2	4:K:88:ARG:CA	2.23	0.68
4:K:143:ASP:O	4:K:144:PHE:HD1	1.77	0.68
4:J:87:PRO:HB2	4:J:88:ARG:CA	2.24	0.67
3:I:202:ARG:NH1	3:I:216:LYS:HB2	2.08	0.67
2:H:122:VAL:HG21	2:H:493:ILE:HB	1.77	0.67
3:D:305:ALA:HB2	3:D:314:ARG:HD3	1.77	0.67
3:D:1261:LEU:HA	3:D:1306:LEU:HD22	1.76	0.67
2:C:122:VAL:HG21	2:C:493:ILE:HB	1.76	0.67
3:I:1261:LEU:HA	3:I:1306:LEU:HD22	1.75	0.67
1:F:46:ILE:HG12	1:G:35:PHE:CE1	2.30	0.67
3:I:425:ARG:CZ	3:I:459:ALA:HB2	2.24	0.67
3:D:113:HIS:CE1	3:D:239:LEU:HG	2.30	0.67
3:D:114:ILE:HG12	3:D:304:ASP:HA	1.77	0.67
3:D:127:LEU:HD13	3:D:234:PRO:HB3	1.78	0.66
2:C:12[A]:ARG:HH11	2:C:12[A]:ARG:CG	2.03	0.66
2:C:211:ARG:HA	2:C:215:TYR:O	1.96	0.66
2:H:211:ARG:HA	2:H:215:TYR:O	1.96	0.66
3:I:202:ARG:HH12	3:I:216:LYS:HB2	1.61	0.66
3:I:303:VAL:HA	3:I:306:LEU:HD12	1.77	0.66
3:I:365:GLN:O	3:I:450:HIS:CE1	2.48	0.66
3:I:315:ALA:HB3	3:I:324:LEU:HD23	1.78	0.66
3:I:536:LEU:HD13	3:I:574:VAL:HG13	1.78	0.66
3:D:421:VAL:HG23	3:D:439:PRO:HG3	1.78	0.66
2:C:1333:LEU:HD23	3:D:307:LEU:HB3	1.78	0.66
1:A:70:THR:HG21	2:C:755:LYS:HD3	1.77	0.66
2:C:1329:GLU:HG2	3:D:245:LEU:HD21	1.78	0.66
3:I:978:ARG:HH12	3:I:1198:VAL:HA	1.61	0.66
2:H:226:GLU:CB	2:H:337:PHE:HE2	2.07	0.66
3:I:189:LEU:HA	3:I:192:MET:HB2	1.78	0.66
3:I:327:LEU:O	3:I:331:ILE:HG12	1.95	0.65
1:G:51:MET:HB3	1:G:179:PRO:HD2	1.78	0.65
3:D:978:ARG:HH12	3:D:1198:VAL:HA	1.59	0.65
1:F:48:LEU:HD11	2:H:1087:TYR:OH	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:228:VAL:HG23	3:I:1341:ARG:CZ	2.26	0.65
4:K:107:GLU:HB2	4:K:145:ASN:HB3	1.77	0.65
1:A:179:PRO:HG3	1:A:211:ILE:HD12	1.79	0.65
3:D:398:LYS:HG2	2:H:901:LEU:HD22	1.79	0.65
3:D:105:ILE:HD13	4:K:18:PHE:CE2	2.32	0.65
2:H:592:ARG:HG3	2:H:655:VAL:HG22	1.79	0.65
3:D:24:LEU:HB2	3:D:236:TRP:HB3	1.77	0.65
2:C:1295:SER:HB3	3:D:347:VAL:HG22	1.77	0.64
2:H:675:ASP:OD1	2:H:1107:MET:HB2	1.98	0.64
3:I:119:SER:C	3:I:121:PRO:HD3	2.22	0.64
2:H:189:ASP:HB2	2:H:195:PHE:CE2	2.33	0.64
3:I:421:VAL:HG23	3:I:439:PRO:HG3	1.78	0.64
3:I:425:ARG:HH12	3:I:458:ASN:C	2.05	0.64
3:I:587:LEU:HB2	3:I:589:TYR:CE1	2.32	0.64
3:D:809:VAL:HB	3:D:913:GLU:H	1.61	0.64
2:C:189:ASP:HB2	2:C:195:PHE:CE2	2.33	0.64
3:D:909:ILE:HG22	3:D:910:ASN:H	1.62	0.64
2:H:1331:ARG:O	3:I:243:PRO:HG2	1.97	0.64
3:I:809:VAL:HB	3:I:913:GLU:H	1.61	0.64
2:C:82:VAL:HA	2:C:92:TYR:HE1	1.62	0.64
3:D:303:VAL:HA	3:D:306:LEU:HD12	1.77	0.64
3:D:587:LEU:HB2	3:D:589:TYR:CE1	2.32	0.64
2:H:820:GLU:HB2	2:H:1082:ILE:HG13	1.80	0.64
3:D:24:LEU:HB2	3:D:236:TRP:CB	2.28	0.63
4:K:73:MET:HG2	4:K:74:VAL:O	1.98	0.63
1:B:51:MET:HB3	1:B:179:PRO:HD2	1.78	0.63
2:C:913:VAL:O	2:C:914:LYS:HG3	1.98	0.63
2:H:1291:LEU:HD22	3:I:343:LEU:O	1.98	0.63
3:I:909:ILE:HG22	3:I:910:ASN:H	1.63	0.63
4:K:75:MET:CE	4:K:100:PRO:HG2	2.28	0.63
2:C:592:ARG:HG3	2:C:655:VAL:HG22	1.79	0.63
2:H:1302:THR:HA	2:H:1305:TYR:CD2	2.34	0.63
4:K:108:VAL:O	4:K:111:ILE:HG22	1.98	0.63
1:A:45:ARG:HB2	1:B:38:THR:HG21	1.80	0.63
2:C:820:GLU:HB2	2:C:1082:ILE:HG13	1.81	0.63
2:C:675:ASP:OD1	2:C:1107:MET:HB2	1.98	0.63
3:D:252:LEU:HG	3:I:86:GLU:HB2	1.78	0.63
1:F:179:PRO:HG3	1:F:211:ILE:HD12	1.80	0.63
2:H:557:ARG:HB3	2:H:587:LEU:HD22	1.81	0.63
2:H:85:CYS:HA	2:H:88:ARG:HB2	1.81	0.63
3:I:50:LYS:HB3	3:I:51:PRO:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:269:TYR:HA	3:D:272:VAL:HG23	1.80	0.62
2:C:1302:THR:HA	2:C:1305:TYR:CD2	2.33	0.62
1:F:35:PHE:CE1	1:G:46:ILE:HG12	2.35	0.62
2:H:884:VAL:HG23	2:H:1052:VAL:HG23	1.82	0.62
2:H:1333:LEU:HD13	3:I:115:TRP:HE1	1.64	0.62
3:D:189:LEU:HA	3:D:192:MET:HB2	1.82	0.62
3:I:885:VAL:HB	3:I:1258:ARG:CD	2.25	0.62
2:C:85:CYS:HA	2:C:88:ARG:HB2	1.81	0.62
3:I:1221:LEU:HG	3:I:1229:VAL:HG21	1.82	0.62
1:A:74:VAL:O	2:C:729:ALA:HB2	2.00	0.61
2:C:557:ARG:HB3	2:C:587:LEU:HD22	1.82	0.61
3:I:365:GLN:O	3:I:450:HIS:HE1	1.83	0.61
2:H:96:LEU:HD11	2:H:127:ILE:HD12	1.83	0.61
2:C:876:GLU:HG2	2:C:927:THR:HG22	1.82	0.61
2:C:903:ARG:HB2	3:I:395:LYS:HZ2	1.64	0.61
3:D:97:VAL:HG21	3:I:47:ARG:HD3	1.82	0.61
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.01	0.61
3:I:269:TYR:HA	3:I:272:VAL:HG23	1.80	0.61
2:C:884:VAL:HG23	2:C:1052:VAL:HG23	1.81	0.61
3:I:807:LEU:HD22	3:I:1262:ARG:HH12	1.66	0.61
3:I:1238:GLN:O	3:I:1242:ARG:HB2	2.01	0.61
3:I:408:VAL:O	3:I:412:LEU:HG	2.01	0.61
3:D:807:LEU:HD22	3:D:1262:ARG:HH12	1.65	0.61
2:C:848:GLU:HG2	2:C:889:PRO:HD3	1.81	0.61
3:D:408:VAL:O	3:D:412:LEU:HG	2.01	0.61
4:K:160:VAL:HG21	4:K:178:VAL:HG11	1.82	0.61
3:D:81:ARG:NH1	2:H:890:LYS:H	1.98	0.61
3:D:395:LYS:O	3:D:398:LYS:HG3	2.01	0.61
3:D:1173:ARG:HB3	3:D:1190:ILE:O	2.00	0.61
3:D:1221:LEU:HG	3:D:1229:VAL:HG21	1.82	0.61
1:F:46:ILE:HG12	1:G:35:PHE:HE1	1.64	0.61
2:H:1332:SER:HA	3:I:243:PRO:HB2	1.83	0.61
2:C:802:VAL:HG21	2:C:1230:MET:HB2	1.83	0.61
3:D:982:LEU:O	3:D:994:SER:HB2	2.00	0.61
3:I:425:ARG:CZ	3:I:457:TYR:HB3	2.31	0.61
3:I:1173:ARG:HB3	3:I:1190:ILE:O	2.01	0.61
3:D:116:PHE:HB3	3:D:237:MET:HE3	1.82	0.60
3:D:205:LEU:HD13	3:D:212:THR:HG21	1.83	0.60
2:H:855:PRO:HD2	2:H:886:LYS:HD2	1.82	0.60
2:H:1295:SER:HB3	3:I:347:VAL:HG22	1.82	0.60
2:C:1330:ILE:HD11	3:D:1332:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:LEU:HD11	2:C:127:ILE:HD12	1.81	0.60
3:I:78:LEU:HD13	3:I:81:ARG:NH2	2.16	0.60
2:H:453:ILE:HD11	2:H:587:LEU:HG	1.83	0.60
3:I:982:LEU:O	3:I:994:SER:HB2	2.01	0.60
3:D:605:LEU:O	3:D:609:TYR:HD2	1.85	0.60
2:C:1137:GLU:HA	2:C:1141:LEU:HD12	1.83	0.60
2:H:802:VAL:HG21	2:H:1230:MET:HB2	1.83	0.60
3:I:309:ASN:HB2	3:I:324:LEU:HD13	1.83	0.60
2:H:1333:LEU:HD22	3:I:115:TRP:NE1	2.16	0.60
3:I:605:LEU:O	3:I:609:TYR:HD2	1.85	0.60
3:I:1241:TYR:HB2	3:I:1248:ILE:HD11	1.82	0.60
3:D:81:ARG:HA	3:D:92:VAL:HB	1.84	0.60
2:H:1107:MET:HE3	3:I:740:LEU:HG	1.84	0.60
3:I:1238:GLN:HG3	3:I:1253:ILE:CD1	2.31	0.60
3:I:1331:VAL:HA	3:I:1334:GLU:HB2	1.83	0.60
3:D:1256:ILE:O	3:D:1260:MET:HG2	2.02	0.59
1:F:107:ILE:HD11	1:F:136:GLU:HG2	1.84	0.59
3:D:1238:GLN:HG3	3:D:1253:ILE:CD1	2.32	0.59
2:H:35:PHE:HZ	2:H:456:VAL:HB	1.66	0.59
3:I:984:LEU:HD12	3:I:993:GLU:HB2	1.84	0.59
2:C:194:LEU:HD11	2:C:433:ILE:HD11	1.83	0.59
3:I:227:PHE:C	3:I:1341:ARG:HH12	2.10	0.59
3:I:1256:ILE:O	3:I:1260:MET:HG2	2.02	0.59
3:I:597:GLY:HA2	3:I:600:ALA:HB3	1.84	0.59
4:J:160:VAL:HG21	4:J:178:VAL:HG11	1.83	0.59
2:C:453:ILE:HD11	2:C:587:LEU:HG	1.84	0.59
3:D:78:LEU:HD13	3:D:81:ARG:HH21	1.67	0.59
3:D:885:VAL:CB	3:D:1258:ARG:HD3	2.26	0.59
3:I:226:ALA:HB1	3:I:1341:ARG:CZ	2.33	0.59
3:D:90:VAL:HA	3:I:260:PHE:HE1	1.68	0.59
3:D:597:GLY:HA2	3:D:600:ALA:HB3	1.85	0.59
3:D:797:THR:O	3:D:801:VAL:HG23	2.03	0.59
4:J:95:GLY:HA3	4:J:102:PRO:HG2	1.84	0.59
1:A:48:LEU:HB2	2:C:1083:GLU:HG2	1.84	0.59
1:F:234:LEU:HD13	1:G:13:LEU:H	1.68	0.59
2:H:1295:SER:HA	2:H:1301:ARG:NH2	2.18	0.59
2:C:82:VAL:O	2:C:92:TYR:OH	2.21	0.58
2:C:1295:SER:HA	2:C:1301:ARG:NH2	2.18	0.58
3:D:239:LEU:HD22	3:D:241:VAL:O	2.03	0.58
3:D:275:ARG:HB3	3:D:299:LEU:HD22	1.85	0.58
1:A:101:THR:O	1:A:115:ILE:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1241:TYR:HB2	3:D:1248:ILE:HD11	1.84	0.58
2:H:226:GLU:HB2	2:H:337:PHE:CD2	2.37	0.58
3:I:550:VAL:HB	3:I:552:ILE:HG13	1.85	0.58
2:C:855:PRO:HG3	2:C:914:LYS:HD3	1.85	0.58
1:F:234:LEU:HB3	1:G:13:LEU:HD12	1.83	0.58
3:D:86:GLU:HB3	2:H:1253:LEU:HD21	1.85	0.58
3:D:1001:ALA:CA	3:D:1020:TRP:HE1	2.02	0.58
2:H:1137:GLU:HA	2:H:1141:LEU:HD12	1.84	0.58
3:D:40:LYS:HZ2	3:I:61:ILE:HD11	1.68	0.58
2:H:1326:LEU:HG	3:I:341:ASN:ND2	2.18	0.58
3:I:797:THR:O	3:I:801:VAL:HG23	2.04	0.58
2:C:697:LYS:HZ3	2:C:791:LEU:HB2	1.68	0.58
3:D:189:LEU:HD22	3:D:234:PRO:HB2	1.85	0.58
2:H:562:GLU:HG2	2:H:683:ALA:HB1	1.85	0.58
2:C:731:ARG:HG2	2:C:752:ASN:HA	1.86	0.58
3:D:169:LEU:HB3	3:D:176:PHE:HZ	1.63	0.58
2:C:35:PHE:HZ	2:C:456:VAL:HB	1.66	0.57
3:D:550:VAL:HB	3:D:552:ILE:HG13	1.85	0.57
2:H:194:LEU:HD11	2:H:433:ILE:HD11	1.84	0.57
2:H:524:ILE:HD11	2:H:712:SER:HB3	1.87	0.57
3:D:247:PRO:CB	3:I:53:ARG:HH12	2.03	0.57
2:H:845:LEU:HB2	2:H:890:LYS:HG2	1.86	0.57
3:I:932:MET:HA	3:I:1139:PRO:HD3	1.86	0.57
3:D:1331:VAL:HA	3:D:1334:GLU:HB2	1.84	0.57
3:I:384:LYS:HD3	3:I:411:ILE:HG22	1.85	0.57
1:A:159:ILE:O	1:A:162:GLU:HG3	2.05	0.57
3:D:885:VAL:HB	3:D:1258:ARG:CD	2.25	0.57
2:H:145:ILE:HG23	2:H:511:LEU:HB3	1.86	0.57
2:C:176:ILE:HD11	2:C:428:VAL:HG11	1.86	0.57
2:C:524:ILE:HD11	2:C:712:SER:HB3	1.87	0.57
3:D:984:LEU:HD12	3:D:993:GLU:HB2	1.86	0.57
2:C:367:TYR:OH	2:C:384:LEU:C	2.48	0.57
2:C:562:GLU:HG2	2:C:683:ALA:HB1	1.86	0.57
3:D:81:ARG:HH12	2:H:890:LYS:N	2.02	0.57
3:D:194:LEU:HD13	3:D:231:GLY:O	2.04	0.57
1:F:104:LYS:HE2	1:F:114:ASP:HB2	1.86	0.57
3:D:1220:ILE:HG22	3:D:1229:VAL:HG22	1.86	0.57
3:D:113:HIS:CD2	3:D:239:LEU:HG	2.40	0.57
4:K:107:GLU:HG2	4:K:135:ARG:CG	2.24	0.57
2:C:904:ALA:HB3	3:I:395:LYS:HD2	1.85	0.56
3:D:70:CYS:HB2	3:D:75:TYR:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:LEU:HD23	1:G:28:LEU:HG	1.87	0.56
2:H:225:PHE:HE2	2:H:347:ILE:HB	1.69	0.56
2:C:765:ILE:HG23	2:C:787:PRO:HG3	1.86	0.56
2:C:1330:ILE:CD1	3:D:1332:LEU:HD22	2.35	0.56
2:H:765:ILE:HG23	2:H:787:PRO:HG3	1.86	0.56
3:I:105:ILE:HG21	4:J:18:PHE:HE2	1.70	0.56
2:H:893:THR:O	2:H:894:GLN:HB2	2.06	0.56
2:H:1123:GLY:HA3	2:H:1204:LEU:HD11	1.87	0.56
2:H:1293:VAL:HG22	2:H:1315:MET:HE2	1.87	0.56
2:C:1115:THR:HB	2:C:1228:GLY:HA3	1.88	0.56
3:D:514:THR:HB	3:D:576:ARG:HE	1.70	0.56
2:H:715:THR:HG22	2:H:786:GLY:H	1.70	0.56
2:H:731:ARG:HG2	2:H:752:ASN:HA	1.87	0.56
2:C:1289:GLU:HA	2:C:1293:VAL:HB	1.87	0.56
2:C:404:LYS:HD2	2:C:452:ARG:HH21	1.71	0.56
3:D:81:ARG:NH1	2:H:890:LYS:N	2.54	0.56
3:D:592:VAL:HG11	3:D:604:MET:HE2	1.88	0.56
2:H:848:GLU:HA	2:H:889:PRO:HD3	1.87	0.56
3:I:514:THR:HB	3:I:576:ARG:HE	1.71	0.56
2:H:176:ILE:HD11	2:H:428:VAL:HG11	1.88	0.56
2:H:367:TYR:OH	2:H:384:LEU:C	2.48	0.56
3:I:198:CYS:SG	3:I:216:LYS:HD3	2.45	0.56
2:C:224:PHE:CE1	2:C:347:ILE:HD13	2.40	0.56
4:J:39:PHE:HZ	4:J:79:SER:HG	1.53	0.56
4:K:23:ALA:HA	4:K:26:LEU:HD12	1.87	0.56
3:I:580:TRP:HE1	3:I:590:SER:HA	1.71	0.56
3:I:661:VAL:HG23	3:I:685:ILE:HG22	1.88	0.56
3:I:1220:ILE:HG22	3:I:1229:VAL:HG22	1.88	0.56
3:I:1316:THR:OG1	3:I:1322:ALA:HB2	2.06	0.56
1:B:91:ARG:HG3	1:B:210:THR:HB	1.87	0.55
2:C:145:ILE:HG23	2:C:511:LEU:HB3	1.88	0.55
2:C:390:PHE:HA	2:C:419:ILE:HG23	1.88	0.55
3:D:885:VAL:HG22	3:D:899:TYR:CD1	2.41	0.55
2:H:390:PHE:HA	2:H:419:ILE:HG23	1.87	0.55
3:D:252:LEU:HD12	3:I:75:TYR:OH	2.07	0.55
3:D:932:MET:HA	3:D:1139:PRO:HD3	1.88	0.55
3:D:1316:THR:OG1	3:D:1322:ALA:HB2	2.05	0.55
4:K:95:GLY:HA3	4:K:102:PRO:HG2	1.88	0.55
3:D:668:PHE:CZ	3:D:678:ARG:HB3	2.41	0.55
3:D:749:LYS:HE3	3:D:755:ILE:HG12	1.88	0.55
2:H:1115:THR:HB	2:H:1228:GLY:HA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:535:ARG:HG2	3:D:538:ARG:HH12	1.67	0.55
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.07	0.55
2:C:1333:LEU:HD13	3:D:115:TRP:HE1	1.71	0.55
2:C:1333:LEU:HD22	3:D:115:TRP:NE1	2.22	0.55
3:I:114:ILE:HD12	3:I:307:LEU:HB2	1.88	0.55
4:J:106:LYS:HB2	4:J:143:ASP:HA	1.88	0.55
4:K:87:PRO:CB	4:K:88:ARG:HA	2.34	0.55
1:B:179:PRO:HA	1:B:209:GLY:CA	2.33	0.55
2:C:1333:LEU:HD22	3:D:115:TRP:HE1	1.71	0.55
3:D:661:VAL:HG23	3:D:685:ILE:HG22	1.89	0.55
4:J:23:ALA:HA	4:J:26:LEU:HD12	1.86	0.55
1:A:104:LYS:HE2	1:A:114:ASP:HB2	1.89	0.55
3:I:668:PHE:CZ	3:I:678:ARG:HB3	2.41	0.55
3:I:78:LEU:HB3	3:I:81:ARG:HH21	1.72	0.55
3:I:885:VAL:HG22	3:I:899:TYR:CD1	2.41	0.55
2:C:715:THR:HG22	2:C:786:GLY:H	1.71	0.55
3:D:194:LEU:HD21	3:D:232:ASN:O	2.07	0.55
1:G:91:ARG:HG3	1:G:210:THR:HB	1.88	0.55
3:I:81:ARG:HA	3:I:92:VAL:HB	1.88	0.55
3:I:206:ASN:HA	3:I:209:ASN:O	2.07	0.55
2:C:496:LYS:HG2	4:J:102:PRO:HB3	1.89	0.54
2:C:1109:ILE:HA	2:C:1112:ILE:HD12	1.90	0.54
2:C:1256:GLN:HB3	2:C:1298:VAL:HG23	1.90	0.54
2:C:1323:PHE:CE1	3:D:1352:ILE:HG23	2.42	0.54
3:D:81:ARG:NH2	2:H:913:VAL:HG11	2.22	0.54
3:D:309:ASN:ND2	3:D:326:SER:HB3	2.22	0.54
3:D:380:PHE:HE2	3:D:472:LEU:HD22	1.72	0.54
3:D:331:ILE:HG12	3:D:337:ARG:NH2	2.22	0.54
1:G:89:ALA:HB1	1:G:210:THR:HG23	1.89	0.54
2:H:404:LYS:HD2	2:H:452:ARG:HH21	1.70	0.54
2:C:144:VAL:HB	2:C:515:MET:SD	2.47	0.54
2:C:818:VAL:HB	2:C:1079:ILE:HG12	1.89	0.54
3:D:189:LEU:HD13	3:D:234:PRO:O	2.07	0.54
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	1.89	0.54
2:H:561:ILE:HA	2:H:680:LEU:HD23	1.90	0.54
1:B:43:LEU:HA	1:B:46:ILE:HD12	1.89	0.54
1:B:179:PRO:HG3	1:B:211:ILE:HD12	1.88	0.54
3:I:79:LYS:HB3	3:I:80:HIS:CD2	2.43	0.54
1:A:43:LEU:HA	1:A:46:ILE:HD12	1.90	0.54
1:A:75:GLN:HE21	2:C:727:VAL:HG11	1.72	0.54
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:395:LYS:HE2	2:H:905:ILE:HD12	1.90	0.54
1:G:43:LEU:HA	1:G:46:ILE:HD12	1.88	0.54
3:I:1323:ALA:HB1	3:I:1332:LEU:HD23	1.90	0.54
2:C:92:TYR:O	2:C:128:PRO:HA	2.08	0.54
3:D:576:ARG:HD3	3:D:593:ASN:HB3	1.90	0.54
2:H:1256:GLN:HB3	2:H:1298:VAL:HG23	1.90	0.54
4:J:92:PHE:CD1	4:J:100:PRO:HG3	2.43	0.54
4:K:27:ARG:HA	4:K:30:ILE:HD12	1.90	0.54
2:C:890:LYS:HD3	3:I:77:ARG:HA	1.89	0.54
3:D:587:LEU:HB3	3:D:588:PRO:HD2	1.89	0.54
3:D:1238:GLN:HG3	3:D:1253:ILE:HD13	1.90	0.54
2:H:1289:GLU:HA	2:H:1293:VAL:HB	1.89	0.54
2:H:1330:ILE:CD1	3:I:1332:LEU:HD22	2.37	0.54
1:B:13:LEU:HD23	1:B:28:LEU:HG	1.89	0.54
2:C:1101:LEU:HD13	3:D:504:GLN:HB3	1.89	0.54
3:D:806:ASP:HA	3:D:1347:LEU:HG	1.90	0.54
2:H:160:ASP:HB3	2:H:164:THR:HG21	1.90	0.54
3:I:1317:GLU:HB2	3:I:1344:LEU:HD11	1.90	0.54
2:C:1255:THR:HG22	2:C:1325:VAL:HG21	1.89	0.53
3:D:580:TRP:HE1	3:D:590:SER:HA	1.71	0.53
3:D:1072:LYS:NZ	3:D:1170:LYS:HE3	2.23	0.53
1:F:43:LEU:HA	1:F:46:ILE:HD12	1.90	0.53
2:H:144:VAL:HB	2:H:515:MET:SD	2.47	0.53
3:I:1001:ALA:CA	3:I:1020:TRP:HE1	2.03	0.53
3:I:1178:THR:HG22	3:I:1187:GLU:HG2	1.90	0.53
2:H:897:PRO:O	2:H:901:LEU:HG	2.08	0.53
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.07	0.53
2:C:473:ARG:HD3	4:J:74:VAL:HG21	1.90	0.53
3:D:264:ASP:HB3	3:D:325:LYS:HD2	1.90	0.53
3:D:807:LEU:CD2	3:D:1262:ARG:HH12	2.22	0.53
1:B:48:LEU:HD21	3:D:534:GLU:OE2	2.08	0.53
2:C:12[A]:ARG:NH1	2:C:12[A]:ARG:CG	2.66	0.53
2:C:496:LYS:HD3	4:J:102:PRO:HD3	1.91	0.53
2:C:561:ILE:HA	2:C:680:LEU:HD23	1.91	0.53
2:C:887:VAL:HG22	2:C:914:LYS:HG2	1.91	0.53
3:D:233:LYS:HB2	3:D:236:TRP:CD1	2.44	0.53
2:H:1109:ILE:HA	2:H:1112:ILE:HD12	1.89	0.53
2:C:1333:LEU:O	3:D:307:LEU:HD13	2.09	0.53
3:D:69:GLU:HG2	3:D:76:LYS:HA	1.90	0.53
3:D:1317:GLU:HB2	3:D:1344:LEU:HD11	1.90	0.53
2:C:20:GLN:HG3	2:C:1157:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1246:ARG:HD2	2:C:1266:GLY:H	1.74	0.53
3:D:395:LYS:HE3	2:H:902:LEU:HA	1.91	0.53
2:H:1333:LEU:HD22	3:I:115:TRP:HE1	1.72	0.53
2:H:1333:LEU:HD21	3:I:327:LEU:HB2	1.90	0.53
3:I:807:LEU:CD2	3:I:1262:ARG:HH12	2.21	0.53
2:C:473:ARG:CD	4:J:74:VAL:HG21	2.38	0.53
3:D:1323:ALA:HB1	3:D:1332:LEU:HD23	1.90	0.53
2:H:818:VAL:HB	2:H:1079:ILE:HG12	1.90	0.53
3:I:69:GLU:HG2	3:I:76:LYS:HA	1.90	0.53
3:I:233:LYS:HB2	3:I:236:TRP:CD1	2.44	0.53
1:B:182:ARG:NH2	3:D:581:MET:HG3	2.24	0.53
2:C:1333:LEU:HD11	3:D:331:ILE:HD11	1.91	0.53
1:G:179:PRO:HA	1:G:209:GLY:CA	2.32	0.53
4:J:87:PRO:CB	4:J:88:ARG:HA	2.36	0.53
2:C:160:ASP:HB3	2:C:164:THR:HG21	1.91	0.53
2:C:1328:LYS:NZ	3:D:99:ARG:HB3	2.24	0.53
2:H:1246:ARG:HD2	2:H:1266:GLY:H	1.74	0.53
3:I:576:ARG:HD3	3:I:593:ASN:HB3	1.90	0.52
2:C:680:LEU:HD13	3:D:783:LEU:HD11	1.90	0.52
3:D:194:LEU:HD11	3:D:233:LYS:N	2.24	0.52
3:I:59:ALA:O	3:I:90:VAL:HG22	2.08	0.52
2:H:92:TYR:O	2:H:128:PRO:HA	2.09	0.52
3:I:309:ASN:HD22	3:I:324:LEU:HB2	1.73	0.52
4:K:105:ASP:O	4:K:107:GLU:N	2.43	0.52
3:D:357:VAL:HG12	3:D:358:GLY:N	2.25	0.52
2:H:172:TYR:CD2	2:H:436:ARG:HD2	2.45	0.52
3:I:535:ARG:HG2	3:I:538:ARG:HH12	1.68	0.52
2:C:172:TYR:CD2	2:C:436:ARG:HD2	2.45	0.52
2:C:1258:PRO:HB3	2:C:1265:PHE:CD2	2.44	0.52
3:D:890:THR:HG1	3:D:895:CYS:HG	1.58	0.52
3:I:70:CYS:HB2	3:I:75:TYR:HB2	1.91	0.52
1:F:48:LEU:CD1	2:H:1087:TYR:OH	2.57	0.52
2:H:186:PHE:HE1	2:H:209:ILE:HD12	1.74	0.52
3:I:53:ARG:HA	3:I:59:ALA:HB3	1.91	0.52
4:K:90:MET:HB3	4:K:91:GLY:HA3	1.91	0.52
2:C:82:VAL:HA	2:C:92:TYR:CE1	2.42	0.52
2:H:96:LEU:HB2	2:H:124:MET:HB2	1.92	0.52
3:I:533:ALA:HA	3:I:578:ILE:HG12	1.91	0.52
3:I:806:ASP:HA	3:I:1347:LEU:HG	1.90	0.52
3:I:277:ASN:HB3	3:I:281:ARG:HD2	1.92	0.52
3:I:536:LEU:HD13	3:I:574:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HD23	1:B:115:ILE:HG12	1.91	0.52
3:D:422:LEU:HB2	3:D:469:HIS:HB2	1.92	0.52
1:G:48:LEU:HG	1:G:183:ILE:HD12	1.91	0.52
3:I:902:ASP:C	3:I:903:LEU:HG	2.35	0.52
3:I:885:VAL:CB	3:I:1258:ARG:HD3	2.25	0.51
3:D:902:ASP:C	3:D:903:LEU:HG	2.35	0.51
3:I:1241:TYR:HB2	3:I:1248:ILE:CD1	2.40	0.51
1:A:107:ILE:HD11	1:A:136:GLU:HG2	1.91	0.51
2:C:577:VAL:HG23	2:C:661:VAL:O	2.10	0.51
2:C:1086:PRO:HA	2:C:1215:GLY:H	1.75	0.51
3:D:536:LEU:HD13	3:D:574:VAL:CG1	2.40	0.51
1:G:45:ARG:HH21	2:H:1219:GLU:HG3	1.75	0.51
2:H:577:VAL:HG23	2:H:661:VAL:O	2.10	0.51
3:I:314:ARG:HD3	3:I:315:ALA:H	1.74	0.51
3:D:114:ILE:HD12	3:D:307:LEU:HB2	1.93	0.51
2:H:1086:PRO:HA	2:H:1215:GLY:H	1.75	0.51
2:H:60:GLN:HG2	2:H:67:GLU:HG2	1.93	0.51
3:I:105:ILE:HG21	4:J:18:PHE:CE2	2.45	0.51
3:I:1238:GLN:HG3	3:I:1253:ILE:HD13	1.90	0.51
3:D:123:ARG:HH12	3:D:1333:THR:CB	2.23	0.51
3:D:1178:THR:HG22	3:D:1187:GLU:HG2	1.92	0.51
2:H:841:ARG:HH11	2:H:1047:LEU:HD22	1.75	0.51
2:H:1280:ALA:C	2:H:1282:GLY:H	2.18	0.51
3:I:592:VAL:HG11	3:I:604:MET:HE2	1.91	0.51
4:K:29:HIS:CB	4:K:82:LEU:HG	2.25	0.51
1:F:234:LEU:CB	1:G:13:LEU:HD12	2.40	0.51
2:C:310:ILE:HG23	2:C:325:LEU:HD22	1.93	0.51
3:D:78:LEU:HD13	3:D:81:ARG:NH2	2.25	0.51
2:H:1258:PRO:HB3	2:H:1265:PHE:CD2	2.46	0.51
3:I:386:GLU:HG2	3:I:394:ILE:HA	1.93	0.51
2:C:189:ASP:HB2	2:C:195:PHE:HE2	1.76	0.51
3:D:381:ILE:HG23	3:D:412:LEU:HD21	1.93	0.51
3:D:1241:TYR:HB2	3:D:1248:ILE:CD1	2.41	0.51
2:H:876:GLU:HG2	2:H:927:THR:HG22	1.93	0.51
3:I:395:LYS:C	3:I:397:ALA:H	2.18	0.51
1:A:166:ARG:H	1:A:167:PRO:HD3	1.76	0.51
2:C:10:ARG:HD2	2:C:697:LYS:HZ2	1.76	0.51
2:C:96:LEU:HB2	2:C:124:MET:HB2	1.92	0.51
2:C:889:PRO:O	3:I:78:LEU:CD1	2.59	0.51
3:D:27:PRO:HB3	3:D:240:THR:OG1	2.11	0.51
3:D:93:THR:HG22	2:H:890:LYS:NZ	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:202:ARG:HD3	3:D:216:LYS:HG3	1.93	0.51
3:D:734:ALA:HA	3:D:737:ILE:HD12	1.93	0.51
3:I:228:VAL:HG23	3:I:1341:ARG:NH1	2.26	0.51
1:B:48:LEU:HG	1:B:183:ILE:HD12	1.92	0.50
3:D:113:HIS:CD2	3:D:237:MET:O	2.63	0.50
2:H:1328:LYS:HA	2:H:1331:ARG:HD2	1.93	0.50
3:I:59:ALA:CB	3:I:71:LEU:HD11	2.41	0.50
3:I:357:VAL:HG12	3:I:358:GLY:N	2.25	0.50
3:I:425:ARG:NH2	3:I:457:TYR:CB	2.73	0.50
2:C:1077:SER:HB2	3:D:357:VAL:HB	1.92	0.50
2:C:1224:PRO:O	3:D:638:SER:HB3	2.11	0.50
2:C:1280:ALA:C	2:C:1282:GLY:H	2.19	0.50
3:D:79:LYS:HB3	3:D:80:HIS:CD2	2.46	0.50
2:C:186:PHE:HE1	2:C:209:ILE:HD12	1.76	0.50
3:D:531:LYS:HD3	3:D:535:ARG:HH21	1.76	0.50
3:I:136:GLU:O	3:I:312:ARG:NH2	2.44	0.50
3:D:452:LEU:HG	3:D:625:MET:SD	2.51	0.50
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.93	0.50
2:H:310:ILE:HG23	2:H:325:LEU:HD22	1.92	0.50
3:I:667:GLN:HG2	3:I:672:LEU:HD12	1.93	0.50
2:C:1291:LEU:HD22	3:D:343:LEU:O	2.11	0.50
3:D:226:ALA:CB	3:D:227:PHE:CA	2.87	0.50
2:H:697:LYS:HZ3	2:H:791:LEU:HB2	1.75	0.50
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.94	0.50
3:D:1326:GLN:HB2	3:D:1331:VAL:HG21	1.94	0.50
2:C:1328:LYS:HA	2:C:1331:ARG:HD2	1.93	0.50
3:D:331:ILE:HG21	3:D:1332:LEU:HD11	1.92	0.50
3:D:667:GLN:HG2	3:D:672:LEU:HD12	1.94	0.50
3:I:169:LEU:O	3:I:173:GLY:CA	2.60	0.50
1:A:16:ILE:HG12	1:A:26:VAL:HG13	1.94	0.50
2:C:1294:LYS:HZ2	3:D:349:TYR:HE2	1.59	0.50
3:D:799:ARG:O	3:D:803:VAL:HG23	2.12	0.50
2:C:92:TYR:CD2	2:C:137:VAL:HB	2.47	0.50
2:H:189:ASP:HB2	2:H:195:PHE:HE2	1.76	0.50
4:J:75:MET:HE3	4:J:75:MET:HA	1.94	0.50
2:C:519:ASN:HD21	2:C:689:ALA:HB3	1.76	0.49
3:I:139:LEU:HD13	3:I:185:ILE:HD11	1.94	0.49
3:I:364:HIS:HB3	3:I:487:THR:HG22	1.93	0.49
3:I:600:ALA:HA	3:I:603:LYS:HB2	1.94	0.49
1:A:74:VAL:O	2:C:729:ALA:N	2.46	0.49
3:D:272:VAL:CG2	3:D:306:LEU:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:364:HIS:HB3	3:D:487:THR:HG22	1.93	0.49
3:D:378:LYS:HA	3:D:381:ILE:HD12	1.93	0.49
1:B:182:ARG:HH22	3:D:581:MET:CG	2.22	0.49
2:C:724:VAL:HG22	2:C:734:ILE:HG12	1.94	0.49
1:G:179:PRO:HG3	1:G:211:ILE:HD12	1.95	0.49
4:J:27:ARG:HA	4:J:30:ILE:HD12	1.94	0.49
3:D:978:ARG:NH1	3:D:1198:VAL:HA	2.27	0.49
2:H:870:ILE:HD12	2:H:944:ARG:HD2	1.95	0.49
3:D:242:LEU:HD22	3:D:303:VAL:HG11	1.92	0.49
3:D:281:ARG:HG2	3:I:107:LEU:CD1	2.42	0.49
3:D:600:ALA:HA	3:D:603:LYS:HB2	1.94	0.49
2:H:895:LEU:HD22	2:H:900:LYS:HG3	1.95	0.49
3:I:750:PRO:HA	3:I:781:LYS:HE2	1.94	0.49
1:A:101:THR:HA	1:A:142:MET:O	2.13	0.49
2:C:224:PHE:CZ	2:C:347:ILE:HG21	2.48	0.49
3:D:337:ARG:HB3	3:D:341:ASN:ND2	2.27	0.49
3:D:366:CYS:HB2	3:D:437:PHE:HB2	1.94	0.49
1:F:16:ILE:HG12	1:F:26:VAL:HG13	1.94	0.49
2:H:122:VAL:HG22	2:H:490:GLN:HA	1.94	0.49
2:H:321:LEU:O	2:H:325:LEU:HG	2.12	0.49
2:H:724:VAL:HG22	2:H:734:ILE:HG12	1.94	0.49
2:H:1255:THR:HG22	2:H:1325:VAL:HG21	1.93	0.49
3:I:422:LEU:HB2	3:I:469:HIS:HB2	1.94	0.49
3:I:580:TRP:HE1	3:I:593:ASN:HB2	1.77	0.49
1:A:48:LEU:HG	1:A:183:ILE:HD12	1.95	0.49
2:C:122:VAL:HG22	2:C:490:GLN:HA	1.94	0.49
2:C:321:LEU:O	2:C:325:LEU:HG	2.13	0.49
2:C:367:TYR:HA	2:C:370:MET:HB2	1.95	0.49
3:D:113:HIS:CD2	3:D:239:LEU:N	2.81	0.49
1:G:101:THR:HA	1:G:142:MET:O	2.13	0.49
2:H:851:THR:HG23	2:H:886:LYS:H	1.78	0.49
2:H:1281:TYR:HD1	3:I:484:MET:HG3	1.76	0.49
3:I:425:ARG:CZ	3:I:457:TYR:CB	2.91	0.49
3:I:430:HIS:CE1	3:I:925:GLU:HB2	2.48	0.49
3:I:749:LYS:HE3	3:I:755:ILE:HG12	1.95	0.49
3:D:185:ILE:HA	3:D:188:LEU:HG	1.95	0.49
1:F:48:LEU:HG	1:F:183:ILE:HD12	1.94	0.49
2:H:367:TYR:HA	2:H:370:MET:HB2	1.95	0.49
4:J:174:ASP:O	4:J:178:VAL:HG22	2.13	0.49
2:C:802:VAL:HA	2:C:1096:ILE:O	2.12	0.49
3:I:62:PHE:CD1	3:I:247:PRO:HD3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:363:LEU:HD23	3:I:450:HIS:HB3	1.94	0.49
3:I:506:VAL:HG22	3:I:629:PHE:CE1	2.48	0.49
4:J:159:LYS:HE3	4:J:170:PRO:HB2	1.94	0.49
2:C:841:ARG:HH11	2:C:1047:LEU:HD22	1.76	0.49
1:F:101:THR:HA	1:F:142:MET:O	2.13	0.49
2:H:519:ASN:HD21	2:H:689:ALA:HB3	1.77	0.49
2:H:870:ILE:HG23	2:H:884:VAL:HG22	1.95	0.49
2:C:60:GLN:HG2	2:C:67:GLU:HG2	1.94	0.48
2:C:870:ILE:HG23	2:C:884:VAL:HG22	1.94	0.48
3:D:81:ARG:CZ	2:H:890:LYS:HB2	2.42	0.48
3:D:90:VAL:HA	3:I:260:PHE:CE1	2.48	0.48
3:D:106:GLU:OE2	3:D:273:ILE:HG12	2.13	0.48
3:D:1002:VAL:HG23	3:D:1020:TRP:CZ2	2.48	0.48
3:I:531:LYS:HD3	3:I:535:ARG:HH21	1.78	0.48
2:H:810:TYR:HB3	2:H:817:LEU:CD2	2.43	0.48
2:H:854:ILE:HD13	2:H:865:LEU:HD13	1.94	0.48
3:I:452:LEU:HG	3:I:625:MET:SD	2.53	0.48
3:I:660:GLU:HB3	3:I:685:ILE:CG2	2.44	0.48
4:K:174:ASP:O	4:K:178:VAL:HG22	2.13	0.48
2:C:117:ILE:HD11	2:C:485:ASP:HB3	1.94	0.48
2:C:1279:GLU:HA	2:C:1287:LEU:HD11	1.95	0.48
3:I:59:ALA:HB2	3:I:71:LEU:HD11	1.94	0.48
3:I:70:CYS:SG	3:I:90:VAL:HB	2.53	0.48
3:I:661:VAL:HG21	3:I:686:TRP:CD1	2.49	0.48
3:D:386:GLU:HG2	3:D:394:ILE:HA	1.95	0.48
1:F:210:THR:O	1:F:211:ILE:HG13	2.14	0.48
3:I:56:LEU:HD11	3:I:270:ARG:HG3	1.94	0.48
3:D:430:HIS:CE1	3:D:925:GLU:HB2	2.48	0.48
3:D:512:TYR:HA	3:D:515:ARG:CZ	2.44	0.48
3:I:799:ARG:O	3:I:803:VAL:HG23	2.13	0.48
3:D:30:ILE:HG21	3:D:243:PRO:HG3	1.94	0.48
3:D:79:LYS:HA	2:H:915:ASP:CG	2.38	0.48
3:D:366:CYS:HB3	3:D:439:PRO:HA	1.95	0.48
3:D:661:VAL:HG21	3:D:686:TRP:CD1	2.49	0.48
1:F:42:ALA:HA	1:G:38:THR:HG22	1.94	0.48
1:G:16:ILE:HG12	1:G:26:VAL:HG13	1.95	0.48
3:I:416:ILE:HG23	3:I:439:PRO:HB2	1.95	0.48
1:A:60:GLU:HG3	1:A:170:ARG:HG3	1.96	0.48
2:C:675:ASP:CG	2:C:1107:MET:HB2	2.38	0.48
3:D:368:LEU:HD21	3:D:421:VAL:HG21	1.96	0.48
1:B:101:THR:HA	1:B:142:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:851:THR:HG23	2:C:886:LYS:H	1.79	0.48
3:D:394:ILE:HG22	2:H:901:LEU:HD23	1.96	0.48
3:D:580:TRP:HE1	3:D:593:ASN:HB2	1.78	0.48
2:H:802:VAL:HA	2:H:1096:ILE:O	2.12	0.48
2:H:819:SER:HB3	2:H:1085:MET:HE2	1.96	0.48
2:C:38:PHE:HD1	2:C:48:GLY:HA2	1.79	0.48
3:D:275:ARG:CZ	3:D:302:ALA:HB3	2.44	0.48
2:H:366:ILE:O	2:H:370:MET:HG2	2.14	0.48
2:H:831:ILE:HG12	2:H:1057:LYS:HG2	1.95	0.48
3:I:512:TYR:HA	3:I:515:ARG:CZ	2.44	0.48
3:I:612:LEU:HB3	3:I:616:PRO:HG2	1.95	0.48
3:I:1002:VAL:HG23	3:I:1020:TRP:CZ2	2.48	0.48
2:C:843:THR:HB	3:I:81:ARG:CZ	2.44	0.48
3:D:416:ILE:HG23	3:D:439:PRO:HB2	1.96	0.48
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.96	0.48
3:I:1326:GLN:HB2	3:I:1331:VAL:HG21	1.96	0.48
2:C:741:MET:HG2	2:C:747:GLY:HA2	1.96	0.47
2:C:1277:ALA:HB1	2:C:1281:TYR:HE2	1.79	0.47
3:D:212:THR:HG22	3:D:215:LYS:HD2	1.96	0.47
2:H:38:PHE:HD1	2:H:48:GLY:HA2	1.79	0.47
4:K:141:PHE:HB3	4:K:162:VAL:HG21	1.96	0.47
1:A:210:THR:O	1:A:211:ILE:HG13	2.14	0.47
3:D:202:ARG:HG2	3:D:212:THR:HB	1.95	0.47
3:D:272:VAL:CG2	3:D:306:LEU:CD1	2.79	0.47
2:H:1277:ALA:HB1	2:H:1281:TYR:HE2	1.79	0.47
2:H:1330:ILE:HD11	3:I:1332:LEU:HD22	1.95	0.47
3:I:425:ARG:CZ	3:I:459:ALA:CB	2.92	0.47
3:I:978:ARG:NH1	3:I:1198:VAL:HA	2.27	0.47
2:C:559:CYS:SG	2:C:662:SER:N	2.87	0.47
2:H:12[B]:ARG:HD2	2:H:1183:ALA:HB2	1.95	0.47
3:I:68:TYR:CG	3:I:78:LEU:CD2	2.98	0.47
3:I:114:ILE:CG1	3:I:304:ASP:HA	2.42	0.47
3:I:381:ILE:HG12	3:I:412:LEU:HD22	1.96	0.47
3:I:660:GLU:HB3	3:I:685:ILE:HG21	1.96	0.47
3:I:896:ALA:HA	3:I:899:TYR:CE2	2.49	0.47
1:A:74:VAL:O	2:C:729:ALA:CB	2.62	0.47
2:C:810:TYR:HB3	2:C:817:LEU:CD2	2.44	0.47
3:D:107:LEU:HD23	3:D:241:VAL:HG22	1.96	0.47
3:D:424:ASN:HD21	3:D:434:ILE:HG12	1.79	0.47
3:D:660:GLU:HB3	3:D:685:ILE:CG2	2.44	0.47
2:H:675:ASP:CG	2:H:1107:MET:HB2	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:812:PHE:HB2	3:I:357:VAL:HG22	1.95	0.47
2:H:944:ARG:HA	2:H:947:GLU:HB2	1.96	0.47
2:C:366:ILE:O	2:C:370:MET:HG2	2.14	0.47
3:D:71:LEU:CD2	3:I:51:PRO:HD3	2.44	0.47
3:D:896:ALA:HA	3:D:899:TYR:CE2	2.49	0.47
2:C:174:ALA:HB2	2:C:432:LEU:CD2	2.45	0.47
3:D:78:LEU:HB3	3:D:81:ARG:HH21	1.78	0.47
1:G:33:ARG:NH2	1:G:196:THR:OG1	2.47	0.47
2:H:524:ILE:HG21	2:H:528:ARG:HH21	1.79	0.47
2:H:857:VAL:H	2:H:858:GLY:HA3	1.80	0.47
2:C:819:SER:HB3	2:C:1085:MET:HE2	1.95	0.47
3:D:35:PHE:CZ	3:D:101:ARG:HG2	2.50	0.47
3:D:506:VAL:HG22	3:D:629:PHE:CE1	2.47	0.47
3:D:660:GLU:HB3	3:D:685:ILE:HG21	1.97	0.47
2:H:559:CYS:SG	2:H:662:SER:N	2.87	0.47
3:I:366:CYS:HB3	3:I:439:PRO:HA	1.95	0.47
4:K:111:ILE:HD12	4:K:135:ARG:HH12	1.80	0.47
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	1.96	0.47
3:D:809:VAL:HG23	3:D:915:ILE:HD11	1.96	0.47
2:H:591:TYR:HB3	2:H:652:TYR:HB3	1.97	0.47
1:B:152:TYR:CZ	3:D:538:ARG:CZ	2.98	0.47
2:C:565:GLU:HA	2:C:569:ILE:HG12	1.97	0.47
2:C:895:LEU:HB2	2:H:1302:THR:HG21	1.96	0.47
2:C:902:LEU:HB3	2:C:912:ASP:CG	2.40	0.47
1:F:107:ILE:HG13	1:F:136:GLU:HA	1.97	0.47
2:H:12[B]:ARG:CZ	2:H:703:GLY:HA2	2.45	0.47
3:I:424:ASN:HD21	3:I:434:ILE:HG12	1.79	0.47
2:C:1246:ARG:HD2	2:C:1266:GLY:N	2.30	0.47
3:D:1221:LEU:HG	3:D:1229:VAL:HG11	1.97	0.47
3:I:357:VAL:HG12	3:I:358:GLY:H	1.80	0.47
3:I:381:ILE:HG23	3:I:412:LEU:HD21	1.96	0.47
3:I:575:GLY:HA2	3:I:578:ILE:HD12	1.96	0.47
3:I:1172:LYS:HG3	3:I:1173:ARG:H	1.79	0.47
3:D:268:LEU:C	3:D:306:LEU:HD21	2.40	0.46
3:D:564:VAL:HG12	3:D:565:ALA:H	1.80	0.46
3:I:366:CYS:HB2	3:I:437:PHE:HB2	1.95	0.46
2:C:591:TYR:HB3	2:C:652:TYR:HB3	1.97	0.46
3:D:268:LEU:O	3:D:306:LEU:HD21	2.14	0.46
2:H:741:MET:HG2	2:H:747:GLY:HA2	1.96	0.46
2:H:1226:THR:HG23	3:I:638:SER:HB2	1.97	0.46
3:I:185:ILE:HA	3:I:188:LEU:HG	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:564:VAL:HG12	3:I:565:ALA:H	1.80	0.46
2:C:841:ARG:HD3	2:C:1047:LEU:HD13	1.97	0.46
2:C:1132:LEU:HD13	2:C:1177:ARG:NE	2.30	0.46
3:D:903:LEU:HD13	3:D:909:ILE:HG13	1.97	0.46
2:H:3:TYR:CE2	2:H:1159:VAL:HG11	2.50	0.46
2:H:225:PHE:CE2	2:H:347:ILE:HB	2.49	0.46
3:I:809:VAL:HG23	3:I:915:ILE:HD11	1.96	0.46
3:I:903:LEU:HD13	3:I:909:ILE:HG13	1.98	0.46
3:D:94:GLN:HB3	3:D:95:THR:H	1.57	0.46
3:D:662:ALA:HA	3:D:665:GLN:HB2	1.98	0.46
2:H:556:GLY:HA2	2:H:660:VAL:HA	1.98	0.46
3:I:396:ALA:O	3:I:400:MET:HG2	2.15	0.46
3:I:534:GLU:O	3:I:538:ARG:N	2.46	0.46
2:C:944:ARG:HA	2:C:947:GLU:HB2	1.98	0.46
3:D:37:GLU:H	3:D:105:ILE:CD1	2.29	0.46
2:H:1279:GLU:HA	2:H:1287:LEU:HD11	1.96	0.46
2:H:1324:ASN:HB3	2:H:1328:LYS:HE3	1.98	0.46
3:I:587:LEU:HB3	3:I:588:PRO:HD2	1.98	0.46
1:A:166:ARG:N	1:A:167:PRO:HD3	2.30	0.46
3:D:533:ALA:HA	3:D:578:ILE:HG12	1.96	0.46
2:H:565:GLU:HA	2:H:569:ILE:HG12	1.97	0.46
2:H:1196:LYS:HA	2:H:1199:LEU:HD12	1.96	0.46
2:H:1246:ARG:HD2	2:H:1266:GLY:N	2.30	0.46
3:I:368:LEU:HD21	3:I:421:VAL:HG21	1.97	0.46
3:I:378:LYS:HA	3:I:381:ILE:HD12	1.97	0.46
2:C:805:MET:CE	2:C:806:PRO:HD2	2.37	0.46
3:D:242:LEU:HD22	3:D:303:VAL:CG1	2.44	0.46
3:D:338:PHE:HA	3:D:342:LEU:HB2	1.97	0.46
3:D:900:GLY:HA3	3:D:1251:LYS:HE2	1.96	0.46
3:I:797:THR:HG22	3:I:924:GLY:CA	2.46	0.46
2:C:473:ARG:HH11	4:J:74:VAL:HG21	1.80	0.46
2:C:767:GLN:HA	2:C:786:GLY:HA2	1.97	0.46
3:D:252:LEU:CG	3:I:86:GLU:HB2	2.44	0.46
3:D:593:ASN:HD22	3:D:593:ASN:HA	1.53	0.46
3:D:1072:LYS:HZ2	3:D:1170:LYS:HE3	1.81	0.46
2:C:174:ALA:HB2	2:C:432:LEU:HD22	1.97	0.46
3:D:331:ILE:HG12	3:D:337:ARG:CZ	2.46	0.46
2:H:672:GLU:HA	3:I:772:TYR:OH	2.16	0.46
3:I:307:LEU:O	3:I:328:ALA:HB2	2.16	0.46
1:A:48:LEU:HD11	2:C:1087:TYR:OH	2.16	0.46
1:B:113:ALA:O	1:B:115:ILE:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:851:THR:HA	2:C:887:VAL:HG21	1.98	0.46
3:D:575:GLY:HA2	3:D:578:ILE:HD12	1.98	0.46
3:D:814:CYS:SG	3:D:898:CYS:N	2.89	0.46
3:D:885:VAL:HG13	3:D:894:VAL:HG11	1.98	0.46
3:D:896:ALA:HA	3:D:899:TYR:HE2	1.81	0.46
2:H:936:ARG:HB2	2:H:1047:LEU:HD23	1.98	0.46
2:H:1107:MET:CE	3:I:740:LEU:HG	2.45	0.46
3:I:785:ASP:HB3	3:I:789:LYS:HZ2	1.81	0.46
3:I:923:ILE:HD13	3:I:1256:ILE:HD11	1.99	0.46
4:J:141:PHE:HB3	4:J:162:VAL:HG21	1.98	0.46
3:D:357:VAL:HG12	3:D:358:GLY:H	1.81	0.45
2:H:766:ASN:H	2:H:787:PRO:HB3	1.80	0.45
2:H:851:THR:HA	2:H:887:VAL:HG21	1.98	0.45
3:I:885:VAL:HG13	3:I:894:VAL:HG11	1.97	0.45
1:B:80:GLU:O	3:D:551:ARG:NH2	2.48	0.45
2:C:556:GLY:HA2	2:C:660:VAL:HA	1.98	0.45
2:C:766:ASN:H	2:C:787:PRO:HB3	1.80	0.45
3:D:131:PRO:HB3	3:D:159:ILE:HD11	1.98	0.45
3:I:429:LEU:HD22	3:I:797:THR:HG21	1.98	0.45
3:I:814:CYS:SG	3:I:898:CYS:N	2.89	0.45
3:D:609:TYR:HA	3:D:617:THR:HG21	1.99	0.45
2:H:117:ILE:HD11	2:H:485:ASP:HB3	1.99	0.45
3:I:1270:GLY:HA3	3:I:1298:VAL:HG13	1.97	0.45
3:D:797:THR:HG22	3:D:924:GLY:CA	2.47	0.45
2:H:767:GLN:HA	2:H:786:GLY:HA2	1.97	0.45
2:H:810:TYR:HA	3:I:357:VAL:HG11	1.97	0.45
2:H:841:ARG:HD3	2:H:1047:LEU:HD13	1.97	0.45
2:H:1132:LEU:HD13	2:H:1177:ARG:NE	2.31	0.45
3:I:206:ASN:HD21	3:I:213:LYS:HD2	1.81	0.45
3:I:580:TRP:HA	3:I:580:TRP:CE3	2.51	0.45
3:D:96:LYS:HE3	2:H:892:GLU:HB3	1.97	0.45
3:D:1270:GLY:HA3	3:D:1298:VAL:HG13	1.99	0.45
1:F:184:ALA:HB2	2:H:1091:GLY:HA3	1.96	0.45
2:H:103:VAL:HG13	2:H:113:THR:HG22	1.98	0.45
4:K:15:PHE:HB2	4:K:89:VAL:HB	1.97	0.45
1:B:176:CYS:SG	3:D:535:ARG:NH2	2.89	0.45
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.99	0.45
3:D:139:LEU:HA	3:D:181:GLY:HA2	1.98	0.45
1:F:30:PRO:HA	1:F:198:LEU:HD13	1.99	0.45
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.31	0.45
1:B:191:ARG:NE	3:D:441:LEU:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:VAL:HG13	2:C:113:THR:HG22	1.98	0.45
2:C:1293:VAL:HG22	2:C:1315:MET:HE2	1.98	0.45
2:C:1334:GLY:HA2	3:D:239:LEU:HD21	1.98	0.45
3:D:396:ALA:O	3:D:400:MET:HG2	2.16	0.45
3:I:44:ILE:HG21	3:I:260:PHE:CE2	2.52	0.45
3:I:803:VAL:HG21	3:I:1309:ILE:HG12	1.98	0.45
3:I:896:ALA:HA	3:I:899:TYR:HE2	1.81	0.45
3:I:933:ARG:HH21	3:I:1240:VAL:HG13	1.82	0.45
3:I:975:ILE:HB	3:I:1001:ALA:HB3	1.99	0.45
2:C:889:PRO:O	3:I:78:LEU:HD11	2.17	0.45
1:F:88:LEU:HD21	1:F:130:ILE:HG12	1.99	0.45
2:H:1101:LEU:HD13	3:I:504:GLN:HB3	1.98	0.45
3:I:121:PRO:HG2	3:I:124:ILE:HD12	1.99	0.45
3:I:609:TYR:HA	3:I:617:THR:HG21	1.98	0.45
2:C:557:ARG:HG3	2:C:589:THR:HG23	1.99	0.45
3:D:123:ARG:NH2	3:D:1333:THR:OG1	2.49	0.45
3:D:260:PHE:CD2	3:I:75:TYR:CD1	3.05	0.45
3:D:395:LYS:HD3	2:H:905:ILE:N	2.31	0.45
3:D:1002:VAL:H	3:D:1020:TRP:HE1	1.65	0.45
2:H:390:PHE:HA	2:H:419:ILE:CG2	2.47	0.45
3:D:770:LEU:HA	3:D:773:PHE:CD2	2.52	0.45
3:D:1172:LYS:HG2	3:D:1173:ARG:H	1.81	0.45
2:H:174:ALA:HB2	2:H:432:LEU:CD2	2.46	0.45
2:H:174:ALA:HB2	2:H:432:LEU:HD22	1.98	0.45
1:A:11:PRO:HG2	1:B:230:ALA:HB3	1.98	0.44
2:C:854:ILE:HG23	2:C:886:LYS:HD2	1.98	0.44
2:C:888:THR:OG1	2:C:915:ASP:OD2	2.36	0.44
3:D:25:ALA:HB1	3:D:30:ILE:CG1	2.47	0.44
3:D:239:LEU:HD13	3:D:242:LEU:HA	1.99	0.44
3:D:515:ARG:NH2	3:D:724:MET:HB3	2.32	0.44
2:C:1333:LEU:HA	3:D:307:LEU:HD22	1.99	0.44
3:D:550:VAL:O	3:D:569:LEU:HA	2.17	0.44
3:D:580:TRP:CE3	3:D:580:TRP:HA	2.52	0.44
3:D:923:ILE:HD13	3:D:1256:ILE:HD11	1.99	0.44
3:D:1002:VAL:H	3:D:1020:TRP:NE1	2.15	0.44
2:H:855:PRO:HB3	2:H:914:LYS:CD	2.44	0.44
3:I:515:ARG:NH2	3:I:724:MET:HB3	2.32	0.44
3:I:1221:LEU:HG	3:I:1229:VAL:HG11	1.97	0.44
3:D:398:LYS:HD3	2:H:901:LEU:HB3	1.98	0.44
3:I:900:GLY:HA3	3:I:1251:LYS:HE2	1.99	0.44
3:I:1002:VAL:H	3:I:1020:TRP:HE1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:70:CYS:SG	3:D:90:VAL:HB	2.58	0.44
3:D:512:TYR:HA	3:D:515:ARG:NH1	2.33	0.44
3:D:545:HIS:CD2	3:D:574:VAL:HG11	2.53	0.44
3:D:1323:ALA:HB1	3:D:1332:LEU:CD2	2.48	0.44
1:F:230:ALA:HB3	1:G:11:PRO:HG2	2.00	0.44
2:H:61:SER:HB3	2:H:479:LEU:HB3	2.00	0.44
2:H:848:GLU:HG2	2:H:889:PRO:HD3	2.00	0.44
3:I:550:VAL:O	3:I:569:LEU:HA	2.18	0.44
3:I:1002:VAL:H	3:I:1020:TRP:NE1	2.15	0.44
2:C:896:THR:HB	2:C:897:PRO:CD	2.43	0.44
2:C:936:ARG:HB2	2:C:1047:LEU:HD23	1.99	0.44
3:D:71:LEU:HD13	3:I:98:ARG:HH22	1.83	0.44
3:D:114:ILE:CG1	3:D:304:ASP:HA	2.44	0.44
2:H:292:ILE:O	2:H:322:LEU:HD11	2.17	0.44
2:H:557:ARG:HG3	2:H:589:THR:HG23	1.99	0.44
3:I:545:HIS:CD2	3:I:574:VAL:HG11	2.53	0.44
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.00	0.44
2:C:805:MET:HE2	3:D:637:ALA:N	2.33	0.44
3:D:113:HIS:CD2	3:D:238:ILE:CA	2.94	0.44
3:D:600:ALA:O	3:D:604:MET:N	2.50	0.44
3:I:662:ALA:HA	3:I:665:GLN:HB2	1.99	0.44
2:C:1029:LEU:HD22	2:C:1033:ARG:HH21	1.82	0.44
2:H:136:PHE:HB2	2:H:143:ARG:O	2.18	0.44
2:H:564:PRO:HD2	2:H:572:ILE:O	2.18	0.44
2:C:397:LEU:HB2	2:C:402:ARG:HE	1.83	0.44
2:C:1323:PHE:CD1	3:D:341:ASN:HB3	2.52	0.44
3:D:975:ILE:HB	3:D:1001:ALA:HB3	1.99	0.44
3:D:1226:VAL:HG22	3:D:1304:ARG:HH22	1.83	0.44
2:H:582:ASN:HB2	2:H:586:PHE:H	1.83	0.44
2:H:1117:LEU:HG	2:H:1195:ILE:HG23	2.00	0.44
4:K:87:PRO:HG2	4:K:88:ARG:HG2	2.00	0.44
1:A:107:ILE:HG13	1:A:136:GLU:HA	1.99	0.43
2:C:136:PHE:HB2	2:C:143:ARG:O	2.18	0.43
2:C:161:LYS:HG2	2:C:170:VAL:HG13	2.00	0.43
3:D:229:GLN:NE2	3:D:1341:ARG:HB2	2.33	0.43
3:D:507:VAL:HG13	3:D:511:TYR:HE2	1.83	0.43
3:D:1179:PRO:HB2	3:D:1180:VAL:H	1.58	0.43
3:I:770:LEU:HA	3:I:773:PHE:CD2	2.52	0.43
4:K:143:ASP:C	4:K:144:PHE:HD1	2.26	0.43
3:D:429:LEU:HD22	3:D:797:THR:HG21	1.99	0.43
3:D:836:ARG:HG2	3:D:871:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1177:ILE:O	3:D:1187:GLU:HA	2.18	0.43
3:D:1261:LEU:HD22	3:D:1306:LEU:HD13	2.00	0.43
1:F:101:THR:O	1:F:115:ILE:HG23	2.18	0.43
2:H:854:ILE:HG23	2:H:886:LYS:HD2	1.98	0.43
3:I:68:TYR:CB	3:I:78:LEU:HD23	2.48	0.43
3:I:309:ASN:ND2	3:I:324:LEU:HB2	2.33	0.43
3:I:470:VAL:HA	3:I:471:PRO:HD3	1.88	0.43
2:C:38:PHE:CD2	2:C:457:GLY:HA3	2.54	0.43
2:C:73:TYR:HD1	2:C:98:VAL:HG22	1.83	0.43
3:D:370:LYS:HE2	3:D:443:GLU:HB3	2.00	0.43
3:D:803:VAL:HG21	3:D:1309:ILE:HG12	1.99	0.43
2:H:1029:LEU:HD22	2:H:1033:ARG:HH21	1.82	0.43
3:I:836:ARG:HG2	3:I:871:LEU:HD22	1.99	0.43
3:I:857:LEU:HD13	3:I:860:ARG:HD2	2.00	0.43
1:A:46:ILE:HG12	1:B:35:PHE:HE1	1.83	0.43
3:D:110:PRO:HB2	3:D:111:THR:H	1.68	0.43
3:I:492:SER:HB3	3:I:499:ILE:HG13	2.00	0.43
3:I:1261:LEU:HD22	3:I:1306:LEU:HD13	1.99	0.43
4:K:128:PHE:CD2	4:K:158:LEU:HD11	2.53	0.43
1:A:45:ARG:NH2	1:B:37:HIS:HB3	2.34	0.43
2:C:211:ARG:HG3	2:C:220:ILE:HD11	2.01	0.43
2:C:1256:GLN:HG3	3:D:99:ARG:NH1	2.33	0.43
3:D:75:TYR:N	3:D:75:TYR:CD2	2.87	0.43
3:D:534:GLU:O	3:D:538:ARG:N	2.47	0.43
2:H:397:LEU:HB2	2:H:402:ARG:HE	1.84	0.43
3:I:380:PHE:HE2	3:I:472:LEU:HD22	1.82	0.43
3:I:424:ASN:ND2	3:I:434:ILE:HG12	2.34	0.43
3:I:600:ALA:O	3:I:604:MET:N	2.50	0.43
3:I:1234:VAL:HG21	3:I:1254:GLU:HG2	2.01	0.43
4:J:10:TYR:CD2	4:J:73:MET:HB3	2.53	0.43
2:C:1278:LEU:HG	3:D:434:ILE:HD13	2.00	0.43
2:H:38:PHE:CD2	2:H:457:GLY:HA3	2.53	0.43
2:H:73:TYR:HD1	2:H:98:VAL:HG22	1.84	0.43
3:I:355:ILE:HG21	3:I:461:PHE:HB3	2.00	0.43
3:I:357:VAL:CG1	3:I:358:GLY:N	2.81	0.43
2:C:153:PRO:O	2:C:452:ARG:NH2	2.52	0.43
3:D:394:ILE:HG21	2:H:900:LYS:O	2.19	0.43
2:H:798:GLN:OE1	2:H:827:ARG:HB3	2.18	0.43
2:H:1127:LYS:HD2	2:H:1202:GLY:HA2	2.00	0.43
3:I:512:TYR:HA	3:I:515:ARG:NH1	2.33	0.43
1:A:44:ARG:HH21	1:A:185:TYR:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:LEU:HD13	3:D:234:PRO:CB	2.47	0.43
3:D:202:ARG:HB2	3:D:216:LYS:HE3	2.01	0.43
3:D:355:ILE:HG21	3:D:461:PHE:HB3	2.00	0.43
3:D:356:THR:HG23	3:D:446:ALA:CB	2.49	0.43
3:D:527:LEU:HD12	3:D:532:GLU:HG2	2.00	0.43
3:D:563:LEU:HD22	3:D:585:LYS:HB3	2.01	0.43
3:D:697:MET:HE2	3:D:741:ALA:HB1	2.00	0.43
3:D:769:VAL:HG12	3:D:770:LEU:HD23	2.01	0.43
1:F:46:ILE:HD13	1:F:224:LEU:HG	2.01	0.43
2:H:226:GLU:HB3	2:H:337:PHE:HE2	1.80	0.43
2:C:551:HIS:H	2:C:554:HIS:HD2	1.67	0.43
2:C:582:ASN:HB2	2:C:586:PHE:H	1.83	0.43
3:D:580:TRP:HA	3:D:580:TRP:HE3	1.84	0.43
3:I:275:ARG:HB3	3:I:299:LEU:HD22	2.01	0.43
3:I:1167:LYS:HD2	3:I:1176:VAL:HB	2.00	0.43
3:I:1351:VAL:HG22	3:I:1357:ILE:HD11	2.00	0.43
2:C:390:PHE:HA	2:C:419:ILE:CG2	2.47	0.43
2:C:727:VAL:HG13	2:C:732:ILE:HG12	2.01	0.43
3:D:452:LEU:HD22	3:D:500:ILE:HG23	2.01	0.43
1:F:39:LEU:HD22	1:G:228:LEU:HD21	2.01	0.43
1:F:60:GLU:CG	1:F:170:ARG:HG3	2.49	0.43
2:H:696:ASP:O	2:H:697:LYS:HB2	2.19	0.43
2:H:847:PRO:C	2:H:889:PRO:HG3	2.44	0.43
2:H:1101:LEU:HD22	3:I:504:GLN:HB3	2.00	0.43
2:H:1247:SER:HB3	3:I:375:GLU:O	2.19	0.43
2:H:1281:TYR:CD1	3:I:484:MET:HG3	2.53	0.43
3:I:511:TYR:HD1	3:I:596:LEU:HD22	1.84	0.43
3:I:580:TRP:HA	3:I:580:TRP:HE3	1.84	0.43
4:J:144:PHE:HB3	4:J:162:VAL:HG13	2.00	0.43
2:C:86:GLN:N	2:C:92:TYR:OH	2.51	0.42
2:C:798:GLN:OE1	2:C:827:ARG:HB3	2.18	0.42
2:C:805:MET:HE2	3:D:637:ALA:H	1.83	0.42
2:C:850:ILE:HG12	2:C:1048:LYS:HE2	2.00	0.42
2:C:889:PRO:O	3:I:78:LEU:HD12	2.18	0.42
2:C:1077:SER:CB	3:D:357:VAL:HB	2.48	0.42
1:F:234:LEU:CD1	1:G:13:LEU:H	2.31	0.42
3:I:356:THR:OG1	3:I:448:GLN:HA	2.19	0.42
3:I:1177:ILE:O	3:I:1187:GLU:HA	2.18	0.42
3:I:1248:ILE:H	3:I:1248:ILE:HG13	1.74	0.42
3:I:1323:ALA:HB1	3:I:1332:LEU:CD2	2.48	0.42
3:D:357:VAL:CG1	3:D:358:GLY:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.00	0.42
3:D:785:ASP:HB3	3:D:789:LYS:HZ2	1.84	0.42
3:D:1167:LYS:HD2	3:D:1176:VAL:HB	2.01	0.42
1:G:38:THR:O	1:G:40:GLY:N	2.46	0.42
2:H:697:LYS:HE2	2:H:790:ASP:CB	2.32	0.42
2:H:1278:LEU:HG	3:I:434:ILE:HD13	2.00	0.42
2:H:1323:PHE:CE1	3:I:1352:ILE:HG23	2.54	0.42
3:I:858:VAL:HB	3:I:859:PRO:HD3	2.00	0.42
2:C:564:PRO:HD2	2:C:572:ILE:O	2.18	0.42
2:C:723:VAL:HA	2:C:776:PRO:HA	2.01	0.42
2:C:889:PRO:C	3:I:78:LEU:CD1	2.89	0.42
3:D:295:GLU:O	3:D:299:LEU:N	2.52	0.42
3:D:381:ILE:HG12	3:D:412:LEU:HD22	2.01	0.42
3:D:424:ASN:ND2	3:D:434:ILE:HG12	2.34	0.42
1:F:33:ARG:HE	1:F:197:ASP:HB2	1.84	0.42
2:H:161:LYS:HG2	2:H:170:VAL:HG13	2.00	0.42
3:I:139:LEU:CD1	3:I:185:ILE:HD11	2.48	0.42
3:I:356:THR:HG23	3:I:446:ALA:CB	2.49	0.42
3:I:825:VAL:HG22	3:I:838:ARG:NH2	2.34	0.42
1:B:102:LEU:HB2	1:B:142:MET:HB2	2.02	0.42
2:C:1117:LEU:HG	2:C:1195:ILE:HG23	2.00	0.42
2:C:1174:GLU:HA	2:C:1177:ARG:CZ	2.49	0.42
3:D:272:VAL:CG2	3:D:306:LEU:HD11	2.31	0.42
3:D:583:VAL:HG22	3:D:589:TYR:CE1	2.54	0.42
3:D:1221:LEU:HD22	3:D:1306:LEU:CD1	2.49	0.42
1:F:30:PRO:HB3	1:F:195:ARG:NH1	2.34	0.42
2:H:524:ILE:CG2	2:H:528:ARG:HH21	2.32	0.42
2:H:851:THR:CG2	2:H:886:LYS:H	2.32	0.42
3:I:950:ILE:HD12	3:I:1018:ALA:HB3	2.01	0.42
2:C:768:MET:HE3	2:C:769:PRO:HD2	2.01	0.42
2:C:845:LEU:HB2	3:I:81:ARG:HH12	1.84	0.42
2:C:1323:PHE:CD1	3:D:1352:ILE:HG23	2.55	0.42
2:C:1324:ASN:HB3	2:C:1328:LYS:HE3	2.00	0.42
3:D:339:ARG:HA	3:D:343:LEU:HD12	2.00	0.42
1:G:211:ILE:HG21	1:G:216:ALA:HB2	2.01	0.42
2:H:1330:ILE:HD13	3:I:1332:LEU:HD22	2.00	0.42
3:I:744:ARG:NH2	3:I:772:TYR:OH	2.53	0.42
4:J:128:PHE:CD2	4:J:158:LEU:HD11	2.54	0.42
2:C:1072:ASN:CG	2:C:1111:GLN:HE22	2.28	0.42
3:D:744:ARG:NH2	3:D:772:TYR:OH	2.52	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ARG:HE	1:G:210:THR:HB	1.85	0.42
1:G:102:LEU:HB2	1:G:142:MET:HB2	2.02	0.42
2:H:153:PRO:O	2:H:452:ARG:NH2	2.52	0.42
2:H:850:ILE:HG12	2:H:1048:LYS:HE2	2.00	0.42
3:I:356:THR:HG23	3:I:446:ALA:HB1	2.02	0.42
3:I:429:LEU:HB2	3:I:925:GLU:HG3	2.01	0.42
3:I:507:VAL:HG13	3:I:511:TYR:HE2	1.85	0.42
3:I:583:VAL:HG22	3:I:589:TYR:CE1	2.53	0.42
3:I:1234:VAL:HG21	3:I:1254:GLU:CG	2.49	0.42
3:D:950:ILE:HD12	3:D:1018:ALA:HB3	2.01	0.42
1:F:44:ARG:HH21	1:F:185:TYR:HB2	1.84	0.42
1:G:44:ARG:HH21	1:G:185:TYR:HB2	1.85	0.42
2:H:98:VAL:HG12	2:H:100:LEU:HG	2.00	0.42
2:H:551:HIS:H	2:H:554:HIS:HD2	1.68	0.42
2:H:805:MET:CE	2:H:806:PRO:HD2	2.37	0.42
3:I:295:GLU:O	3:I:299:LEU:N	2.52	0.42
3:I:426:ALA:HB3	3:I:427:PRO:HD3	2.00	0.42
2:C:855:PRO:HG3	2:C:914:LYS:CD	2.48	0.42
3:D:857:LEU:HD13	3:D:860:ARG:HD2	2.02	0.42
1:F:107:ILE:CG1	1:F:136:GLU:HA	2.49	0.42
2:H:727:VAL:HG13	2:H:732:ILE:HG12	2.01	0.42
2:H:1298:VAL:O	2:H:1302:THR:HG23	2.20	0.42
3:I:339:ARG:HA	3:I:343:LEU:HD12	2.01	0.42
3:I:734:ALA:HA	3:I:737:ILE:HD12	2.02	0.42
1:B:83:LEU:HD21	3:D:526:VAL:O	2.20	0.42
1:B:91:ARG:HE	1:B:210:THR:HB	1.85	0.42
2:C:696:ASP:O	2:C:697:LYS:HB2	2.20	0.42
3:D:1191:PRO:O	3:D:1192:LYS:HB2	2.19	0.42
2:H:896:THR:HB	2:H:897:PRO:CD	2.46	0.42
2:H:960:LEU:O	2:H:964:LEU:HG	2.20	0.42
2:H:1072:ASN:CG	2:H:1111:GLN:HE22	2.28	0.42
2:H:1198:LEU:HD23	2:H:1201:LEU:HD12	2.02	0.42
3:I:1321:SER:CB	3:I:1348:LYS:HB3	2.50	0.42
1:A:60:GLU:CG	1:A:170:ARG:HG3	2.50	0.42
1:B:9:LEU:HD12	1:B:195:ARG:HH22	1.84	0.42
2:C:38:PHE:HA	2:C:48:GLY:HA3	2.02	0.42
2:C:960:LEU:O	2:C:964:LEU:HG	2.20	0.42
2:C:1328:LYS:HZ3	3:D:99:ARG:HB3	1.84	0.42
3:D:356:THR:OG1	3:D:448:GLN:HA	2.19	0.42
3:D:808:VAL:HG21	3:D:1347:LEU:HD21	2.01	0.42
2:H:448:LEU:HD23	2:H:451:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1163:VAL:CG2	3:I:1204:VAL:HB	2.50	0.42
4:K:10:TYR:CD2	4:K:73:MET:HB3	2.55	0.42
1:A:61:ILE:HB	1:A:64:VAL:O	2.20	0.41
1:A:107:ILE:CG1	1:A:136:GLU:HA	2.50	0.41
2:C:843:THR:HG22	3:I:78:LEU:O	2.20	0.41
3:D:694:SER:HB2	3:D:738:ARG:HD3	2.02	0.41
3:D:825:VAL:HG22	3:D:838:ARG:NH2	2.35	0.41
3:I:56:LEU:HD13	3:I:266:ASN:ND2	2.35	0.41
3:I:1172:LYS:HG3	3:I:1173:ARG:N	2.35	0.41
1:B:211:ILE:HG21	1:B:216:ALA:HB2	2.02	0.41
2:C:98:VAL:HG12	2:C:100:LEU:HG	2.01	0.41
2:C:448:LEU:HD23	2:C:451:ARG:HD2	2.01	0.41
3:D:492:SER:HB3	3:D:499:ILE:HG13	2.02	0.41
3:D:587:LEU:HD11	3:D:608:CYS:SG	2.60	0.41
3:D:903:LEU:HD22	3:D:909:ILE:HG13	2.02	0.41
2:H:1174:GLU:HA	2:H:1177:ARG:CZ	2.50	0.41
3:I:425:ARG:NH2	3:I:459:ALA:CB	2.84	0.41
3:I:490:ILE:HA	3:I:500:ILE:HD12	2.02	0.41
3:I:518:VAL:HG11	3:I:707:ILE:HD13	2.02	0.41
3:I:527:LEU:HD12	3:I:532:GLU:HG2	2.02	0.41
1:A:166:ARG:N	1:A:167:PRO:CD	2.83	0.41
3:D:31:ARG:HA	3:D:34:SER:OG	2.20	0.41
3:D:233:LYS:HD2	3:D:236:TRP:HE1	1.86	0.41
3:D:858:VAL:HB	3:D:859:PRO:HD3	2.01	0.41
3:D:1145:PHE:HB3	3:D:1309:ILE:HD12	2.02	0.41
1:F:61:ILE:HB	1:F:64:VAL:O	2.20	0.41
2:H:723:VAL:HA	2:H:776:PRO:HA	2.02	0.41
3:I:65:VAL:CG2	3:I:71:LEU:HD22	2.33	0.41
2:C:810:TYR:CE2	3:D:359:PRO:HG2	2.55	0.41
3:D:37:GLU:H	3:D:105:ILE:HG13	1.85	0.41
3:D:89:GLY:O	3:I:252:LEU:HD12	2.19	0.41
3:D:534:GLU:HB3	3:D:538:ARG:NE	2.35	0.41
3:D:655:SER:HA	3:D:658:GLU:HB2	2.02	0.41
1:G:125:LYS:HA	1:G:126:PRO:HD3	1.91	0.41
2:H:768:MET:HE3	2:H:769:PRO:HD2	2.02	0.41
3:I:899:TYR:CE1	3:I:915:ILE:HD13	2.56	0.41
1:A:30:PRO:HA	1:A:198:LEU:HD13	2.01	0.41
1:B:44:ARG:HH21	1:B:185:TYR:HB2	1.84	0.41
2:C:1127:LYS:HD2	2:C:1202:GLY:HA2	2.02	0.41
3:D:1351:VAL:HG22	3:D:1357:ILE:HD11	2.02	0.41
2:H:237:LEU:HD13	2:H:292:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:551:HIS:H	2:H:554:HIS:CD2	2.38	0.41
1:B:104:LYS:HE2	1:B:114:ASP:HB2	2.01	0.41
2:C:1198:LEU:HD23	2:C:1201:LEU:HD12	2.03	0.41
2:C:1280:ALA:HB1	3:D:431:ARG:NE	2.35	0.41
3:D:356:THR:HG23	3:D:446:ALA:HB1	2.02	0.41
3:D:429:LEU:HB2	3:D:925:GLU:HG3	2.02	0.41
2:H:19:PRO:HB2	2:H:20:GLN:CG	2.47	0.41
2:H:177:ILE:HG12	2:H:183:TRP:HZ3	1.84	0.41
2:H:211:ARG:HG3	2:H:220:ILE:HD11	2.01	0.41
3:D:1068:THR:O	3:D:1072:LYS:HE3	2.21	0.41
3:D:1248:ILE:H	3:D:1248:ILE:HG13	1.73	0.41
2:H:89:GLY:HA2	2:H:140:GLY:HA3	2.03	0.41
2:H:909:LYS:HE3	2:H:914:LYS:HG2	2.01	0.41
4:K:12:VAL:HG22	4:K:92:PHE:CD1	2.54	0.41
1:A:33:ARG:HE	1:A:197:ASP:HB2	1.85	0.41
2:C:551:HIS:H	2:C:554:HIS:CD2	2.38	0.41
2:C:1334:GLY:CA	3:D:239:LEU:HD21	2.51	0.41
1:G:113:ALA:O	1:G:115:ILE:N	2.46	0.41
1:G:210:THR:O	1:G:211:ILE:HG13	2.20	0.41
2:H:38:PHE:HA	2:H:48:GLY:HA3	2.02	0.41
2:H:303:ASP:HB2	2:H:308:GLU:H	1.86	0.41
2:H:401:GLY:HA2	2:H:452:ARG:HH22	1.85	0.41
3:I:532:GLU:O	3:I:533:ALA:C	2.64	0.41
3:I:1003:LEU:HD23	3:I:1018:ALA:HB2	2.02	0.41
1:B:182:ARG:NH2	3:D:530:PRO:HA	2.36	0.41
2:C:155:VAL:HG23	2:C:405:PHE:CD1	2.56	0.41
2:C:303:ASP:HB2	2:C:308:GLU:H	1.86	0.41
2:C:850:ILE:H	2:C:850:ILE:HG13	1.73	0.41
2:C:1280:ALA:C	2:C:1282:GLY:N	2.79	0.41
2:C:1323:PHE:CE1	3:D:341:ASN:HB3	2.56	0.41
3:D:105:ILE:HD13	4:K:18:PHE:HE2	1.83	0.41
3:D:123:ARG:HA	3:D:126:LEU:HD12	2.03	0.41
3:D:689:ALA:HA	3:D:692:ARG:HB2	2.03	0.41
3:D:809:VAL:N	3:D:915:ILE:HD11	2.36	0.41
3:D:1163:VAL:CG2	3:D:1204:VAL:HB	2.51	0.41
1:F:29:GLU:HB2	1:F:30:PRO:HD3	2.03	0.41
1:F:60:GLU:HA	1:F:169:GLY:O	2.21	0.41
2:H:321:LEU:C	2:H:325:LEU:HG	2.46	0.41
2:H:855:PRO:CB	2:H:914:LYS:HD3	2.45	0.41
3:I:233:LYS:HD2	3:I:236:TRP:HE1	1.85	0.41
3:I:347:VAL:HG12	3:I:348:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:452:LEU:HG	3:I:625:MET:HE2	2.03	0.41
3:I:755:ILE:H	3:I:755:ILE:HG13	1.63	0.41
3:I:808:VAL:HG21	3:I:1347:LEU:HD21	2.02	0.41
4:J:125:LYS:HD3	4:J:127:LEU:HD12	2.02	0.41
3:D:452:LEU:HD13	3:D:500:ILE:HG23	2.02	0.41
3:D:515:ARG:NH1	3:D:724:MET:HG3	2.36	0.41
2:H:561:ILE:CD1	2:H:661:VAL:HG22	2.51	0.41
3:I:75:TYR:N	3:I:75:TYR:CD2	2.89	0.41
3:I:592:VAL:HG21	3:I:604:MET:SD	2.61	0.41
4:K:10:TYR:HD2	4:K:73:MET:HE2	1.85	0.41
2:C:177:ILE:HG12	2:C:183:TRP:HZ3	1.86	0.40
2:C:321:LEU:C	2:C:325:LEU:HG	2.46	0.40
2:C:680:LEU:CD1	3:D:783:LEU:HD11	2.51	0.40
3:D:490:ILE:HA	3:D:500:ILE:HD12	2.03	0.40
2:H:805:MET:HE2	3:I:637:ALA:H	1.86	0.40
2:H:963:GLU:O	2:H:967:LEU:HG	2.22	0.40
2:H:1257:GLN:NE2	3:I:340:GLN:O	2.54	0.40
2:H:1280:ALA:C	2:H:1282:GLY:N	2.79	0.40
3:I:61:ILE:HG23	3:I:103:GLY:HA3	2.04	0.40
3:I:370:LYS:HE2	3:I:443:GLU:HB3	2.03	0.40
3:I:506:VAL:HG13	3:I:625:MET:HA	2.03	0.40
3:I:534:GLU:HB3	3:I:538:ARG:NE	2.36	0.40
3:I:1002:VAL:N	3:I:1020:TRP:HE1	2.19	0.40
1:A:29:GLU:HB2	1:A:30:PRO:HD3	2.03	0.40
1:A:102:LEU:HB2	1:A:142:MET:HB2	2.03	0.40
1:B:61:ILE:HB	1:B:64:VAL:O	2.21	0.40
2:C:1298:VAL:O	2:C:1302:THR:HG23	2.21	0.40
3:D:312:ARG:HD2	3:D:314:ARG:NH2	2.36	0.40
3:D:429:LEU:HD12	3:D:925:GLU:HG2	2.03	0.40
3:D:824:PRO:HG3	3:D:835:LEU:HG	2.04	0.40
3:I:50:LYS:HB3	3:I:51:PRO:CD	2.49	0.40
3:I:110:PRO:HB2	3:I:111:THR:H	1.72	0.40
3:I:809:VAL:N	3:I:915:ILE:HD11	2.36	0.40
3:I:824:PRO:HG3	3:I:835:LEU:HG	2.03	0.40
3:I:1163:VAL:HG21	3:I:1204:VAL:HB	2.02	0.40
3:D:923:ILE:HA	3:D:926:PRO:HG2	2.04	0.40
1:F:102:LEU:HB2	1:F:142:MET:HB2	2.03	0.40
3:I:587:LEU:HD11	3:I:608:CYS:SG	2.62	0.40
3:I:960:LEU:HD13	3:I:963:VAL:HG21	2.03	0.40
4:J:10:TYR:HD2	4:J:73:MET:HE2	1.87	0.40
2:C:19:PRO:HA	2:C:1157:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1171:ARG:HA	2:C:1174:GLU:HB2	2.04	0.40
3:D:844:THR:HG21	3:D:856:ILE:HG21	2.04	0.40
1:G:61:ILE:HB	1:G:64:VAL:O	2.21	0.40
2:H:1171:ARG:HA	2:H:1174:GLU:HB2	2.04	0.40
3:I:1191:PRO:O	3:I:1192:LYS:HB2	2.20	0.40
2:C:367:TYR:CE2	2:C:381:ALA:HA	2.56	0.40
2:C:1196:LYS:HA	2:C:1199:LEU:HB2	2.03	0.40
3:D:93:THR:HA	2:H:890:LYS:HZ3	1.87	0.40
3:D:282:LEU:HG	4:J:21:ARG:HH21	1.86	0.40
2:H:7:GLU:C	2:H:9:LYS:H	2.30	0.40
2:H:120:GLN:HB3	2:H:490:GLN:HG3	2.04	0.40
2:H:225:PHE:HB3	2:H:226:GLU:H	1.65	0.40
3:I:452:LEU:HD22	3:I:500:ILE:HG23	2.04	0.40
3:I:675:ALA:HA	3:I:678:ARG:HD2	2.04	0.40
3:I:1145:PHE:HB3	3:I:1309:ILE:HD12	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:184:ALA:O	3:D:191:SER:OG[2_957]	2.03	0.17
3:D:1183:SER:OG	3:D:1183:SER:OG[2_957]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/242 (92%)	182 (82%)	29 (13%)	12 (5%)	1	15
1	B	211/242 (87%)	175 (83%)	27 (13%)	9 (4%)	2	17
1	F	223/242 (92%)	183 (82%)	28 (13%)	12 (5%)	1	15
1	G	212/242 (88%)	177 (84%)	26 (12%)	9 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1316/1342 (98%)	1108 (84%)	172 (13%)	36 (3%)	4	25
2	H	1316/1342 (98%)	1110 (84%)	168 (13%)	38 (3%)	3	23
3	D	1294/1407 (92%)	1023 (79%)	190 (15%)	81 (6%)	1	13
3	I	1300/1407 (92%)	1024 (79%)	197 (15%)	79 (6%)	1	13
4	J	141/181 (78%)	123 (87%)	15 (11%)	3 (2%)	5	30
4	K	141/181 (78%)	117 (83%)	18 (13%)	6 (4%)	2	17
All	All	6377/6828 (93%)	5222 (82%)	870 (14%)	285 (4%)	2	17

All (285) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	67	GLU
1	A	114	ASP
1	A	155	ALA
1	B	114	ASP
1	B	193	GLU
2	C	58	PRO
2	C	842	ASP
2	C	851	THR
2	C	890	LYS
2	C	1216	ARG
2	C	1317	PRO
3	D	37	GLU
3	D	98	ARG
3	D	110	PRO
3	D	112	ALA
3	D	173	GLY
3	D	178	ALA
3	D	323	PRO
3	D	587	LEU
3	D	1179	PRO
3	D	1180	VAL
1	F	15	ASP
1	F	67	GLU
1	F	114	ASP
1	G	114	ASP
1	G	193	GLU
2	H	58	PRO
2	H	228	VAL

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Mol	Chain	Res	Type
2	H	311	CYS
2	H	842	ASP
2	H	851	THR
2	H	890	LYS
2	H	894	GLN
2	H	1216	ARG
3	I	65	VAL
3	I	110	PRO
3	I	323	PRO
3	I	461	PHE
3	I	587	LEU
3	I	741	ALA
3	I	1179	PRO
3	I	1180	VAL
4	J	34	ASN
4	J	87	PRO
4	K	74	VAL
4	K	87	PRO
4	K	93	ILE
4	K	106	LYS
1	A	111	THR
1	A	119	GLY
1	B	39	LEU
1	B	111	THR
1	B	119	GLY
2	C	117	ILE
2	C	311	CYS
2	C	796	LEU
2	C	818	VAL
2	C	855	PRO
2	C	1077	SER
3	D	129	ASP
3	D	257	GLY
3	D	347	VAL
3	D	354	VAL
3	D	357	VAL
3	D	434	ILE
3	D	458	ASN
3	D	461	PHE
3	D	519	ASN
3	D	545	HIS
3	D	589	TYR

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Mol	Chain	Res	Type
3	D	741	ALA
3	D	828	GLY
3	D	855	ASP
3	D	915	ILE
3	D	1192	LYS
3	D	1274	PHE
3	D	1299	GLY
1	F	111	THR
1	F	119	GLY
1	F	136	GLU
1	F	163	GLU
1	G	39	LEU
1	G	111	THR
1	G	119	GLY
2	H	117	ILE
2	H	796	LEU
2	H	818	VAL
2	H	895	LEU
2	H	1077	SER
2	H	1317	PRO
3	I	112	ALA
3	I	120	LEU
3	I	347	VAL
3	I	354	VAL
3	I	357	VAL
3	I	434	ILE
3	I	458	ASN
3	I	519	ASN
3	I	586	GLY
3	I	589	TYR
3	I	734	ALA
3	I	828	GLY
3	I	855	ASP
3	I	915	ILE
3	I	1192	LYS
3	I	1274	PHE
3	I	1299	GLY
1	A	38	THR
1	A	136	GLU
1	A	154	PRO
2	C	8	LYS
2	C	487	LEU

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Mol	Chain	Res	Type
2	C	555	TYR
2	C	596	ASP
3	D	36	GLY
3	D	67	ASP
3	D	95	THR
3	D	177	ASP
3	D	286	ALA
3	D	359	PRO
3	D	404	GLU
3	D	471	PRO
3	D	560	ASN
3	D	586	GLY
3	D	625	MET
3	D	637	ALA
3	D	758	PRO
3	D	840	LEU
3	D	859	PRO
3	D	905	ARG
3	D	933	ARG
3	D	1128	SER
3	D	1134	ILE
3	D	1173	ARG
3	D	1342	ASP
1	F	38	THR
2	H	8	LYS
2	H	225	PHE
2	H	487	LEU
2	H	555	TYR
2	H	596	ASP
3	I	67	ASP
3	I	359	PRO
3	I	471	PRO
3	I	545	HIS
3	I	560	ASN
3	I	625	MET
3	I	637	ALA
3	I	840	LEU
3	I	859	PRO
3	I	863	LEU
3	I	905	ARG
3	I	933	ARG
3	I	1128	SER

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Mol	Chain	Res	Type
3	I	1245	GLY
4	K	34	ASN
2	C	488	MET
2	C	854	ILE
3	D	176	PHE
3	D	346	ARG
3	D	532	GLU
3	D	561	GLY
3	D	580	TRP
3	D	583	VAL
3	D	710	ASP
3	D	847	ASP
3	D	850	LYS
3	D	863	LEU
3	D	1245	GLY
3	D	1291	GLU
3	D	1327	GLU
2	H	111	GLU
2	H	201	ARG
2	H	488	MET
2	H	854	ILE
2	H	887	VAL
3	I	95	THR
3	I	258	GLY
3	I	286	ALA
3	I	315	ALA
3	I	404	GLU
3	I	532	GLU
3	I	561	GLY
3	I	583	VAL
3	I	710	ASP
3	I	758	PRO
3	I	847	ASP
3	I	850	LYS
3	I	1134	ILE
3	I	1173	ARG
3	I	1291	GLU
3	I	1327	GLU
3	I	1342	ASP
4	K	105	ASP
1	A	30	PRO
1	B	13	LEU

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Mol	Chain	Res	Type
1	B	30	PRO
2	C	111	GLU
2	C	201	ARG
2	C	224	PHE
2	C	398	SER
2	C	638	SER
2	C	740	GLU
2	C	748	ILE
2	C	887	VAL
2	C	1138	VAL
2	C	1247	SER
2	C	1281	TYR
3	D	106	GLU
3	D	113	HIS
3	D	179	LYS
3	D	805	GLN
3	D	908	ILE
3	D	971	GLY
3	D	1175	LEU
3	D	1352	ILE
1	F	30	PRO
1	F	166	ARG
1	G	13	LEU
1	G	30	PRO
2	H	638	SER
2	H	740	GLU
2	H	748	ILE
2	H	1138	VAL
2	H	1247	SER
2	H	1281	TYR
3	I	227	PHE
3	I	346	ARG
3	I	580	TRP
3	I	805	GLN
3	I	908	ILE
3	I	1175	LEU
4	J	35	MET
1	A	167	PRO
2	C	746	ALA
3	D	427	PRO
3	D	706	VAL
3	D	1178	THR

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Mol	Chain	Res	Type
3	I	106	GLU
3	I	177	ASP
3	I	211	GLU
3	I	427	PRO
3	I	500	ILE
3	I	706	VAL
3	I	971	GLY
3	I	1178	THR
3	I	1352	ILE
2	C	162	GLY
2	C	873	ILE
3	D	500	ILE
3	D	529	GLY
3	D	1118	GLY
3	I	529	GLY
2	C	544	GLY
2	C	655	VAL
2	C	1071	GLY
3	D	451	PRO
3	D	524	GLY
2	H	162	GLY
2	H	544	GLY
2	H	655	VAL
2	H	1071	GLY
3	I	1118	GLY
3	D	358	GLY
3	D	433	GLY
3	D	671	GLY
2	H	627	GLY
3	I	358	GLY
3	I	433	GLY
3	I	451	PRO
3	I	524	GLY
3	I	671	GLY
1	A	126	PRO
1	F	126	PRO
1	F	167	PRO
1	G	14	VAL
2	H	292	ILE
2	H	873	ILE
2	H	891	GLY
3	I	257	GLY

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Mol	Chain	Res	Type
1	B	14	VAL
1	B	126	PRO
2	C	896	THR
1	G	126	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	193/208 (93%)	190 (98%)	3 (2%)	55	70
1	B	184/208 (88%)	181 (98%)	3 (2%)	55	70
1	F	193/208 (93%)	190 (98%)	3 (2%)	55	70
1	G	185/208 (89%)	182 (98%)	3 (2%)	55	70
2	C	1137/1157 (98%)	1109 (98%)	28 (2%)	42	63
2	H	1137/1157 (98%)	1111 (98%)	26 (2%)	44	64
3	D	1087/1168 (93%)	1029 (95%)	58 (5%)	20	41
3	I	1091/1168 (93%)	1039 (95%)	52 (5%)	23	44
4	J	128/158 (81%)	123 (96%)	5 (4%)	28	49
4	K	128/158 (81%)	121 (94%)	7 (6%)	19	41
All	All	5463/5798 (94%)	5275 (97%)	188 (3%)	32	54

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	45	ARG
1	A	134	THR
1	B	5	VAL
1	B	14	VAL
1	B	134	THR
2	C	12[A]	ARG
2	C	12[B]	ARG
2	C	21	VAL

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Mol	Chain	Res	Type
2	C	39	ILE
2	C	59	ILE
2	C	85	CYS
2	C	102	LEU
2	C	117	ILE
2	C	208	ILE
2	C	217	THR
2	C	364	VAL
2	C	400	VAL
2	C	675	ASP
2	C	690	VAL
2	C	739	ASP
2	C	833	ILE
2	C	850	ILE
2	C	877	VAL
2	C	901	LEU
2	C	1041	ASP
2	C	1046	VAL
2	C	1047	LEU
2	C	1101	LEU
2	C	1107	MET
2	C	1141	LEU
2	C	1216	ARG
2	C	1233	LEU
2	C	1259	LEU
3	D	70	CYS
3	D	75	TYR
3	D	95	THR
3	D	114	ILE
3	D	139	LEU
3	D	159	ILE
3	D	185	ILE
3	D	188	LEU
3	D	189	LEU
3	D	193	ASP
3	D	194	LEU
3	D	240	THR
3	D	272	VAL
3	D	299	LEU
3	D	307	LEU
3	D	324	LEU
3	D	331	ILE

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Mol	Chain	Res	Type
3	D	337	ARG
3	D	342	LEU
3	D	354	VAL
3	D	357	VAL
3	D	415	VAL
3	D	416	ILE
3	D	422	LEU
3	D	430	HIS
3	D	442	ILE
3	D	450	HIS
3	D	460	ASP
3	D	470	VAL
3	D	526	VAL
3	D	536	LEU
3	D	550	VAL
3	D	564	VAL
3	D	572	THR
3	D	580	TRP
3	D	592	VAL
3	D	593	ASN
3	D	685	ILE
3	D	755	ILE
3	D	814	CYS
3	D	825	VAL
3	D	826	ILE
3	D	903	LEU
3	D	908	ILE
3	D	915	ILE
3	D	917	VAL
3	D	1031	VAL
3	D	1155	ILE
3	D	1181	ASP
3	D	1198	VAL
3	D	1229	VAL
3	D	1241	TYR
3	D	1248	ILE
3	D	1265	THR
3	D	1280	VAL
3	D	1309	ILE
3	D	1344	LEU
3	D	1347	LEU
1	F	28	LEU

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Mol	Chain	Res	Type
1	F	45	ARG
1	F	134	THR
1	G	5	VAL
1	G	14	VAL
1	G	134	THR
2	H	12[A]	ARG
2	H	12[B]	ARG
2	H	21	VAL
2	H	59	ILE
2	H	85	CYS
2	H	102	LEU
2	H	208	ILE
2	H	217	THR
2	H	364	VAL
2	H	400	VAL
2	H	675	ASP
2	H	690	VAL
2	H	739	ASP
2	H	833	ILE
2	H	850	ILE
2	H	866	ASP
2	H	877	VAL
2	H	1041	ASP
2	H	1046	VAL
2	H	1047	LEU
2	H	1101	LEU
2	H	1107	MET
2	H	1141	LEU
2	H	1216	ARG
2	H	1233	LEU
2	H	1259	LEU
3	I	61	ILE
3	I	70	CYS
3	I	95	THR
3	I	139	LEU
3	I	188	LEU
3	I	193	ASP
3	I	213	LYS
3	I	240	THR
3	I	275	ARG
3	I	299	LEU
3	I	307	LEU

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Mol	Chain	Res	Type
3	I	314	ARG
3	I	342	LEU
3	I	354	VAL
3	I	357	VAL
3	I	415	VAL
3	I	416	ILE
3	I	422	LEU
3	I	430	HIS
3	I	442	ILE
3	I	460	ASP
3	I	470	VAL
3	I	526	VAL
3	I	536	LEU
3	I	550	VAL
3	I	564	VAL
3	I	572	THR
3	I	580	TRP
3	I	587	LEU
3	I	592	VAL
3	I	641	ILE
3	I	685	ILE
3	I	755	ILE
3	I	814	CYS
3	I	825	VAL
3	I	826	ILE
3	I	903	LEU
3	I	908	ILE
3	I	915	ILE
3	I	917	VAL
3	I	1031	VAL
3	I	1155	ILE
3	I	1181	ASP
3	I	1198	VAL
3	I	1229	VAL
3	I	1241	TYR
3	I	1248	ILE
3	I	1265	THR
3	I	1280	VAL
3	I	1309	ILE
3	I	1344	LEU
3	I	1347	LEU
4	J	35	MET

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Mol	Chain	Res	Type
4	J	82	LEU
4	J	88	ARG
4	J	113	ASN
4	J	164	ILE
4	K	35	MET
4	K	76	ASN
4	K	77	ASP
4	K	82	LEU
4	K	96	THR
4	K	115	LEU
4	K	164	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	41	ASN
1	A	75	GLN
1	A	103	ASN
1	A	160	HIS
1	A	208	ASN
1	B	23	HIS
1	B	41	ASN
1	B	103	ASN
2	C	46	GLN
2	C	120	GLN
2	C	148	GLN
2	C	193	ASN
2	C	273	HIS
2	C	447	HIS
2	C	519	ASN
2	C	554	HIS
2	C	568	ASN
2	C	580	GLN
2	C	622	ASN
2	C	725	GLN
2	C	761	GLN
2	C	767	GLN
2	C	922	ASN
2	C	1099	ASN
2	C	1111	GLN
2	C	1157	GLN

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Mol	Chain	Res	Type
2	C	1236	ASN
2	C	1257	GLN
2	C	1288	GLN
2	C	1314	GLN
3	D	80	HIS
3	D	113	HIS
3	D	206	ASN
3	D	229	GLN
3	D	276	ASN
3	D	294	ASN
3	D	341	ASN
3	D	495	ASN
3	D	519	ASN
3	D	593	ASN
3	D	700	ASN
3	D	762	ASN
3	D	768	ASN
3	D	777	HIS
3	D	1249	ASN
3	D	1252	HIS
3	D	1268	ASN
3	D	1366	HIS
1	F	23	HIS
1	F	41	ASN
1	F	75	GLN
1	F	103	ASN
1	F	160	HIS
1	F	208	ASN
1	G	23	HIS
1	G	41	ASN
1	G	103	ASN
2	H	120	GLN
2	H	148	GLN
2	H	193	ASN
2	H	273	HIS
2	H	447	HIS
2	H	519	ASN
2	H	554	HIS
2	H	568	ASN
2	H	580	GLN
2	H	620	ASN
2	H	622	ASN

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Mol	Chain	Res	Type
2	H	649	GLN
2	H	725	GLN
2	H	761	GLN
2	H	767	GLN
2	H	922	ASN
2	H	1111	GLN
2	H	1236	ASN
2	H	1256	GLN
2	H	1257	GLN
2	H	1264	GLN
2	H	1268	GLN
2	H	1288	GLN
3	I	94	GLN
3	I	113	HIS
3	I	206	ASN
3	I	274	ASN
3	I	276	ASN
3	I	294	ASN
3	I	300	GLN
3	I	309	ASN
3	I	341	ASN
3	I	495	ASN
3	I	519	ASN
3	I	700	ASN
3	I	736	GLN
3	I	762	ASN
3	I	768	ASN
3	I	1249	ASN
3	I	1252	HIS
3	I	1268	ASN
3	I	1366	HIS
4	J	13	GLN
4	K	29	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	225/242 (92%)	-0.67	3 (1%) 75 64	267, 330, 380, 416	0
1	B	215/242 (88%)	-0.53	4 (1%) 66 56	266, 335, 388, 430	0
1	F	225/242 (92%)	-0.50	6 (2%) 56 48	248, 320, 383, 403	0
1	G	216/242 (89%)	-0.44	9 (4%) 40 40	279, 337, 380, 412	0
2	C	1319/1342 (98%)	-0.61	16 (1%) 76 65	153, 313, 384, 510	1 (0%)
2	H	1319/1342 (98%)	-0.58	8 (0%) 85 76	164, 315, 383, 482	1 (0%)
3	D	1302/1407 (92%)	-0.61	9 (0%) 84 74	230, 326, 424, 473	0
3	I	1306/1407 (92%)	-0.63	7 (0%) 87 78	231, 332, 431, 492	0
4	J	147/181 (81%)	-0.60	0 100 100	300, 384, 446, 483	0
4	K	147/181 (81%)	-0.56	4 (2%) 56 48	324, 413, 469, 491	0
All	All	6421/6828 (94%)	-0.60	66 (1%) 79 68	153, 324, 419, 510	2 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	72	SER	15.0
1	G	57	THR	8.9
1	F	97	GLU	5.9
3	D	234	PRO	5.4
2	C	1123	GLY	5.0
4	K	102	PRO	4.6
1	B	87	GLY	4.4
2	C	635	THR	4.3
3	I	757	THR	4.0
2	C	128	PRO	3.9
2	H	454	ARG	3.7
3	D	1082	ASP	3.7
4	K	96	THR	3.5

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Mol	Chain	Res	Type	RSRZ
3	I	812	ASP	3.4
2	C	962	GLU	3.3
1	F	56	VAL	3.2
2	H	535	PRO	3.1
3	I	235	GLU	3.1
1	F	149	GLY	3.0
1	B	82	LEU	3.0
3	D	189	LEU	3.0
2	C	644	LEU	3.0
1	F	98	VAL	2.8
2	H	1250	SER	2.8
2	C	1122	LYS	2.7
3	D	127	LEU	2.7
2	H	788	SER	2.7
2	C	1239	VAL	2.7
3	I	992	LYS	2.7
4	K	46	THR	2.7
1	A	98	VAL	2.6
1	G	146	VAL	2.6
2	C	127	ILE	2.6
1	A	97	GLU	2.5
2	C	500	ALA	2.5
1	F	54	CYS	2.4
3	D	745	GLY	2.4
1	G	88	LEU	2.4
2	C	319	LEU	2.4
2	C	1124	ILE	2.4
2	H	1299	ASN	2.4
3	I	423	LEU	2.4
2	H	789	THR	2.3
1	G	56	VAL	2.3
1	B	85	LEU	2.3
1	F	148	ARG	2.3
2	C	129	LEU	2.3
3	I	758	PRO	2.3
1	B	149	GLY	2.2
3	D	1083	ALA	2.2
1	G	5	VAL	2.2
3	I	1107	VAL	2.2
1	G	144	ILE	2.2
1	G	210	THR	2.2
1	G	89	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	530	ILE	2.1
2	C	174	ALA	2.1
3	D	193	ASP	2.1
3	D	747	MET	2.1
2	C	1210	ILE	2.1
3	D	1261	LEU	2.1
1	G	52	PRO	2.1
2	C	963	GLU	2.1
1	A	172	LEU	2.1
2	H	73	TYR	2.0
4	K	45	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.