



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:35 PM UTC

PDB ID : 4LK0 / pdb_00004lk0
Title : Crystal Structure Analysis of the E.coli holoenzyme/T7 Gp2 complex
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-05
Resolution : 3.91 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

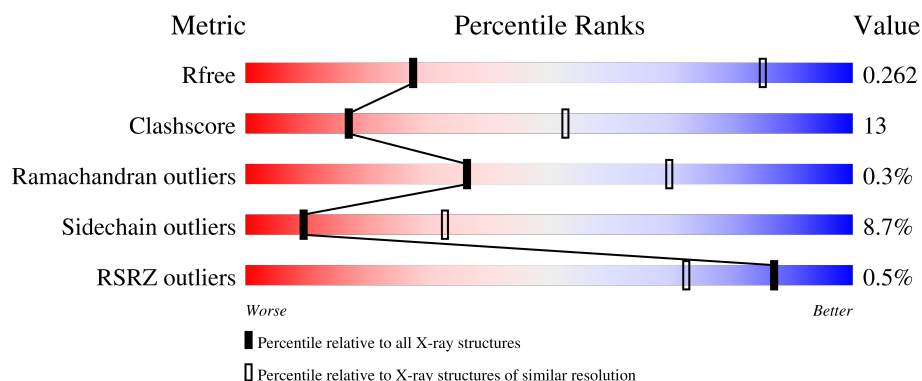
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 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	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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	239	2% 57% 35% • 6%
1	B	239	% 62% 26% • 8%
1	G	239	% 58% 37% • 5%
1	H	239	58% 28% • 9%
2	C	1342	% 66% 30% •

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Mol	Chain	Length	Quality of chain
2	I	1342	67% 29% •
3	D	1407	62% 30% • •
3	J	1407	62% 28% • 6%
4	E	91	77% 19% • •
4	K	91	70% 14% • 13%
5	F	522	58% 29% • 10%
5	L	522	56% 31% • 10%
6	M	64	2% 50% 25% 5% 20%
6	N	64	45% 31% • 20%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58505 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	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP C9QXI7
A	236	VAL	-	expression tag	UNP C9QXI7
A	237	LEU	-	expression tag	UNP C9QXI7
A	238	PHE	-	expression tag	UNP C9QXI7
A	239	GLN	-	expression tag	UNP C9QXI7
B	235	GLU	-	expression tag	UNP C9QXI7
B	236	VAL	-	expression tag	UNP C9QXI7
B	237	LEU	-	expression tag	UNP C9QXI7
B	238	PHE	-	expression tag	UNP C9QXI7
B	239	GLN	-	expression tag	UNP C9QXI7
G	235	GLU	-	expression tag	UNP C9QXI7
G	236	VAL	-	expression tag	UNP C9QXI7
G	237	LEU	-	expression tag	UNP C9QXI7
G	238	PHE	-	expression tag	UNP C9QXI7
G	239	GLN	-	expression tag	UNP C9QXI7
H	235	GLU	-	expression tag	UNP C9QXI7
H	236	VAL	-	expression tag	UNP C9QXI7
H	237	LEU	-	expression tag	UNP C9QXI7
H	238	PHE	-	expression tag	UNP C9QXI7
H	239	GLN	-	expression tag	UNP C9QXI7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1345	Total	C	N	O	S	0	0	0
			10447	6560	1864	1974	49			
3	J	1325	Total	C	N	O	S	0	0	0
			10295	6470	1831	1945	49			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	470	Total	C	N	O	S	0	0	0
			3822	2394	680	725	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called Bacterial RNA polymerase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	51	Total	C	N	O	S	0	0	0
			413	268	65	79	1			
6	N	51	Total	C	N	O	S	0	0	0
			413	268	65	79	1			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Mg 1	0	0
7	J	1	Total 1	Mg 1	0	0

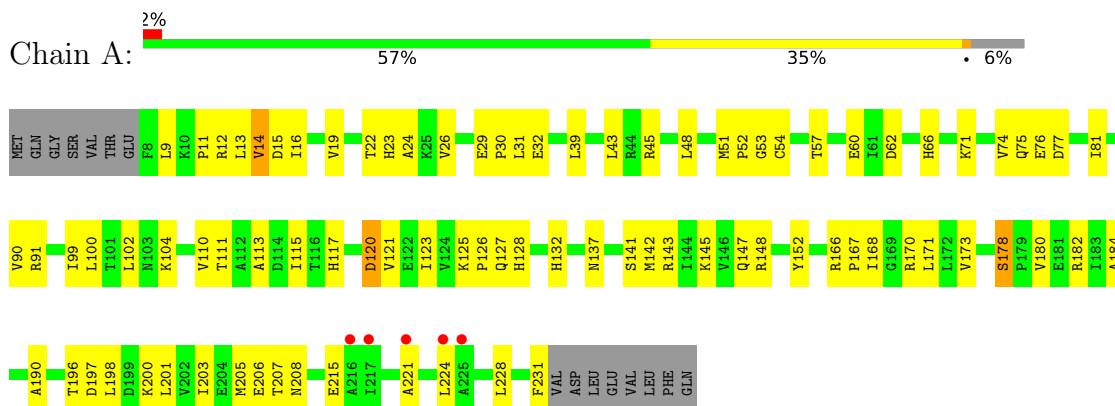
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total 2	Zn 2	0	0
8	J	2	Total 2	Zn 2	0	0

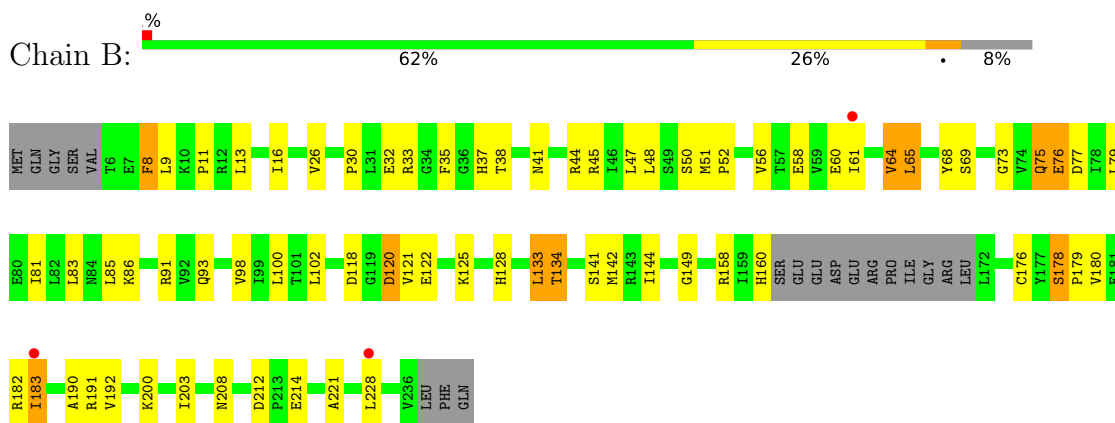
3 Residue-property plots

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.

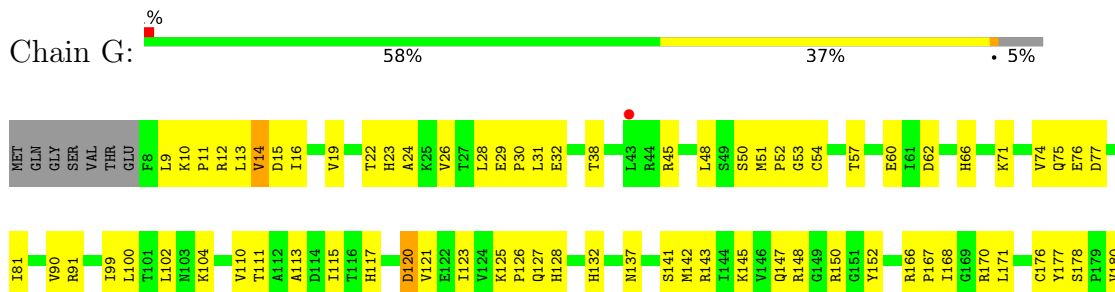
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



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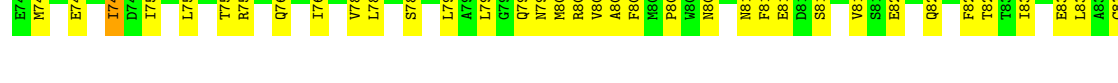
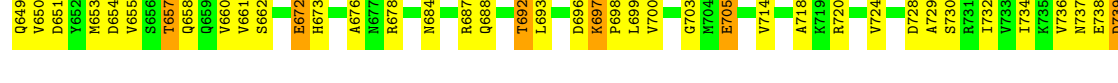
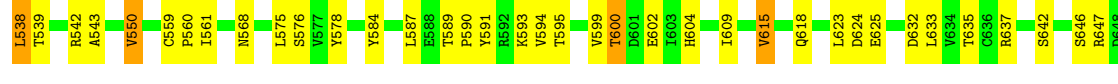
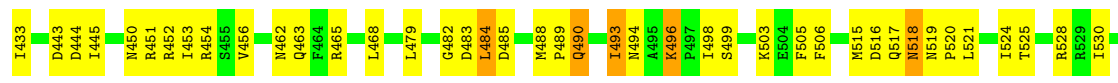
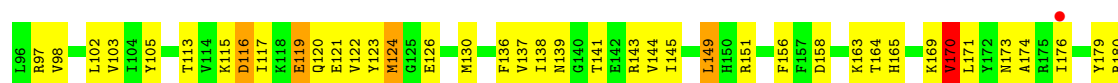


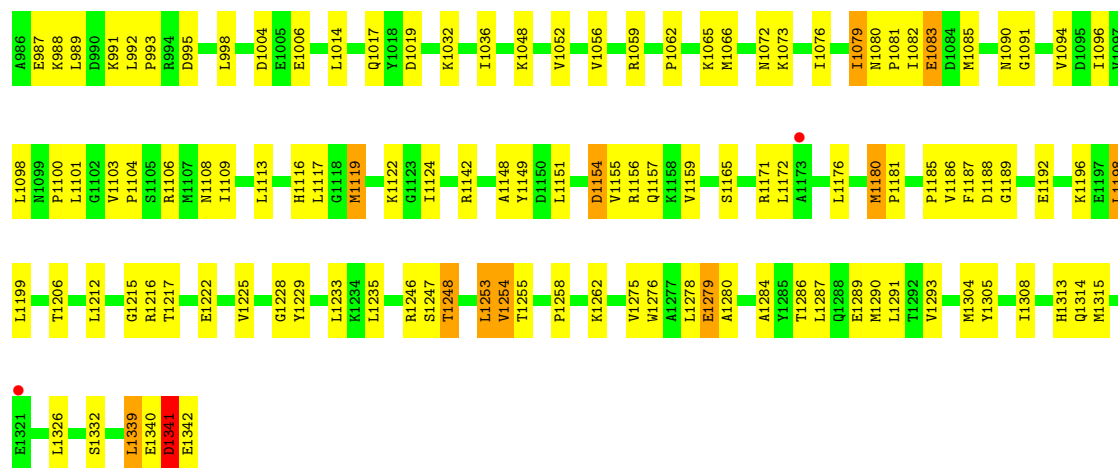


• Molecule 1: DNA-directed RNA polymerase subunit alpha

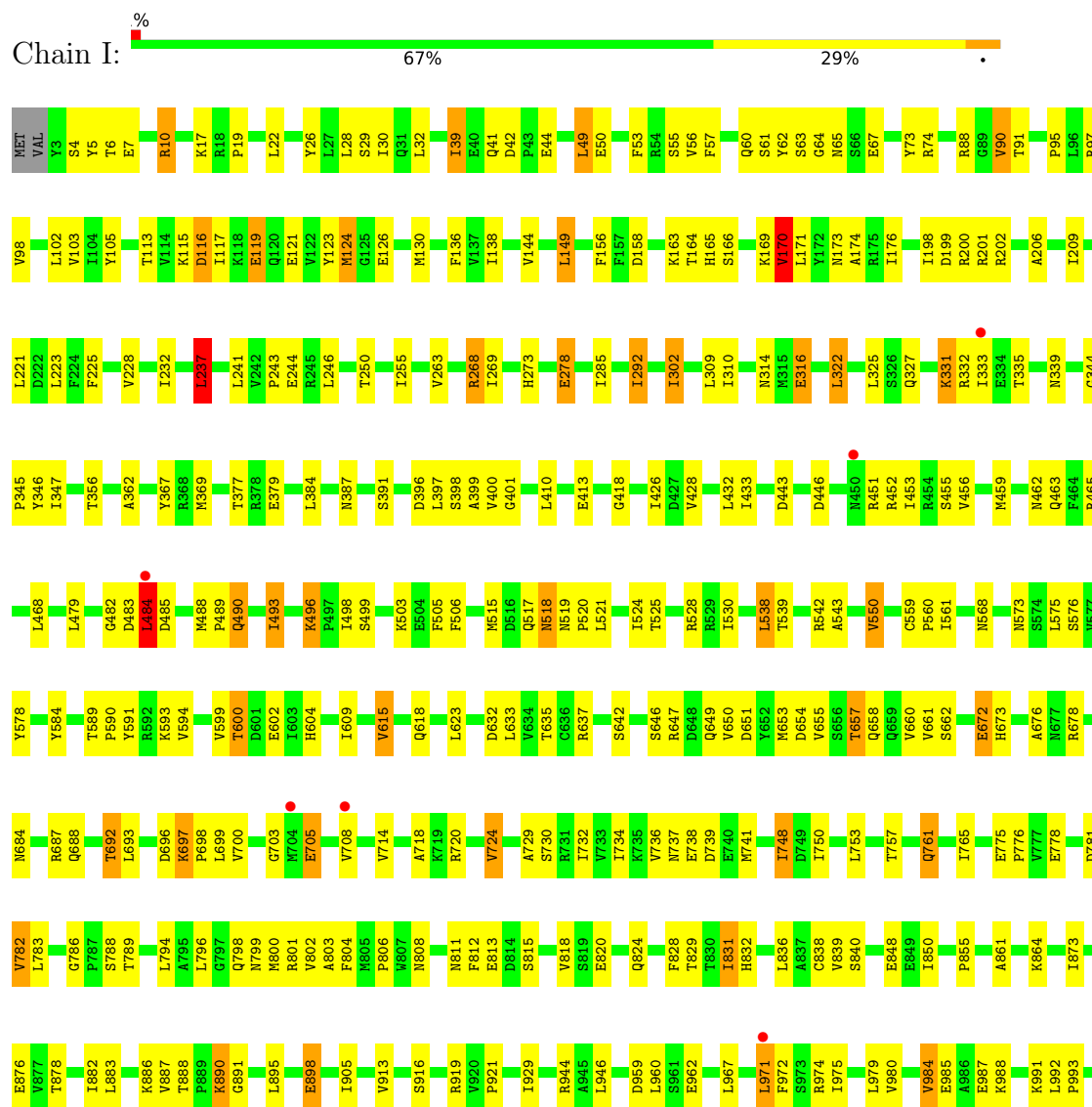


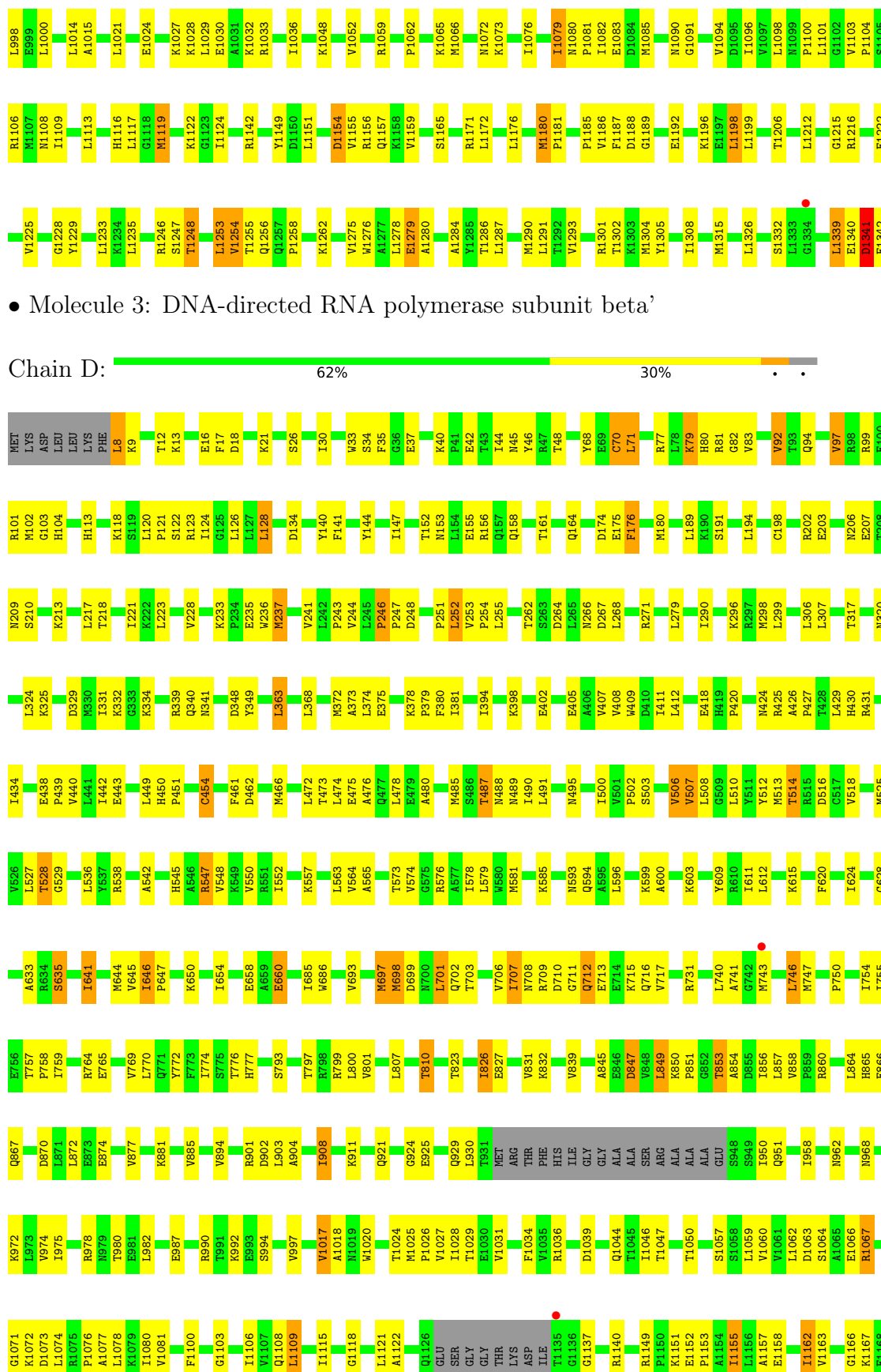
• Molecule 2: DNA-directed RNA polymerase subunit beta





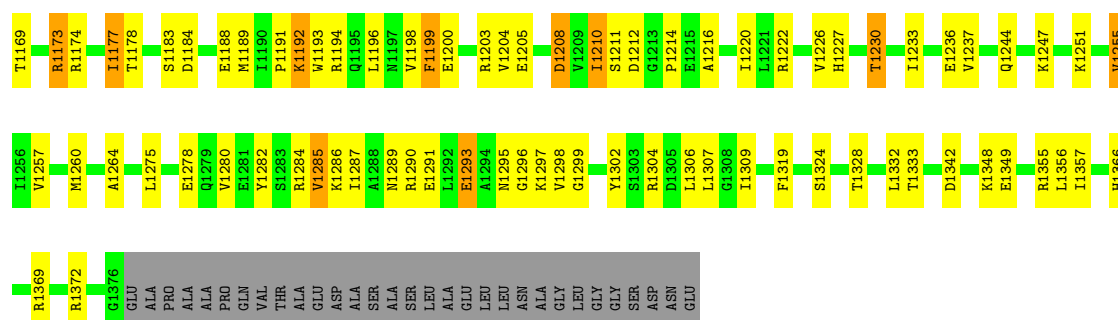
● Molecule 2: DNA-directed RNA polymerase subunit beta





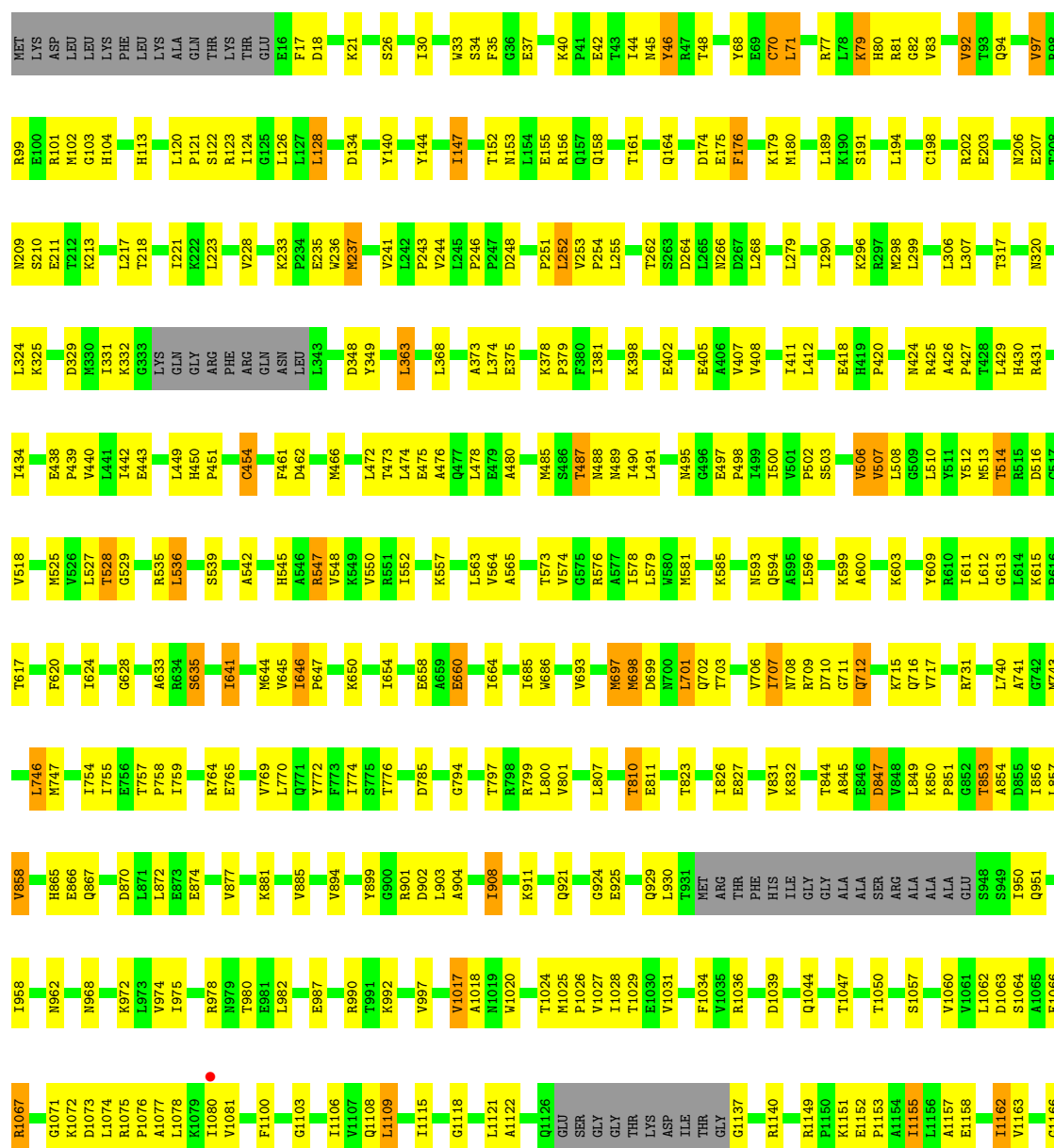
• Molecule 3: DNA-directed RNA polymerase subunit beta'

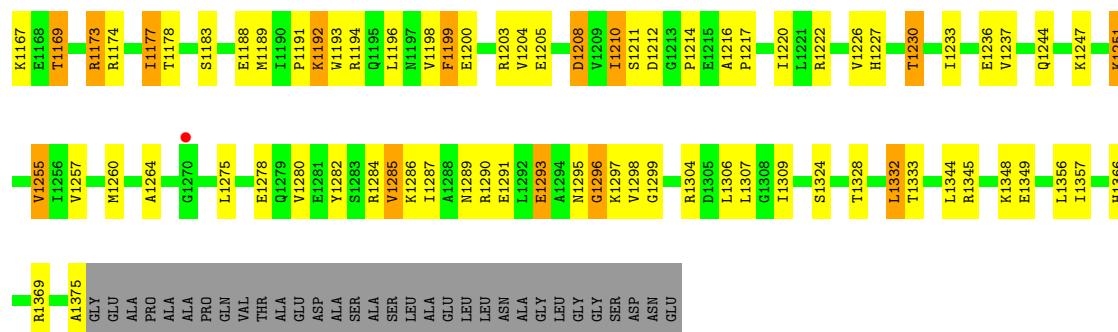
Chain D:



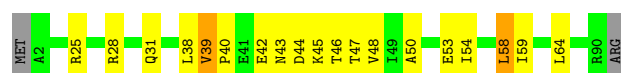
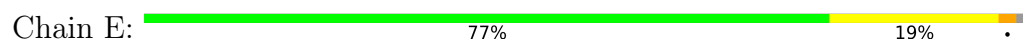
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 62% 28% 6%

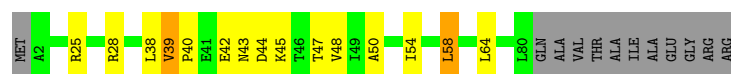




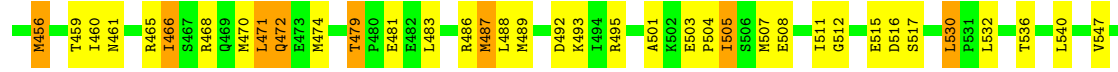
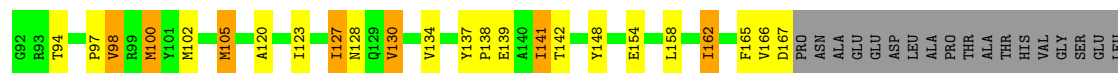
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 4: DNA-directed RNA polymerase subunit omega

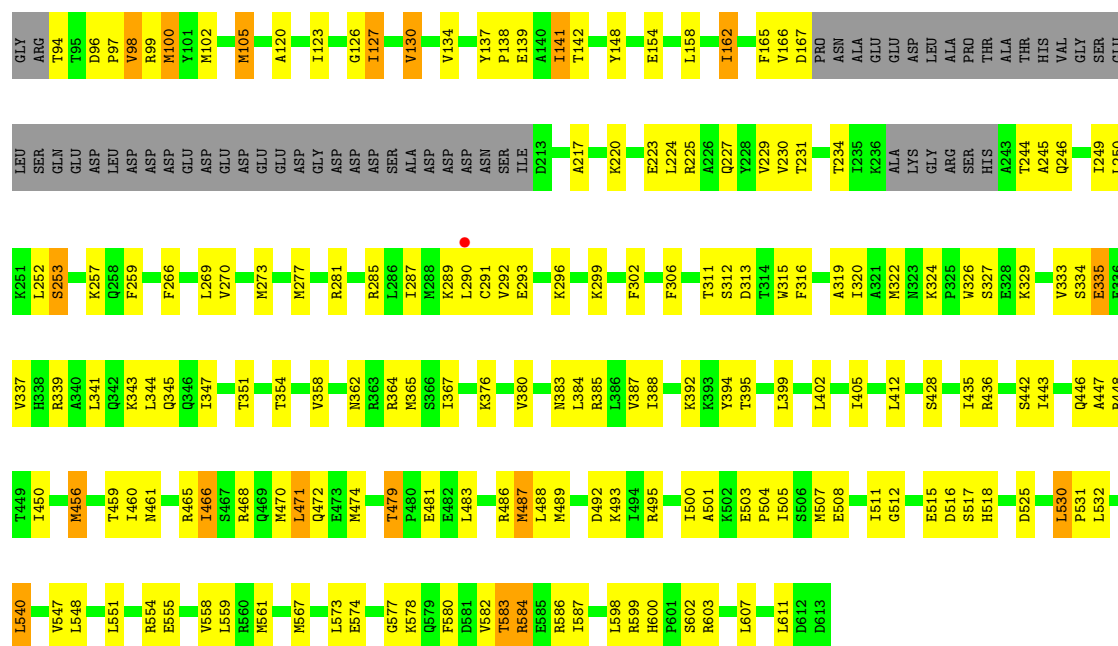


- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L:  56% 31% 10%

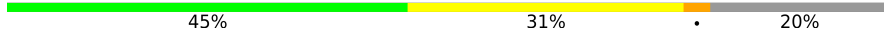


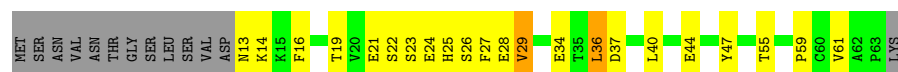
• Molecule 6: Bacterial RNA polymerase inhibitor

Chain M:  2% 50% 25% 5% 20%



• Molecule 6: Bacterial RNA polymerase inhibitor

Chain N:  45% 31% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.36Å 206.28Å 308.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.94 – 3.91 39.94 – 3.91	Depositor EDS
% Data completeness (in resolution range)	92.8 (39.94-3.91) 92.7 (39.94-3.91)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.87Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.219 , 0.260 0.219 , 0.262	Depositor DCC
R_{free} test set	5166 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	120.8	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	58505	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/1751	0.84	3/2373 (0.1%)
1	B	0.38	1/1707 (0.1%)	0.86	0/2314
1	G	0.34	0/1771	0.85	1/2401 (0.0%)
1	H	0.39	1/1686 (0.1%)	0.85	1/2285 (0.0%)
2	C	0.34	0/10739	0.80	7/14489 (0.0%)
2	I	0.34	0/10735	0.80	7/14484 (0.0%)
3	D	0.33	0/10603	0.80	9/14316 (0.1%)
3	J	0.33	0/10450	0.80	10/14112 (0.1%)
4	E	0.35	0/693	0.78	0/935
4	K	0.33	0/629	0.77	0/847
5	F	0.34	0/3873	0.81	1/5206 (0.0%)
5	L	0.35	0/3872	0.81	4/5205 (0.1%)
6	M	0.42	0/426	0.76	0/583
6	N	0.41	0/426	0.77	0/583
All	All	0.34	2/59361 (0.0%)	0.81	43/80133 (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
3	D	0	1
3	J	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	178	SER	C-N	6.56	1.41	1.33
1	B	178	SER	C-N	-5.13	1.27	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1210	ILE	N-CA-C	-6.66	106.23	112.83
2	I	42	ASP	CA-C-N	6.34	126.03	119.56
2	I	42	ASP	C-N-CA	6.34	126.03	119.56
2	I	199	ASP	CB-CA-C	-6.20	109.42	116.54
2	C	199	ASP	CB-CA-C	-6.08	109.55	116.54
2	I	482	GLY	N-CA-C	5.83	118.63	111.93
2	C	482	GLY	N-CA-C	5.78	118.58	111.93
2	C	237	LEU	N-CA-C	5.70	118.33	110.35
2	I	237	LEU	N-CA-C	5.70	118.32	110.35
1	H	8	PHE	N-CA-C	5.69	117.62	109.14
3	D	1278	GLU	N-CA-C	5.64	117.83	110.43
3	J	1278	GLU	N-CA-C	5.63	117.80	110.43
1	G	29	GLU	N-CA-C	5.60	119.86	112.35
3	D	246	PRO	CA-C-N	5.60	125.26	119.05
3	D	246	PRO	C-N-CA	5.60	125.26	119.05
3	J	246	PRO	CA-C-N	5.59	125.25	119.05
3	J	246	PRO	C-N-CA	5.59	125.25	119.05
1	A	29	GLU	N-CA-C	5.54	119.78	112.35
3	D	40	LYS	CA-C-N	5.52	125.61	119.87
3	D	40	LYS	C-N-CA	5.52	125.61	119.87
3	J	40	LYS	CA-C-N	5.48	125.57	119.87
3	J	40	LYS	C-N-CA	5.48	125.57	119.87
3	D	1210	ILE	N-CA-C	-5.45	106.52	113.22
3	D	1067	ARG	N-CA-C	5.41	117.27	110.24
3	J	1067	ARG	N-CA-C	5.40	117.26	110.24
2	C	42	ASP	CA-C-N	5.37	126.55	119.84
2	C	42	ASP	C-N-CA	5.37	126.55	119.84
3	J	450	HIS	CA-C-N	5.37	125.01	119.05
3	J	450	HIS	C-N-CA	5.37	125.01	119.05
3	D	450	HIS	CA-C-N	5.36	125.00	119.05
3	D	450	HIS	C-N-CA	5.36	125.00	119.05
5	L	96	ASP	CA-C-N	5.16	124.82	119.56
5	L	96	ASP	C-N-CA	5.16	124.82	119.56
5	L	383	ASN	N-CA-C	5.10	119.20	112.92
2	C	1341	ASP	N-CA-C	5.09	115.54	108.00
2	I	1154	ASP	N-CA-C	5.09	116.87	110.91
3	J	1169	THR	N-CA-C	5.09	117.73	110.24
2	C	1154	ASP	N-CA-C	5.07	116.85	110.91
5	L	584	ARG	CB-CA-C	-5.07	109.24	116.34
5	F	383	ASN	N-CA-C	5.06	119.15	112.92
2	I	1341	ASP	N-CA-C	5.04	115.45	108.00
1	A	178	SER	CA-C-N	5.02	124.32	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	SER	C-N-CA	5.02	124.32	118.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1296	GLY	Peptide
3	J	1296	GLY	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	1730	0	1756	55	0
1	B	1687	0	1700	47	0
1	G	1750	0	1764	60	0
1	H	1667	0	1689	51	0
2	C	10570	0	10582	285	0
2	I	10566	0	10576	267	0
3	D	10447	0	10672	317	0
3	J	10295	0	10511	302	0
4	E	691	0	695	15	0
4	K	627	0	634	12	0
5	F	3822	0	3885	108	0
5	L	3821	0	3884	112	0
6	M	413	0	389	11	0
6	N	413	0	389	14	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	58505	0	59126	1492	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 13.

All (1492) 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:D:206:ASN:ND2	3:J:1183:SER:OG	2.04	0.90
3:D:1183:SER:OG	3:J:206:ASN:ND2	2.08	0.87
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.60	0.83
2:C:452:ARG:NH1	2:C:584:TYR:O	2.11	0.83
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.60	0.81
3:D:418:GLU:HG3	4:E:45:LYS:H	1.44	0.81
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.64	0.80
2:I:452:ARG:NH1	2:I:584:TYR:O	2.12	0.80
5:F:448:ARG:NH2	5:F:501:ALA:O	2.15	0.80
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.64	0.80
3:J:418:GLU:HG3	4:K:45:LYS:H	1.44	0.80
5:L:448:ARG:NH2	5:L:501:ALA:O	2.15	0.78
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.65	0.78
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.65	0.78
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.66	0.78
3:D:1044:GLN:HB3	3:D:1071:GLY:HA3	1.65	0.77
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.50	0.77
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.66	0.77
1:H:182:ARG:HD2	3:J:581:MET:HE1	1.66	0.77
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.66	0.77
6:M:19:THR:HG22	6:M:28:GLU:HG2	1.67	0.76
2:I:398:SER:OG	2:I:399:ALA:N	2.17	0.76
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.66	0.76
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.50	0.76
6:N:19:THR:HG22	6:N:28:GLU:HG2	1.66	0.76
2:C:398:SER:OG	2:C:399:ALA:N	2.18	0.75
1:G:113:ALA:HB2	1:G:126:PRO:HB3	1.68	0.75
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.68	0.75
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.52	0.74
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.68	0.74
5:F:515:GLU:HG2	5:F:516:ASP:H	1.52	0.74
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.51	0.74
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.68	0.74
2:I:166:SER:HB2	6:N:23:SER:H	1.51	0.74
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.70	0.74
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.68	0.73
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.70	0.73
3:J:1064:SER:HB2	3:J:1173:ARG:HH12	1.54	0.73
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.70	0.73
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.70	0.73
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.71	0.73
5:L:515:GLU:HG2	5:L:516:ASP:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.53	0.72
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.72	0.72
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.72	0.71
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.72	0.71
2:C:684:ASN:OD1	2:C:687:ARG:NH2	2.23	0.71
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.72	0.71
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.73	0.71
3:D:1188:GLU:HG2	6:M:59:PRO:HD2	1.71	0.71
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.54	0.71
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.71	0.70
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.73	0.70
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.73	0.70
3:D:251:PRO:HD2	5:F:507:MET:HE1	1.74	0.70
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.73	0.70
3:J:1188:GLU:HG2	6:N:59:PRO:HD2	1.73	0.69
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.73	0.69
3:D:152:THR:OG1	3:D:153:ASN:N	2.24	0.69
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.74	0.69
2:I:166:SER:HA	6:N:23:SER:HB3	1.74	0.69
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.74	0.69
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.73	0.69
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.58	0.69
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.74	0.68
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	1.74	0.68
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.58	0.68
2:C:516:ASP:OD1	2:C:516:ASP:O	2.11	0.68
3:D:123:ARG:HB3	3:D:237:MET:HE1	1.75	0.68
5:F:492:ASP:HA	5:F:495:ARG:HH12	1.58	0.68
5:L:492:ASP:HA	5:L:495:ARG:HH12	1.57	0.68
3:J:123:ARG:HB3	3:J:237:MET:HE1	1.75	0.67
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.60	0.67
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.77	0.67
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.74	0.67
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.76	0.67
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.76	0.67
1:A:224:LEU:HD22	1:B:228:LEU:HD11	1.77	0.67
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.77	0.67
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.77	0.67
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.77	0.66
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.60	0.66
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.60	0.66
5:F:134:VAL:HG22	5:F:273:MET:HE1	1.77	0.66
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.28	0.66
3:D:1152:GLU:HG2	3:D:1194:ARG:HH21	1.60	0.66
1:H:60:GLU:HA	1:H:171:LEU:HD23	1.76	0.66
3:J:152:THR:OG1	3:J:153:ASN:N	2.24	0.66
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.79	0.65
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.77	0.65
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.60	0.65
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.78	0.65
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.76	0.65
2:C:243:PRO:HG2	2:C:278:GLU:HG3	1.78	0.65
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.60	0.65
2:I:292:ILE:HD12	2:I:322:LEU:HD11	1.78	0.65
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.78	0.65
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.78	0.65
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.79	0.65
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	1.79	0.64
3:J:1152:GLU:HG2	3:J:1194:ARG:HH21	1.60	0.64
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.77	0.64
3:D:557:LYS:HA	3:D:563:LEU:HA	1.78	0.64
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.79	0.64
3:D:1264:ALA:HB2	3:D:1280:VAL:HG22	1.79	0.64
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.80	0.64
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.80	0.64
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.79	0.64
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.80	0.64
2:C:292:ILE:HD12	2:C:322:LEU:HD11	1.80	0.64
3:D:885:VAL:HG21	3:D:1255:VAL:HG12	1.80	0.64
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.78	0.64
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.31	0.64
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.80	0.64
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.80	0.64
2:I:243:PRO:HG2	2:I:278:GLU:HG3	1.78	0.64
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.79	0.64
5:L:126:GLY:O	5:L:130:VAL:HG13	1.97	0.64
3:J:510:LEU:O	3:J:514:THR:OG1	2.16	0.63
3:D:485:MET:HG3	3:D:487:THR:HG23	1.80	0.63
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.80	0.63
3:D:1060:VAL:HG22	3:D:1106:ILE:HG23	1.79	0.63
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.79	0.63
3:D:510:LEU:O	3:D:514:THR:OG1	2.16	0.63
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.80	0.63
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.80	0.63
3:J:1264:ALA:HB2	3:J:1280:VAL:CG2	2.29	0.63
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.79	0.63
5:L:583:THR:HG22	5:L:584:ARG:H	1.64	0.63
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.80	0.63
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.79	0.62
3:J:485:MET:HG3	3:J:487:THR:HG23	1.81	0.62
3:J:557:LYS:HA	3:J:563:LEU:HA	1.78	0.62
1:A:166:ARG:O	1:A:168:ILE:N	2.32	0.62
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.82	0.62
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.80	0.62
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.79	0.62
3:D:1264:ALA:HB2	3:D:1280:VAL:CG2	2.29	0.62
1:G:12:ARG:H	1:G:30:PRO:HD2	1.63	0.62
5:L:548:LEU:HD23	5:L:551:LEU:HD12	1.81	0.62
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.82	0.62
2:I:237:LEU:HD22	2:I:237:LEU:H	1.64	0.62
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.82	0.62
1:A:12:ARG:H	1:A:30:PRO:HD2	1.64	0.62
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.80	0.62
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.65	0.62
1:G:166:ARG:O	1:G:168:ILE:N	2.33	0.62
2:C:237:LEU:H	2:C:237:LEU:HD22	1.64	0.62
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.82	0.62
3:J:885:VAL:HG21	3:J:1255:VAL:HG12	1.81	0.62
5:L:561:MET:HA	5:L:567:MET:HE1	1.81	0.62
1:A:74:VAL:HG22	1:A:76:GLU:H	1.65	0.61
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.81	0.61
1:A:45:ARG:HG2	1:B:38:THR:HB	1.83	0.61
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.82	0.61
3:D:1297:LYS:HG3	3:D:1299:GLY:H	1.65	0.61
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.83	0.61
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.66	0.61
5:F:583:THR:HG22	5:F:584:ARG:H	1.64	0.61
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	1.83	0.61
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.81	0.61
5:F:561:MET:HA	5:F:567:MET:HE1	1.83	0.61
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.82	0.61
2:C:1066:MET:HE2	2:C:1076:ILE:HB	1.83	0.61
1:G:45:ARG:HG2	1:H:38:THR:HB	1.82	0.61
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.81	0.61
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.82	0.61
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.83	0.61
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.35	0.61
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.82	0.61
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.65	0.60
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.82	0.60
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.36	0.60
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	1.83	0.60
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.83	0.60
2:C:123:TYR:HB3	5:F:472:GLN:HB2	1.83	0.60
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.82	0.60
1:H:48:LEU:HD21	3:J:539:SER:HB3	1.83	0.60
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.82	0.60
3:D:1050:THR:HG23	3:D:1057:SER:HB3	1.83	0.60
3:D:1108:GLN:HG3	3:D:1109:LEU:HD13	1.83	0.60
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.84	0.60
1:G:74:VAL:HG22	1:G:76:GLU:H	1.66	0.60
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.84	0.60
1:G:182:ARG:H	1:G:206:GLU:HB3	1.67	0.60
3:J:45:ASN:HB3	3:J:48:THR:O	2.02	0.60
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.84	0.60
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.84	0.60
3:D:218:THR:HA	3:D:221:ILE:HG22	1.83	0.60
3:J:218:THR:HA	3:J:221:ILE:HG22	1.83	0.59
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.83	0.59
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.83	0.59
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.35	0.59
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.83	0.59
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.82	0.59
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.35	0.59
1:A:182:ARG:H	1:A:206:GLU:HB3	1.67	0.59
3:D:424:ASN:HD22	3:D:434:ILE:HG12	1.67	0.59
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.84	0.59
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.83	0.59
3:D:1162:ILE:O	3:D:1178:THR:OG1	2.19	0.59
3:J:1191:PRO:HB2	3:J:1193:TRP:CD1	2.38	0.59
3:D:853:THR:HG22	3:D:854:ALA:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.85	0.59
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.84	0.59
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.85	0.59
3:D:978:ARG:HH21	3:D:1199:PHE:HE1	1.49	0.59
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.37	0.59
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.18	0.59
5:L:479:THR:HG23	5:L:481:GLU:H	1.68	0.59
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.84	0.59
2:I:103:VAL:HB	2:I:113:THR:HG21	1.84	0.58
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.83	0.58
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.38	0.58
3:J:251:PRO:HD2	5:L:507:MET:HE1	1.83	0.58
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.84	0.58
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.85	0.58
5:F:479:THR:HG23	5:F:481:GLU:H	1.68	0.58
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.17	0.58
2:C:255:ILE:HB	2:C:263:VAL:HB	1.85	0.58
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.84	0.58
1:H:51:MET:HE3	1:H:52:PRO:HD2	1.85	0.58
2:I:255:ILE:HB	2:I:263:VAL:HB	1.85	0.58
2:I:1066:MET:HE2	2:I:1076:ILE:HB	1.83	0.58
3:D:45:ASN:HB3	3:D:48:THR:O	2.02	0.58
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.86	0.58
2:C:250:THR:HA	2:C:268:ARG:HA	1.86	0.58
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.86	0.58
2:I:1278:LEU:HD12	2:I:1287:LEU:HD12	1.86	0.58
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.18	0.58
3:D:1191:PRO:HB2	3:D:1193:TRP:CD1	2.38	0.58
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.34	0.58
2:I:538:LEU:HD22	2:I:543:ALA:HB2	1.85	0.58
1:B:51:MET:HE3	1:B:52:PRO:HD2	1.86	0.58
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.85	0.58
1:G:23:HIS:HB2	1:G:205:MET:O	2.04	0.58
3:J:709:ARG:C	3:J:711:GLY:H	2.12	0.58
1:A:23:HIS:HB2	1:A:205:MET:O	2.04	0.58
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.85	0.58
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.85	0.57
5:F:547:VAL:HG11	5:F:607:LEU:HD11	1.86	0.57
2:I:518:ASN:OD1	2:I:518:ASN:N	2.35	0.57
2:I:1073:LYS:HD3	3:J:462:ASP:HB2	1.85	0.57
1:B:182:ARG:HD2	3:D:581:MET:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.86	0.57
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.86	0.57
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.85	0.57
2:C:232:ILE:HG13	2:C:331:LYS:O	2.05	0.57
2:I:166:SER:HB2	6:N:23:SER:N	2.19	0.57
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.86	0.57
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.87	0.57
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.68	0.57
3:D:827:GLU:HG2	3:D:832:LYS:HD2	1.86	0.57
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.86	0.57
3:D:495:ASN:ND2	3:D:1247:LYS:O	2.37	0.57
2:I:232:ILE:HG13	2:I:331:LYS:O	2.05	0.57
3:J:1297:LYS:HG3	3:J:1299:GLY:H	1.68	0.57
2:C:103:VAL:HB	2:C:113:THR:HG21	1.84	0.57
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.87	0.57
2:C:518:ASN:OD1	2:C:518:ASN:N	2.36	0.57
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	1.86	0.57
1:G:26:VAL:HG23	1:G:203:ILE:HB	1.87	0.57
3:J:1189:MET:HE3	6:N:36:LEU:HB3	1.86	0.57
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.70	0.57
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.87	0.57
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.87	0.57
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.70	0.57
2:C:1278:LEU:HD12	2:C:1287:LEU:HD12	1.87	0.56
3:D:1026:PRO:HB2	3:D:1028:ILE:HG23	1.86	0.56
2:I:560:PRO:HB3	3:J:776:THR:HG21	1.87	0.56
3:J:34:SER:OG	3:J:104:HIS:ND1	2.24	0.56
3:J:1063:ASP:HB3	3:J:1103:GLY:HA3	1.87	0.56
2:C:615:VAL:HG13	2:C:651:ASP:H	1.70	0.56
3:D:77:ARG:HG3	3:D:79:LYS:H	1.69	0.56
3:D:325:LYS:HG2	3:D:329:ASP:HB2	1.88	0.56
3:D:1077:ALA:HA	3:D:1100:PHE:HA	1.87	0.56
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.70	0.56
1:G:50:SER:HB3	1:H:8:PHE:HZ	1.70	0.56
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.87	0.56
2:I:615:VAL:HG13	2:I:651:ASP:H	1.70	0.56
2:I:992:LEU:HD11	2:I:1000:LEU:HD11	1.86	0.56
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.87	0.56
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.86	0.56
3:D:17:PHE:O	3:D:1369:ARG:NH2	2.34	0.56
3:D:709:ARG:C	3:D:711:GLY:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1063:ASP:HB3	3:D:1103:GLY:HA3	1.87	0.56
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.87	0.56
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.86	0.56
3:J:77:ARG:HG3	3:J:79:LYS:H	1.70	0.56
3:J:1077:ALA:HA	3:J:1100:PHE:HA	1.87	0.56
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.87	0.56
3:D:381:ILE:HD11	3:D:412:LEU:HD12	1.87	0.56
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.88	0.56
2:I:1085:MET:HA	2:I:1085:MET:HE2	1.88	0.56
3:J:853:THR:HG22	3:J:854:ALA:H	1.70	0.56
2:I:488:MET:O	2:I:490:GLN:N	2.35	0.56
3:J:325:LYS:HG2	3:J:329:ASP:HB2	1.88	0.56
3:J:827:GLU:HG2	3:J:832:LYS:HD2	1.86	0.56
3:J:1151:LYS:NZ	6:N:22:SER:O	2.39	0.56
3:J:1192:LYS:HG2	3:J:1196:LEU:HD11	1.88	0.56
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.88	0.56
3:D:847:ASP:HB3	3:D:856:ILE:HG23	1.87	0.56
2:I:967:LEU:HD21	2:I:1021:LEU:HD13	1.87	0.56
5:L:166:VAL:O	5:L:167:ASP:HB2	2.05	0.56
2:I:250:THR:HA	2:I:268:ARG:HA	1.86	0.56
2:I:808:ASN:H	3:J:633:ALA:HB2	1.69	0.56
3:J:424:ASN:HD22	3:J:434:ILE:HG12	1.69	0.56
3:J:490:ILE:HG22	3:J:500:ILE:HG13	1.88	0.56
3:J:1100:PHE:HB2	3:J:1200:GLU:CD	2.30	0.56
5:L:316:PHE:HZ	5:L:334:SER:HA	1.71	0.56
1:A:26:VAL:HG23	1:A:203:ILE:HB	1.87	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.69	0.56
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.88	0.56
3:J:381:ILE:HD11	3:J:412:LEU:HD12	1.86	0.56
3:J:1211:SER:OG	3:J:1212:ASP:N	2.39	0.56
2:I:19:PRO:HA	2:I:1156:ARG:HD3	1.87	0.56
3:D:1198:VAL:HG22	3:D:1199:PHE:H	1.70	0.56
3:J:495:ASN:ND2	3:J:1247:LYS:O	2.39	0.56
5:L:281:ARG:O	5:L:285:ARG:HG3	2.06	0.56
2:C:19:PRO:HA	2:C:1156:ARG:HD3	1.87	0.55
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.87	0.55
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.87	0.55
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.88	0.55
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.87	0.55
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.88	0.55
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.87	0.55
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.71	0.55
5:L:530:LEU:H	5:L:530:LEU:HD23	1.71	0.55
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.87	0.55
3:D:1192:LYS:HG2	3:D:1196:LEU:HD11	1.89	0.55
5:F:511:ILE:HG13	5:F:512:GLY:H	1.72	0.55
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.87	0.55
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.88	0.55
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.22	0.55
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.88	0.55
5:F:530:LEU:HD23	5:F:530:LEU:H	1.71	0.55
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.89	0.55
3:J:1198:VAL:HG22	3:J:1199:PHE:H	1.70	0.55
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.89	0.55
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.87	0.55
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.89	0.55
5:L:470:MET:O	5:L:474:MET:HB2	2.07	0.55
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.88	0.55
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.89	0.55
5:F:281:ARG:O	5:F:285:ARG:HG3	2.07	0.55
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.88	0.55
5:L:511:ILE:HG13	5:L:512:GLY:H	1.72	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.55
5:F:554:ARG:HB2	5:F:580:PHE:HE2	1.72	0.55
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.89	0.55
3:J:847:ASP:HB3	3:J:856:ILE:HG23	1.87	0.55
5:L:551:LEU:HD11	5:L:598:LEU:HD11	1.89	0.55
2:C:39:ILE:HA	2:C:49:LEU:HD12	1.89	0.55
2:C:1085:MET:HE2	2:C:1085:MET:HA	1.89	0.55
3:D:1029:THR:HG21	3:D:1080:ILE:HD11	1.89	0.55
3:D:1211:SER:OG	3:D:1212:ASP:N	2.39	0.55
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.88	0.55
5:L:97:PRO:HA	5:L:100:MET:HG3	1.89	0.55
2:C:149:LEU:HD21	2:C:451:ARG:NH1	2.22	0.55
4:E:38:LEU:HD23	4:E:58:LEU:HD13	1.87	0.55
5:F:316:PHE:HZ	5:F:334:SER:HA	1.71	0.55
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.89	0.55
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.89	0.55
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.88	0.55
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.90	0.54
5:F:316:PHE:O	5:F:320:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1191:PRO:HB2	3:J:1193:TRP:HD1	1.72	0.54
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.90	0.54
3:D:490:ILE:HG22	3:D:500:ILE:HG13	1.89	0.54
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.90	0.54
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.89	0.54
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.73	0.54
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.89	0.54
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.89	0.54
2:I:41:GLN:NE2	2:I:73:TYR:O	2.40	0.54
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.89	0.54
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.72	0.54
5:F:551:LEU:HD11	5:F:598:LEU:HD11	1.89	0.54
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.90	0.54
2:I:39:ILE:HA	2:I:49:LEU:HD12	1.89	0.54
2:I:149:LEU:HD21	2:I:451:ARG:NH1	2.23	0.54
2:C:41:GLN:NE2	2:C:73:TYR:O	2.41	0.54
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.73	0.54
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.41	0.54
3:J:968:ASN:HB3	3:J:1118:GLY:HA3	1.88	0.54
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.90	0.54
2:C:515:MET:HE3	2:C:517:GLN:HB2	1.89	0.54
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.88	0.54
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.89	0.54
1:G:19:VAL:HG12	1:G:24:ALA:HA	1.90	0.54
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.90	0.54
5:F:577:GLY:HA3	5:F:583:THR:HA	1.90	0.54
6:M:21:GLU:HG3	6:M:26:SER:HB3	1.90	0.54
2:C:736:VAL:HG23	2:C:748:ILE:HA	1.89	0.54
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.89	0.54
5:L:489:MET:HE2	5:L:493:LYS:HG3	1.90	0.54
1:A:60:GLU:OE1	1:A:143:ARG:NH2	2.41	0.54
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.89	0.54
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.90	0.54
5:L:554:ARG:HB2	5:L:580:PHE:HE2	1.72	0.54
3:D:1191:PRO:HB2	3:D:1193:TRP:HD1	1.72	0.54
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.23	0.54
2:I:515:MET:HE3	2:I:517:GLN:HB2	1.89	0.54
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.72	0.54
5:L:316:PHE:O	5:L:320:ILE:HG13	2.08	0.54
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.43	0.53
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.41	0.53
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.90	0.53
2:C:815:SER:HB3	3:D:461:PHE:HB3	1.90	0.53
3:D:1167:LYS:HG3	3:D:1174:ARG:HD2	1.91	0.53
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.91	0.53
3:D:978:ARG:HB2	3:D:1199:PHE:CZ	2.43	0.53
3:D:1189:MET:HE3	6:M:36:LEU:HB3	1.89	0.53
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.89	0.53
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.90	0.53
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.90	0.53
5:L:130:VAL:HB	5:L:365:MET:HG3	1.90	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.90	0.53
1:B:8:PHE:HD1	1:B:9:LEU:H	1.55	0.53
5:F:97:PRO:HA	5:F:100:MET:HG3	1.90	0.53
5:F:234:THR:O	5:F:245:ALA:HB2	2.09	0.53
2:I:91:THR:HG21	2:I:503:LYS:HE2	1.90	0.53
6:N:21:GLU:HG3	6:N:26:SER:HB3	1.90	0.53
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.90	0.53
2:C:120:GLN:HG2	2:C:121:GLU:H	1.73	0.53
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.90	0.53
2:C:818:VAL:HG13	2:C:1096:ILE:HG12	1.90	0.53
5:F:270:VAL:HA	5:F:273:MET:HE3	1.89	0.53
5:F:470:MET:O	5:F:474:MET:HB2	2.07	0.53
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.91	0.53
2:I:593:LYS:HB3	2:I:602:GLU:HG3	1.89	0.53
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.89	0.53
2:I:815:SER:HB3	3:J:461:PHE:HB3	1.90	0.53
3:J:1167:LYS:HG3	3:J:1174:ARG:HD2	1.90	0.53
5:L:270:VAL:HA	5:L:273:MET:HE3	1.90	0.53
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	1.91	0.53
2:C:1247:SER:HB3	3:D:375:GLU:O	2.09	0.53
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.91	0.53
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.91	0.53
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.90	0.53
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.90	0.53
1:G:60:GLU:OE1	1:G:143:ARG:NH2	2.42	0.53
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.90	0.53
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.43	0.53
4:K:42:GLU:O	4:K:43:ASN:HB2	2.08	0.53
5:L:234:THR:O	5:L:245:ALA:HB2	2.09	0.53
1:B:75:GLN:OE1	1:B:76:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:387:ASN:HA	2:C:391:SER:HB2	1.91	0.53
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.39	0.53
3:D:1039:ASP:OD1	3:D:1074:LEU:HB3	2.09	0.53
2:I:387:ASN:HA	2:I:391:SER:HB2	1.90	0.53
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.90	0.53
3:D:425:ARG:HG2	3:D:426:ALA:H	1.74	0.53
3:D:968:ASN:HB3	3:D:1118:GLY:HA3	1.90	0.53
1:G:102:LEU:HD12	1:G:142:MET:HE3	1.91	0.53
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.90	0.53
5:L:577:GLY:HA3	5:L:583:THR:HA	1.91	0.53
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.89	0.53
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.91	0.53
3:D:1191:PRO:HD3	6:M:55:THR:O	2.08	0.53
4:E:42:GLU:O	4:E:43:ASN:HB2	2.09	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.07	0.53
1:A:14:VAL:HG22	1:A:15:ASP:H	1.74	0.52
1:H:75:GLN:OE1	1:H:76:GLU:HG3	2.09	0.52
2:I:356:THR:HG21	2:I:362:ALA:HA	1.90	0.52
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	1.91	0.52
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.74	0.52
3:D:1151:LYS:NZ	6:M:22:SER:O	2.42	0.52
2:I:455:SER:O	2:I:459:MET:HE3	2.09	0.52
2:I:1247:SER:OG	2:I:1248:THR:N	2.42	0.52
1:H:125:LYS:HE2	1:H:128:HIS:HB2	1.92	0.52
2:I:818:VAL:HG13	2:I:1096:ILE:HG12	1.91	0.52
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.91	0.52
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.92	0.52
3:J:475:GLU:OE2	4:K:28:ARG:NH2	2.39	0.52
1:B:64:VAL:HG12	1:B:65:LEU:H	1.74	0.52
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.92	0.52
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.91	0.52
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.90	0.52
5:F:489:MET:HE2	5:F:493:LYS:HG3	1.92	0.52
1:G:14:VAL:HG22	1:G:15:ASP:H	1.74	0.52
3:J:425:ARG:HG2	3:J:426:ALA:H	1.74	0.52
3:D:1078:LEU:HD13	3:D:1121:LEU:HD22	1.91	0.52
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.91	0.52
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.92	0.52
2:C:861:ALA:HB1	2:C:882:ILE:HD13	1.91	0.52
2:I:5:TYR:CE1	2:I:776:PRO:HB2	2.44	0.52
3:J:332:LYS:HG2	3:J:1328:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.92	0.52
1:B:125:LYS:HE2	1:B:128:HIS:HB2	1.91	0.52
2:C:703:GLY:N	2:C:705:GLU:OE2	2.42	0.52
3:D:198:CYS:O	3:D:202:ARG:HG3	2.10	0.52
3:D:974:VAL:HG21	3:D:1118:GLY:HA2	1.92	0.52
2:C:356:THR:HG21	2:C:362:ALA:HA	1.91	0.52
1:G:50:SER:HB3	1:H:8:PHE:CZ	2.45	0.52
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.74	0.52
2:I:980:VAL:O	2:I:984:VAL:HB	2.10	0.52
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.91	0.52
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.91	0.52
3:J:1029:THR:HG21	3:J:1080:ILE:HD11	1.91	0.52
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.92	0.52
1:H:64:VAL:HG12	1:H:65:LEU:H	1.75	0.52
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.92	0.52
2:I:600:THR:HB	2:I:602:GLU:HG2	1.92	0.52
2:I:1247:SER:HB3	3:J:375:GLU:O	2.10	0.52
3:J:502:PRO:HB2	3:J:507:VAL:HG12	1.92	0.52
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.90	0.51
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.91	0.51
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.92	0.51
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.93	0.51
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.90	0.51
2:I:861:ALA:HB1	2:I:882:ILE:HD13	1.91	0.51
3:J:474:LEU:O	3:J:478:LEU:HD12	2.10	0.51
3:D:474:LEU:O	3:D:478:LEU:HD12	2.10	0.51
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.92	0.51
1:G:74:VAL:HG23	1:G:132:HIS:O	2.10	0.51
3:J:198:CYS:O	3:J:202:ARG:HG3	2.11	0.51
3:J:697:MET:HG3	3:J:698:MET:N	2.26	0.51
3:J:1039:ASP:OD1	3:J:1074:LEU:HB3	2.09	0.51
2:C:600:THR:HB	2:C:602:GLU:HG2	1.93	0.51
3:D:699:ASP:HA	3:D:702:GLN:HG2	1.92	0.51
5:F:130:VAL:HB	5:F:365:MET:HG3	1.93	0.51
2:I:804:PHE:HB3	2:I:1100:PRO:HG3	1.91	0.51
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.93	0.51
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.92	0.51
2:I:864:LYS:NZ	2:I:876:GLU:O	2.43	0.51
3:J:810:THR:O	3:J:911:LYS:HE3	2.10	0.51
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.92	0.51
3:D:901:ARG:HA	3:D:908:ILE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:119:GLU:HB2	2:I:489:PRO:HD2	1.92	0.51
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.91	0.51
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.91	0.51
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.93	0.51
3:J:901:ARG:HA	3:J:908:ILE:HA	1.92	0.51
5:L:289:LYS:HE3	5:L:293:GLU:HG2	1.93	0.51
3:D:810:THR:O	3:D:911:LYS:HE3	2.10	0.51
5:F:289:LYS:HE3	5:F:293:GLU:HG2	1.92	0.51
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.76	0.51
5:F:158:LEU:HD22	5:F:162:ILE:HD11	1.93	0.51
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.93	0.51
2:C:864:LYS:NZ	2:C:876:GLU:O	2.43	0.51
1:G:120:ASP:OD2	1:G:120:ASP:N	2.44	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.11	0.51
3:J:978:ARG:HB2	3:J:1199:PHE:CZ	2.46	0.51
1:B:191:ARG:NH2	3:D:409:TRP:HB3	2.26	0.51
3:D:34:SER:OG	3:D:104:HIS:ND1	2.26	0.51
3:D:1100:PHE:HB2	3:D:1200:GLU:CD	2.36	0.51
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.93	0.51
1:A:74:VAL:HG23	1:A:132:HIS:O	2.10	0.50
3:D:847:ASP:OD1	3:D:847:ASP:N	2.44	0.50
5:L:158:LEU:HD22	5:L:162:ILE:HD11	1.93	0.50
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.92	0.50
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.76	0.50
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.93	0.50
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.94	0.50
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	1.93	0.50
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	0.50
3:D:644:MET:HE3	3:D:764:ARG:HG3	1.93	0.50
5:F:245:ALA:O	5:F:249:ILE:HG13	2.12	0.50
2:C:331:LYS:HB2	2:C:332:ARG:NH2	2.26	0.50
2:C:1314:GLN:HG2	4:E:28:ARG:NH1	2.27	0.50
3:D:1064:SER:HB2	3:D:1173:ARG:HH12	1.77	0.50
3:J:478:LEU:HG	4:K:47:THR:HG23	1.94	0.50
3:J:1162:ILE:O	3:J:1178:THR:OG1	2.18	0.50
1:A:120:ASP:N	1:A:120:ASP:OD2	2.44	0.50
3:D:1077:ALA:HB2	3:D:1100:PHE:CD1	2.47	0.50
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.93	0.50
2:C:225:PHE:HE1	2:C:345:PRO:HA	1.77	0.50
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.93	0.50
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.93	0.50
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.47	0.50
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.46	0.50
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.94	0.50
3:J:699:ASP:HA	3:J:702:GLN:HG2	1.92	0.50
3:J:847:ASP:OD1	3:J:847:ASP:N	2.43	0.50
2:C:55:SER:OG	2:C:56:VAL:N	2.45	0.50
2:C:206:ALA:O	2:C:209:ILE:HG22	2.11	0.50
2:C:632:ASP:HA	2:C:647:ARG:HB2	1.93	0.50
3:D:697:MET:HG3	3:D:698:MET:N	2.26	0.50
3:D:902:ASP:OD1	3:D:903:LEU:N	2.45	0.50
1:H:102:LEU:O	1:H:141:SER:OG	2.28	0.50
2:I:331:LYS:HB2	2:I:332:ARG:NH2	2.26	0.50
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.12	0.50
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.47	0.50
2:C:170:VAL:HG23	2:C:171:LEU:N	2.27	0.49
3:D:576:ARG:NH1	3:D:593:ASN:O	2.44	0.49
3:D:870:ASP:O	3:D:874:GLU:HG2	2.12	0.49
2:I:30:ILE:HD12	2:I:30:ILE:H	1.77	0.49
2:I:170:VAL:HG23	2:I:171:LEU:N	2.27	0.49
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	1.93	0.49
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.12	0.49
3:D:298:MET:SD	5:F:402:LEU:HB3	2.52	0.49
3:D:564:VAL:HG12	3:D:565:ALA:H	1.77	0.49
3:D:708:ASN:HB3	3:D:712:GLN:O	2.11	0.49
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.93	0.49
5:F:343:LYS:HD2	5:F:343:LYS:H	1.76	0.49
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.76	0.49
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.93	0.49
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.95	0.49
3:D:1227:HIS:ND1	3:J:1293:GLU:HG2	2.27	0.49
5:F:141:ILE:HG21	5:F:252:LEU:HD11	1.93	0.49
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.47	0.49
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.93	0.49
3:J:644:MET:HE3	3:J:764:ARG:HG3	1.94	0.49
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.48	0.49
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.77	0.49
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.94	0.49
3:J:451:PRO:O	3:J:454:CYS:HB2	2.13	0.49
3:J:902:ASP:OD1	3:J:903:LEU:N	2.46	0.49
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:829:THR:HG23	2:C:1059:ARG:HA	1.95	0.49
3:D:332:LYS:HG2	3:D:1328:THR:HB	1.92	0.49
3:D:826:ILE:HD12	3:D:994:SER:HB2	1.94	0.49
3:D:1349:GLU:H	3:D:1349:GLU:CD	2.20	0.49
5:F:461:ASN:O	5:F:465:ARG:HG2	2.12	0.49
2:I:632:ASP:HA	2:I:647:ARG:HB2	1.94	0.49
3:J:564:VAL:HG12	3:J:565:ALA:H	1.78	0.49
1:A:102:LEU:HD12	1:A:142:MET:HE3	1.93	0.49
1:A:197:ASP:OD1	1:A:197:ASP:N	2.45	0.49
2:C:30:ILE:HD12	2:C:30:ILE:H	1.76	0.49
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.26	0.49
2:C:1106:ARG:NE	3:D:731:ARG:HH21	2.10	0.49
5:F:442:SER:O	5:F:446:GLN:HG2	2.12	0.49
4:K:25:ARG:HD3	4:K:64:LEU:HD13	1.93	0.49
1:B:44:ARG:HG3	1:B:183:ILE:HB	1.94	0.49
3:D:755:ILE:HG22	3:D:757:THR:H	1.78	0.49
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.12	0.49
5:F:250:LEU:O	5:F:253:SER:OG	2.27	0.49
1:G:197:ASP:OD1	1:G:197:ASP:N	2.45	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
3:J:708:ASN:HB3	3:J:712:GLN:O	2.12	0.49
3:D:398:LYS:O	3:D:402:GLU:HB2	2.13	0.49
3:D:451:PRO:O	3:D:454:CYS:HB2	2.13	0.49
3:D:845:ALA:HB3	3:D:881:LYS:HB3	1.95	0.49
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.94	0.49
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.77	0.49
5:L:245:ALA:O	5:L:249:ILE:HG13	2.12	0.49
5:L:343:LYS:O	5:L:347:ILE:HG13	2.13	0.49
5:F:343:LYS:O	5:F:347:ILE:HG13	2.13	0.49
1:H:44:ARG:HG3	1:H:183:ILE:HB	1.94	0.49
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.48	0.49
3:J:576:ARG:NH1	3:J:593:ASN:O	2.45	0.49
6:N:16:PHE:HD1	6:N:59:PRO:HA	1.78	0.49
3:D:850:LYS:HG2	3:D:851:PRO:HD2	1.95	0.48
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.48	0.48
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.77	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.13	0.48
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.13	0.48
5:L:470:MET:HG3	5:L:486:ARG:HH22	1.78	0.48
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.95	0.48
3:D:978:ARG:HB2	3:D:1199:PHE:HZ	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.95	0.48
2:I:528:ARG:NH2	2:I:576:SER:O	2.46	0.48
2:I:738:GLU:HA	2:I:741:MET:HE2	1.95	0.48
2:I:818:VAL:HG21	2:I:1066:MET:HE1	1.95	0.48
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.10	0.48
5:L:250:LEU:O	5:L:253:SER:OG	2.28	0.48
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.96	0.48
3:D:478:LEU:HG	4:E:47:THR:HG23	1.94	0.48
2:I:55:SER:OG	2:I:56:VAL:N	2.46	0.48
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.14	0.48
3:J:398:LYS:O	3:J:402:GLU:HB2	2.13	0.48
2:C:444:ASP:O	2:C:450:ASN:ND2	2.39	0.48
2:C:802:VAL:HG23	2:C:1098:LEU:HD13	1.94	0.48
2:I:232:ILE:HD11	2:I:333:ILE:HD11	1.96	0.48
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.95	0.48
3:J:870:ASP:O	3:J:874:GLU:HG2	2.13	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.94	0.48
3:J:1062:LEU:CD2	3:J:1066:GLU:HB3	2.44	0.48
2:C:232:ILE:HD11	2:C:333:ILE:HD11	1.95	0.48
2:C:1149:TYR:OH	2:C:1176:LEU:HD11	2.14	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.95	0.48
2:C:1246:ARG:NH2	3:D:348:ASP:OD1	2.46	0.48
3:D:807:LEU:HD11	3:D:894:VAL:HG23	1.95	0.48
3:D:1264:ALA:CB	3:D:1280:VAL:HG22	2.44	0.48
3:J:298:MET:SD	5:L:402:LEU:HB3	2.53	0.48
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.95	0.48
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.95	0.48
2:C:692:THR:OG1	2:C:693:LEU:N	2.46	0.48
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.95	0.48
2:C:739:ASP:OD1	2:C:739:ASP:N	2.43	0.48
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.96	0.48
3:D:1226:VAL:HG23	3:J:1296:GLY:HA2	1.96	0.48
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.94	0.48
2:I:1246:ARG:NH2	3:J:348:ASP:OD1	2.46	0.48
3:J:17:PHE:O	3:J:1369:ARG:NH2	2.38	0.48
3:J:99:ARG:HA	3:J:248:ASP:HB2	1.96	0.48
1:B:73:GLY:O	1:B:134:THR:N	2.35	0.48
2:C:528:ARG:NH2	2:C:576:SER:O	2.47	0.48
3:D:1067:ARG:HH22	3:D:1076:PRO:HD3	1.79	0.48
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.96	0.48
3:J:755:ILE:HG22	3:J:757:THR:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1349:GLU:H	3:J:1349:GLU:CD	2.19	0.48
5:L:138:PRO:O	5:L:142:THR:HG23	2.14	0.48
5:L:141:ILE:HG21	5:L:252:LEU:HD11	1.94	0.48
5:L:319:ALA:HA	5:L:322:MET:HG3	1.94	0.48
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.96	0.48
1:G:207:THR:HG22	1:G:208:ASN:H	1.79	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.96	0.48
3:J:1062:LEU:HD21	3:J:1066:GLU:HB3	1.95	0.48
1:A:57:THR:OG1	1:A:147:GLN:HG2	2.14	0.48
1:B:61:ILE:HB	1:B:64:VAL:O	2.14	0.48
5:F:98:VAL:O	5:F:102:MET:HB2	2.14	0.48
5:F:130:VAL:O	5:F:134:VAL:HG23	2.14	0.48
2:I:4:SER:OG	2:I:5:TYR:N	2.47	0.48
2:I:703:GLY:N	2:I:705:GLU:OE2	2.43	0.48
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.95	0.48
3:J:525:MET:O	3:J:548:VAL:HG13	2.14	0.48
3:J:807:LEU:HD11	3:J:894:VAL:HG23	1.96	0.48
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.47	0.48
3:J:1067:ARG:HH22	3:J:1076:PRO:HD3	1.79	0.48
3:J:1264:ALA:CB	3:J:1280:VAL:HG22	2.44	0.48
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.96	0.47
5:F:319:ALA:HA	5:F:322:MET:HG3	1.95	0.47
1:H:181:GLU:HA	3:J:535:ARG:NH2	2.29	0.47
3:J:845:ALA:HB3	3:J:881:LYS:HB3	1.96	0.47
1:B:16:ILE:HG13	1:B:26:VAL:HG22	1.96	0.47
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.79	0.47
2:C:890:LYS:NZ	2:C:891:GLY:O	2.47	0.47
1:G:10:LYS:HE2	1:H:229:GLU:HB3	1.95	0.47
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.79	0.47
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.96	0.47
3:J:161:THR:HG22	3:J:164:GLN:CD	2.39	0.47
5:L:130:VAL:O	5:L:134:VAL:HG23	2.14	0.47
3:D:475:GLU:CD	4:E:28:ARG:HH22	2.23	0.47
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.96	0.47
5:F:138:PRO:O	5:F:142:THR:HG23	2.14	0.47
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.13	0.47
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.96	0.47
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.97	0.47
3:D:144:TYR:CD1	3:D:180:MET:HB3	2.50	0.47
3:D:405:GLU:O	3:D:408:VAL:HG22	2.14	0.47
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:850:LYS:HG2	3:J:851:PRO:HD2	1.95	0.47
1:B:68:TYR:O	1:B:69:SER:OG	2.32	0.47
2:C:151:ARG:HG2	2:C:445:ILE:HG23	1.97	0.47
2:C:225:PHE:CE1	2:C:345:PRO:HA	2.50	0.47
3:D:525:MET:O	3:D:548:VAL:HG13	2.13	0.47
3:D:1062:LEU:HD21	3:D:1066:GLU:HB3	1.95	0.47
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.96	0.47
2:I:5:TYR:CD2	2:I:778:GLU:HB2	2.50	0.47
2:I:499:SER:O	2:I:503:LYS:HB2	2.15	0.47
2:I:890:LYS:NZ	2:I:891:GLY:O	2.47	0.47
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.96	0.47
3:J:122:SER:O	3:J:126:LEU:HG	2.15	0.47
3:J:1064:SER:HB2	3:J:1173:ARG:NH1	2.25	0.47
6:M:16:PHE:HD1	6:M:59:PRO:HA	1.78	0.47
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.97	0.47
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.79	0.47
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.97	0.47
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.46	0.47
5:L:220:LYS:O	5:L:223:GLU:HB3	2.15	0.47
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.96	0.47
2:C:4:SER:OG	2:C:5:TYR:N	2.47	0.47
2:C:818:VAL:HG21	2:C:1066:MET:HE1	1.96	0.47
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.96	0.47
3:D:442:ILE:HG22	3:D:443:GLU:O	2.15	0.47
3:D:853:THR:HG21	3:J:1375:ALA:CB	2.45	0.47
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.48	0.47
3:D:1062:LEU:CD2	3:D:1066:GLU:HB3	2.44	0.47
3:D:1189:MET:HE1	6:M:37:ASP:HA	1.96	0.47
3:D:1282:TYR:O	3:D:1285:VAL:HG12	2.15	0.47
5:F:598:LEU:HA	5:F:603:ARG:HB2	1.96	0.47
1:H:61:ILE:HB	1:H:64:VAL:O	2.14	0.47
3:J:1260:MET:HG2	3:J:1307:LEU:O	2.14	0.47
5:L:515:GLU:C	5:L:517:SER:H	2.23	0.47
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.97	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.97	0.47
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.97	0.47
1:G:75:GLN:HA	2:I:729:ALA:N	2.30	0.47
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.97	0.47
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.45	0.47
3:J:174:ASP:C	3:J:176:PHE:H	2.22	0.47
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:98:VAL:O	5:L:102:MET:HB2	2.15	0.47
2:C:499:SER:O	2:C:503:LYS:HB2	2.15	0.47
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.96	0.47
3:D:1153:PRO:HA	3:D:1214:PRO:O	2.15	0.47
5:F:470:MET:HG3	5:F:486:ARG:HH22	1.78	0.47
5:L:598:LEU:HA	5:L:603:ARG:HB2	1.97	0.47
1:A:45:ARG:NE	2:C:1083:GLU:HB3	2.29	0.47
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.49	0.47
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.97	0.47
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.47
2:C:883:LEU:HD22	2:C:1052:VAL:HG11	1.97	0.47
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.15	0.47
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.14	0.47
1:H:73:GLY:CA	1:H:134:THR:HG22	2.44	0.47
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.50	0.47
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.96	0.47
2:C:120:GLN:HG2	2:C:121:GLU:HG2	1.96	0.46
2:C:494:ASN:HD21	5:F:468:ARG:HG2	1.80	0.46
3:J:442:ILE:HG22	3:J:443:GLU:O	2.15	0.46
1:A:207:THR:HG22	1:A:208:ASN:H	1.80	0.46
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.45	0.46
2:C:1253:LEU:HD11	3:D:251:PRO:HG2	1.96	0.46
3:D:574:VAL:O	3:D:578:ILE:HG13	2.16	0.46
3:D:1260:MET:HG2	3:D:1307:LEU:O	2.15	0.46
2:I:1116:HIS:O	2:I:1119:MET:HB3	2.15	0.46
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.97	0.46
5:L:547:VAL:HG21	5:L:607:LEU:HD11	1.98	0.46
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.98	0.46
2:C:1113:LEU:HD11	3:D:641:ILE:HG13	1.97	0.46
3:D:122:SER:O	3:D:126:LEU:HG	2.15	0.46
3:D:161:THR:HG22	3:D:164:GLN:CD	2.40	0.46
3:D:290:ILE:HD12	3:D:290:ILE:H	1.81	0.46
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.97	0.46
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.97	0.46
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.96	0.46
3:J:156:ARG:NH2	3:J:191:SER:OG	2.48	0.46
6:N:40:LEU:O	6:N:44:GLU:HG2	2.16	0.46
2:C:1247:SER:OG	2:C:1248:THR:N	2.44	0.46
2:C:1279:GLU:HG3	3:D:1357:ILE:HD13	1.97	0.46
3:D:654:ILE:O	3:D:658:GLU:HB2	2.16	0.46
1:G:201:LEU:HG	1:G:203:ILE:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:90:VAL:HG12	2:I:91:THR:H	1.80	0.46
5:L:456:MET:O	5:L:460:ILE:HG13	2.15	0.46
6:M:40:LEU:O	6:M:44:GLU:HG2	2.15	0.46
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.97	0.46
2:C:855:PRO:HG3	2:C:913:VAL:HG13	1.97	0.46
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.98	0.46
2:I:5:TYR:HD2	2:I:778:GLU:HB2	1.80	0.46
2:I:223:LEU:HD22	2:I:426:ILE:HG21	1.97	0.46
2:C:136:PHE:O	2:C:143:ARG:N	2.37	0.46
2:C:379:GLU:CD	2:C:379:GLU:H	2.23	0.46
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.97	0.46
3:D:156:ARG:NH2	3:D:191:SER:OG	2.47	0.46
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.97	0.46
1:G:75:GLN:HA	2:I:729:ALA:H	1.80	0.46
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.97	0.46
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.49	0.46
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.50	0.46
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.96	0.46
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.97	0.46
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.96	0.46
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.98	0.46
3:J:574:VAL:O	3:J:578:ILE:HG13	2.16	0.46
1:B:47:LEU:HB3	1:B:180:VAL:HG11	1.98	0.46
1:B:75:GLN:H	1:B:75:GLN:HG3	1.60	0.46
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.97	0.46
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.97	0.46
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.49	0.46
2:I:379:GLU:H	2:I:379:GLU:CD	2.24	0.46
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.80	0.46
2:I:1113:LEU:HD11	3:J:641:ILE:HG13	1.97	0.46
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.46	0.46
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.59	0.46
2:C:738:GLU:HA	2:C:741:MET:HE2	1.96	0.46
3:D:174:ASP:C	3:D:176:PHE:H	2.23	0.46
5:F:456:MET:O	5:F:460:ILE:HG13	2.15	0.46
3:J:405:GLU:O	3:J:408:VAL:HG22	2.15	0.46
5:L:311:THR:HB	5:L:345:GLN:HG2	1.98	0.46
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.49	0.46
5:F:515:GLU:C	5:F:517:SER:H	2.23	0.46
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.81	0.46
3:J:144:TYR:CD1	3:J:180:MET:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:473:THR:HG23	3:J:476:ALA:H	1.81	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.46
2:C:223:LEU:HD22	2:C:426:ILE:HG21	1.98	0.46
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.80	0.46
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.70	0.46
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.98	0.46
3:D:650:LYS:O	3:D:654:ILE:HG13	2.16	0.46
3:J:1158:GLU:OE2	3:J:1222:ARG:NH1	2.48	0.46
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.81	0.45
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.45	0.45
2:I:705:GLU:O	2:I:794:LEU:N	2.49	0.45
2:I:883:LEU:HD22	2:I:1052:VAL:HG11	1.97	0.45
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.98	0.45
1:B:44:ARG:NH2	3:D:538:ARG:HH21	2.14	0.45
2:C:90:VAL:HG12	2:C:91:THR:H	1.79	0.45
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.97	0.45
4:E:50:ALA:O	4:E:54:ILE:HG12	2.16	0.45
5:F:311:THR:HB	5:F:345:GLN:HG2	1.99	0.45
5:F:446:GLN:O	5:F:448:ARG:N	2.49	0.45
2:I:960:LEU:HD13	2:I:960:LEU:HA	1.87	0.45
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.97	0.45
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.31	0.45
2:C:123:TYR:OH	2:C:126:GLU:HG3	2.17	0.45
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.96	0.45
2:C:1142:ARG:HH22	2:C:1165:SER:HA	1.81	0.45
3:D:1078:LEU:HB2	3:D:1121:LEU:HD13	1.98	0.45
3:D:1158:GLU:OE2	3:D:1222:ARG:NH1	2.50	0.45
3:D:1167:LYS:O	3:D:1169:THR:N	2.50	0.45
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.31	0.45
2:I:1279:GLU:HG3	3:J:1357:ILE:HD13	1.98	0.45
3:J:475:GLU:CD	4:K:28:ARG:HH22	2.23	0.45
3:J:1062:LEU:O	3:J:1067:ARG:NE	2.45	0.45
6:N:19:THR:OG1	6:N:55:THR:HB	2.17	0.45
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.52	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.52	0.45
3:D:600:ALA:O	3:D:603:LYS:HG2	2.16	0.45
1:H:30:PRO:HB3	1:H:192:VAL:HG21	1.98	0.45
2:I:5:TYR:HB2	2:I:781:ASP:OD1	2.17	0.45
3:J:650:LYS:O	3:J:654:ILE:HG13	2.16	0.45
3:J:654:ILE:O	3:J:658:GLU:HB2	2.16	0.45
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1167:LYS:O	3:J:1169:THR:N	2.49	0.45
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.47	0.45
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.51	0.45
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	1.99	0.45
3:J:363:LEU:HD21	3:J:487:THR:HA	1.97	0.45
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.51	0.45
2:C:705:GLU:O	2:C:794:LEU:N	2.49	0.45
3:D:1027:VAL:HG21	3:D:1122:ALA:HB3	1.97	0.45
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.17	0.45
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.49	0.45
3:J:211:GLU:HG3	6:N:13:ASN:O	2.16	0.45
3:J:378:LYS:HB3	3:J:379:PRO:HD3	1.99	0.45
3:J:424:ASN:ND2	3:J:434:ILE:HG12	2.31	0.45
5:L:446:GLN:O	5:L:448:ARG:N	2.50	0.45
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.27	0.45
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.47	0.45
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.47	0.45
3:J:950:ILE:HG13	3:J:1020:TRP:CZ3	2.52	0.45
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.17	0.45
6:N:29:VAL:HG21	6:N:47:TYR:OH	2.17	0.45
1:B:73:GLY:CA	1:B:134:THR:HG22	2.44	0.45
2:C:976:ARG:O	2:C:980:VAL:HG23	2.16	0.45
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.17	0.45
3:D:1166:GLY:O	3:D:1174:ARG:HB2	2.17	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.17	0.45
2:C:519:ASN:OD1	2:C:521:LEU:N	2.50	0.45
2:C:1326:LEU:HD11	3:D:331:ILE:HG23	1.98	0.45
3:D:473:THR:HG23	3:D:476:ALA:H	1.81	0.45
3:D:1257:VAL:HA	3:D:1260:MET:HE3	1.99	0.45
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.81	0.45
5:F:580:PHE:C	5:F:582:VAL:H	2.25	0.45
3:J:770:LEU:HD22	3:J:770:LEU:H	1.81	0.45
3:J:1064:SER:O	3:J:1072:LYS:HE2	2.17	0.45
3:J:1078:LEU:HB2	3:J:1121:LEU:HD13	1.98	0.45
5:L:580:PHE:C	5:L:582:VAL:H	2.25	0.45
2:C:121:GLU:H	2:C:121:GLU:HG2	1.59	0.45
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.99	0.45
1:H:32:GLU:HB2	1:H:35:PHE:CD1	2.52	0.45
2:I:98:VAL:HG21	2:I:124:MET:HE3	1.99	0.45
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.52	0.45
2:I:971:LEU:HD22	2:I:1021:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.98	0.45
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.98	0.44
3:D:1302:TYR:CZ	3:J:1297:LYS:HD3	2.52	0.44
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.65	0.44
3:J:600:ALA:O	3:J:603:LYS:HG2	2.16	0.44
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.65	0.44
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.65	0.44
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.53	0.44
1:A:104:LYS:HG2	1:A:110:VAL:HG22	2.00	0.44
2:C:971:LEU:HD23	2:C:975:ILE:HD11	1.99	0.44
3:D:418:GLU:H	4:E:45:LYS:NZ	2.15	0.44
2:I:831:ILE:C	2:I:832:HIS:HD2	2.25	0.44
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.99	0.44
5:L:442:SER:O	5:L:446:GLN:HG2	2.18	0.44
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.43	0.44
6:M:19:THR:OG1	6:M:55:THR:HB	2.16	0.44
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.72	0.44
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.99	0.44
3:D:958:ILE:HD11	3:D:1017:VAL:HG11	2.00	0.44
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.98	0.44
5:F:220:LYS:O	5:F:223:GLU:HB3	2.17	0.44
5:F:335:GLU:O	5:F:339:ARG:HG2	2.18	0.44
5:F:354:THR:O	5:F:358:VAL:HG23	2.16	0.44
1:H:47:LEU:HB3	1:H:180:VAL:HG11	1.99	0.44
1:H:172:LEU:HD12	1:H:172:LEU:H	1.82	0.44
1:H:196:THR:HG23	3:J:443:GLU:HG3	2.00	0.44
2:I:174:ALA:HB2	2:I:432:LEU:HD13	2.00	0.44
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.00	0.44
3:J:233:LYS:HB3	3:J:235:GLU:OE2	2.17	0.44
3:J:1282:TYR:O	3:J:1285:VAL:HG12	2.17	0.44
2:C:62:TYR:C	2:C:64:GLY:H	2.26	0.44
3:D:334:LYS:HB3	5:F:516:ASP:OD2	2.16	0.44
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.17	0.44
1:H:81:ILE:O	1:H:85:LEU:HG	2.18	0.44
1:H:93:GLN:HB2	1:H:120:ASP:HB3	2.00	0.44
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.97	0.44
2:I:396:ASP:OD1	2:I:418:GLY:HA3	2.18	0.44
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.32	0.44
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.98	0.44
3:J:743:MET:HB2	3:J:759:ILE:O	2.17	0.44
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLN:HB2	1:B:120:ASP:HB3	1.99	0.44
1:B:178:SER:HA	1:B:179:PRO:HD3	1.71	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
5:F:253:SER:O	5:F:257:LYS:HG3	2.17	0.44
2:I:992:LEU:HB2	2:I:993:PRO:HD2	1.99	0.44
3:J:794:GLY:O	3:J:797:THR:OG1	2.31	0.44
1:A:231:PHE:CE1	1:B:221:ALA:HB3	2.53	0.44
2:C:657:THR:HG23	2:C:658:GLN:HG3	2.00	0.44
3:D:430:HIS:CE1	3:D:925:GLU:HG3	2.52	0.44
3:D:706:VAL:HG12	3:D:715:LYS:HB3	2.00	0.44
3:D:950:ILE:HG13	3:D:1020:TRP:CZ3	2.52	0.44
4:E:44:ASP:HB3	4:E:48:VAL:HB	2.00	0.44
1:H:79:LEU:HD23	1:H:79:LEU:H	1.82	0.44
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.53	0.44
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.99	0.44
3:J:418:GLU:H	4:K:45:LYS:NZ	2.15	0.44
3:J:613:GLY:O	3:J:617:THR:OG1	2.33	0.44
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.17	0.44
4:K:44:ASP:HB3	4:K:48:VAL:HB	2.00	0.44
1:B:30:PRO:HB3	1:B:192:VAL:HG21	1.99	0.44
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.32	0.44
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.16	0.44
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.87	0.44
3:D:363:LEU:HD21	3:D:487:THR:HA	1.98	0.44
3:D:440:VAL:O	3:D:442:ILE:HG12	2.18	0.44
3:D:490:ILE:HD11	3:D:609:TYR:CE2	2.53	0.44
3:D:800:LEU:HD12	3:D:1309:ILE:HD13	2.00	0.44
2:I:62:TYR:C	2:I:64:GLY:H	2.25	0.44
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.47	0.44
2:I:1326:LEU:HD11	3:J:331:ILE:HG23	1.99	0.44
3:J:490:ILE:HD11	3:J:609:TYR:CE2	2.53	0.44
3:J:958:ILE:HG23	3:J:982:LEU:HD11	2.00	0.44
5:L:312:SER:OG	5:L:313:ASP:N	2.51	0.44
1:A:51:MET:HE3	1:A:52:PRO:HD2	2.00	0.44
1:B:52:PRO:HA	1:B:149:GLY:O	2.18	0.44
1:B:102:LEU:O	1:B:141:SER:OG	2.29	0.44
2:C:137:VAL:HA	2:C:141:THR:O	2.18	0.44
2:C:980:VAL:HG13	2:C:984:VAL:HG23	1.99	0.44
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.00	0.44
3:D:18:ASP:OD1	3:D:18:ASP:N	2.50	0.44
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.18	0.44
5:F:324:LYS:HB2	5:F:327:SER:HB2	2.00	0.44
1:G:51:MET:HE3	1:G:52:PRO:HD2	2.00	0.44
2:I:594:VAL:HG22	2:I:599:VAL:HA	2.00	0.44
2:I:657:THR:HG23	2:I:658:GLN:HG3	2.00	0.44
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.00	0.44
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.53	0.44
5:L:335:GLU:O	5:L:339:ARG:HG2	2.17	0.44
1:B:79:LEU:HD23	1:B:79:LEU:H	1.84	0.43
2:C:396:ASP:OD1	2:C:418:GLY:HA3	2.18	0.43
2:C:403:MET:HG3	2:C:584:TYR:CZ	2.53	0.43
2:C:594:VAL:HG22	2:C:599:VAL:HA	2.00	0.43
3:D:124:ILE:HG23	3:D:189:LEU:HD11	2.00	0.43
3:D:743:MET:HB2	3:D:759:ILE:O	2.17	0.43
5:F:468:ARG:O	5:F:471:LEU:HB2	2.18	0.43
1:G:11:PRO:HB3	1:G:31:LEU:HD23	2.00	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.00	0.43
2:I:905:ILE:O	5:L:599:ARG:NH1	2.51	0.43
2:I:1142:ARG:HH22	2:I:1165:SER:HA	1.82	0.43
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.16	0.43
3:J:290:ILE:H	3:J:290:ILE:HD12	1.81	0.43
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.89	0.43
3:J:697:MET:SD	3:J:741:ALA:HB3	2.58	0.43
3:J:702:GLN:HG3	3:J:703:THR:N	2.33	0.43
3:J:747:MET:HB2	3:J:774:ILE:HG22	2.00	0.43
3:J:990:ARG:NH1	3:J:992:LYS:HD3	2.33	0.43
3:J:1257:VAL:HA	3:J:1260:MET:HE3	1.99	0.43
5:L:354:THR:O	5:L:358:VAL:HG23	2.18	0.43
2:C:174:ALA:HB2	2:C:432:LEU:HD13	2.01	0.43
3:D:394:ILE:HG21	5:F:536:THR:HA	2.00	0.43
3:D:518:VAL:O	3:D:547:ARG:NH1	2.51	0.43
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	2.00	0.43
3:D:1062:LEU:O	3:D:1067:ARG:NE	2.45	0.43
1:G:16:ILE:HG23	1:G:26:VAL:HG12	2.00	0.43
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.98	0.43
5:L:287:ILE:HG23	5:L:337:VAL:HG13	2.00	0.43
5:L:461:ASN:O	5:L:465:ARG:HG2	2.17	0.43
5:L:468:ARG:O	5:L:471:LEU:HB2	2.18	0.43
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.99	0.43
1:B:81:ILE:O	1:B:85:LEU:HG	2.18	0.43
2:C:905:ILE:O	5:F:599:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:747:MET:HB2	3:D:774:ILE:HG22	2.00	0.43
3:D:1067:ARG:HB2	3:D:1072:LYS:HG3	2.00	0.43
5:F:312:SER:OG	5:F:313:ASP:N	2.51	0.43
2:I:4:SER:HB3	2:I:7:GLU:CD	2.43	0.43
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.43
2:I:703:GLY:H	2:I:705:GLU:CD	2.25	0.43
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.18	0.43
3:J:1067:ARG:HB2	3:J:1072:LYS:HG3	2.01	0.43
2:C:703:GLY:H	2:C:705:GLU:CD	2.25	0.43
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.48	0.43
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.43
5:F:137:TYR:CE1	5:F:139:GLU:HB2	2.53	0.43
5:F:302:PHE:O	5:F:306:PHE:HB2	2.18	0.43
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.43	0.43
3:J:46:TYR:O	5:L:500:ILE:HG21	2.18	0.43
3:J:440:VAL:O	3:J:442:ILE:HG12	2.18	0.43
5:L:253:SER:O	5:L:257:LYS:HG3	2.18	0.43
6:M:29:VAL:HG21	6:M:47:TYR:OH	2.17	0.43
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.18	0.43
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.01	0.43
3:D:958:ILE:HG23	3:D:982:LEU:HD11	2.01	0.43
3:D:1064:SER:O	3:D:1072:LYS:HE2	2.18	0.43
3:D:1177:ILE:H	3:D:1177:ILE:HG13	1.69	0.43
1:G:137:ASN:OD1	1:G:137:ASN:N	2.51	0.43
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.99	0.43
2:I:517:GLN:O	2:I:761:GLN:HB2	2.19	0.43
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.18	0.43
3:J:518:VAL:O	3:J:547:ARG:NH1	2.51	0.43
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.18	0.43
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	2.00	0.43
3:D:712:GLN:H	3:D:712:GLN:CD	2.26	0.43
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.51	0.43
5:F:394:TYR:HB3	5:F:443:ILE:HD11	2.01	0.43
1:G:53:GLY:O	1:G:148:ARG:HG3	2.19	0.43
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	2.00	0.43
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.83	0.43
1:A:77:ASP:O	1:A:81:ILE:HG13	2.19	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.59	0.43
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	2.00	0.43
3:D:26:SER:HB2	3:D:236:TRP:CE2	2.54	0.43
3:D:339:ARG:O	3:D:341:ASN:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:512:TYR:CD2	3:D:635:SER:HB2	2.53	0.43
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.01	0.43
3:D:564:VAL:HG12	3:D:565:ALA:N	2.34	0.43
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.58	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.54	0.43
2:I:1302:THR:HG22	5:L:531:PRO:HB3	2.00	0.43
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.18	0.43
2:I:1332:SER:HA	3:J:102:MET:HE1	2.01	0.43
3:J:527:LEU:HD21	3:J:536:LEU:HG	2.01	0.43
3:J:746:LEU:HD13	3:J:754:ILE:HD11	2.00	0.43
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.00	0.43
3:J:1227:HIS:O	3:J:1230:THR:HG22	2.19	0.43
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.19	0.43
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	0.43
5:L:555:GLU:HA	5:L:558:VAL:HG12	2.01	0.43
2:C:3:TYR:HB3	2:C:4:SER:H	1.64	0.43
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.99	0.43
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	1.99	0.43
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.54	0.43
3:D:1227:HIS:O	3:D:1230:THR:HG22	2.19	0.43
2:I:339:ASN:O	2:I:344:GLY:HA2	2.18	0.43
2:I:697:LYS:HG2	2:I:698:PRO:O	2.19	0.43
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	2.01	0.43
2:I:1286:THR:O	2:I:1290:MET:HB2	2.19	0.43
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.87	0.43
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	2.00	0.43
1:A:53:GLY:O	1:A:148:ARG:HG3	2.19	0.43
2:C:4:SER:HB3	2:C:7:GLU:CD	2.44	0.43
3:D:339:ARG:C	3:D:341:ASN:H	2.27	0.43
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.87	0.43
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.43
3:D:990:ARG:NH1	3:D:992:LYS:HD3	2.34	0.43
2:I:708:VAL:HG11	2:I:794:LEU:HD22	2.01	0.43
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	2.01	0.43
2:I:1339:LEU:HB3	3:J:17:PHE:CD1	2.54	0.43
1:A:90:VAL:HG22	1:A:91:ARG:H	1.84	0.43
2:C:985:GLU:O	2:C:989:LEU:HB2	2.18	0.43
3:D:702:GLN:HG3	3:D:703:THR:N	2.34	0.43
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.84	0.43
2:I:519:ASN:OD1	2:I:521:LEU:N	2.51	0.43
3:J:124:ILE:HG23	3:J:189:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.43
3:J:702:GLN:HG3	3:J:703:THR:H	1.83	0.43
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.00	0.43
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	2.01	0.43
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.51	0.43
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.81	0.43
5:L:266:PHE:HA	5:L:269:LEU:HD12	2.00	0.43
5:L:324:LYS:HB2	5:L:327:SER:HB2	2.01	0.43
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.84	0.42
2:C:1109:ILE:HG12	3:D:644:MET:HE1	2.01	0.42
2:C:1339:LEU:HB3	3:D:17:PHE:CD1	2.54	0.42
5:F:141:ILE:H	5:F:141:ILE:HG12	1.68	0.42
5:F:266:PHE:HA	5:F:269:LEU:HD12	2.00	0.42
5:F:573:LEU:H	5:F:573:LEU:HD23	1.83	0.42
5:F:584:ARG:NH1	5:F:584:ARG:HA	2.34	0.42
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.87	0.42
1:A:117:HIS:NE2	1:A:121:VAL:O	2.53	0.42
2:C:53:PHE:O	2:C:57:PHE:HB2	2.19	0.42
2:C:316:GLU:CD	2:C:316:GLU:H	2.27	0.42
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.92	0.42
2:C:980:VAL:O	2:C:984:VAL:HB	2.19	0.42
3:D:746:LEU:HD13	3:D:754:ILE:HD11	2.00	0.42
2:I:228:VAL:HB	2:I:335:THR:OG1	2.19	0.42
2:I:637:ARG:HA	2:I:642:SER:HA	2.01	0.42
2:I:946:LEU:HD23	2:I:946:LEU:HA	1.85	0.42
3:J:712:GLN:CD	3:J:712:GLN:H	2.26	0.42
5:L:296:LYS:HA	5:L:296:LYS:HD3	1.79	0.42
2:C:637:ARG:HA	2:C:642:SER:HA	2.00	0.42
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.42
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	2.01	0.42
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.18	0.42
3:D:1031:VAL:HG23	3:D:1080:ILE:HG21	2.00	0.42
2:I:316:GLU:H	2:I:316:GLU:CD	2.27	0.42
3:J:94:GLN:O	3:J:97:VAL:HG23	2.19	0.42
3:J:512:TYR:CD2	3:J:635:SER:HB2	2.54	0.42
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.91	0.42
3:J:1155:ILE:HD12	3:J:1210:ILE:HB	2.02	0.42
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.02	0.42
1:A:208:ASN:OD1	1:A:208:ASN:N	2.49	0.42
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.27	0.42
2:C:179:TYR:HE1	2:C:454:ARG:HH21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.88	0.42
2:C:1253:LEU:CD1	3:D:251:PRO:HG2	2.50	0.42
3:D:8:LEU:HD23	3:D:9:LYS:N	2.34	0.42
3:D:264:ASP:OD2	3:D:264:ASP:N	2.52	0.42
3:D:1046:ILE:HD12	3:D:1059:LEU:HD13	2.02	0.42
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.29	0.42
5:F:227:GLN:HA	5:F:230:VAL:HG12	2.01	0.42
5:F:577:GLY:HA3	5:F:583:THR:HG23	2.01	0.42
1:G:90:VAL:HG22	1:G:91:ARG:H	1.84	0.42
2:I:91:THR:HG21	2:I:503:LYS:CE	2.49	0.42
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.49	0.42
3:J:81:ARG:HG3	3:J:82:GLY:H	1.83	0.42
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.94	0.42
2:C:946:LEU:HD23	2:C:946:LEU:HA	1.86	0.42
3:D:203:GLU:O	3:D:207:GLU:HG2	2.19	0.42
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	2.01	0.42
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.84	0.42
2:I:88:ARG:NH1	2:I:88:ARG:HB2	2.34	0.42
2:I:653:MET:HG2	2:I:654:ASP:N	2.35	0.42
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	2.02	0.42
5:L:105:MET:HE3	5:L:384:LEU:HB2	2.01	0.42
1:B:11:PRO:HB3	1:B:30:PRO:O	2.19	0.42
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.51	0.42
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.20	0.42
3:D:424:ASN:ND2	3:D:434:ILE:HG12	2.33	0.42
2:I:1109:ILE:HG12	3:J:644:MET:HE1	2.01	0.42
3:J:480:ALA:O	3:J:485:MET:N	2.52	0.42
5:L:302:PHE:O	5:L:306:PHE:HB2	2.19	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.34	0.42
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.84	0.42
2:C:520:PRO:HG3	2:C:714:VAL:HG11	2.01	0.42
2:C:676:ALA:HB2	3:D:772:TYR:HE1	1.85	0.42
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	2.01	0.42
3:D:1063:ASP:O	3:D:1067:ARG:HG3	2.20	0.42
5:F:505:ILE:HD12	5:F:505:ILE:HA	1.84	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.42
2:I:347:ILE:HD11	2:I:433:ILE:HD11	2.02	0.42
5:L:137:TYR:CE1	5:L:139:GLU:HB2	2.54	0.42
5:L:364:ARG:HA	5:L:367:ILE:HD12	2.02	0.42
5:L:394:TYR:HB3	5:L:443:ILE:HD11	2.00	0.42
1:A:11:PRO:HB3	1:A:31:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:ILE:HG22	2:C:139:ASN:N	2.34	0.42
2:C:452:ARG:HG2	2:C:453:ILE:N	2.35	0.42
2:C:484:LEU:CD1	2:C:485:ASP:H	2.32	0.42
3:D:118:LYS:HD2	3:D:118:LYS:HA	1.81	0.42
3:D:702:GLN:HG3	3:D:703:THR:H	1.83	0.42
5:F:120:ALA:HA	5:F:123:ILE:HD12	2.02	0.42
1:G:125:LYS:HE2	1:G:128:HIS:HB2	2.01	0.42
2:I:672:GLU:H	2:I:672:GLU:HG3	1.57	0.42
3:J:203:GLU:O	3:J:207:GLU:HG2	2.20	0.42
5:L:577:GLY:HA3	5:L:583:THR:HG23	2.01	0.42
3:D:12:THR:HG22	3:D:13:LYS:HG2	2.02	0.42
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.42
3:D:750:PRO:HA	3:D:777:HIS:NE2	2.35	0.42
5:F:291:CYS:O	5:F:296:LYS:N	2.53	0.42
2:I:53:PHE:O	2:I:57:PHE:HB2	2.20	0.42
2:I:676:ALA:HB2	3:J:772:TYR:HE1	1.85	0.42
2:I:975:ILE:O	2:I:979:LEU:HB2	2.19	0.42
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.02	0.42
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.35	0.42
5:L:291:CYS:O	5:L:296:LYS:N	2.53	0.42
5:L:516:ASP:C	5:L:518:HIS:H	2.28	0.42
5:L:584:ARG:HA	5:L:584:ARG:NH1	2.34	0.42
1:A:75:GLN:HA	2:C:729:ALA:H	1.85	0.42
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.35	0.42
2:C:521:LEU:HA	2:C:524:ILE:HG22	2.02	0.42
2:C:848:GLU:HG2	2:C:888:THR:HG22	2.02	0.42
2:C:925:SER:O	2:C:1056:VAL:HG13	2.20	0.42
3:D:70:CYS:SG	3:D:71:LEU:N	2.92	0.42
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.95	0.42
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.35	0.42
5:F:387:VAL:HG22	5:F:435:ILE:HD13	2.02	0.42
2:I:130:MET:HE3	2:I:136:PHE:CE2	2.54	0.42
2:I:898:GLU:HB3	5:L:540:LEU:HD22	2.02	0.42
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.01	0.42
5:L:227:GLN:HA	5:L:230:VAL:HG12	2.01	0.42
5:L:344:LEU:HD12	5:L:344:LEU:HA	1.85	0.42
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.02	0.41
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	2.02	0.41
3:D:9:LYS:HE2	3:D:9:LYS:HB3	1.93	0.41
3:D:44:ILE:HD13	3:D:252:LEU:HD13	2.02	0.41
3:D:418:GLU:O	3:D:420:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:480:ALA:O	3:D:485:MET:N	2.52	0.41
3:D:645:VAL:HB	3:D:701:LEU:HD23	2.02	0.41
3:D:697:MET:SD	3:D:741:ALA:HB3	2.60	0.41
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.34	0.41
5:F:287:ILE:HG23	5:F:337:VAL:HG13	2.01	0.41
5:F:376:LYS:O	5:F:380:VAL:HG23	2.20	0.41
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.27	0.41
2:I:446:ASP:OD1	2:I:446:ASP:N	2.53	0.41
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.88	0.41
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.50	0.41
5:L:584:ARG:O	5:L:587:ILE:HG22	2.20	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.87	0.41
2:C:88:ARG:HB2	2:C:88:ARG:NH1	2.35	0.41
2:C:198:ILE:O	2:C:201:ARG:HB2	2.20	0.41
2:C:1286:THR:O	2:C:1290:MET:HB2	2.20	0.41
3:D:425:ARG:HG2	3:D:426:ALA:N	2.35	0.41
3:D:620:PHE:O	3:D:624:ILE:HG13	2.20	0.41
3:D:644:MET:SD	3:D:740:LEU:HD23	2.60	0.41
5:F:441:ARG:O	5:F:445:ASP:HB2	2.20	0.41
5:F:550:GLY:HA3	5:F:603:ARG:NH1	2.36	0.41
1:G:45:ARG:NH1	1:H:34:GLY:O	2.52	0.41
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.55	0.41
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.20	0.41
2:I:452:ARG:HG2	2:I:453:ILE:N	2.35	0.41
2:I:730:SER:O	2:I:753:LEU:HB2	2.20	0.41
2:I:1028:LYS:HB2	2:I:1028:LYS:HE2	1.71	0.41
3:J:564:VAL:HG12	3:J:565:ALA:N	2.35	0.41
5:L:573:LEU:HD23	5:L:573:LEU:H	1.84	0.41
2:C:130:MET:HE3	2:C:136:PHE:CE2	2.54	0.41
3:D:372:MET:HE2	3:D:372:MET:HB3	1.89	0.41
3:D:528:THR:HG23	3:D:529:GLY:H	1.85	0.41
3:D:712:GLN:HG2	3:D:713:GLU:H	1.85	0.41
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.50	0.41
5:F:225:ARG:O	5:F:229:VAL:HG13	2.20	0.41
1:G:111:THR:HB	1:G:126:PRO:O	2.21	0.41
1:H:11:PRO:HB3	1:H:30:PRO:O	2.20	0.41
3:J:147:ILE:HD11	3:J:179:LYS:HG2	2.03	0.41
3:J:155:GLU:HB2	3:J:158:GLN:HB2	2.02	0.41
3:J:449:LEU:HD22	3:J:466:MET:SD	2.60	0.41
3:J:620:PHE:O	3:J:624:ILE:HG13	2.20	0.41
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:551:LEU:HD21	5:L:598:LEU:HD21	2.01	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.19	0.41
2:C:228:VAL:HB	2:C:335:THR:OG1	2.20	0.41
2:C:1293:VAL:HG11	2:C:1304:MET:HE2	2.02	0.41
2:C:1332:SER:HA	3:D:102:MET:HE1	2.00	0.41
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.88	0.41
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	2.02	0.41
5:F:344:LEU:HD12	5:F:344:LEU:HA	1.86	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
2:I:959:ASP:O	2:I:962:GLU:HB2	2.21	0.41
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.47	0.41
5:L:470:MET:HB3	5:L:474:MET:HG3	2.01	0.41
2:C:246:LEU:H	2:C:246:LEU:HD12	1.85	0.41
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.41
2:C:697:LYS:HG2	2:C:698:PRO:O	2.20	0.41
2:C:1124:ILE:HB	2:C:1180:MET:HB2	2.02	0.41
3:D:418:GLU:H	4:E:45:LYS:HZ2	1.69	0.41
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.35	0.41
3:D:709:ARG:O	3:D:711:GLY:N	2.52	0.41
3:D:1024:THR:HG22	3:D:1026:PRO:HD3	2.02	0.41
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	2.02	0.41
5:F:470:MET:HB3	5:F:474:MET:HG3	2.01	0.41
1:G:28:LEU:HD23	1:H:231:PHE:CZ	2.56	0.41
1:G:208:ASN:OD1	1:G:208:ASN:N	2.50	0.41
3:J:407:VAL:O	3:J:411:ILE:HG12	2.20	0.41
3:J:528:THR:HG23	3:J:529:GLY:H	1.85	0.41
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.89	0.41
5:L:120:ALA:HA	5:L:123:ILE:HD12	2.02	0.41
5:L:388:ILE:HG22	5:L:392:LYS:HE3	2.02	0.41
1:A:137:ASN:OD1	1:A:137:ASN:N	2.51	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.51	0.41
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.88	0.41
3:D:155:GLU:HB2	3:D:158:GLN:HB2	2.02	0.41
3:D:449:LEU:HD22	3:D:466:MET:SD	2.61	0.41
5:F:105:MET:HE3	5:F:384:LEU:HB2	2.01	0.41
5:F:561:MET:HE3	5:F:561:MET:HB2	1.88	0.41
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.55	0.41
2:I:169:LYS:O	2:I:170:VAL:HG22	2.18	0.41
2:I:484:LEU:CD1	2:I:485:ASP:H	2.34	0.41
2:I:573:ASN:OD1	2:I:573:ASN:N	2.54	0.41
2:I:848:GLU:HG2	2:I:888:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:264:ASP:OD2	3:J:264:ASP:N	2.53	0.41
3:J:490:ILE:HA	3:J:500:ILE:HG12	2.03	0.41
3:J:644:MET:SD	3:J:740:LEU:HD23	2.60	0.41
3:J:660:GLU:O	3:J:664:ILE:HG12	2.20	0.41
1:A:45:ARG:HG2	1:B:38:THR:CB	2.50	0.41
1:A:111:THR:HB	1:A:126:PRO:O	2.21	0.41
2:C:728:ASP:OD1	2:C:729:ALA:N	2.53	0.41
3:D:1036:ARG:HE	3:D:1081:VAL:HG11	1.86	0.41
1:G:117:HIS:NE2	1:G:121:VAL:O	2.53	0.41
3:J:18:ASP:OD1	3:J:18:ASP:N	2.54	0.41
3:J:1034:PHE:HB2	3:J:1081:VAL:HG23	2.03	0.41
3:J:1036:ARG:HE	3:J:1081:VAL:HG11	1.86	0.41
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.21	0.41
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.34	0.41
5:L:554:ARG:HB2	5:L:580:PHE:CE2	2.55	0.41
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.02	0.41
3:D:1183:SER:OG	3:D:1184:ASP:N	2.51	0.41
4:E:53:GLU:HB3	4:E:59:ILE:HG13	2.03	0.41
5:F:554:ARG:HB2	5:F:580:PHE:CE2	2.55	0.41
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.82	0.41
1:G:115:ILE:H	1:G:115:ILE:HG13	1.70	0.41
1:H:63:GLY:HA3	1:H:71:LYS:HD3	2.03	0.41
2:I:985:GLU:HB3	2:I:988:LYS:HB2	2.03	0.41
2:I:1124:ILE:HB	2:I:1180:MET:HB2	2.02	0.41
2:I:1340:GLU:OE2	3:J:21:LYS:HE3	2.20	0.41
3:J:844:THR:HG21	3:J:858:VAL:HG21	2.02	0.41
5:L:466:ILE:HD11	5:L:487:MET:HE3	2.03	0.41
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.41
2:C:403:MET:HE2	2:C:584:TYR:CD1	2.56	0.41
2:C:462:ASN:O	2:C:465:ARG:HB3	2.21	0.41
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.03	0.41
2:C:624:ASP:OD1	2:C:625:GLU:HG3	2.21	0.41
2:C:1340:GLU:OE2	3:D:21:LYS:HE3	2.21	0.41
3:D:94:GLN:O	3:D:97:VAL:HG23	2.20	0.41
3:D:860:ARG:HD2	3:D:860:ARG:HA	1.89	0.41
4:E:31:GLN:HB2	4:E:46:THR:HG21	2.03	0.41
5:F:466:ILE:H	5:F:466:ILE:HG13	1.41	0.41
1:G:221:ALA:HB1	1:H:228:LEU:HD22	2.02	0.41
1:H:108:GLY:HA2	1:H:109:PRO:HD3	1.92	0.41
2:I:496:LYS:HA	2:I:499:SER:HB3	2.03	0.41
2:I:980:VAL:HG13	2:I:984:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	2.02	0.41
2:I:1293:VAL:HG21	2:I:1315:MET:HE3	2.03	0.41
3:J:646:ILE:HG22	3:J:647:PRO:HD2	2.03	0.41
5:L:224:LEU:HB2	5:L:259:PHE:CZ	2.56	0.41
2:C:91:THR:HG21	2:C:503:LYS:CE	2.50	0.41
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.21	0.41
2:C:730:SER:O	2:C:753:LEU:HB2	2.20	0.41
3:D:646:ILE:HG22	3:D:647:PRO:HD2	2.02	0.41
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.03	0.41
1:H:59:VAL:O	1:H:171:LEU:HA	2.21	0.41
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.51	0.41
2:I:786:GLY:N	2:I:789:THR:OG1	2.42	0.41
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.20	0.41
3:J:70:CYS:SG	3:J:71:LEU:N	2.94	0.41
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.56	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.87	0.41
3:J:262:THR:HG1	3:J:266:ASN:ND2	2.19	0.41
3:J:645:VAL:HB	3:J:701:LEU:HD23	2.02	0.41
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.03	0.41
5:L:269:LEU:O	5:L:273:MET:HG3	2.20	0.41
5:L:600:HIS:O	5:L:602:SER:N	2.47	0.41
1:A:39:LEU:O	1:A:43:LEU:HG	2.22	0.40
3:D:849:LEU:HD22	3:D:849:LEU:H	1.86	0.40
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.78	0.40
2:I:246:LEU:HD12	2:I:246:LEU:H	1.85	0.40
2:I:724:VAL:HG23	2:I:775:GLU:O	2.21	0.40
3:J:123:ARG:HA	3:J:123:ARG:HD3	1.87	0.40
3:J:418:GLU:O	3:J:420:PRO:HD3	2.21	0.40
3:J:425:ARG:HG2	3:J:426:ALA:N	2.35	0.40
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.87	0.40
3:J:488:ASN:HD22	3:J:488:ASN:HA	1.68	0.40
3:J:810:THR:HG23	3:J:811:GLU:H	1.87	0.40
3:J:1177:ILE:H	3:J:1177:ILE:HG13	1.69	0.40
3:J:1332:LEU:HD13	3:J:1332:LEU:HA	1.93	0.40
5:L:376:LYS:O	5:L:380:VAL:HG23	2.22	0.40
1:A:125:LYS:HE2	1:A:128:HIS:HB2	2.02	0.40
2:C:519:ASN:HA	2:C:520:PRO:HD3	1.95	0.40
2:C:758:ARG:HD2	2:C:835:GLU:HB2	2.04	0.40
2:C:992:LEU:HB2	2:C:993:PRO:HD2	2.03	0.40
3:D:16:GLU:OE2	3:D:1355:ARG:NH2	2.53	0.40
3:D:267:ASP:OD1	3:D:271:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:793:SER:O	3:D:797:THR:HG23	2.21	0.40
5:F:127:ILE:O	5:F:128:ASN:C	2.63	0.40
5:F:364:ARG:HA	5:F:367:ILE:HD12	2.02	0.40
5:F:584:ARG:O	5:F:587:ILE:HG22	2.21	0.40
1:G:38:THR:OG1	1:H:45:ARG:HD3	2.21	0.40
1:H:182:ARG:NH1	3:J:581:MET:SD	2.94	0.40
2:I:521:LEU:HA	2:I:524:ILE:HG22	2.02	0.40
3:J:262:THR:C	5:L:507:MET:HB2	2.46	0.40
3:J:709:ARG:O	3:J:711:GLY:N	2.53	0.40
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.21	0.40
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.21	0.40
5:L:225:ARG:O	5:L:229:VAL:HG13	2.21	0.40
5:L:561:MET:HE3	5:L:561:MET:HB2	1.87	0.40
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.57	0.40
3:D:140:TYR:HB3	5:F:100:MET:SD	2.61	0.40
3:D:141:PHE:HA	3:D:180:MET:HE2	2.04	0.40
5:F:339:ARG:HA	5:F:339:ARG:HD2	1.97	0.40
5:F:551:LEU:HD21	5:F:598:LEU:HD21	2.03	0.40
1:G:152:TYR:CZ	2:I:824:GLN:HA	2.57	0.40
1:G:176:CYS:O	1:G:177:TYR:C	2.65	0.40
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.56	0.40
3:J:44:ILE:HD13	3:J:252:LEU:HD13	2.03	0.40
3:J:103:GLY:C	3:J:244:VAL:HG22	2.46	0.40
3:J:140:TYR:HB3	5:L:100:MET:SD	2.61	0.40
6:N:13:ASN:N	6:N:34:GLU:HG2	2.36	0.40
1:A:60:GLU:HB2	1:A:170:ARG:HG2	2.03	0.40
2:C:232:ILE:HD12	2:C:330:HIS:O	2.21	0.40
2:C:496:LYS:HA	2:C:499:SER:HB3	2.03	0.40
2:C:1289:GLU:HB3	2:C:1315:MET:SD	2.61	0.40
5:F:388:ILE:HG22	5:F:392:LYS:HE3	2.02	0.40
5:F:466:ILE:HD11	5:F:487:MET:HE3	2.02	0.40
1:G:11:PRO:HD2	1:H:227:GLN:HA	2.02	0.40
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.86	0.40
2:I:462:ASN:O	2:I:465:ARG:HB3	2.21	0.40
3:J:124:ILE:O	3:J:128:LEU:HG	2.22	0.40
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.21	0.40
5:L:139:GLU:HG3	5:L:351:THR:HA	2.03	0.40
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.94	0.40
1:B:41:ASN:CG	2:C:1217:THR:HA	2.47	0.40
1:B:212:ASP:OD1	1:B:214:GLU:HB3	2.22	0.40
2:C:32:LEU:HA	2:C:130:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:363:LEU:HB3	2:C:381:ALA:HB1	2.04	0.40
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.47	0.40
2:C:1148:ALA:HB1	2:C:1180:MET:HE2	2.03	0.40
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.22	0.40
3:D:103:GLY:C	3:D:244:VAL:HG22	2.47	0.40
3:D:124:ILE:O	3:D:128:LEU:HG	2.21	0.40
3:D:407:VAL:O	3:D:411:ILE:HG12	2.21	0.40
3:D:488:ASN:HD22	3:D:488:ASN:HA	1.67	0.40
3:D:746:LEU:HB2	3:D:754:ILE:HD11	2.04	0.40
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.21	0.40
5:F:555:GLU:HA	5:F:558:VAL:HG12	2.02	0.40
1:G:60:GLU:HB2	1:G:170:ARG:HG2	2.03	0.40
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	2.02	0.40
3:J:1075:ARG:HH21	3:J:1166:GLY:HA2	1.87	0.40
5:L:394:TYR:OH	5:L:436:ARG:HG2	2.21	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	222/239 (93%)	197 (89%)	21 (10%)	4 (2%)	6	34
1	B	216/239 (90%)	189 (88%)	27 (12%)	0	100	100
1	G	226/239 (95%)	202 (89%)	20 (9%)	4 (2%)	6	34
1	H	213/239 (89%)	187 (88%)	26 (12%)	0	100	100
2	C	1338/1342 (100%)	1213 (91%)	121 (9%)	4 (0%)	36	70
2	I	1338/1342 (100%)	1216 (91%)	117 (9%)	5 (0%)	30	65
3	D	1339/1407 (95%)	1217 (91%)	120 (9%)	2 (0%)	48	81
3	J	1317/1407 (94%)	1201 (91%)	115 (9%)	1 (0%)	48	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	70 (91%)	7 (9%)	0	100	100
5	F	464/522 (89%)	415 (89%)	48 (10%)	1 (0%)	43	75
5	L	463/522 (89%)	415 (90%)	47 (10%)	1 (0%)	43	75
6	M	49/64 (77%)	42 (86%)	7 (14%)	0	100	100
6	N	49/64 (77%)	42 (86%)	7 (14%)	0	100	100
All	All	7398/7808 (95%)	6685 (90%)	691 (9%)	22 (0%)	36	70

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	170	VAL
2	I	170	VAL
3	D	340	GLN
1	G	167	PRO
2	I	484	LEU
1	A	14	VAL
1	A	167	PRO
1	A	196	THR
2	C	63	SER
2	C	697	LYS
1	G	14	VAL
1	G	196	THR
2	I	63	SER
2	I	697	LYS
5	F	447	ALA
5	L	447	ALA
2	C	1186	VAL
2	I	1186	VAL
1	A	178	SER
3	D	826	ILE
1	G	178	SER
3	J	826	ILE

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	191/206 (93%)	180 (94%)	11 (6%)	18	43
1	B	184/206 (89%)	164 (89%)	20 (11%)	6	23
1	G	191/206 (93%)	180 (94%)	11 (6%)	18	43
1	H	183/206 (89%)	164 (90%)	19 (10%)	7	25
2	C	1155/1157 (100%)	1045 (90%)	110 (10%)	8	28
2	I	1154/1157 (100%)	1046 (91%)	108 (9%)	8	29
3	D	1125/1168 (96%)	1032 (92%)	93 (8%)	10	34
3	J	1110/1168 (95%)	1016 (92%)	94 (8%)	10	33
4	E	72/75 (96%)	70 (97%)	2 (3%)	38	59
4	K	67/75 (89%)	65 (97%)	2 (3%)	36	57
5	F	417/462 (90%)	383 (92%)	34 (8%)	10	34
5	L	418/462 (90%)	383 (92%)	35 (8%)	10	33
6	M	44/56 (79%)	36 (82%)	8 (18%)	2	11
6	N	44/56 (79%)	36 (82%)	8 (18%)	2	11
All	All	6355/6660 (95%)	5800 (91%)	555 (9%)	9	33

All (555) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	22	THR
1	A	54	CYS
1	A	62	ASP
1	A	71	LYS
1	A	120	ASP
1	A	127	GLN
1	A	141	SER
1	A	215	GLU
1	A	228	LEU
1	B	8	PHE
1	B	13	LEU
1	B	45	ARG
1	B	50	SER
1	B	58	GLU

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Mol	Chain	Res	Type
1	B	60	GLU
1	B	64	VAL
1	B	65	LEU
1	B	75	GLN
1	B	76	GLU
1	B	77	ASP
1	B	120	ASP
1	B	133	LEU
1	B	134	THR
1	B	142	MET
1	B	158	ARG
1	B	160	HIS
1	B	176	CYS
1	B	183	ILE
1	B	203	ILE
2	C	10	ARG
2	C	22	LEU
2	C	29	SER
2	C	32	LEU
2	C	39	ILE
2	C	44	GLU
2	C	49	LEU
2	C	90	VAL
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	119	GLU
2	C	124	MET
2	C	149	LEU
2	C	164	THR
2	C	165	HIS
2	C	170	VAL
2	C	237	LEU
2	C	244	GLU
2	C	268	ARG
2	C	278	GLU
2	C	285	ILE
2	C	292	ILE
2	C	302	ILE
2	C	316	GLU
2	C	322	LEU
2	C	327	GLN

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Mol	Chain	Res	Type
2	C	331	LYS
2	C	377	THR
2	C	410	LEU
2	C	413	GLU
2	C	443	ASP
2	C	483	ASP
2	C	484	LEU
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	518	ASN
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
2	C	550	VAL
2	C	561	ILE
2	C	568	ASN
2	C	589	THR
2	C	600	THR
2	C	604	HIS
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	635	THR
2	C	650	VAL
2	C	655	VAL
2	C	657	THR
2	C	672	GLU
2	C	692	THR
2	C	699	LEU
2	C	705	GLU
2	C	724	VAL
2	C	737	ASN
2	C	739	ASP
2	C	748	ILE
2	C	750	ILE
2	C	761	GLN
2	C	782	VAL
2	C	788	SER
2	C	799	ASN

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Mol	Chain	Res	Type
2	C	800	MET
2	C	828	PHE
2	C	831	ILE
2	C	839	VAL
2	C	878	THR
2	C	890	LYS
2	C	895	LEU
2	C	898	GLU
2	C	919	ARG
2	C	929	ILE
2	C	966	ILE
2	C	974	ARG
2	C	976	ARG
2	C	979	LEU
2	C	984	VAL
2	C	995	ASP
2	C	998	LEU
2	C	1004	ASP
2	C	1006	GLU
2	C	1019	ASP
2	C	1079	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1090	ASN
2	C	1103	VAL
2	C	1108	ASN
2	C	1119	MET
2	C	1155	VAL
2	C	1171	ARG
2	C	1172	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1222	GLU
2	C	1233	LEU
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1279	GLU
2	C	1291	LEU
2	C	1339	LEU
2	C	1341	ASP
3	D	8	LEU

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Mol	Chain	Res	Type
3	D	33	TRP
3	D	42	GLU
3	D	46	TYR
3	D	70	CYS
3	D	71	LEU
3	D	79	LYS
3	D	92	VAL
3	D	97	VAL
3	D	128	LEU
3	D	134	ASP
3	D	147	ILE
3	D	175	GLU
3	D	176	PHE
3	D	209	ASN
3	D	217	LEU
3	D	237	MET
3	D	241	VAL
3	D	252	LEU
3	D	255	LEU
3	D	299	LEU
3	D	324	LEU
3	D	363	LEU
3	D	374	LEU
3	D	429	LEU
3	D	454	CYS
3	D	472	LEU
3	D	487	THR
3	D	506	VAL
3	D	507	VAL
3	D	514	THR
3	D	528	THR
3	D	545	HIS
3	D	547	ARG
3	D	552	ILE
3	D	594	GLN
3	D	596	LEU
3	D	615	LYS
3	D	635	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	686	TRP

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Mol	Chain	Res	Type
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	746	LEU
3	D	769	VAL
3	D	810	THR
3	D	823	THR
3	D	831	VAL
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	908	ILE
3	D	929	GLN
3	D	951	GLN
3	D	962	ASN
3	D	972	LYS
3	D	987	GLU
3	D	997	VAL
3	D	1017	VAL
3	D	1025	MET
3	D	1047	THR
3	D	1073	ASP
3	D	1109	LEU
3	D	1115	ILE
3	D	1155	ILE
3	D	1162	ILE
3	D	1173	ARG
3	D	1177	ILE
3	D	1192	LYS
3	D	1199	PHE
3	D	1204	VAL
3	D	1208	ASP
3	D	1220	ILE
3	D	1230	THR
3	D	1251	LYS
3	D	1255	VAL

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Mol	Chain	Res	Type
3	D	1275	LEU
3	D	1285	VAL
3	D	1293	GLU
3	D	1306	LEU
3	D	1324	SER
3	D	1332	LEU
3	D	1333	THR
3	D	1366	HIS
4	E	39	VAL
4	E	58	LEU
5	F	94	THR
5	F	98	VAL
5	F	100	MET
5	F	105	MET
5	F	127	ILE
5	F	130	VAL
5	F	141	ILE
5	F	154	GLU
5	F	162	ILE
5	F	244	THR
5	F	246	GLN
5	F	253	SER
5	F	335	GLU
5	F	395	THR
5	F	399	LEU
5	F	428	SER
5	F	456	MET
5	F	459	THR
5	F	466	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	483	LEU
5	F	487	MET
5	F	488	LEU
5	F	505	ILE
5	F	508	GLU
5	F	530	LEU
5	F	540	LEU
5	F	574	GLU
5	F	578	LYS
5	F	583	THR

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Mol	Chain	Res	Type
5	F	586	ARG
5	F	611	LEU
1	G	9	LEU
1	G	13	LEU
1	G	22	THR
1	G	54	CYS
1	G	62	ASP
1	G	71	LYS
1	G	120	ASP
1	G	127	GLN
1	G	141	SER
1	G	215	GLU
1	G	228	LEU
1	H	7	GLU
1	H	13	LEU
1	H	45	ARG
1	H	50	SER
1	H	58	GLU
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	76	GLU
1	H	77	ASP
1	H	120	ASP
1	H	133	LEU
1	H	134	THR
1	H	142	MET
1	H	158	ARG
1	H	176	CYS
1	H	183	ILE
1	H	203	ILE
2	I	10	ARG
2	I	22	LEU
2	I	29	SER
2	I	32	LEU
2	I	39	ILE
2	I	44	GLU
2	I	49	LEU
2	I	90	VAL
2	I	115	LYS
2	I	116	ASP

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Mol	Chain	Res	Type
2	I	117	ILE
2	I	119	GLU
2	I	124	MET
2	I	149	LEU
2	I	164	THR
2	I	165	HIS
2	I	170	VAL
2	I	200	ARG
2	I	237	LEU
2	I	244	GLU
2	I	268	ARG
2	I	278	GLU
2	I	285	ILE
2	I	292	ILE
2	I	302	ILE
2	I	316	GLU
2	I	322	LEU
2	I	327	GLN
2	I	331	LYS
2	I	377	THR
2	I	400	VAL
2	I	410	LEU
2	I	413	GLU
2	I	443	ASP
2	I	483	ASP
2	I	484	LEU
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
2	I	550	VAL
2	I	561	ILE
2	I	568	ASN
2	I	589	THR
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL

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Mol	Chain	Res	Type
2	I	623	LEU
2	I	633	LEU
2	I	635	THR
2	I	650	VAL
2	I	655	VAL
2	I	657	THR
2	I	672	GLU
2	I	684	ASN
2	I	692	THR
2	I	699	LEU
2	I	705	GLU
2	I	724	VAL
2	I	737	ASN
2	I	739	ASP
2	I	748	ILE
2	I	750	ILE
2	I	761	GLN
2	I	782	VAL
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	828	PHE
2	I	831	ILE
2	I	839	VAL
2	I	878	THR
2	I	890	LYS
2	I	895	LEU
2	I	898	GLU
2	I	919	ARG
2	I	929	ILE
2	I	971	LEU
2	I	972	PHE
2	I	984	VAL
2	I	1027	LYS
2	I	1029	LEU
2	I	1079	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1090	ASN
2	I	1103	VAL
2	I	1108	ASN
2	I	1119	MET

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Mol	Chain	Res	Type
2	I	1155	VAL
2	I	1171	ARG
2	I	1172	LEU
2	I	1180	MET
2	I	1198	LEU
2	I	1222	GLU
2	I	1233	LEU
2	I	1248	THR
2	I	1253	LEU
2	I	1254	VAL
2	I	1279	GLU
2	I	1291	LEU
2	I	1339	LEU
2	I	1341	ASP
3	J	33	TRP
3	J	42	GLU
3	J	46	TYR
3	J	70	CYS
3	J	71	LEU
3	J	79	LYS
3	J	92	VAL
3	J	97	VAL
3	J	128	LEU
3	J	134	ASP
3	J	147	ILE
3	J	175	GLU
3	J	176	PHE
3	J	209	ASN
3	J	217	LEU
3	J	237	MET
3	J	241	VAL
3	J	252	LEU
3	J	255	LEU
3	J	299	LEU
3	J	324	LEU
3	J	363	LEU
3	J	374	LEU
3	J	429	LEU
3	J	454	CYS
3	J	472	LEU
3	J	487	THR
3	J	506	VAL

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Mol	Chain	Res	Type
3	J	507	VAL
3	J	514	THR
3	J	528	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	552	ILE
3	J	594	GLN
3	J	596	LEU
3	J	615	LYS
3	J	635	SER
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	686	TRP
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	746	LEU
3	J	769	VAL
3	J	785	ASP
3	J	810	THR
3	J	823	THR
3	J	831	VAL
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	908	ILE
3	J	929	GLN
3	J	951	GLN
3	J	962	ASN
3	J	972	LYS
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1025	MET

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Mol	Chain	Res	Type
3	J	1047	THR
3	J	1073	ASP
3	J	1109	LEU
3	J	1115	ILE
3	J	1155	ILE
3	J	1162	ILE
3	J	1173	ARG
3	J	1177	ILE
3	J	1192	LYS
3	J	1199	PHE
3	J	1204	VAL
3	J	1208	ASP
3	J	1220	ILE
3	J	1230	THR
3	J	1251	LYS
3	J	1255	VAL
3	J	1275	LEU
3	J	1285	VAL
3	J	1293	GLU
3	J	1306	LEU
3	J	1324	SER
3	J	1332	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	39	VAL
4	K	58	LEU
5	L	94	THR
5	L	98	VAL
5	L	100	MET
5	L	105	MET
5	L	127	ILE
5	L	130	VAL
5	L	141	ILE
5	L	154	GLU
5	L	162	ILE
5	L	244	THR
5	L	246	GLN
5	L	253	SER
5	L	335	GLU
5	L	395	THR
5	L	399	LEU
5	L	428	SER

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Mol	Chain	Res	Type
5	L	450	ILE
5	L	456	MET
5	L	459	THR
5	L	466	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	483	LEU
5	L	487	MET
5	L	488	LEU
5	L	505	ILE
5	L	508	GLU
5	L	530	LEU
5	L	540	LEU
5	L	574	GLU
5	L	578	LYS
5	L	583	THR
5	L	586	ARG
5	L	611	LEU
6	M	14	LYS
6	M	24	GLU
6	M	25	HIS
6	M	27	PHE
6	M	29	VAL
6	M	36	LEU
6	M	37	ASP
6	M	61	VAL
6	N	14	LYS
6	N	24	GLU
6	N	25	HIS
6	N	27	PHE
6	N	29	VAL
6	N	36	LEU
6	N	37	ASP
6	N	61	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	B	66	HIS
1	B	137	ASN

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Mol	Chain	Res	Type
2	C	580	GLN
2	C	659	GLN
2	C	686	GLN
2	C	725	GLN
2	C	761	GLN
2	C	955	GLN
2	C	1008	GLN
2	C	1009	ASN
2	C	1017	GLN
2	C	1090	ASN
2	C	1136	GLN
2	C	1236	ASN
2	C	1264	GLN
3	D	186	GLN
3	D	196	GLN
3	D	206	ASN
3	D	519	ASN
3	D	594	GLN
3	D	665	GLN
3	D	667	GLN
3	D	708	ASN
3	D	739	GLN
3	D	875	ASN
3	D	1010	GLN
3	D	1044	GLN
3	D	1098	GLN
3	D	1268	ASN
3	D	1367	GLN
4	E	7	GLN
5	F	131	GLN
5	F	294	GLN
5	F	301	ASN
5	F	317	ASN
5	F	338	HIS
5	F	362	ASN
5	F	461	ASN
5	F	545	HIS
1	H	66	HIS
1	H	137	ASN
1	H	208	ASN
2	I	20	GLN
2	I	31	GLN

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Mol	Chain	Res	Type
2	I	686	GLN
2	I	725	GLN
2	I	752	ASN
2	I	761	GLN
2	I	1136	GLN
2	I	1236	ASN
2	I	1264	GLN
2	I	1299	ASN
3	J	186	GLN
3	J	196	GLN
3	J	206	ASN
3	J	266	ASN
3	J	519	ASN
3	J	594	GLN
3	J	665	GLN
3	J	667	GLN
3	J	708	ASN
3	J	716	GLN
3	J	739	GLN
3	J	792	ASN
3	J	875	ASN
3	J	1010	GLN
3	J	1044	GLN
3	J	1098	GLN
3	J	1367	GLN
4	K	43	ASN
5	L	131	GLN
5	L	294	GLN
5	L	301	ASN
5	L	317	ASN
5	L	338	HIS
5	L	362	ASN
5	L	446	GLN
5	L	461	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	224/239 (93%)	-0.25	5 (2%) 62 44	48, 85, 138, 169	0
1	B	220/239 (92%)	-0.29	3 (1%) 73 53	46, 110, 148, 166	0
1	G	228/239 (95%)	-0.28	3 (1%) 75 55	48, 94, 141, 167	0
1	H	217/239 (90%)	-0.19	1 (0%) 87 72	48, 111, 150, 167	0
2	C	1340/1342 (99%)	-0.32	8 (0%) 85 70	12, 74, 129, 163	0
2	I	1340/1342 (99%)	-0.36	7 (0%) 87 72	12, 78, 143, 189	0
3	D	1345/1407 (95%)	-0.38	2 (0%) 92 87	13, 61, 142, 194	0
3	J	1325/1407 (94%)	-0.45	2 (0%) 91 81	10, 63, 139, 195	0
4	E	89/91 (97%)	-0.44	0 100 100	30, 77, 122, 138	0
4	K	79/91 (86%)	-0.50	0 100 100	32, 76, 121, 164	0
5	F	470/522 (90%)	-0.43	4 (0%) 81 62	25, 98, 147, 179	0
5	L	469/522 (89%)	-0.40	1 (0%) 91 81	28, 96, 150, 181	0
6	M	51/64 (79%)	-0.45	1 (1%) 65 45	66, 115, 146, 158	0
6	N	51/64 (79%)	-0.50	0 100 100	64, 112, 143, 149	0
All	All	7448/7808 (95%)	-0.37	37 (0%) 87 72	10, 79, 142, 195	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	4.0
2	I	450	ASN	3.5
2	C	184	LEU	3.0
2	C	317	LEU	3.0
5	L	290	LEU	3.0
5	F	259	PHE	3.0
5	F	255	VAL	2.9
2	C	929	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	221	ALA	2.9
2	I	484	LEU	2.9
1	A	217	ILE	2.8
1	H	228	LEU	2.8
2	C	1321	GLU	2.8
2	I	704	MET	2.8
1	G	224	LEU	2.7
1	B	228	LEU	2.6
1	B	61	ILE	2.6
2	C	1173	ALA	2.5
2	I	333	ILE	2.5
3	D	1135	THR	2.4
2	I	1334	GLY	2.4
6	M	63	PRO	2.4
1	G	43	LEU	2.4
1	G	221	ALA	2.3
1	A	224	LEU	2.3
3	J	1270	GLY	2.3
3	J	1080	ILE	2.3
2	C	405	PHE	2.3
2	I	971	LEU	2.2
2	I	708	VAL	2.2
5	F	446	GLN	2.1
2	C	176	ILE	2.1
1	B	183	ILE	2.1
2	C	883	LEU	2.1
3	D	743	MET	2.1
1	A	225	ALA	2.0
5	F	243	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	J	1501	1/1	0.61	0.14	40,40,40,40	0
7	MG	D	1501	1/1	0.70	0.12	41,41,41,41	0
8	ZN	D	1502	1/1	0.99	0.14	193,193,193,193	0
8	ZN	J	1502	1/1	0.99	0.02	71,71,71,71	0
8	ZN	D	1503	1/1	1.00	0.07	36,36,36,36	0
8	ZN	J	1503	1/1	1.00	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.