



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:32 PM UTC

PDB ID : 4TMA / pdb_00004tma
Title : Crystal structure of gyrase bound to its inhibitor YacG
Authors : Vos, S.M.; Lyubimov, A.Y.; Hershey, D.M.; Schoeffler, A.J.; Berger, J.M.
Deposited on : 2014-05-31
Resolution : 3.30 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

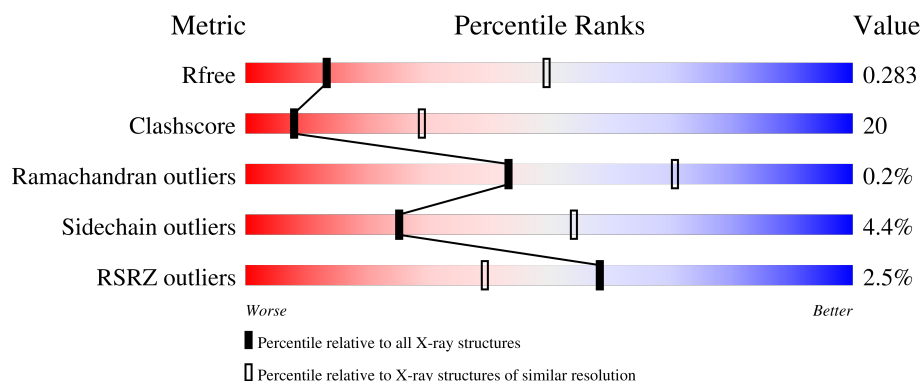
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	525	2% 54% 37% 5%
1	C	525	3% 55% 30% 10%
1	E	525	2% 64% 26% 7%
1	G	525	3% 63% 26% 8%
2	B	417	2% 49% 32% 7% 10%

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Mol	Chain	Length	Quality of chain
2	D	417	% 41% 16% • 40%
2	F	417	% 53% 31% 5% 11%
2	H	417	2% 35% 18% • 44%
3	I	65	2% 48% 22% • 28%
3	J	65	3% 66% 17% 5% 12%
3	K	65	2% 40% 40% 5% 15%
3	L	65	2% 42% 25% 8% 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26792 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 gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3983	2510	711	747	15			
1	C	475	Total	C	N	O	S	0	0	0
			3733	2345	672	701	15			
1	E	486	Total	C	N	O	S	0	1	0
			3841	2413	698	715	15			
1	G	483	Total	C	N	O	S	0	0	0
			3800	2391	682	713	14			

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	374	Total	C	N	O	S	0	0	0
			2995	1875	527	579	14			
2	D	251	Total	C	N	O	S	0	0	0
			1990	1252	347	379	12			
2	F	371	Total	C	N	O	S	0	0	0
			2971	1863	523	571	14			
2	H	233	Total	C	N	O	S	0	1	0
			1863	1170	326	356	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	385	SER	-	expression tag	UNP U6NGU8
B	386	ASN	-	expression tag	UNP U6NGU8
B	387	ALA	-	expression tag	UNP U6NGU8
B	458	TYR	PHE	engineered mutation	UNP U6NGU8
D	385	SER	-	expression tag	UNP U6NGU8
D	386	ASN	-	expression tag	UNP U6NGU8
D	387	ALA	-	expression tag	UNP U6NGU8
D	458	TYR	PHE	engineered mutation	UNP U6NGU8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	385	SER	-	expression tag	UNP U6NGU8
F	386	ASN	-	expression tag	UNP U6NGU8
F	387	ALA	-	expression tag	UNP U6NGU8
F	458	TYR	PHE	engineered mutation	UNP U6NGU8
H	385	SER	-	expression tag	UNP U6NGU8
H	386	ASN	-	expression tag	UNP U6NGU8
H	387	ALA	-	expression tag	UNP U6NGU8
H	458	TYR	PHE	engineered mutation	UNP U6NGU8

- Molecule 3 is a protein called DNA gyrase inhibitor YacG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	47	Total	C	N	O	S	0	0	0
			363	230	63	66	4			
3	J	57	Total	C	N	O	S	0	0	0
			446	279	74	89	4			
3	K	55	Total	C	N	O	S	0	0	0
			430	270	72	84	4			
3	L	48	Total	C	N	O	S	0	0	0
			371	234	64	69	4			

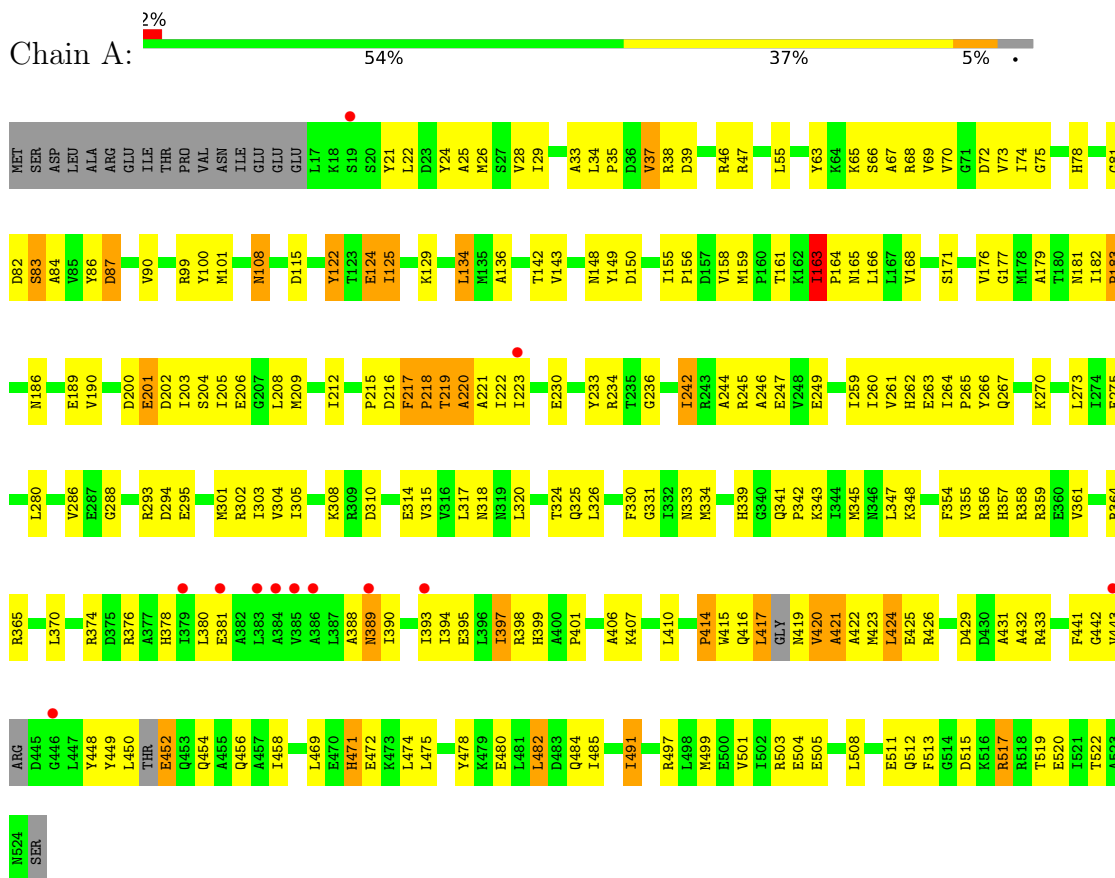
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

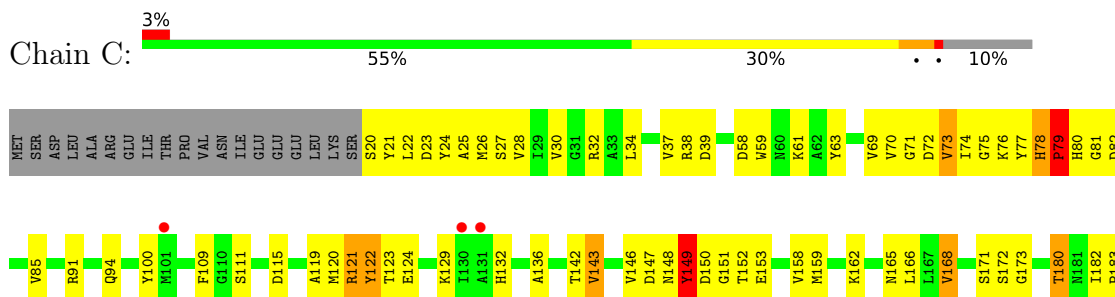
3 Residue-property plots

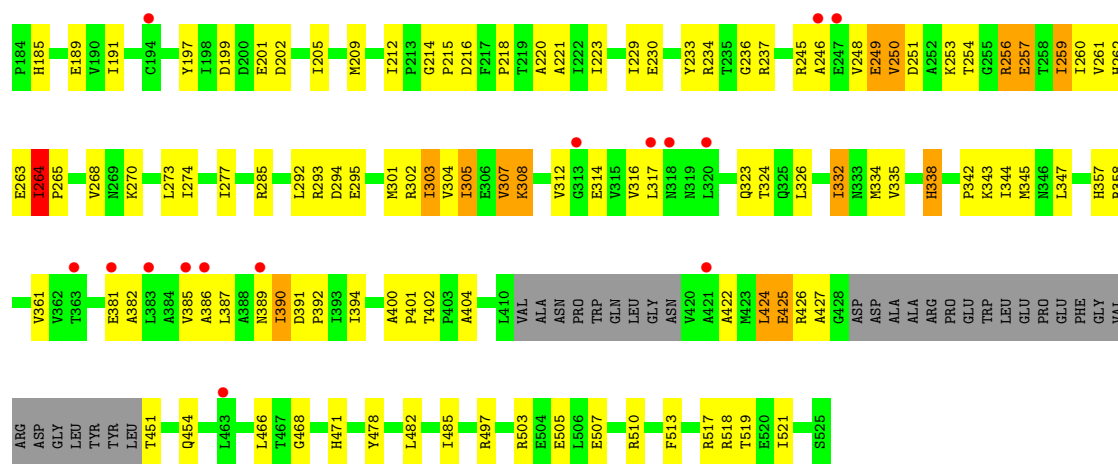
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 gyrase subunit A

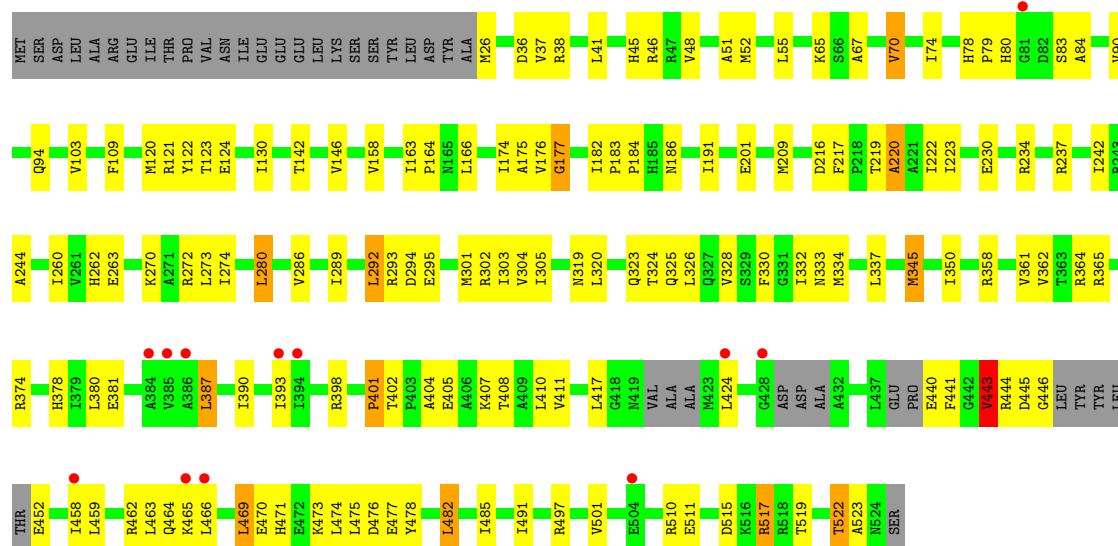


• Molecule 1: DNA gyrase subunit A

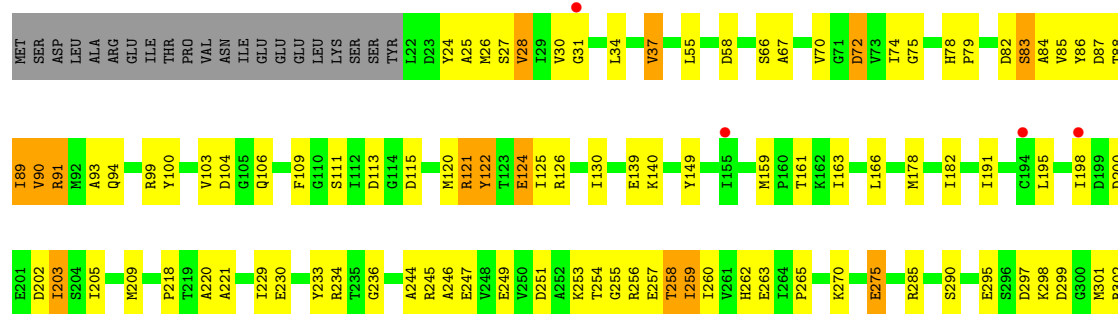


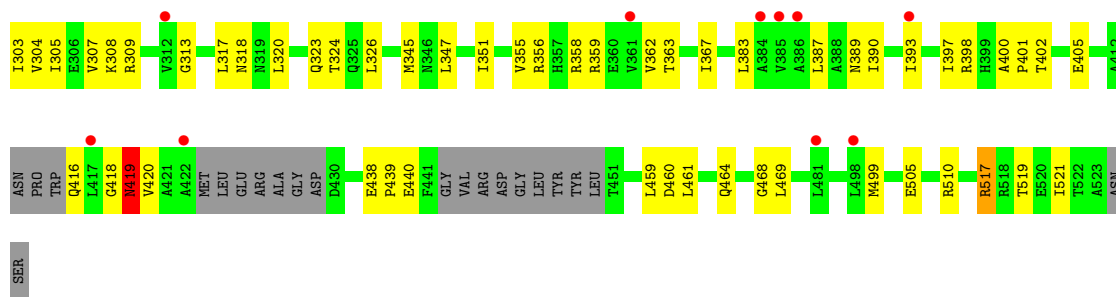


• Molecule 1: DNA gyrase subunit A

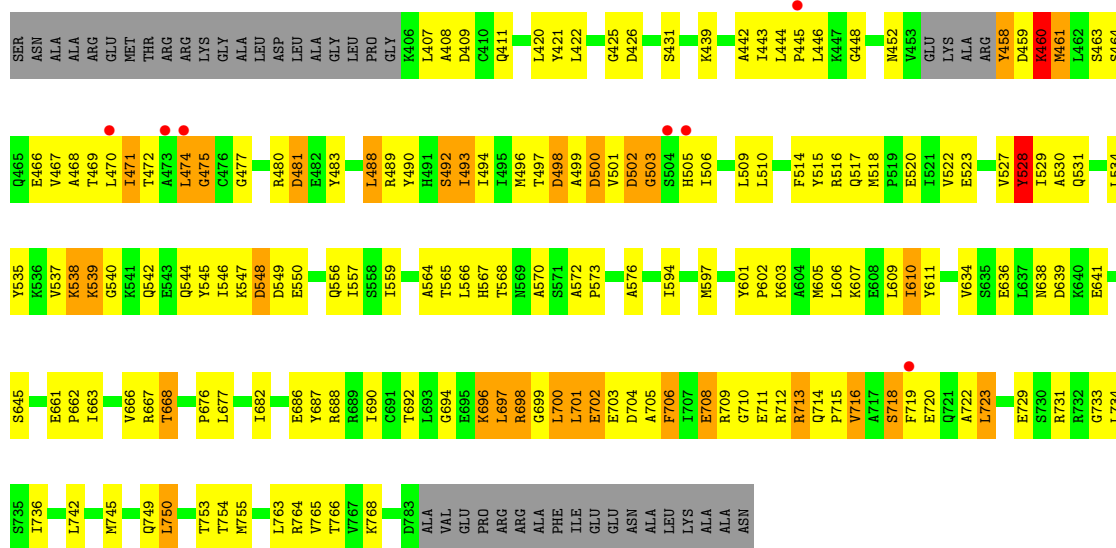


• Molecule 1: DNA gyrase subunit A

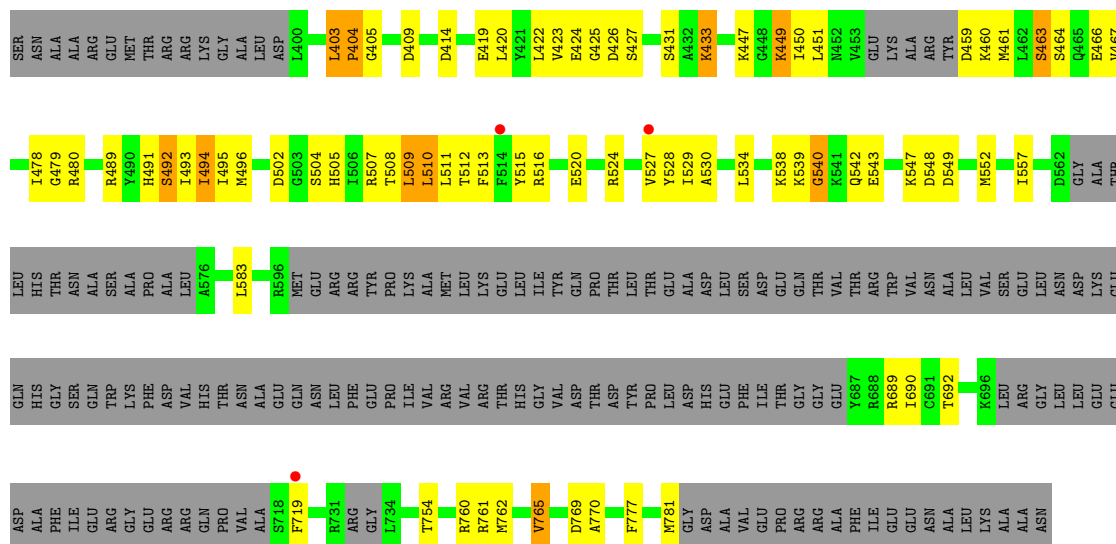




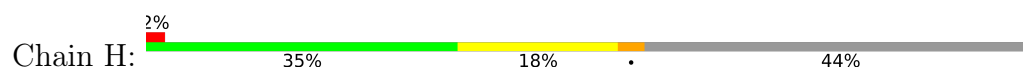
• Molecule 2: DNA gyrase subunit B



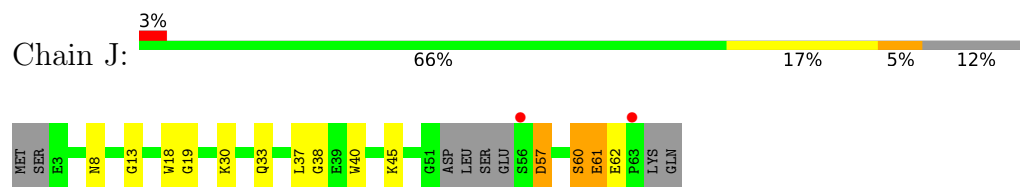
• Molecule 2: DNA gyrase subunit B



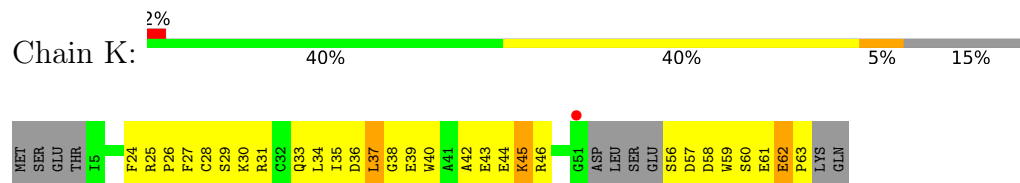
Chain F: 53% 31% 5% 11%



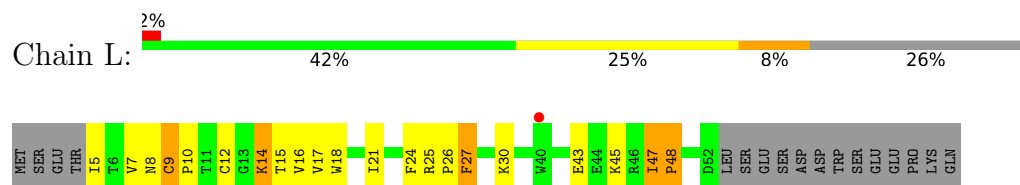
• Molecule 3: DNA gyrase inhibitor YacG



• Molecule 3: DNA gyrase inhibitor YacG



• Molecule 3: DNA gyrase inhibitor YacG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.21Å 114.46Å 462.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.30 49.32 – 3.30	Depositor EDS
% Data completeness (in resolution range)	77.7 (49.32-3.30) 77.6 (49.32-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.243 , 0.283 0.244 , 0.283	Depositor DCC
R_{free} test set	3399 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	109.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 101.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26792	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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

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	0.82	7/4044 (0.2%)	1.12	36/5466 (0.7%)
1	C	0.61	5/3785 (0.1%)	0.98	26/5111 (0.5%)
1	E	0.63	1/3896 (0.0%)	0.94	15/5258 (0.3%)
1	G	0.53	3/3855 (0.1%)	0.88	11/5209 (0.2%)
2	B	0.68	3/3046 (0.1%)	1.13	33/4111 (0.8%)
2	D	0.52	0/2015	0.99	14/2705 (0.5%)
2	F	0.56	0/3021	1.08	24/4074 (0.6%)
2	H	0.60	1/1887 (0.1%)	1.02	9/2534 (0.4%)
3	I	0.86	0/372	1.21	5/504 (1.0%)
3	J	0.49	1/457 (0.2%)	0.92	4/620 (0.6%)
3	K	0.86	1/441 (0.2%)	0.97	2/598 (0.3%)
3	L	0.92	3/380 (0.8%)	1.20	6/515 (1.2%)
All	All	0.65	25/27199 (0.1%)	1.02	185/36705 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	1
2	H	0	1
All	All	0	3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	63	PRO	N-CD	-15.47	1.26	1.47
2	B	502	ASP	CA-C	10.56	1.67	1.52
3	L	26	PRO	N-CD	9.34	1.60	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	ASN	CA-C	8.19	1.62	1.53
1	E	70	VAL	C-O	-7.59	1.15	1.24
1	A	264	ILE	CA-C	-6.49	1.46	1.52
3	J	61	GLU	CA-C	6.48	1.61	1.52
1	G	88	THR	C-O	-6.48	1.16	1.24
1	A	264	ILE	C-O	-6.34	1.16	1.24
1	G	304	VAL	CA-C	-6.14	1.45	1.52
1	A	183	PRO	C-N	6.07	1.41	1.33
1	A	303	ILE	C-O	-5.80	1.17	1.24
3	L	47	ILE	C-N	5.78	1.40	1.33
1	C	303	ILE	C-O	-5.74	1.17	1.24
3	L	48	PRO	N-CD	5.49	1.55	1.47
1	G	89	ILE	C-O	-5.44	1.17	1.24
1	C	264	ILE	CA-C	-5.33	1.47	1.52
1	C	305	ILE	C-O	-5.32	1.17	1.24
2	H	496	MET	CA-C	5.26	1.59	1.52
1	A	218	PRO	N-CD	5.24	1.55	1.47
2	B	493	ILE	CA-C	-5.20	1.46	1.52
1	A	217	PHE	C-N	5.18	1.41	1.34
2	B	488	LEU	CA-C	-5.14	1.46	1.52
1	C	79	PRO	N-CD	5.07	1.54	1.47
1	A	163	ILE	C-N	5.00	1.40	1.34

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	VAL	N-CA-C	19.41	128.77	110.53
2	B	475	GLY	N-CA-C	14.64	134.84	115.36
1	A	414	PRO	CB-CA-C	-13.53	93.91	111.23
1	C	307	VAL	N-CA-C	13.11	127.94	108.54
2	F	603	LYS	N-CA-C	12.96	132.76	111.37
2	F	604	ALA	N-CA-C	12.87	126.75	111.82
2	H	460	LYS	N-CA-C	12.22	128.64	108.73
3	I	28	CYS	O-C-N	-12.17	107.99	122.11
2	B	697	LEU	N-CA-C	11.54	127.97	113.43
2	F	528	TYR	CA-C-N	11.20	136.47	120.91
2	F	528	TYR	C-N-CA	11.20	136.47	120.91
2	H	448	GLY	N-CA-C	10.88	126.69	112.77
1	A	432	ALA	N-CA-C	-10.69	97.53	114.09
1	G	259	ILE	N-CA-C	-9.84	95.97	109.55
2	B	547	LYS	N-CA-C	9.76	122.00	111.36
2	F	611	TYR	N-CA-C	9.69	121.60	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ALA	N-CA-C	9.21	121.39	111.36
1	E	219	THR	CB-CA-C	-9.16	97.16	111.17
2	B	461	MET	N-CA-C	9.04	124.14	109.94
2	B	700	LEU	N-CA-C	8.89	124.54	111.02
2	H	493	ILE	N-CA-C	8.87	120.50	107.37
1	E	177	GLY	N-CA-C	8.57	122.86	112.49
1	A	417	LEU	N-CA-CB	-8.57	95.93	110.50
2	D	466	GLU	N-CA-C	8.46	120.51	111.28
1	A	424	LEU	N-CA-C	-8.28	101.95	110.97
3	I	27	PHE	O-C-N	-8.23	113.84	123.06
1	A	419	ASN	N-CA-C	8.20	133.96	111.00
2	D	404	PRO	N-CA-C	8.10	123.51	111.03
3	I	47	ILE	CB-CA-C	-8.09	96.64	111.36
2	F	654	ASN	N-CA-C	-8.05	99.15	110.50
2	D	449	LYS	N-CA-C	8.04	121.83	110.50
2	B	668	THR	N-CA-C	7.89	119.97	111.36
2	D	447	LYS	N-CA-C	7.82	121.30	109.41
2	H	765	VAL	N-CA-CB	7.81	119.69	110.95
1	A	424	LEU	N-CA-CB	7.79	121.29	109.91
1	C	122	TYR	N-CA-C	7.76	121.23	111.69
2	B	460	LYS	N-CA-C	7.72	127.24	110.80
2	B	503	GLY	N-CA-C	7.62	122.13	112.83
2	B	528	TYR	CA-C-N	7.62	133.80	122.91
2	B	528	TYR	C-N-CA	7.62	133.80	122.91
2	F	501	VAL	N-CA-C	7.60	117.72	110.42
2	D	491	HIS	N-CA-C	-7.59	104.15	113.41
1	A	399	HIS	N-CA-C	7.54	119.50	111.28
1	C	307	VAL	CB-CA-C	-7.47	102.34	111.08
3	J	60	SER	N-CA-C	7.40	120.79	111.24
2	B	713	ARG	N-CA-C	7.39	121.17	109.50
1	G	256	ARG	N-CA-C	-7.38	97.70	109.59
2	B	699	GLY	N-CA-C	-7.36	104.58	113.99
1	A	389	ASN	N-CA-C	7.24	120.74	110.68
2	F	652	HIS	N-CA-C	7.24	121.22	107.75
1	C	259	ILE	CB-CA-C	-7.20	100.10	110.83
1	C	120	MET	N-CA-C	-7.16	103.80	112.54
3	J	62	GLU	N-CA-CB	7.14	123.32	111.17
3	L	47	ILE	CA-C-N	-7.14	113.46	120.52
3	L	47	ILE	C-N-CA	-7.14	113.46	120.52
1	E	443	VAL	N-CA-C	7.12	117.88	110.62
2	B	539	LYS	N-CA-C	7.11	120.36	108.20
2	H	450	ILE	N-CA-C	7.08	124.07	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	418	GLY	N-CA-C	7.07	122.91	111.38
1	C	25	ALA	N-CA-C	-7.06	103.67	111.36
1	C	304	VAL	N-CA-C	7.05	118.73	107.73
2	F	529	ILE	N-CA-C	7.05	118.67	109.58
2	B	701	LEU	N-CA-C	-7.03	100.59	110.50
1	A	390	ILE	N-CA-C	6.96	117.57	110.82
1	A	429	ASP	N-CA-C	-6.95	99.09	109.86
2	D	492	SER	N-CA-C	6.91	119.79	108.52
2	D	510	LEU	N-CA-C	-6.89	103.70	111.07
2	B	459	ASP	N-CA-C	6.89	120.16	109.07
2	F	528	TYR	O-C-N	6.87	131.05	123.22
2	H	449	LYS	N-CA-C	6.83	125.34	110.80
1	A	201	GLU	N-CA-C	-6.79	101.57	110.53
1	A	419	ASN	CB-CA-C	6.79	123.00	110.10
1	A	431	ALA	N-CA-C	6.78	119.57	108.52
2	B	718	SER	N-CA-C	6.73	118.03	108.74
1	G	258	THR	CA-C-N	6.65	132.26	121.62
1	G	258	THR	C-N-CA	6.65	132.26	121.62
1	E	220	ALA	N-CA-C	6.59	119.68	108.67
2	B	458	TYR	N-CA-C	6.58	129.44	111.00
2	B	502	ASP	CA-C-O	6.58	129.92	120.51
1	G	83	SER	N-CA-C	-6.58	105.65	113.21
1	C	424	LEU	N-CA-C	-6.56	104.13	111.28
1	A	125	ILE	N-CA-C	6.54	117.77	108.42
1	C	27	SER	N-CA-C	6.49	118.35	111.28
1	E	84	ALA	N-CA-C	-6.46	104.16	111.07
2	B	474	LEU	N-CA-C	-6.39	104.31	111.28
2	H	497	THR	N-CA-C	-6.34	99.92	108.86
2	F	600	ARG	N-CA-C	6.33	118.18	111.28
1	C	424	LEU	N-CA-CB	6.30	119.38	110.12
1	E	219	THR	N-CA-C	-6.27	106.33	112.97
2	F	602	PRO	N-CA-C	6.25	121.03	111.15
1	G	122	TYR	N-CA-C	-6.25	104.62	112.93
2	B	500	ASP	N-CA-C	-6.15	100.20	109.79
1	C	236	GLY	N-CA-C	-6.14	107.39	114.69
2	H	587	TYR	N-CA-C	6.09	118.42	111.11
1	A	471	HIS	N-CA-C	-6.07	104.35	110.97
2	B	716	VAL	N-CA-C	6.07	116.58	108.27
1	A	183	PRO	CA-C-N	-6.06	112.88	120.51
1	A	183	PRO	C-N-CA	-6.06	112.88	120.51
1	E	303	ILE	CA-C-N	-6.06	117.21	122.96
1	E	303	ILE	C-N-CA	-6.06	117.21	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	538	LYS	N-CA-C	6.05	117.34	107.23
2	B	528	TYR	O-C-N	6.03	130.25	123.19
1	C	148	ASN	CB-CA-C	6.03	123.94	112.43
1	A	419	ASN	N-CA-CB	-6.01	100.28	110.50
2	B	498	ASP	N-CA-C	5.99	118.60	111.71
3	L	27	PHE	N-CA-C	5.98	118.56	109.95
3	K	63	PRO	N-CD-CG	5.96	112.15	103.20
2	B	502	ASP	N-CA-C	5.95	123.48	110.80
2	F	603	LYS	CB-CA-C	-5.93	100.89	110.74
3	L	14	LYS	N-CA-C	-5.93	98.84	108.52
1	E	292	LEU	N-CA-C	-5.93	98.61	108.75
1	G	419	ASN	N-CA-C	5.93	119.61	111.54
2	D	513	PHE	N-CA-C	-5.91	104.84	111.28
3	I	20	GLU	N-CA-C	-5.90	106.06	113.20
1	A	339	HIS	CB-CA-C	-5.90	98.68	110.42
1	A	304	VAL	CB-CA-C	-5.88	103.85	110.96
2	F	529	ILE	CB-CA-C	-5.87	102.34	111.26
1	E	304	VAL	N-CA-CB	-5.85	106.80	112.65
1	C	73	VAL	N-CA-C	-5.85	105.03	110.53
1	E	304	VAL	N-CA-C	5.84	115.24	106.42
1	C	249	GLU	N-CA-C	5.81	117.85	108.32
1	C	149	TYR	N-CA-C	-5.81	98.42	110.80
3	J	61	GLU	CB-CA-C	-5.79	98.89	110.42
1	A	452	GLU	N-CA-CB	-5.79	100.65	110.50
1	C	305	ILE	N-CA-C	5.77	121.33	109.34
3	K	45	LYS	N-CA-C	5.75	118.12	107.99
2	D	509	LEU	N-CA-C	-5.72	105.19	111.82
2	B	713	ARG	N-CA-CB	-5.69	101.01	111.37
2	F	651	VAL	N-CA-C	5.66	116.03	108.11
1	A	452	GLU	N-CA-C	5.64	126.78	111.00
2	D	539	LYS	N-CA-C	-5.62	105.16	111.28
3	J	61	GLU	CA-C-O	5.61	128.54	120.51
2	B	570	ALA	CB-CA-C	-5.60	110.10	116.54
2	B	488	LEU	N-CA-C	-5.59	100.57	109.96
1	A	208	LEU	N-CA-C	-5.58	105.19	111.28
3	L	9	CYS	CA-C-N	5.58	126.82	119.84
3	L	9	CYS	C-N-CA	5.58	126.82	119.84
1	E	452	GLU	N-CA-C	5.54	126.51	111.00
1	C	78	HIS	CA-C-N	-5.51	112.95	119.84
1	C	78	HIS	C-N-CA	-5.51	112.95	119.84
1	A	356	ARG	N-CA-C	-5.51	105.28	111.28
1	C	308	LYS	N-CA-C	-5.50	103.23	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	666	VAL	N-CA-C	5.50	116.03	108.12
1	E	244	ALA	N-CA-C	-5.46	103.69	110.41
2	F	604	ALA	N-CA-CB	-5.44	101.84	110.28
2	B	492	SER	CA-C-N	-5.43	112.19	121.97
2	B	492	SER	C-N-CA	-5.43	112.19	121.97
1	G	90	VAL	CB-CA-C	-5.37	104.98	112.02
2	D	447	LYS	N-CA-CB	-5.37	102.90	111.43
2	F	456	ALA	N-CA-CB	-5.33	102.11	110.69
2	B	698	ARG	CA-C-O	5.30	125.88	119.31
1	E	175	ALA	N-CA-C	-5.30	100.68	108.79
2	D	414	ASP	CA-C-N	5.29	124.92	119.05
2	D	414	ASP	C-N-CA	5.29	124.92	119.05
1	C	389	ASN	CA-C-O	5.29	129.45	122.63
2	F	597	MET	N-CA-C	-5.29	106.81	113.20
1	A	122	TYR	N-CA-C	-5.27	106.91	113.55
1	C	425	GLU	CA-C-N	5.27	127.78	120.29
1	C	425	GLU	C-N-CA	5.27	127.78	120.29
2	F	404	PRO	CA-N-CD	-5.27	104.62	112.00
1	A	217	PHE	CA-C-N	-5.27	113.20	119.05
1	A	217	PHE	C-N-CA	-5.27	113.20	119.05
2	F	617	GLU	N-CA-C	-5.26	105.44	111.07
1	A	425	GLU	CA-C-N	5.26	127.75	120.29
1	A	425	GLU	C-N-CA	5.26	127.75	120.29
1	C	390	ILE	N-CA-C	5.26	120.27	109.34
1	C	148	ASN	N-CA-C	-5.25	101.66	109.96
1	A	206	GLU	N-CA-C	-5.24	105.57	111.28
1	A	397	ILE	N-CA-C	-5.22	104.44	111.44
2	F	414	ASP	CA-C-N	5.21	124.66	119.24
2	F	414	ASP	C-N-CA	5.21	124.66	119.24
1	A	236	GLY	N-CA-C	-5.20	108.29	114.48
2	H	585	SER	N-CA-C	-5.20	105.52	111.14
1	A	425	GLU	N-CA-C	5.18	117.01	111.36
2	F	601	TYR	N-CA-C	-5.17	101.15	109.58
1	C	389	ASN	CB-CA-C	-5.16	104.38	112.12
1	G	303	ILE	N-CA-C	5.15	115.27	107.80
1	E	522	THR	CB-CA-C	-5.14	100.85	109.48
2	B	509	LEU	N-CA-C	-5.13	105.69	111.28
1	C	308	LYS	N-CA-CB	5.12	117.25	110.29
1	A	441	PHE	N-CA-C	5.11	118.04	110.48
1	G	236	GLY	N-CA-C	-5.11	107.76	115.32
2	F	684	GLY	N-CA-C	5.07	118.38	112.50
2	D	463	SER	N-CA-C	5.06	117.21	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	47	ILE	N-CA-C	5.01	119.70	108.88

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	251	ASP	Peptide
2	D	540	GLY	Peptide
2	H	449	LYS	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	3983	0	4040	195	1
1	C	3733	0	3810	156	1
1	E	3841	0	3910	127	14
1	G	3800	0	3867	111	0
2	B	2995	0	2972	165	1
2	D	1990	0	2013	85	0
2	F	2971	0	2959	133	14
2	H	1863	0	1887	74	1
3	I	363	0	357	17	0
3	J	446	0	416	12	0
3	K	430	0	404	38	0
3	L	371	0	362	19	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
All	All	26792	0	26997	1056	16

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 20.

All (1056) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:760:ARG:HD3	2:D:762:MET:CE	1.40	1.52
2:D:760:ARG:CD	2:D:762:MET:HE3	1.49	1.41
2:D:760:ARG:NH1	2:D:762:MET:HE1	1.34	1.40
1:G:257:GLU:OE2	1:G:313:GLY:N	1.61	1.31
1:G:255:GLY:O	1:G:309:ARG:HD3	1.17	1.27
2:D:760:ARG:CD	2:D:762:MET:CE	2.09	1.25
1:E:380:LEU:HD11	1:E:477:GLU:HG2	1.14	1.14
2:H:561:LEU:HD13	2:H:581:GLU:HG2	1.32	1.10
1:A:270:LYS:NZ	1:A:294:ASP:OD2	1.84	1.09
1:C:250:VAL:HG22	1:C:256:ARG:O	1.49	1.09
1:E:380:LEU:CD1	1:E:477:GLU:HG2	1.84	1.08
1:A:417:LEU:HB3	1:A:421:ALA:HB2	1.25	1.08
2:D:538:LYS:HG3	2:D:543:GLU:HB3	1.36	1.07
1:G:257:GLU:OE2	1:G:313:GLY:CA	2.02	1.07
1:A:471:HIS:CE1	1:A:475:LEU:HD21	1.88	1.06
1:A:55:LEU:HD11	1:A:72:ASP:OD2	1.54	1.06
2:D:760:ARG:HD3	2:D:762:MET:HE2	1.33	1.06
1:G:255:GLY:O	1:G:309:ARG:CD	2.02	1.06
2:B:463:SER:O	2:B:467:VAL:HG23	1.55	1.05
1:A:482:LEU:HD23	1:A:485:ILE:HD11	1.38	1.04
1:E:381:GLU:HG2	1:E:424:LEU:HD23	1.39	1.03
2:B:572:ALA:HB1	2:B:573:PRO:HD2	1.38	1.02
2:D:760:ARG:NH1	2:D:762:MET:CE	2.23	1.01
1:E:417:LEU:O	1:E:417:LEU:HD23	1.61	1.00
1:A:108:ASN:ND2	2:D:427:SER:O	1.95	0.99
2:D:760:ARG:HH11	2:D:762:MET:CE	1.75	0.98
2:F:659:LEU:HD12	2:F:659:LEU:H	1.30	0.97
2:D:760:ARG:HD2	2:D:762:MET:HE3	1.46	0.96
2:H:480:ARG:NH2	2:H:523:GLU:OE2	1.97	0.96
2:D:760:ARG:HD3	2:D:762:MET:HE3	0.98	0.96
1:A:471:HIS:CD2	1:A:475:LEU:HD11	2.00	0.95
1:C:264:ILE:HG12	1:C:301:MET:HE1	1.47	0.94
2:B:463:SER:HB3	2:B:466:GLU:HB2	1.49	0.94
2:D:760:ARG:CZ	2:D:762:MET:HE1	1.97	0.93
1:E:380:LEU:HD11	1:E:477:GLU:CG	1.96	0.92
2:H:509:LEU:HD11	3:L:47:ILE:HD11	1.49	0.92
2:F:699:GLY:C	2:F:700:LEU:HD12	1.95	0.92
2:H:561:LEU:HB2	2:H:581:GLU:HG3	1.49	0.92
2:B:565:THR:HG22	2:B:576:ALA:HB2	1.47	0.92
1:C:307:VAL:HG12	1:C:308:LYS:O	1.68	0.91
2:D:538:LYS:CG	2:D:543:GLU:HB3	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:GLU:HG3	1:E:478:TYR:HE2	1.33	0.90
1:C:72:ASP:O	1:C:76:LYS:HG3	1.71	0.90
2:F:596:ARG:HH11	2:F:597:MET:HE2	1.32	0.89
2:D:449:LYS:HD2	2:D:461:MET:HE2	1.54	0.89
1:A:471:HIS:NE2	1:A:475:LEU:HD11	1.87	0.89
1:A:25:ALA:O	1:A:29:ILE:HG13	1.74	0.88
2:D:760:ARG:HH11	2:D:762:MET:HE1	1.09	0.88
1:G:91:ARG:HH21	1:G:91:ARG:HG3	1.38	0.87
1:A:26:MET:SD	1:A:176:VAL:HG21	2.15	0.87
1:G:257:GLU:OE2	1:G:313:GLY:HA3	1.74	0.87
2:B:474:LEU:HD21	2:B:514:PHE:CE1	2.10	0.87
1:C:30:VAL:HG13	1:C:34:LEU:HD12	1.56	0.86
2:D:494:ILE:CG2	2:D:530:ALA:HB2	2.04	0.86
2:D:493:ILE:HG13	2:D:527:VAL:HA	1.56	0.86
2:H:509:LEU:CD1	3:L:47:ILE:HD11	2.05	0.86
1:A:270:LYS:HD2	1:A:301:MET:HE2	1.56	0.86
1:G:86:TYR:O	1:G:90:VAL:HG23	1.75	0.86
2:F:612:GLN:O	2:F:698:ARG:NH1	2.08	0.85
2:B:559:ILE:O	2:B:709:ARG:NH2	2.10	0.85
1:E:381:GLU:HG2	1:E:424:LEU:CD2	2.06	0.84
1:A:417:LEU:HB3	1:A:421:ALA:CB	2.06	0.84
1:A:69:VAL:O	1:A:73:VAL:HG23	1.76	0.84
1:C:270:LYS:HD3	1:C:301:MET:HE3	1.59	0.84
2:D:493:ILE:C	2:D:494:ILE:HD13	2.02	0.84
2:B:611:TYR:O	2:B:698:ARG:CD	2.25	0.84
1:G:99:ARG:NH1	1:G:100:TYR:OH	2.11	0.84
1:A:186:ASN:O	1:A:190:VAL:HG23	1.77	0.84
2:B:408:ALA:HB2	2:B:444:LEU:HD13	1.58	0.83
2:H:495:ILE:HG22	2:H:495:ILE:O	1.77	0.83
1:A:99:ARG:HA	1:A:218:PRO:HG3	1.60	0.83
3:K:37:LEU:HD12	3:K:37:LEU:O	1.77	0.82
1:A:70:VAL:O	1:A:74:ILE:HG13	1.78	0.82
2:B:694:GLY:C	2:B:698:ARG:NH1	2.38	0.81
2:F:702:GLU:HG2	2:F:703:GLU:H	1.45	0.81
3:I:30:LYS:NZ	3:I:33:GLN:OE1	2.14	0.80
1:A:324:THR:HG22	1:A:325:GLN:N	1.96	0.80
2:D:504:SER:O	2:D:508:THR:HG23	1.80	0.80
2:B:474:LEU:HD21	2:B:514:PHE:HE1	1.45	0.80
2:D:529:ILE:O	2:D:762:MET:HB3	1.81	0.80
2:F:457:ARG:HH21	2:F:457:ARG:HG3	1.46	0.80
2:B:468:ALA:O	2:B:471:ILE:HG22	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:656:GLU:CB	2:F:657:GLN:HA	2.10	0.79
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.47	0.79
1:E:324:THR:HG22	1:E:325:GLN:N	1.98	0.79
2:B:714:GLN:CG	2:B:715:PRO:HD2	2.13	0.79
1:E:471:HIS:O	1:E:475:LEU:HD13	1.82	0.79
2:B:611:TYR:O	2:B:698:ARG:HD3	1.82	0.78
2:F:528:TYR:CE1	2:F:764:ARG:HB2	2.18	0.78
1:G:257:GLU:O	1:G:307:VAL:HB	1.83	0.78
1:C:317:LEU:HD12	1:C:317:LEU:O	1.83	0.78
2:D:760:ARG:CZ	2:D:762:MET:CE	2.61	0.78
1:A:176:VAL:HG13	1:A:177:GLY:N	1.99	0.78
2:B:610:ILE:HG22	2:B:690:ILE:HG23	1.65	0.78
1:C:81:GLY:HA3	3:K:58:ASP:O	1.84	0.78
2:D:479:GLY:HA2	3:K:33:GLN:NE2	1.97	0.77
3:J:61:GLU:O	3:J:61:GLU:HG2	1.84	0.77
2:B:708:GLU:HB2	2:B:713:ARG:HG2	1.64	0.77
1:E:79:PRO:HB2	1:G:121:ARG:HB3	1.65	0.77
1:C:74:ILE:O	1:C:79:PRO:HB3	1.85	0.77
2:F:493:ILE:HD11	2:F:527:VAL:HG22	1.65	0.77
2:B:697:LEU:HD11	2:B:719:PHE:CG	2.20	0.77
2:D:493:ILE:HD11	2:D:527:VAL:HB	1.66	0.77
1:C:264:ILE:HB	1:C:265:PRO:HD2	1.67	0.77
2:H:528:TYR:HB3	2:H:762:MET:HE3	1.66	0.76
2:B:564:ALA:HB2	2:B:709:ARG:HA	1.67	0.76
2:H:561:LEU:HB2	2:H:581:GLU:CG	2.15	0.76
1:C:80:HIS:O	3:K:57:ASP:HB2	1.85	0.76
2:F:699:GLY:O	2:F:700:LEU:HD12	1.85	0.76
1:A:55:LEU:HD21	1:A:72:ASP:OD2	1.86	0.75
2:B:488:LEU:HD23	2:B:490:TYR:H	1.50	0.75
1:C:76:LYS:HE2	1:C:153:GLU:OE2	1.86	0.75
1:A:38:ARG:NH1	1:A:158:VAL:HG21	2.01	0.75
2:F:653:THR:HG22	2:F:654:ASN:O	1.86	0.75
2:B:464:SER:HB3	3:I:43:GLU:HG2	1.69	0.75
1:C:150:ASP:OD1	1:C:151:GLY:N	2.20	0.75
1:A:83:SER:OG	3:K:62:GLU:OE1	2.04	0.74
1:A:324:THR:HG22	1:A:325:GLN:H	1.52	0.74
2:B:500:ASP:OD1	2:B:502:ASP:N	2.19	0.74
2:F:657:GLN:O	2:F:657:GLN:HG2	1.87	0.74
1:C:250:VAL:HG22	1:C:256:ARG:C	2.12	0.74
1:A:420:VAL:HG12	1:A:471:HIS:CE1	2.23	0.74
2:H:496:MET:HE1	2:H:755:MET:SD	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:LYS:HE2	3:I:46:ARG:HD2	1.68	0.74
1:E:381:GLU:CG	1:E:424:LEU:HD23	2.18	0.73
1:G:74:ILE:HA	1:G:78:HIS:O	1.89	0.73
2:F:457:ARG:HG3	2:F:457:ARG:NH2	2.03	0.73
2:H:561:LEU:CD1	2:H:581:GLU:HG2	2.16	0.73
1:E:381:GLU:HG3	1:E:478:TYR:CE2	2.20	0.73
3:K:27:PHE:CE2	3:K:33:GLN:HG3	2.24	0.73
1:G:290:SER:HB3	1:G:308:LYS:HB3	1.70	0.72
1:E:121:ARG:HB3	1:G:79:PRO:HB2	1.71	0.72
1:A:66:SER:O	1:A:70:VAL:HG23	1.90	0.72
1:A:471:HIS:NE2	1:A:475:LEU:HD21	2.05	0.72
2:B:611:TYR:O	2:B:698:ARG:HD2	1.89	0.72
2:F:596:ARG:NH1	2:F:597:MET:HE2	2.03	0.72
1:C:245:ARG:HG3	1:C:245:ARG:NH1	2.02	0.72
2:D:760:ARG:NE	2:D:762:MET:CE	2.53	0.71
2:F:559:ILE:HG22	2:F:730:SER:HB2	1.72	0.71
1:C:119:ALA:CB	1:C:121:ARG:HG2	2.20	0.71
1:C:293:ARG:NH1	1:C:295:GLU:OE2	2.21	0.71
2:F:659:LEU:HD12	2:F:659:LEU:N	2.04	0.71
1:G:31:GLY:O	1:G:34:LEU:O	2.09	0.71
2:B:719:PHE:CE2	2:B:723:LEU:HD22	2.25	0.71
1:A:259:ILE:HD13	1:A:317:LEU:CD1	2.21	0.71
2:B:745:MET:HE3	2:B:750:LEU:HD12	1.71	0.71
2:F:596:ARG:HH11	2:F:597:MET:CE	2.04	0.71
2:B:488:LEU:HD23	2:B:490:TYR:N	2.06	0.71
2:D:529:ILE:HG13	2:D:765:VAL:CG1	2.20	0.70
2:F:494:ILE:HA	2:F:528:TYR:O	1.92	0.70
2:H:495:ILE:HG22	2:H:497:THR:HG22	1.72	0.70
2:F:438:ARG:HH22	1:G:299:ASP:HB2	1.56	0.70
3:K:62:GLU:HA	3:K:62:GLU:OE2	1.91	0.70
2:B:408:ALA:CB	2:B:444:LEU:HD13	2.21	0.70
2:F:529:ILE:O	2:F:762:MET:HB2	1.91	0.70
2:H:419:GLU:OE1	2:H:760:ARG:NH1	2.23	0.70
2:B:548:ASP:OD1	2:B:550:GLU:HB3	1.91	0.69
1:C:197:TYR:OH	1:C:201:GLU:OE2	2.04	0.69
1:E:469:LEU:HD13	1:E:469:LEU:C	2.17	0.69
1:A:212:ILE:HD11	1:A:347:LEU:HD21	1.74	0.69
1:C:38:ARG:HD2	1:C:158:VAL:HG11	1.74	0.69
2:B:712:ARG:HD3	2:B:729:GLU:OE1	1.93	0.69
1:G:120:MET:HG2	1:G:120:MET:O	1.91	0.69
2:F:591:GLN:O	2:F:594:ILE:HG12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:CD1	1:A:72:ASP:OD2	2.37	0.69
2:D:403:LEU:N	2:D:404:PRO:CD	2.56	0.69
2:B:537:VAL:HG12	2:B:736:ILE:HG22	1.75	0.69
1:A:39:ASP:O	1:A:165:ASN:ND2	2.21	0.69
1:E:471:HIS:HD2	1:E:475:LEU:HD13	1.59	0.68
2:F:454:GLU:HG3	2:H:451:LEU:HG	1.75	0.68
2:F:596:ARG:NH1	2:F:597:MET:CE	2.57	0.68
1:A:249:GLU:OE2	1:A:260:ILE:HD12	1.94	0.68
2:B:539:LYS:HB2	2:B:734:LEU:HB3	1.75	0.68
2:F:616:THR:HG22	2:F:618:ALA:H	1.59	0.68
1:C:246:ALA:HA	1:C:261:VAL:HA	1.75	0.68
2:B:488:LEU:HD21	2:B:490:TYR:O	1.95	0.67
1:A:81:GLY:O	3:K:61:GLU:HB2	1.93	0.67
1:A:99:ARG:HH12	1:A:515:ASP:HB3	1.59	0.67
1:E:469:LEU:HD13	1:E:469:LEU:O	1.93	0.67
1:A:398:ARG:NH2	1:C:391:ASP:OD2	2.28	0.67
2:B:714:GLN:HG2	2:B:715:PRO:HD2	1.75	0.67
1:C:249:GLU:O	1:C:249:GLU:HG3	1.94	0.67
2:H:461:MET:SD	3:L:45:LYS:O	2.53	0.67
1:A:259:ILE:HG22	1:A:260:ILE:N	2.10	0.67
1:G:416:GLN:O	1:G:416:GLN:HG2	1.94	0.67
1:A:359:ARG:HG2	1:A:499:MET:HE1	1.77	0.67
1:A:478:TYR:CE2	1:A:482:LEU:CD1	2.78	0.67
2:B:564:ALA:CB	2:B:709:ARG:HA	2.25	0.67
2:D:494:ILE:HD13	2:D:494:ILE:N	2.10	0.67
2:B:422:LEU:HD13	2:B:510:LEU:HD22	1.75	0.66
2:F:569:ASN:ND2	2:F:570:ALA:HB2	2.10	0.66
2:H:459:ASP:OD1	3:L:48:PRO:HA	1.96	0.66
2:D:419:GLU:HB3	2:D:492:SER:HB2	1.76	0.66
1:A:143:VAL:HG21	1:A:158:VAL:HB	1.76	0.66
2:B:602:PRO:HD2	2:B:605:MET:HE2	1.76	0.66
2:F:705:ALA:HB3	2:F:716:VAL:O	1.94	0.66
2:B:694:GLY:HA3	2:B:698:ARG:HH12	1.60	0.66
2:F:494:ILE:HG12	2:F:762:MET:HE1	1.78	0.66
1:C:119:ALA:HB1	1:C:121:ARG:HG2	1.76	0.66
2:H:419:GLU:CD	2:H:760:ARG:HH12	2.04	0.66
1:A:259:ILE:O	1:A:260:ILE:HG13	1.96	0.66
2:D:505:HIS:O	2:D:509:LEU:HG	1.96	0.66
1:E:473:LYS:O	1:E:476:ASP:HB2	1.95	0.66
2:H:494:ILE:HA	2:H:528:TYR:O	1.96	0.66
1:A:86:TYR:O	1:A:90:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:ILE:O	1:C:394:ILE:HG13	1.95	0.66
1:G:419:ASN:O	1:G:420:VAL:HG22	1.96	0.66
2:B:572:ALA:HB1	2:B:573:PRO:CD	2.20	0.65
1:A:416:GLN:C	1:A:417:LEU:HD12	2.21	0.65
2:D:529:ILE:HG13	2:D:765:VAL:HG12	1.77	0.65
2:B:425:GLY:N	2:B:446:LEU:O	2.29	0.65
1:A:200:ASP:O	1:A:203:ILE:HB	1.96	0.65
2:B:708:GLU:CB	2:B:713:ARG:HG2	2.26	0.65
1:C:250:VAL:HG23	1:C:257:GLU:HG2	1.77	0.65
2:F:656:GLU:HB3	2:F:657:GLN:HA	1.79	0.65
2:B:634:VAL:O	2:B:638:ASN:ND2	2.30	0.65
1:C:82:ASP:OD2	3:K:60:SER:HB3	1.96	0.65
1:E:324:THR:HG22	1:E:325:GLN:H	1.61	0.65
1:E:74:ILE:HA	1:E:78:HIS:O	1.97	0.64
3:L:7:VAL:HG21	3:L:18:TRP:HE3	1.62	0.64
1:A:324:THR:CG2	1:A:325:GLN:H	2.09	0.64
1:C:250:VAL:CG2	1:C:256:ARG:O	2.37	0.64
1:E:37:VAL:HA	1:E:166:LEU:HD22	1.79	0.64
1:E:273:LEU:HD11	1:E:324:THR:HG22	1.80	0.64
2:B:488:LEU:CD2	2:B:490:TYR:H	2.11	0.64
1:C:265:PRO:HG2	1:C:268:VAL:HG21	1.78	0.64
2:B:714:GLN:HG2	2:B:715:PRO:CD	2.26	0.64
2:F:616:THR:H	2:F:619:ASP:HB2	1.63	0.64
1:A:482:LEU:CD2	1:A:485:ILE:HD11	2.21	0.64
1:E:324:THR:CG2	1:E:325:GLN:N	2.61	0.64
1:G:259:ILE:HB	1:G:305:ILE:HB	1.79	0.64
1:A:74:ILE:HA	1:A:78:HIS:O	1.98	0.64
1:A:201:GLU:O	1:A:202:ASP:HB2	1.98	0.64
1:C:386:ALA:O	1:C:390:ILE:HG13	1.98	0.64
1:A:65:LYS:NZ	1:A:122:TYR:O	2.29	0.63
1:A:324:THR:CG2	1:A:325:GLN:N	2.61	0.63
2:B:718:SER:OG	2:B:719:PHE:N	2.29	0.63
2:H:480:ARG:CZ	3:L:25:ARG:HD2	2.28	0.63
3:K:37:LEU:HD12	3:K:37:LEU:C	2.23	0.63
2:B:408:ALA:CA	2:B:444:LEU:HD13	2.29	0.63
1:E:191:ILE:HG21	1:E:510:ARG:HB2	1.79	0.63
1:G:121:ARG:NH2	1:G:122:TYR:CZ	2.66	0.63
1:A:420:VAL:HG12	1:A:471:HIS:NE2	2.13	0.63
1:E:470:GLU:OE1	1:E:470:GLU:HA	1.98	0.63
2:B:502:ASP:O	2:B:506:ILE:HD12	1.99	0.63
3:L:7:VAL:HG21	3:L:18:TRP:CE3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:616:THR:HG22	2:F:617:GLU:N	2.13	0.63
1:A:478:TYR:CE2	1:A:482:LEU:HD11	2.34	0.63
2:D:493:ILE:HD11	2:D:527:VAL:CB	2.28	0.63
2:F:603:LYS:HG3	2:F:604:ALA:H	1.63	0.62
1:A:215:PRO:HG2	1:A:223:ILE:CD1	2.29	0.62
2:F:603:LYS:HG3	2:F:604:ALA:N	2.14	0.62
1:A:83:SER:O	1:A:87:ASP:HB2	2.00	0.62
1:A:242:ILE:HD11	1:A:330:PHE:HB2	1.80	0.62
1:A:273:LEU:HD21	1:A:326:LEU:HD21	1.81	0.62
2:D:494:ILE:HA	2:D:528:TYR:O	1.99	0.62
1:G:91:ARG:HG3	1:G:91:ARG:NH2	2.08	0.62
1:A:82:ASP:C	1:A:84:ALA:H	2.07	0.62
2:F:680:GLU:O	2:F:684:GLY:N	2.33	0.62
2:F:705:ALA:HB3	2:F:716:VAL:HG23	1.81	0.62
2:H:495:ILE:HG21	2:H:507:ARG:HG3	1.81	0.62
1:E:273:LEU:HD11	1:E:324:THR:CG2	2.30	0.62
1:E:475:LEU:HD12	1:E:475:LEU:N	2.15	0.62
1:A:395:GLU:O	1:A:398:ARG:HB3	1.99	0.62
1:E:380:LEU:HD22	1:E:474:LEU:HD11	1.82	0.62
2:H:509:LEU:HD11	3:L:47:ILE:CD1	2.28	0.62
2:H:523:GLU:O	2:H:525:GLY:N	2.32	0.62
2:B:564:ALA:HB2	2:B:709:ARG:HG3	1.82	0.61
2:B:568:THR:O	2:B:705:ALA:HB2	2.00	0.61
1:A:33:ALA:O	1:A:34:LEU:HD23	2.01	0.61
1:C:312:VAL:O	1:C:316:VAL:HG23	2.00	0.61
2:F:421:TYR:HB2	2:F:443:ILE:HD13	1.82	0.61
2:D:478:ILE:HD13	3:K:37:LEU:CD2	2.30	0.61
1:G:191:ILE:HG21	1:G:510:ARG:HB2	1.82	0.61
2:H:538:LYS:HG2	2:H:543:GLU:HA	1.83	0.61
1:A:259:ILE:HD13	1:A:317:LEU:HD12	1.82	0.61
1:A:280:LEU:HB3	1:A:286:VAL:HG12	1.81	0.61
2:D:512:THR:HG21	2:D:777:PHE:HD2	1.65	0.61
2:F:656:GLU:CG	2:F:657:GLN:HA	2.29	0.61
1:E:324:THR:CG2	1:E:325:GLN:H	2.13	0.61
1:A:189:GLU:HB3	1:A:212:ILE:HG22	1.82	0.61
1:A:471:HIS:O	1:A:472:GLU:C	2.43	0.61
2:B:464:SER:HB3	3:I:43:GLU:CG	2.30	0.61
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.64	0.61
2:B:488:LEU:HD21	2:B:490:TYR:C	2.25	0.61
1:G:67:ALA:HB2	1:G:120:MET:O	2.00	0.61
2:B:475:GLY:HA3	2:B:489:ARG:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:714:GLN:HG3	2:B:715:PRO:HD2	1.82	0.61
2:D:494:ILE:HG22	2:D:530:ALA:HB2	1.83	0.61
2:F:702:GLU:HG2	2:F:703:GLU:N	2.15	0.61
2:H:761:ARG:NH1	2:H:762:MET:O	2.34	0.61
1:C:121:ARG:HG3	1:C:122:TYR:CE1	2.36	0.61
1:E:65:LYS:NZ	1:E:122:TYR:O	2.31	0.60
3:K:39:GLU:HB3	3:K:44:GLU:HB2	1.83	0.60
1:C:427:ALA:HB1	1:C:482:LEU:HD13	1.82	0.60
2:B:594:ILE:HG22	2:B:603:LYS:HG3	1.82	0.60
2:F:607:LYS:O	2:F:610:ILE:HG13	2.01	0.60
2:F:656:GLU:HG2	2:F:657:GLN:HA	1.83	0.60
1:A:21:TYR:O	1:A:24:TYR:HB3	2.01	0.60
1:A:26:MET:HE1	1:A:176:VAL:HG22	1.83	0.60
2:B:488:LEU:HD23	2:B:488:LEU:C	2.27	0.60
1:E:444:ARG:O	1:E:445:ASP:HB2	2.01	0.60
1:C:358:ARG:NH2	1:C:505:GLU:OE1	2.34	0.60
1:G:82:ASP:C	1:G:84:ALA:H	2.09	0.60
1:A:244:ALA:HB2	1:A:265:PRO:HD3	1.82	0.60
2:B:611:TYR:CE1	2:B:697:LEU:HD22	2.36	0.60
1:C:381:GLU:O	1:C:385:VAL:HG23	2.01	0.60
1:E:471:HIS:CD2	1:E:475:LEU:HD13	2.37	0.60
1:C:332:ILE:HD11	1:C:334:MET:HE3	1.83	0.60
1:G:75:GLY:O	1:G:149:TYR:OH	2.15	0.60
2:B:715:PRO:C	2:B:716:VAL:HG13	2.27	0.60
1:E:390:ILE:HG21	1:G:398:ARG:HH12	1.66	0.60
1:E:417:LEU:O	1:E:417:LEU:CD2	2.44	0.60
2:B:564:ALA:HB2	2:B:709:ARG:CG	2.32	0.59
2:B:696:LYS:O	2:B:700:LEU:HD22	2.02	0.59
1:C:305:ILE:HG22	1:C:305:ILE:O	2.01	0.59
2:B:694:GLY:CA	2:B:698:ARG:HH12	2.14	0.59
1:C:230:GLU:HG2	1:C:234:ARG:HH12	1.68	0.59
2:D:460:LYS:HE3	2:D:502:ASP:CG	2.26	0.59
1:E:260:ILE:HD13	1:E:302:ARG:NH1	2.18	0.59
1:E:273:LEU:CD1	1:E:324:THR:CG2	2.80	0.59
2:F:659:LEU:H	2:F:659:LEU:CD1	2.05	0.59
1:G:255:GLY:HA3	1:G:309:ARG:NH1	2.17	0.59
2:H:452:ASN:C	2:H:453:VAL:HG23	2.27	0.59
1:E:381:GLU:OE2	1:E:478:TYR:OH	2.12	0.59
1:C:254:THR:HG22	1:C:254:THR:O	2.02	0.59
2:D:479:GLY:HA2	3:K:33:GLN:HE22	1.67	0.59
1:A:358:ARG:NH2	1:A:505:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:ILE:HA	2:B:528:TYR:O	2.03	0.59
2:D:494:ILE:HG21	2:D:530:ALA:HB2	1.84	0.59
1:E:393:ILE:HD13	1:E:458:ILE:HD11	1.84	0.59
1:C:422:ALA:O	1:C:426:ARG:HB2	2.03	0.59
1:G:358:ARG:NH2	1:G:505:GLU:OE1	2.36	0.59
3:I:16:VAL:HG11	3:I:28:CYS:HA	1.84	0.59
2:B:602:PRO:HD2	2:B:605:MET:CE	2.32	0.58
2:B:714:GLN:HG2	2:B:715:PRO:N	2.18	0.58
1:A:259:ILE:HD13	1:A:317:LEU:HD13	1.85	0.58
2:B:463:SER:CB	2:B:466:GLU:HB2	2.29	0.58
2:B:694:GLY:CA	2:B:698:ARG:NH1	2.66	0.58
2:B:409:ASP:O	2:B:442:ALA:HB1	2.04	0.58
1:C:32:ARG:O	1:C:32:ARG:HG2	2.02	0.58
1:G:244:ALA:HB2	1:G:265:PRO:HD3	1.84	0.58
1:A:203:ILE:O	1:A:348:LYS:NZ	2.36	0.58
1:C:245:ARG:O	1:C:245:ARG:HG2	2.02	0.58
2:D:419:GLU:CB	2:D:492:SER:HB2	2.33	0.58
1:A:422:ALA:O	1:A:426:ARG:HB2	2.03	0.58
1:C:324:THR:HB	1:C:326:LEU:HD13	1.85	0.58
1:E:444:ARG:O	1:E:444:ARG:HG3	2.03	0.58
1:C:37:VAL:HA	1:C:166:LEU:HD22	1.85	0.58
1:E:462:ARG:NH2	1:E:464:GLN:OE1	2.36	0.58
1:C:391:ASP:N	1:C:392:PRO:CD	2.66	0.58
3:K:42:ALA:HB3	3:K:44:GLU:HG2	1.86	0.58
2:B:517:GLN:OE1	3:I:33:GLN:NE2	2.37	0.58
2:F:751:TRP:HA	2:F:755:MET:HB2	1.86	0.58
2:B:474:LEU:HD23	2:B:518:MET:SD	2.44	0.57
2:D:515:TYR:HB2	2:D:770:ALA:HB1	1.86	0.57
2:D:420:LEU:HB3	2:D:493:ILE:HG22	1.86	0.57
2:H:751:TRP:HA	2:H:755:MET:HB2	1.85	0.57
1:C:74:ILE:HA	1:C:78:HIS:O	2.04	0.57
1:G:209:MET:HE1	1:G:230:GLU:HA	1.86	0.57
2:B:464:SER:HB2	3:I:41:ALA:O	2.04	0.57
2:B:500:ASP:OD1	2:B:501:VAL:N	2.38	0.57
2:D:479:GLY:CA	3:K:33:GLN:NE2	2.67	0.57
1:A:176:VAL:CG1	1:A:177:GLY:N	2.67	0.57
1:A:295:GLU:OE1	1:A:302:ARG:NH2	2.36	0.57
1:A:342:PRO:C	1:A:343:LYS:HG2	2.30	0.57
1:C:39:ASP:O	1:C:165:ASN:ND2	2.35	0.57
1:G:320:LEU:HB3	1:G:326:LEU:HD12	1.87	0.57
2:H:448:GLY:O	2:H:449:LYS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:CA	1:A:218:PRO:HG3	2.33	0.57
2:F:751:TRP:CE2	1:G:298:LYS:NZ	2.73	0.57
2:H:766:THR:O	2:H:769:ASP:HB2	2.03	0.57
2:F:459:ASP:OD2	2:F:461:MET:HE2	2.05	0.57
2:B:488:LEU:HD23	2:B:489:ARG:N	2.20	0.56
2:B:489:ARG:NH2	2:B:490:TYR:OH	2.38	0.56
2:F:609:LEU:HB3	2:F:690:ILE:HD13	1.87	0.56
1:A:203:ILE:HG23	1:A:204:SER:N	2.20	0.56
1:E:362:VAL:HG13	1:E:365:ARG:HH21	1.69	0.56
1:E:463:LEU:HD12	1:G:461:LEU:HB3	1.85	0.56
2:B:421:TYR:HB2	2:B:443:ILE:HG22	1.87	0.56
2:B:601:TYR:HB3	2:B:605:MET:CE	2.35	0.56
1:C:173:GLY:HA3	1:C:180:THR:H	1.69	0.56
2:H:527:VAL:HB	2:H:765:VAL:CG2	2.35	0.56
1:C:23:ASP:O	1:C:26:MET:HB3	2.05	0.56
1:E:469:LEU:HD11	1:E:473:LYS:HG3	1.88	0.56
1:A:68:ARG:HH12	1:C:76:LYS:CE	2.19	0.56
1:C:149:TYR:CG	1:C:150:ASP:N	2.71	0.56
2:F:512:THR:O	2:F:516:ARG:HG3	2.05	0.56
1:C:162:LYS:HA	1:C:358:ARG:NH1	2.20	0.56
1:E:230:GLU:OE2	1:E:234:ARG:NH1	2.39	0.56
2:B:607:LYS:O	2:B:610:ILE:HG12	2.05	0.56
1:E:471:HIS:HD2	1:E:475:LEU:CD1	2.18	0.56
2:H:463:SER:O	2:H:467:VAL:HG23	2.05	0.56
1:A:164:PRO:O	1:A:166:LEU:N	2.39	0.56
1:C:58:ASP:OD2	1:C:61:LYS:NZ	2.39	0.56
1:C:70:VAL:O	1:C:71:GLY:C	2.49	0.55
1:E:270:LYS:NZ	1:E:294:ASP:OD2	2.39	0.55
1:A:407:LYS:HD2	1:A:452:GLU:HG3	1.88	0.55
2:B:421:TYR:CZ	2:B:494:ILE:HD12	2.41	0.55
2:F:480:ARG:NH2	2:F:523:GLU:OE2	2.29	0.55
1:G:195:LEU:HA	1:G:198:ILE:HG22	1.88	0.55
2:F:406:LYS:HG2	2:F:406:LYS:O	2.07	0.55
3:L:16:VAL:HG11	3:L:27:PHE:O	2.06	0.55
1:A:164:PRO:HB2	1:A:168:VAL:HG23	1.88	0.55
2:B:522:VAL:HG13	2:B:765:VAL:HG23	1.88	0.55
1:C:30:VAL:HG11	1:C:342:PRO:HG3	1.87	0.55
2:F:652:HIS:HB3	2:F:661:GLU:HB3	1.89	0.55
1:A:108:ASN:HB2	2:D:431:SER:HB3	1.89	0.55
2:B:694:GLY:C	2:B:698:ARG:HH12	2.15	0.55
1:A:82:ASP:C	1:A:84:ALA:N	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD13	1:C:401:PRO:HB3	1.88	0.55
1:A:22:LEU:O	1:A:26:MET:HG2	2.06	0.55
2:B:498:ASP:O	2:B:499:ALA:HB3	2.06	0.55
3:K:36:ASP:OD1	3:K:45:LYS:CE	2.55	0.55
3:L:9:CYS:SG	3:L:10:PRO:HD2	2.47	0.54
2:B:408:ALA:CA	2:B:444:LEU:CD1	2.85	0.54
2:F:610:ILE:C	2:F:610:ILE:HD12	2.32	0.54
3:K:31:ARG:O	3:K:35:ILE:HG13	2.06	0.54
1:A:365:ARG:NH2	1:A:505:GLU:OE2	2.33	0.54
1:C:335:VAL:HG22	1:C:344:ILE:HG12	1.90	0.54
1:C:199:ASP:OD1	1:C:503:ARG:NH1	2.41	0.54
1:A:68:ARG:HH12	1:C:76:LYS:HE3	1.72	0.54
1:A:81:GLY:HA3	1:C:82:ASP:OD2	2.07	0.54
2:F:471:ILE:HD11	2:F:478:ILE:HG22	1.89	0.54
2:B:408:ALA:N	2:B:444:LEU:CD1	2.71	0.54
2:B:452:ASN:O	2:B:458:TYR:N	2.41	0.54
2:B:567:HIS:O	2:B:705:ALA:HB1	2.08	0.54
2:B:697:LEU:HD11	2:B:719:PHE:CD1	2.43	0.54
2:B:701:LEU:HD23	2:B:702:GLU:N	2.22	0.54
2:H:531:GLN:NE2	2:H:763:LEU:HB2	2.23	0.54
1:C:273:LEU:O	1:C:277:ILE:HG13	2.08	0.54
1:E:517:ARG:HD3	1:E:519:THR:O	2.07	0.54
3:L:17:VAL:HG11	3:L:21:ILE:HG21	1.90	0.54
1:C:119:ALA:HB3	1:C:121:ARG:HG2	1.89	0.54
2:F:667:ARG:HG2	2:F:672:ASP:HA	1.90	0.54
1:C:301:MET:O	1:C:302:ARG:HG3	2.08	0.53
2:F:745:MET:HB2	2:F:749:GLN:HB2	1.90	0.53
1:G:247:GLU:OE1	1:G:247:GLU:HA	2.08	0.53
2:B:572:ALA:CB	2:B:573:PRO:HD2	2.23	0.53
1:C:69:VAL:O	1:C:70:VAL:C	2.50	0.53
1:C:424:LEU:HD12	1:C:425:GLU:N	2.24	0.53
1:E:280:LEU:HB3	1:E:286:VAL:HG12	1.90	0.53
2:H:580:LEU:O	2:H:583:LEU:HB3	2.07	0.53
1:A:293:ARG:NH1	1:A:295:GLU:OE2	2.41	0.53
1:C:82:ASP:N	1:C:82:ASP:OD1	2.39	0.53
2:F:705:ALA:CB	2:F:716:VAL:HG23	2.38	0.53
3:L:18:TRP:CD1	3:L:18:TRP:C	2.85	0.53
2:D:511:LEU:O	2:D:515:TYR:N	2.36	0.53
2:H:423:VAL:HA	2:H:496:MET:O	2.09	0.53
1:A:471:HIS:O	1:A:474:LEU:N	2.42	0.53
2:D:461:MET:SD	3:K:43:GLU:HB3	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:548:ASP:OD1	2:D:549:ASP:N	2.42	0.53
1:A:209:MET:HE2	1:A:233:TYR:HB2	1.90	0.53
1:G:221:ALA:H	1:G:519:THR:HG22	1.73	0.53
2:B:565:THR:HG22	2:B:576:ALA:CB	2.30	0.53
1:E:80:HIS:ND1	3:J:57:ASP:HB3	2.23	0.53
2:F:409:ASP:OD1	2:F:490:TYR:OH	2.27	0.53
2:F:428:ALA:HB2	2:F:742:LEU:HB3	1.90	0.53
2:D:480:ARG:HD2	3:K:25:ARG:HB2	1.89	0.53
2:D:493:ILE:HD11	2:D:527:VAL:CG1	2.39	0.53
1:A:155:ILE:HD12	1:A:156:PRO:HD2	1.92	0.52
1:A:414:PRO:O	1:A:415:TRP:HD1	1.92	0.52
2:B:527:VAL:O	2:B:765:VAL:HG22	2.08	0.52
1:C:182:ILE:HG12	1:C:334:MET:HG2	1.91	0.52
2:F:702:GLU:CG	2:F:703:GLU:H	2.15	0.52
3:K:27:PHE:CD2	3:K:33:GLN:HG3	2.45	0.52
1:A:517:ARG:HH11	1:A:517:ARG:CG	2.19	0.52
1:A:129:LYS:HB3	1:A:513:PHE:CE1	2.45	0.52
2:B:431:SER:HB3	2:B:750:LEU:HD22	1.90	0.52
2:B:701:LEU:HD13	2:B:718:SER:HA	1.91	0.52
1:E:48:VAL:HG12	1:E:52:MET:HE2	1.91	0.52
2:F:569:ASN:CG	2:F:704:ASP:H	2.17	0.52
1:G:70:VAL:O	1:G:74:ILE:HG13	2.09	0.52
1:G:113:ASP:OD1	1:G:270:LYS:NZ	2.32	0.52
2:D:449:LYS:HG2	2:D:450:ILE:N	2.23	0.52
3:I:16:VAL:HG11	3:I:28:CYS:CA	2.39	0.52
2:B:715:PRO:O	2:B:716:VAL:CG1	2.57	0.52
2:B:719:PHE:HE2	2:B:723:LEU:HD22	1.72	0.52
1:C:270:LYS:NZ	1:C:294:ASP:OD2	2.43	0.52
1:E:220:ALA:HB1	1:E:263:GLU:OE1	2.10	0.52
1:E:380:LEU:HD22	1:E:474:LEU:CD1	2.39	0.52
2:F:716:VAL:HG21	2:F:722:ALA:HB2	1.91	0.52
1:G:89:ILE:HG21	1:G:125:ILE:HD13	1.91	0.52
1:G:99:ARG:NH1	1:G:100:TYR:CZ	2.77	0.52
1:A:417:LEU:HD23	1:A:421:ALA:CB	2.40	0.52
2:D:459:ASP:N	3:K:46:ARG:HD3	2.25	0.52
2:D:760:ARG:CD	2:D:762:MET:HE2	2.10	0.52
1:G:438:GLU:O	1:G:440:GLU:N	2.41	0.52
2:B:516:ARG:HH12	3:I:45:LYS:HZ2	1.57	0.52
2:B:702:GLU:OE1	2:B:702:GLU:HA	2.09	0.52
2:D:777:PHE:O	2:D:781:MET:N	2.43	0.52
2:F:529:ILE:HG12	2:F:765:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:490:TYR:HB2	2:H:493:ILE:HD11	1.92	0.52
2:F:528:TYR:OH	2:F:764:ARG:CZ	2.57	0.52
2:H:528:TYR:CB	2:H:762:MET:HE3	2.40	0.52
1:A:75:GLY:O	1:A:149:TYR:OH	2.18	0.51
2:B:477:GLY:O	2:B:518:MET:HE2	2.10	0.51
2:H:495:ILE:O	2:H:495:ILE:CG2	2.47	0.51
1:C:122:TYR:CD1	1:C:122:TYR:N	2.76	0.51
2:F:599:ARG:HG3	2:F:599:ARG:HH11	1.75	0.51
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.73	0.51
2:F:599:ARG:HG3	2:F:599:ARG:NH1	2.25	0.51
1:A:124:GLU:C	1:A:125:ILE:HG23	2.34	0.51
1:A:259:ILE:CG2	1:A:260:ILE:N	2.73	0.51
2:B:711:GLU:OE2	2:B:711:GLU:HA	2.10	0.51
1:C:250:VAL:HA	1:C:257:GLU:HA	1.93	0.51
1:E:70:VAL:O	1:E:74:ILE:HG13	2.10	0.51
1:E:459:LEU:O	1:G:464:GLN:N	2.43	0.51
1:G:37:VAL:HA	1:G:166:LEU:HD22	1.92	0.51
1:A:501:VAL:O	1:A:504:GLU:HG2	2.11	0.51
1:G:130:ILE:HD12	1:G:130:ILE:H	1.76	0.51
2:H:412:GLU:HG2	2:H:417:LEU:HB2	1.92	0.51
2:B:496:MET:HE2	2:B:742:LEU:HD23	1.91	0.51
2:B:766:THR:HB	2:B:768:LYS:HG2	1.93	0.51
1:C:85:VAL:HG12	1:C:85:VAL:O	2.09	0.51
1:E:38:ARG:HE	1:E:158:VAL:HG11	1.75	0.51
1:E:293:ARG:HD2	1:E:295:GLU:OE2	2.11	0.51
1:E:345:MET:HB3	1:E:350:ILE:HG13	1.93	0.51
1:E:475:LEU:N	1:E:475:LEU:CD1	2.73	0.51
3:J:40:TRP:CD2	3:J:45:LYS:HG3	2.46	0.51
1:A:471:HIS:CD2	1:A:475:LEU:CD1	2.86	0.51
2:B:483:TYR:CD2	2:B:520:GLU:HB2	2.46	0.51
1:C:201:GLU:OE1	1:C:202:ASP:N	2.39	0.51
1:C:381:GLU:OE2	1:C:478:TYR:OH	2.11	0.51
1:G:106:GLN:HB3	1:G:124:GLU:HG3	1.93	0.51
1:A:354:PHE:O	1:A:357:HIS:HB3	2.11	0.51
1:C:451:THR:N	1:C:454:GLN:OE1	2.44	0.51
1:G:420:VAL:HG23	1:G:420:VAL:O	2.11	0.51
2:B:567:HIS:ND1	2:B:706:PHE:HB3	2.25	0.50
1:C:58:ASP:HA	1:C:132:HIS:CE1	2.46	0.50
1:E:401:PRO:HA	1:G:468:GLY:HA3	1.93	0.50
2:F:412:GLU:HG2	2:F:417:LEU:HB2	1.92	0.50
1:G:416:GLN:O	1:G:416:GLN:CG	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLN:O	1:A:417:LEU:HD12	2.11	0.50
1:A:165:ASN:H	1:A:168:VAL:CG2	2.25	0.50
1:A:381:GLU:OE2	1:A:433:ARG:NH2	2.44	0.50
1:E:393:ILE:HG23	1:E:410:LEU:HD21	1.92	0.50
2:H:400:LEU:HD23	2:H:404:PRO:HG3	1.94	0.50
3:L:8:ASN:HA	3:L:15:THR:HA	1.93	0.50
1:A:414:PRO:HA	1:A:448:TYR:O	2.11	0.50
2:F:496:MET:HE1	2:F:750:LEU:HD11	1.93	0.50
2:F:701:LEU:HD23	2:F:705:ALA:HB2	1.93	0.50
3:K:57:ASP:OD1	3:K:57:ASP:N	2.44	0.50
1:C:149:TYR:O	1:C:150:ASP:C	2.54	0.50
2:F:702:GLU:CG	2:F:703:GLU:N	2.73	0.50
2:F:601:TYR:HB2	2:F:606:LEU:HD11	1.94	0.50
2:B:421:TYR:CZ	2:B:755:MET:HE3	2.46	0.50
1:G:91:ARG:NH2	1:G:91:ARG:CG	2.73	0.50
1:A:381:GLU:OE1	1:A:433:ARG:NH1	2.42	0.50
1:A:389:ASN:O	1:A:393:ILE:HG22	2.12	0.50
1:C:189:GLU:OE1	1:C:517:ARG:NH1	2.45	0.50
2:D:754:THR:O	2:D:754:THR:OG1	2.28	0.50
1:E:83:SER:HB3	3:J:60:SER:HB2	1.92	0.50
2:F:438:ARG:HD2	1:G:302:ARG:HH21	1.77	0.50
2:F:465:GLN:O	2:F:469:THR:OG1	2.15	0.50
2:H:497:THR:OG1	2:H:498:ASP:N	2.43	0.50
3:J:30:LYS:NZ	3:J:33:GLN:NE2	2.60	0.50
2:B:697:LEU:C	2:B:697:LEU:HD23	2.37	0.49
1:C:220:ALA:HB3	1:C:263:GLU:CD	2.37	0.49
1:E:176:VAL:HG23	1:E:177:GLY:N	2.26	0.49
2:F:597:MET:O	2:F:600:ARG:HB3	2.11	0.49
1:G:83:SER:O	1:G:87:ASP:HB2	2.12	0.49
1:C:80:HIS:HD1	3:K:56:SER:C	2.19	0.49
1:E:319:ASN:HB3	1:E:323:GLN:NE2	2.28	0.49
1:E:440:GLU:C	1:E:441:PHE:HD2	2.20	0.49
1:G:205:ILE:HD12	1:G:234:ARG:HG2	1.94	0.49
1:A:471:HIS:HE2	1:A:475:LEU:HD11	1.70	0.49
1:C:270:LYS:CD	1:C:301:MET:HE3	2.37	0.49
2:D:549:ASP:HA	2:D:552:MET:HB3	1.95	0.49
2:F:497:THR:C	2:F:498:ASP:O	2.49	0.49
2:F:750:LEU:O	2:F:754:THR:OG1	2.27	0.49
1:E:41:LEU:HB3	1:E:45:HIS:HB2	1.94	0.49
1:G:90:VAL:HG13	1:G:109:PHE:CD2	2.47	0.49
2:H:423:VAL:HG21	2:H:429:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:THR:HG21	1:C:361:VAL:HG13	1.95	0.49
1:C:260:ILE:HA	1:C:303:ILE:O	2.12	0.49
1:A:124:GLU:C	1:A:125:ILE:CG2	2.85	0.49
2:B:446:LEU:HD22	2:B:466:GLU:HG2	1.95	0.49
1:C:58:ASP:HA	1:C:132:HIS:HE1	1.77	0.49
2:D:478:ILE:O	2:D:478:ILE:HD12	2.13	0.49
2:D:504:SER:O	2:D:508:THR:CG2	2.59	0.49
1:E:273:LEU:CD1	1:E:324:THR:HG22	2.42	0.49
1:E:471:HIS:CD2	1:E:475:LEU:CD1	2.95	0.49
2:F:634:VAL:HG21	2:F:649:PHE:HB3	1.93	0.49
2:F:696:LYS:O	2:F:700:LEU:HD13	2.13	0.49
1:A:176:VAL:HG13	1:A:177:GLY:H	1.78	0.49
1:A:342:PRO:O	1:A:343:LYS:HG2	2.13	0.49
1:A:480:GLU:O	1:A:484:GLN:HG2	2.12	0.49
1:C:273:LEU:HD11	1:C:326:LEU:HD12	1.94	0.49
1:C:274:ILE:HG23	1:C:292:LEU:HD11	1.95	0.49
2:F:694:GLY:O	2:F:698:ARG:HB2	2.12	0.49
2:B:708:GLU:O	2:B:708:GLU:HG3	2.13	0.49
1:C:390:ILE:HD13	1:C:466:LEU:HD22	1.94	0.49
1:E:478:TYR:CE1	1:E:482:LEU:HD13	2.47	0.49
1:G:297:ASP:OD2	1:G:298:LYS:HG2	2.13	0.49
2:B:715:PRO:O	2:B:716:VAL:HG13	2.13	0.49
1:E:407:LYS:O	1:E:411:VAL:HG13	2.13	0.49
1:E:471:HIS:CD2	1:E:471:HIS:C	2.91	0.49
2:B:480:ARG:HH21	3:I:25:ARG:HG3	1.78	0.48
2:B:494:ILE:HG22	2:B:530:ALA:HB2	1.94	0.48
2:B:606:LEU:HA	2:B:609:LEU:HB2	1.95	0.48
1:C:218:PRO:HA	1:C:518:ARG:HH21	1.78	0.48
1:C:285:ARG:HH11	1:C:285:ARG:HB3	1.77	0.48
1:G:389:ASN:O	1:G:393:ILE:HG12	2.12	0.48
1:C:152:THR:C	1:C:153:GLU:HG2	2.38	0.48
2:B:534:LEU:HD23	2:B:535:TYR:CE2	2.49	0.48
1:C:285:ARG:HB3	1:C:285:ARG:NH1	2.28	0.48
1:E:270:LYS:CD	1:E:301:MET:HE3	2.43	0.48
3:J:8:ASN:ND2	3:J:13:GLY:O	2.46	0.48
2:B:697:LEU:HD11	2:B:719:PHE:CB	2.44	0.48
1:C:386:ALA:O	1:C:390:ILE:CG1	2.61	0.48
1:G:66:SER:O	1:G:70:VAL:HG23	2.14	0.48
1:G:221:ALA:N	1:G:519:THR:HG22	2.28	0.48
1:A:68:ARG:NH1	1:C:76:LYS:HE3	2.29	0.48
2:B:719:PHE:O	2:B:720:GLU:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:569:ASN:HB2	2:F:704:ASP:O	2.13	0.48
2:F:686:GLU:O	2:F:690:ILE:HG23	2.13	0.48
2:H:527:VAL:HB	2:H:765:VAL:HG22	1.96	0.48
3:J:30:LYS:NZ	3:J:33:GLN:HE21	2.12	0.48
3:K:38:GLY:O	3:K:42:ALA:N	2.43	0.48
2:B:421:TYR:CE1	2:B:494:ILE:HD12	2.49	0.48
2:B:523:GLU:OE2	3:I:18:TRP:HZ2	1.96	0.48
2:B:539:LYS:O	2:B:540:GLY:C	2.56	0.48
2:F:616:THR:CG2	2:F:617:GLU:N	2.75	0.48
1:A:266:TYR:O	1:A:267:GLN:HB2	2.12	0.48
1:E:79:PRO:HG2	1:G:121:ARG:HD2	1.95	0.48
2:F:596:ARG:NH1	2:F:597:MET:HE1	2.28	0.48
2:F:610:ILE:HD11	2:F:611:TYR:CD1	2.48	0.48
3:K:24:PHE:CZ	3:K:30:LYS:HB2	2.48	0.48
3:K:36:ASP:O	3:K:40:TRP:HD1	1.97	0.48
1:A:38:ARG:HD2	1:A:158:VAL:HG11	1.94	0.48
1:A:55:LEU:CD2	1:A:72:ASP:OD2	2.60	0.48
1:A:393:ILE:HG13	1:A:410:LEU:HD21	1.95	0.48
2:B:497:THR:HG21	2:B:503:GLY:O	2.14	0.48
1:C:111:SER:HB3	1:C:115:ASP:HB2	1.95	0.48
1:A:288:GLY:HA2	1:A:308:LYS:HE2	1.95	0.48
1:E:52:MET:HE1	1:E:103:VAL:HG22	1.96	0.48
1:G:121:ARG:NH2	1:G:122:TYR:OH	2.46	0.48
1:G:259:ILE:O	1:G:260:ILE:HG13	2.13	0.48
2:B:411:GLN:HG2	2:B:439:LYS:HA	1.94	0.47
2:F:411:GLN:OE1	1:G:302:ARG:NH2	2.47	0.47
2:F:767:VAL:O	2:F:771:ILE:HG13	2.14	0.47
1:G:111:SER:OG	1:G:115:ASP:OD2	2.32	0.47
1:G:166:LEU:HD11	1:G:182:ILE:HD12	1.96	0.47
2:H:548:ASP:OD1	2:H:549:ASP:N	2.47	0.47
1:A:417:LEU:HD12	1:A:417:LEU:N	2.30	0.47
1:C:63:TYR:HB3	1:C:124:GLU:HB3	1.96	0.47
1:C:74:ILE:HG23	1:C:79:PRO:HA	1.96	0.47
1:E:408:THR:HA	1:E:411:VAL:HG22	1.96	0.47
1:E:443:VAL:O	1:E:444:ARG:C	2.57	0.47
2:H:523:GLU:C	2:H:525:GLY:N	2.70	0.47
2:B:460:LYS:CE	3:I:46:ARG:HD2	2.42	0.47
2:B:564:ALA:HB2	2:B:709:ARG:CA	2.40	0.47
1:E:398:ARG:NH1	1:G:390:ILE:HD12	2.29	0.47
1:E:469:LEU:C	1:E:469:LEU:CD1	2.86	0.47
1:G:275:GLU:O	1:G:275:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HA	1:C:75:GLY:CA	2.45	0.47
2:B:749:GLN:O	2:B:753:THR:HG23	2.14	0.47
2:D:538:LYS:HD3	2:D:540:GLY:HA2	1.95	0.47
1:E:45:HIS:CD2	1:E:45:HIS:H	2.32	0.47
1:E:402:THR:HG22	1:E:404:ALA:H	1.79	0.47
1:A:260:ILE:HG23	1:A:302:ARG:HG3	1.97	0.47
1:E:182:ILE:HG12	1:E:334:MET:HA	1.97	0.47
1:G:139:GLU:OE2	1:G:140:LYS:HE3	2.15	0.47
1:A:181:ASN:ND2	1:A:331:GLY:O	2.39	0.47
2:B:539:LYS:NZ	2:B:733:GLY:HA3	2.30	0.47
1:E:289:ILE:HG23	1:E:305:ILE:CG2	2.45	0.47
1:E:358:ARG:O	1:E:362:VAL:HG23	2.15	0.47
2:F:705:ALA:O	2:F:715:PRO:HA	2.15	0.47
1:G:90:VAL:O	1:G:94:GLN:HG3	2.14	0.47
2:H:496:MET:HA	2:H:530:ALA:HB3	1.96	0.47
1:A:414:PRO:O	1:A:414:PRO:HG2	2.15	0.47
2:B:460:LYS:HE2	2:B:461:MET:HE2	1.96	0.47
2:B:488:LEU:CD2	2:B:490:TYR:N	2.72	0.47
1:C:185:HIS:HA	1:C:216:ASP:H	1.80	0.47
1:C:264:ILE:HB	1:C:265:PRO:CD	2.42	0.47
2:F:404:PRO:HG2	2:F:405:GLY:N	2.30	0.47
2:H:494:ILE:HG12	2:H:528:TYR:HB2	1.95	0.47
1:A:100:TYR:HE1	1:A:515:ASP:OD2	1.98	0.47
2:B:697:LEU:HD23	2:B:697:LEU:O	2.15	0.47
2:D:464:SER:HA	2:D:467:VAL:HG12	1.96	0.47
1:G:55:LEU:HD11	1:G:72:ASP:OD2	2.15	0.47
1:A:21:TYR:O	1:A:22:LEU:C	2.58	0.47
1:C:24:TYR:CE1	1:C:28:VAL:HG23	2.50	0.47
1:C:262:HIS:C	1:C:263:GLU:HG3	2.40	0.47
1:E:237:ARG:NE	1:E:333:ASN:OD1	2.44	0.47
2:H:515:TYR:CD2	2:H:774:ASP:HB2	2.50	0.47
1:A:259:ILE:HB	1:A:305:ILE:HB	1.97	0.46
1:A:401:PRO:HA	1:C:468:GLY:H	1.80	0.46
2:B:470:LEU:CD1	2:B:474:LEU:HD13	2.45	0.46
2:B:516:ARG:NH1	3:I:45:LYS:NZ	2.64	0.46
2:B:715:PRO:C	2:B:716:VAL:CG1	2.88	0.46
1:C:129:LYS:HE3	1:C:513:PHE:HE1	1.80	0.46
1:E:142:THR:C	1:E:364:ARG:HH11	2.24	0.46
2:F:657:GLN:OE1	2:F:657:GLN:N	2.47	0.46
2:H:407:LEU:HD11	2:H:420:LEU:HD11	1.97	0.46
1:A:134:LEU:HG	1:A:163:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:ARG:NH1	3:I:45:LYS:HZ2	2.13	0.46
1:C:301:MET:O	1:C:302:ARG:CG	2.63	0.46
1:E:491:ILE:HG22	1:E:497:ARG:HE	1.80	0.46
2:F:414:ASP:OD2	2:F:417:LEU:HG	2.15	0.46
2:F:595:ASN:O	2:F:598:GLU:HB3	2.15	0.46
1:G:89:ILE:HD13	1:G:125:ILE:CD1	2.45	0.46
1:A:46:ARG:HG2	1:A:159:MET:HE2	1.98	0.46
2:B:445:PRO:O	2:B:446:LEU:HD23	2.15	0.46
1:C:75:GLY:O	1:C:149:TYR:OH	2.30	0.46
1:E:183:PRO:HD3	1:E:332:ILE:HG23	1.97	0.46
1:E:387:LEU:CD2	1:E:471:HIS:HB2	2.46	0.46
2:F:407:LEU:CD1	2:F:444:LEU:HB2	2.45	0.46
2:F:616:THR:HG22	2:F:618:ALA:N	2.29	0.46
1:A:68:ARG:HA	1:C:75:GLY:HA2	1.96	0.46
1:A:165:ASN:N	1:A:168:VAL:HG23	2.30	0.46
1:E:109:PHE:CE1	1:E:123:THR:HB	2.51	0.46
1:E:380:LEU:HD11	1:E:477:GLU:CD	2.39	0.46
1:G:358:ARG:O	1:G:362:VAL:HG22	2.16	0.46
2:H:495:ILE:CG2	2:H:497:THR:HG22	2.44	0.46
3:J:30:LYS:HZ3	3:J:33:GLN:HE21	1.63	0.46
1:A:63:TYR:HB3	1:A:124:GLU:HB2	1.96	0.46
1:A:401:PRO:HA	1:C:468:GLY:N	2.30	0.46
1:C:136:ALA:HB3	1:C:162:LYS:HE2	1.98	0.46
1:E:469:LEU:HB3	1:G:401:PRO:O	2.15	0.46
2:B:556:GLN:CD	2:B:731:ARG:HH12	2.24	0.46
2:F:457:ARG:HH21	2:F:457:ARG:CG	2.19	0.46
2:D:538:LYS:HG2	2:D:542:GLN:O	2.14	0.46
1:A:388:ALA:HB2	1:A:420:VAL:HG21	1.98	0.46
2:B:481:ASP:OD1	2:B:481:ASP:N	2.48	0.46
1:C:38:ARG:HB3	1:C:357:HIS:CD2	2.50	0.46
2:F:517:GLN:HE21	3:J:37:LEU:HB2	1.81	0.46
1:G:419:ASN:C	1:G:420:VAL:HG22	2.41	0.46
2:H:527:VAL:O	2:H:765:VAL:HG22	2.16	0.46
2:B:452:ASN:HB3	2:B:460:LYS:HZ2	1.80	0.46
2:H:537:VAL:HA	2:H:735:SER:O	2.15	0.46
3:L:24:PHE:CZ	3:L:30:LYS:HB2	2.51	0.46
1:A:423:MET:O	1:A:424:LEU:C	2.59	0.46
2:B:611:TYR:HE1	2:B:697:LEU:HD22	1.78	0.46
1:E:36:ASP:OD2	1:E:38:ARG:NH2	2.49	0.46
2:F:528:TYR:CD1	2:F:764:ARG:HB2	2.49	0.46
2:F:737:GLN:HE21	2:F:739:TYR:HE1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:561:LEU:CB	2:H:581:GLU:HG3	2.33	0.46
1:A:209:MET:HE1	1:A:230:GLU:HG2	1.98	0.45
1:A:220:ALA:O	1:A:221:ALA:HB3	2.17	0.45
1:A:305:ILE:HD13	1:A:320:LEU:HD13	1.97	0.45
2:B:474:LEU:CD2	2:B:514:PHE:HE1	2.22	0.45
2:F:494:ILE:HD12	2:F:494:ILE:H	1.81	0.45
1:G:402:THR:HB	1:G:405:GLU:HG3	1.98	0.45
1:A:35:PRO:HG3	1:A:171:SER:OG	2.16	0.45
1:E:184:PRO:HD2	1:E:217:PHE:CD1	2.51	0.45
2:F:492:SER:HA	2:F:526:HIS:O	2.16	0.45
2:F:595:ASN:O	2:F:598:GLU:CB	2.64	0.45
2:F:701:LEU:HD23	2:F:705:ALA:CB	2.46	0.45
2:B:636:GLU:HA	2:B:639:ASP:OD2	2.16	0.45
1:C:264:ILE:CB	1:C:265:PRO:HD2	2.38	0.45
1:E:402:THR:HB	1:E:405:GLU:HG3	1.98	0.45
2:F:532:PRO:HA	2:F:754:THR:HG22	1.98	0.45
1:A:165:ASN:H	1:A:168:VAL:HG23	1.81	0.45
1:A:222:ILE:HG22	1:A:223:ILE:N	2.30	0.45
1:A:275:GLU:HG3	2:D:405:GLY:HA3	1.99	0.45
2:B:470:LEU:HD12	2:B:474:LEU:HD13	1.98	0.45
2:B:515:TYR:OH	3:I:7:VAL:HG11	2.16	0.45
1:C:37:VAL:HG11	1:C:345:MET:SD	2.57	0.45
2:D:495:ILE:HG21	2:D:507:ARG:HG3	1.98	0.45
2:F:515:TYR:HB2	2:F:770:ALA:HB1	1.97	0.45
2:H:523:GLU:C	2:H:525:GLY:H	2.24	0.45
3:K:42:ALA:C	3:K:43:GLU:HG3	2.42	0.45
1:A:161:THR:OG1	1:A:163:ILE:HG12	2.17	0.45
1:C:152:THR:O	1:C:153:GLU:HG2	2.16	0.45
2:D:449:LYS:HD2	2:D:461:MET:CE	2.35	0.45
1:G:246:ALA:CB	1:G:317:LEU:HD11	2.47	0.45
1:A:230:GLU:CD	1:A:234:ARG:HE	2.25	0.45
1:C:191:ILE:HG21	1:C:510:ARG:HB3	1.98	0.45
1:C:482:LEU:HA	1:C:485:ILE:HG12	1.99	0.45
2:F:656:GLU:HB3	2:F:657:GLN:CA	2.46	0.45
2:B:531:GLN:OE1	2:B:763:LEU:HB2	2.17	0.45
2:D:516:ARG:HD3	3:K:36:ASP:OD2	2.17	0.45
1:E:441:PHE:N	1:E:441:PHE:CD2	2.85	0.45
2:H:403:LEU:HD22	2:H:407:LEU:HD22	1.99	0.45
1:A:179:ALA:O	1:A:333:ASN:ND2	2.50	0.45
1:C:143:VAL:HG11	1:C:158:VAL:HB	1.98	0.45
1:G:26:MET:O	1:G:30:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:THR:OG1	1:G:163:ILE:O	2.34	0.45
1:A:230:GLU:OE2	1:A:234:ARG:NE	2.49	0.45
2:B:567:HIS:HB2	2:B:706:PHE:CB	2.45	0.45
1:C:109:PHE:CE1	1:C:123:THR:HB	2.52	0.45
1:C:111:SER:HB3	1:C:115:ASP:OD2	2.17	0.45
1:G:209:MET:HE2	1:G:233:TYR:HD2	1.82	0.45
2:H:729:GLU:OE2	2:H:732:ARG:NH2	2.50	0.45
1:A:217:PHE:HE2	1:A:223:ILE:HD11	1.82	0.45
1:A:394:ILE:O	1:A:398:ARG:HB2	2.17	0.45
1:A:417:LEU:N	1:A:417:LEU:CD1	2.80	0.45
1:G:99:ARG:HG2	1:G:218:PRO:HD3	1.99	0.45
1:G:104:ASP:OD2	1:G:126:ARG:HD2	2.16	0.45
1:G:200:ASP:HB3	1:G:203:ILE:HG13	1.98	0.45
2:H:483:TYR:CE2	2:H:485:PRO:HG3	2.52	0.45
1:E:441:PHE:HD2	1:E:441:PHE:N	2.15	0.44
1:A:397:ILE:HG13	1:A:406:ALA:HB1	1.99	0.44
2:B:471:ILE:HG23	2:B:472:THR:N	2.31	0.44
2:B:567:HIS:HB2	2:B:706:PHE:HB2	1.99	0.44
1:C:212:ILE:HD12	1:C:347:LEU:HD21	1.98	0.44
2:F:546:ILE:HG21	2:F:552:MET:HA	1.98	0.44
1:A:246:ALA:HA	1:A:261:VAL:HA	1.98	0.44
1:C:301:MET:C	1:C:302:ARG:HG3	2.42	0.44
1:E:67:ALA:HB2	1:E:120:MET:HG3	1.99	0.44
1:E:374:ARG:HG2	1:E:485:ILE:HD12	2.00	0.44
1:E:497:ARG:O	1:E:501:VAL:HG23	2.17	0.44
2:H:515:TYR:O	2:H:515:TYR:CD1	2.70	0.44
2:H:765:VAL:O	2:H:765:VAL:HG23	2.18	0.44
1:A:129:LYS:HB3	1:A:513:PHE:HE1	1.81	0.44
2:B:667:ARG:O	2:B:667:ARG:HG2	2.18	0.44
1:C:146:VAL:HG22	1:C:147:ASP:N	2.32	0.44
2:D:479:GLY:HA2	3:K:33:GLN:HE21	1.78	0.44
1:E:319:ASN:HB3	1:E:323:GLN:HE21	1.81	0.44
1:A:28:VAL:HG13	1:A:29:ILE:N	2.31	0.44
2:B:408:ALA:HA	2:B:444:LEU:CD1	2.48	0.44
1:C:259:ILE:HB	1:C:305:ILE:HB	1.99	0.44
2:D:689:ARG:O	2:D:692:THR:OG1	2.30	0.44
2:F:531:GLN:HB2	2:F:761:ARG:O	2.18	0.44
3:K:28:CYS:SG	3:K:29:SER:N	2.91	0.44
1:A:164:PRO:HB2	1:A:168:VAL:CG2	2.48	0.44
1:C:24:TYR:CD1	1:C:24:TYR:O	2.70	0.44
1:C:171:SER:OG	1:C:172:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:LEU:N	2:D:494:ILE:O	2.49	0.44
1:E:90:VAL:O	1:E:94:GLN:HG3	2.17	0.44
2:F:529:ILE:HG22	2:F:530:ALA:O	2.18	0.44
1:G:25:ALA:HA	1:G:28:VAL:HG23	1.99	0.44
3:L:12:CYS:SG	3:L:14:LYS:HG2	2.57	0.44
2:B:662:PRO:HB2	2:B:677:LEU:HD12	1.98	0.44
1:C:214:GLY:C	1:C:517:ARG:HH22	2.26	0.44
1:C:402:THR:HG22	1:C:404:ALA:H	1.81	0.44
2:F:547:LYS:HD2	2:F:761:ARG:NH1	2.33	0.44
2:H:420:LEU:HB3	2:H:493:ILE:HD12	1.99	0.44
2:H:461:MET:CG	2:H:462:LEU:N	2.80	0.44
2:H:580:LEU:O	2:H:584:VAL:HG23	2.17	0.44
2:B:448:GLY:HA3	2:B:506:ILE:HG12	1.98	0.44
2:D:479:GLY:CA	3:K:33:GLN:HE22	2.29	0.44
1:A:314:GLU:O	1:A:318:ASN:ND2	2.51	0.44
1:E:320:LEU:HB3	1:E:326:LEU:HD12	2.00	0.44
1:G:254:THR:HG22	1:G:255:GLY:N	2.33	0.43
1:A:219:THR:O	1:A:220:ALA:HB3	2.18	0.43
1:E:36:ASP:HA	1:E:337:LEU:HB2	2.00	0.43
1:E:466:LEU:HB2	1:G:397:ILE:HG21	2.00	0.43
2:F:603:LYS:CG	2:F:604:ALA:H	2.28	0.43
1:G:285:ARG:HB3	1:G:323:GLN:HE22	1.83	0.43
1:G:517:ARG:HH12	1:G:521:ILE:HD11	1.83	0.43
2:B:661:GLU:HA	2:B:662:PRO:HD3	1.82	0.43
1:G:359:ARG:HD3	1:G:499:MET:HE1	1.98	0.43
3:K:36:ASP:O	3:K:40:TRP:CD1	2.70	0.43
2:B:688:ARG:O	2:B:692:THR:HG23	2.18	0.43
1:C:338:HIS:HB3	1:C:343:LYS:HD3	1.98	0.43
2:F:430:GLY:O	2:F:434:GLN:HG3	2.19	0.43
2:H:515:TYR:CD1	2:H:515:TYR:C	2.96	0.43
3:I:10:PRO:HG2	3:I:27:PHE:CE1	2.52	0.43
1:A:148:ASN:ND2	1:A:150:ASP:OD1	2.47	0.43
1:C:391:ASP:N	1:C:392:PRO:HD2	2.32	0.43
1:E:273:LEU:HD12	1:E:324:THR:CG2	2.48	0.43
2:F:658:ASN:HB3	2:F:659:LEU:H	1.69	0.43
2:F:661:GLU:HA	2:F:662:PRO:HD3	1.89	0.43
1:G:249:GLU:HB2	1:G:258:THR:O	2.19	0.43
3:K:39:GLU:HB2	3:K:45:LYS:HE2	1.99	0.43
2:B:496:MET:HG2	2:B:742:LEU:HD21	2.00	0.43
2:B:597:MET:HE1	2:B:686:GLU:HB3	2.00	0.43
2:B:641:GLU:OE2	2:B:645:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ARG:HH21	1:C:344:ILE:HD11	1.84	0.43
1:C:254:THR:O	1:C:254:THR:CG2	2.66	0.43
2:F:419:GLU:OE2	2:F:760:ARG:NH1	2.32	0.43
3:I:41:ALA:HB3	3:J:38:GLY:HA3	2.01	0.43
1:A:183:PRO:HG3	1:A:330:PHE:CE1	2.54	0.43
1:C:223:ILE:HG21	1:C:229:ILE:HD11	2.00	0.43
2:D:520:GLU:O	2:D:524:ARG:HG2	2.18	0.43
1:E:222:ILE:HG22	1:E:223:ILE:N	2.34	0.43
1:G:70:VAL:HG13	1:G:85:VAL:HB	2.00	0.43
3:L:12:CYS:SG	3:L:14:LYS:CG	3.06	0.43
2:B:538:LYS:HA	2:B:542:GLN:O	2.19	0.43
1:C:387:LEU:HA	1:C:390:ILE:HD11	2.01	0.43
2:D:478:ILE:HD13	3:K:37:LEU:HD23	1.99	0.43
2:D:583:LEU:HD21	2:D:719:PHE:HZ	1.83	0.43
2:F:746:ASN:HB2	2:F:749:GLN:HG3	1.99	0.43
2:H:753:THR:OG1	2:H:754:THR:HG23	2.19	0.43
1:G:58:ASP:OD1	1:G:58:ASP:N	2.51	0.43
3:L:17:VAL:O	3:L:17:VAL:HG13	2.18	0.43
1:A:165:ASN:O	1:A:166:LEU:C	2.57	0.43
2:D:425:GLY:C	2:D:427:SER:H	2.27	0.43
1:A:183:PRO:HB2	1:A:215:PRO:HB3	2.00	0.42
1:A:475:LEU:O	1:A:478:TYR:N	2.51	0.42
2:B:544:GLN:HG2	2:B:545:TYR:N	2.34	0.42
1:C:100:TYR:HD2	1:C:168:VAL:HG13	1.84	0.42
1:E:337:LEU:HD23	1:E:337:LEU:HA	1.88	0.42
1:E:464:GLN:HG3	1:G:459:LEU:HD13	2.01	0.42
2:F:701:LEU:HD12	2:F:701:LEU:N	2.34	0.42
1:G:383:LEU:O	1:G:387:LEU:HG	2.19	0.42
2:H:424:GLU:OE1	2:H:498:ASP:HB2	2.19	0.42
1:A:158:VAL:HG12	1:A:159:MET:N	2.35	0.42
1:C:20:SER:OG	1:C:21:TYR:N	2.50	0.42
1:C:221:ALA:H	1:C:519:THR:HG22	1.84	0.42
1:C:274:ILE:HD13	1:C:294:ASP:HB2	2.00	0.42
1:C:387:LEU:HB3	1:C:471:HIS:CE1	2.55	0.42
1:E:51:ALA:O	1:E:55:LEU:HD13	2.19	0.42
1:E:186:ASN:ND2	1:E:515:ASP:O	2.43	0.42
1:E:469:LEU:CD1	1:E:473:LYS:HG3	2.49	0.42
2:F:656:GLU:CB	2:F:657:GLN:CA	2.91	0.42
2:F:659:LEU:HD22	2:F:679:HIS:CD2	2.54	0.42
1:A:26:MET:HE1	1:A:176:VAL:CG2	2.47	0.42
1:A:203:ILE:HG12	1:A:204:SER:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:MET:HE2	1:A:345:MET:HB3	1.90	0.42
1:A:519:THR:O	1:A:519:THR:HG23	2.19	0.42
1:C:220:ALA:O	1:C:263:GLU:HB3	2.19	0.42
2:D:424:GLU:HB3	2:D:427:SER:HB3	2.01	0.42
2:H:528:TYR:OH	2:H:764:ARG:NH2	2.52	0.42
2:B:709:ARG:O	2:B:710:GLY:C	2.62	0.42
1:E:274:ILE:HD13	1:E:294:ASP:HB2	2.01	0.42
1:A:245:ARG:O	1:A:245:ARG:HG3	2.20	0.42
1:A:450:LEU:HD11	1:A:454:GLN:HB2	2.01	0.42
1:C:59:TRP:HD1	1:C:132:HIS:ND1	2.17	0.42
2:F:610:ILE:CD1	2:F:611:TYR:CD1	3.02	0.42
1:A:315:VAL:HA	1:E:319:ASN:ND2	2.34	0.42
1:A:414:PRO:CA	1:A:448:TYR:O	2.68	0.42
1:C:497:ARG:HA	1:C:497:ARG:HD2	1.88	0.42
1:G:220:ALA:O	1:G:263:GLU:HB3	2.18	0.42
1:A:186:ASN:HB2	1:A:216:ASP:OD2	2.20	0.42
1:A:341:GLN:HA	1:A:342:PRO:HD3	1.83	0.42
2:D:769:ASP:OD1	2:D:769:ASP:N	2.53	0.42
2:F:657:GLN:O	2:F:657:GLN:CG	2.62	0.42
2:H:432:ALA:HB1	2:H:443:ILE:HD12	2.00	0.42
3:J:18:TRP:CD1	3:J:19:GLY:H	2.37	0.42
1:A:182:ILE:HG12	1:A:334:MET:HA	2.02	0.42
1:A:442:GLY:O	1:A:449:TYR:N	2.38	0.42
2:B:609:LEU:HG	2:B:687:TYR:HE1	1.84	0.42
1:C:76:LYS:HB2	1:C:77:TYR:CD1	2.55	0.42
2:D:403:LEU:N	2:D:404:PRO:HD2	2.32	0.42
2:F:537:VAL:HG11	2:F:546:ILE:HD11	2.00	0.42
2:F:566:LEU:HD23	2:F:575:LEU:HD23	2.02	0.42
2:F:593:MET:HE3	2:F:593:MET:HB2	1.85	0.42
2:H:591:GLN:O	2:H:594:ILE:HG13	2.19	0.42
2:B:408:ALA:HA	2:B:444:LEU:HD13	2.01	0.42
2:D:493:ILE:HD11	2:D:527:VAL:HG12	2.01	0.42
1:E:262:HIS:C	1:E:263:GLU:HG3	2.45	0.42
2:F:559:ILE:HD13	2:F:559:ILE:HA	1.89	0.42
2:F:580:LEU:O	2:F:584:VAL:HG23	2.20	0.42
2:F:595:ASN:HA	2:F:598:GLU:HB2	2.02	0.42
1:G:355:VAL:O	1:G:359:ARG:HG3	2.20	0.42
1:G:358:ARG:HD2	1:G:358:ARG:HA	1.81	0.42
1:G:400:ALA:HA	1:G:401:PRO:HD3	1.80	0.42
1:A:209:MET:HE1	1:A:230:GLU:HA	2.00	0.42
2:B:497:THR:CG2	2:B:503:GLY:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:TYR:HD1	1:C:347:LEU:HB2	1.85	0.42
2:D:409:ASP:OD2	2:D:489:ARG:NH2	2.53	0.42
2:D:547:LYS:HG3	2:D:548:ASP:H	1.85	0.42
1:E:209:MET:HE2	1:E:209:MET:HB3	1.94	0.42
2:F:517:GLN:NE2	3:J:33:GLN:OE1	2.53	0.42
2:F:593:MET:SD	2:F:686:GLU:HG3	2.60	0.42
2:H:423:VAL:HG23	2:H:445:PRO:HA	2.02	0.42
1:A:115:ASP:OD1	2:D:433:LYS:NZ	2.45	0.41
1:A:358:ARG:HA	1:A:358:ARG:HD2	1.89	0.41
1:C:24:TYR:CD1	1:C:24:TYR:C	2.96	0.41
1:C:253:LYS:HG3	1:C:253:LYS:O	2.20	0.41
1:C:400:ALA:HA	1:C:401:PRO:HD3	1.87	0.41
1:C:517:ARG:HH21	1:C:521:ILE:HD11	1.84	0.41
1:E:443:VAL:O	1:E:446:GLY:N	2.53	0.41
2:F:436:ARG:HH12	1:G:295:GLU:HA	1.85	0.41
1:G:356:ARG:HG3	1:G:359:ARG:HH21	1.83	0.41
3:K:58:ASP:OD1	3:K:59:TRP:N	2.53	0.41
1:A:247:GLU:O	1:A:260:ILE:N	2.53	0.41
2:B:548:ASP:HB2	2:B:549:ASP:H	1.71	0.41
1:C:173:GLY:N	1:C:180:THR:O	2.52	0.41
1:C:182:ILE:HA	1:C:183:PRO:HD3	1.80	0.41
1:C:478:TYR:CE2	1:C:482:LEU:HD11	2.55	0.41
1:E:469:LEU:O	1:E:469:LEU:HD22	2.20	0.41
2:H:422:LEU:HD23	2:H:444:LEU:HB3	2.03	0.41
2:H:461:MET:HE2	3:L:43:GLU:HA	2.01	0.41
2:H:509:LEU:CD1	3:L:47:ILE:CD1	2.87	0.41
1:A:471:HIS:NE2	1:A:475:LEU:CD1	2.73	0.41
1:C:205:ILE:HG22	1:C:209:MET:HE3	2.01	0.41
1:C:245:ARG:HH11	1:C:245:ARG:CG	2.19	0.41
1:C:382:ALA:HB2	1:C:454:GLN:NE2	2.35	0.41
2:D:423:VAL:HG12	2:D:496:MET:HE2	2.02	0.41
1:E:462:ARG:NH2	1:G:460:ASP:OD1	2.52	0.41
1:G:320:LEU:O	1:G:324:THR:OG1	2.35	0.41
2:B:528:TYR:HE2	2:B:764:ARG:NE	2.17	0.41
2:B:539:LYS:HB2	2:B:734:LEU:HD23	2.01	0.41
2:F:478:ILE:O	2:F:482:GLU:HB2	2.21	0.41
2:F:505:HIS:O	2:F:509:LEU:HG	2.20	0.41
2:F:623:GLU:HB2	2:F:660:PHE:CE2	2.54	0.41
2:B:471:ILE:CG2	2:B:472:THR:N	2.84	0.41
2:B:703:GLU:O	2:B:704:ASP:HB2	2.19	0.41
2:D:510:LEU:HD23	2:D:510:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ASN:HB2	1:E:216:ASP:OD2	2.21	0.41
1:A:142:THR:O	1:A:364:ARG:HD3	2.21	0.41
1:C:91:ARG:HA	1:C:94:GLN:HE21	1.85	0.41
1:C:507:GLU:HA	1:C:510:ARG:HG2	2.01	0.41
1:E:163:ILE:HA	1:E:164:PRO:HD2	1.92	0.41
1:E:182:ILE:HA	1:E:183:PRO:HD3	1.83	0.41
1:G:347:LEU:O	1:G:351:ILE:HG12	2.19	0.41
3:K:35:ILE:O	3:K:39:GLU:HG3	2.20	0.41
2:B:528:TYR:HE2	2:B:764:ARG:CZ	2.33	0.41
1:C:73:VAL:O	1:C:78:HIS:N	2.48	0.41
1:G:82:ASP:C	1:G:84:ALA:N	2.74	0.41
2:H:415:PRO:O	2:H:491:HIS:HB2	2.20	0.41
2:H:515:TYR:HE2	2:H:774:ASP:CG	2.28	0.41
2:H:772:ALA:O	2:H:775:GLN:HG2	2.21	0.41
1:A:262:HIS:C	1:A:263:GLU:HG3	2.46	0.41
1:G:113:ASP:HB2	1:G:115:ASP:OD2	2.20	0.41
1:G:178:MET:SD	1:G:178:MET:N	2.94	0.41
1:G:363:THR:O	1:G:367:ILE:HG13	2.21	0.41
2:H:422:LEU:HA	2:H:444:LEU:O	2.21	0.41
3:K:25:ARG:HA	3:K:26:PRO:HA	1.87	0.41
1:A:189:GLU:OE2	1:A:517:ARG:HD2	2.21	0.41
2:B:502:ASP:O	2:B:505:HIS:HB2	2.20	0.41
2:D:689:ARG:HG3	2:D:690:ILE:H	1.85	0.41
1:E:26:MET:HE1	1:E:177:GLY:HA3	2.03	0.41
1:E:142:THR:C	1:E:364:ARG:NH1	2.78	0.41
1:E:511:GLU:HA	1:E:511:GLU:OE2	2.21	0.41
2:F:626:VAL:HG13	2:F:662:PRO:HG3	2.01	0.41
1:G:383:LEU:HD22	1:G:461:LEU:HD12	2.03	0.41
2:H:727:VAL:O	2:H:731:ARG:HG2	2.21	0.41
1:A:37:VAL:H	1:A:37:VAL:HG12	1.56	0.41
1:A:482:LEU:HA	1:A:485:ILE:HG12	2.02	0.41
2:B:452:ASN:CB	2:B:460:LYS:HZ2	2.34	0.41
2:B:719:PHE:O	2:B:722:ALA:N	2.54	0.41
1:C:185:HIS:CD2	1:C:215:PRO:HA	2.56	0.41
1:E:242:ILE:HD11	1:E:330:PHE:HB2	2.03	0.41
1:E:464:GLN:HB2	1:G:459:LEU:HB3	2.03	0.41
2:F:404:PRO:HG2	2:F:405:GLY:H	1.85	0.41
1:G:259:ILE:HG13	1:G:307:VAL:CG2	2.51	0.41
1:A:217:PHE:CE2	1:A:223:ILE:HD11	2.56	0.40
1:A:245:ARG:NH1	1:A:520:GLU:OE1	2.51	0.40
1:A:370:LEU:O	1:A:374:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:HA	1:A:374:ARG:HD3	1.82	0.40
1:A:491:ILE:HD11	1:A:497:ARG:HE	1.86	0.40
1:A:503:ARG:HB3	1:A:503:ARG:NH1	2.35	0.40
1:C:30:VAL:HG13	1:C:34:LEU:CD1	2.39	0.40
2:D:527:VAL:O	2:D:527:VAL:HG23	2.20	0.40
2:F:524:ARG:HB2	2:F:526:HIS:CD2	2.56	0.40
2:F:597:MET:HG3	2:F:686:GLU:CD	2.47	0.40
1:G:93:ALA:HA	1:G:103:VAL:O	2.21	0.40
1:G:251:ASP:C	1:G:253:LYS:H	2.29	0.40
1:G:285:ARG:HB3	1:G:323:GLN:NE2	2.37	0.40
1:A:310:ASP:OD1	1:A:310:ASP:N	2.53	0.40
1:C:250:VAL:HA	1:C:256:ARG:O	2.22	0.40
2:F:691:CYS:O	2:F:695:GLU:HG3	2.20	0.40
1:G:262:HIS:O	1:G:301:MET:HG3	2.21	0.40
1:A:221:ALA:N	1:A:263:GLU:OE2	2.46	0.40
1:A:508:LEU:O	1:A:512:GLN:HG3	2.22	0.40
2:B:663:ILE:HG12	2:B:676:PRO:HA	2.02	0.40
1:E:522:THR:HG22	1:E:523:ALA:N	2.36	0.40
3:K:36:ASP:OD1	3:K:45:LYS:HE3	2.20	0.40
1:A:47:ARG:HA	1:A:155:ILE:HD11	2.04	0.40
2:B:698:ARG:C	2:B:700:LEU:N	2.78	0.40
2:D:493:ILE:CG1	2:D:527:VAL:HG12	2.52	0.40
1:A:28:VAL:CG1	1:A:29:ILE:N	2.85	0.40
1:A:65:LYS:O	1:A:67:ALA:N	2.54	0.40
1:A:376:ARG:O	1:A:380:LEU:HB2	2.21	0.40
2:B:420:LEU:O	2:B:493:ILE:HA	2.21	0.40
2:D:451:LEU:HD23	2:D:451:LEU:HA	1.96	0.40
2:D:547:LYS:HB3	2:D:761:ARG:NH1	2.37	0.40
1:E:358:ARG:HH12	1:E:361:VAL:HG11	1.87	0.40
1:E:465:LYS:HA	1:E:470:GLU:HG3	2.03	0.40
2:F:742:LEU:HA	2:F:742:LEU:HD23	1.82	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:ASP:OD2	2:F:596:ARG:CZ[3_757]	1.27	0.93
1:E:476:ASP:OD2	2:F:596:ARG:NE[3_757]	1.27	0.93
1:E:476:ASP:CG	2:F:596:ARG:NE[3_757]	1.32	0.88
1:E:476:ASP:CG	2:F:596:ARG:CZ[3_757]	1.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:ASP:CG	2:F:596:ARG:NH2[3_757]	1.39	0.81
1:E:476:ASP:CB	2:F:596:ARG:NH2[3_757]	1.40	0.80
1:E:476:ASP:CB	2:F:596:ARG:CZ[3_757]	1.49	0.71
1:E:473:LYS:NZ	2:F:597:MET:CA[3_757]	1.59	0.61
1:E:473:LYS:NZ	2:F:596:ARG:O[3_757]	1.60	0.60
1:E:476:ASP:OD2	2:F:596:ARG:NH2[3_757]	1.61	0.59
1:E:473:LYS:NZ	2:F:597:MET:N[3_757]	1.74	0.46
1:E:473:LYS:NZ	2:F:596:ARG:C[3_757]	1.77	0.43
1:E:476:ASP:OD1	2:F:596:ARG:NE[3_757]	2.01	0.19
1:E:473:LYS:CE	2:F:596:ARG:O[3_757]	2.12	0.08
1:A:511:GLU:OE1	2:B:573:PRO:O[4_477]	2.13	0.07
1:C:314:GLU:OE1	2:H:491:HIS:ND1[1_545]	2.13	0.07

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	497/525 (95%)	473 (95%)	22 (4%)	2 (0%)	30	60
1	C	469/525 (89%)	438 (93%)	30 (6%)	1 (0%)	43	71
1	E	477/525 (91%)	454 (95%)	22 (5%)	1 (0%)	43	71
1	G	475/525 (90%)	443 (93%)	31 (6%)	1 (0%)	43	71
2	B	370/417 (89%)	341 (92%)	28 (8%)	1 (0%)	36	65
2	D	239/417 (57%)	225 (94%)	13 (5%)	1 (0%)	30	60
2	F	365/417 (88%)	347 (95%)	18 (5%)	0	100	100
2	H	224/417 (54%)	206 (92%)	17 (8%)	1 (0%)	30	60
3	I	45/65 (69%)	42 (93%)	3 (7%)	0	100	100
3	J	53/65 (82%)	50 (94%)	3 (6%)	0	100	100
3	K	51/65 (78%)	47 (92%)	4 (8%)	0	100	100
3	L	46/65 (71%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3311/4028 (82%)	3112 (94%)	191 (6%)	8 (0%)	43 71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ALA
1	E	401	PRO
2	B	696	LYS
1	A	136	ALA
1	G	439	PRO
2	H	524	ARG
1	C	79	PRO
2	D	403	LEU

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	422/440 (96%)	401 (95%)	21 (5%)	22 50
1	C	397/440 (90%)	382 (96%)	15 (4%)	29 57
1	E	407/440 (92%)	389 (96%)	18 (4%)	25 54
1	G	403/440 (92%)	384 (95%)	19 (5%)	23 52
2	B	322/352 (92%)	300 (93%)	22 (7%)	14 42
2	D	214/352 (61%)	207 (97%)	7 (3%)	33 59
2	F	319/352 (91%)	307 (96%)	12 (4%)	29 57
2	H	202/352 (57%)	194 (96%)	8 (4%)	28 56
3	I	41/59 (70%)	40 (98%)	1 (2%)	43 65
3	J	51/59 (86%)	50 (98%)	1 (2%)	48 68
3	K	49/59 (83%)	46 (94%)	3 (6%)	17 45
3	L	42/59 (71%)	41 (98%)	1 (2%)	43 65
All	All	2869/3404 (84%)	2741 (96%)	128 (4%)	25 53

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	83	SER
1	A	87	ASP
1	A	101	MET
1	A	108	ASN
1	A	124	GLU
1	A	134	LEU
1	A	163	ILE
1	A	205	ILE
1	A	219	THR
1	A	242	ILE
1	A	355	VAL
1	A	361	VAL
1	A	378	HIS
1	A	443	VAL
1	A	456	GLN
1	A	458	ILE
1	A	482	LEU
1	A	491	ILE
1	A	517	ARG
1	A	522	THR
2	B	407	LEU
2	B	426	ASP
2	B	460	LYS
2	B	469	THR
2	B	471	ILE
2	B	481	ASP
2	B	492	SER
2	B	528	TYR
2	B	529	ILE
2	B	546	ILE
2	B	548	ASP
2	B	557	ILE
2	B	566	LEU
2	B	610	ILE
2	B	668	THR
2	B	682	ILE
2	B	702	GLU
2	B	706	PHE
2	B	708	GLU
2	B	723	LEU
2	B	750	LEU

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Mol	Chain	Res	Type
2	B	754	THR
1	C	22	LEU
1	C	121	ARG
1	C	143	VAL
1	C	149	TYR
1	C	159	MET
1	C	168	VAL
1	C	180	THR
1	C	248	VAL
1	C	250	VAL
1	C	256	ARG
1	C	257	GLU
1	C	264	ILE
1	C	323	GLN
1	C	332	ILE
1	C	338	HIS
2	D	426	ASP
2	D	433	LYS
2	D	463	SER
2	D	494	ILE
2	D	534	LEU
2	D	557	ILE
2	D	765	VAL
1	E	46	ARG
1	E	124	GLU
1	E	130	ILE
1	E	146	VAL
1	E	174	ILE
1	E	201	GLU
1	E	272[A]	ARG
1	E	272[B]	ARG
1	E	280	LEU
1	E	292	LEU
1	E	328	VAL
1	E	345	MET
1	E	378	HIS
1	E	387	LEU
1	E	443	VAL
1	E	469	LEU
1	E	482	LEU
1	E	517	ARG
2	F	450	ILE

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Mol	Chain	Res	Type
2	F	517	GLN
2	F	550	GLU
2	F	569	ASN
2	F	586	GLU
2	F	592	LYS
2	F	607	LYS
2	F	609	LEU
2	F	610	ILE
2	F	661	GLU
2	F	683	THR
2	F	778	THR
1	G	24	TYR
1	G	27	SER
1	G	28	VAL
1	G	37	VAL
1	G	72	ASP
1	G	91	ARG
1	G	121	ARG
1	G	124	GLU
1	G	159	MET
1	G	202	ASP
1	G	203	ILE
1	G	229	ILE
1	G	245	ARG
1	G	275	GLU
1	G	318	ASN
1	G	345	MET
1	G	419	ASN
1	G	469	LEU
1	G	517	ARG
2	H	423	VAL
2	H	451	LEU
2	H	482	GLU
2	H	491	HIS
2	H	492	SER
2	H	495	ILE
2	H	498	ASP
2	H	584	VAL
3	I	50	SER
3	J	57	ASP
3	K	34	LEU
3	K	37	LEU

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Mol	Chain	Res	Type
3	K	62	GLU
3	L	5	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	192	ASN
1	A	318	ASN
1	A	319	ASN
1	A	338	HIS
1	A	378	HIS
1	A	464	GLN
1	A	484	GLN
2	B	542	GLN
2	B	556	GLN
2	B	624	GLN
2	B	749	GLN
1	C	94	GLN
1	C	106	GLN
1	C	211	HIS
1	C	454	GLN
1	C	456	GLN
1	C	464	GLN
2	D	411	GLN
2	D	434	GLN
2	D	437	ASN
2	D	517	GLN
2	D	531	GLN
2	D	556	GLN
2	D	749	GLN
2	D	775	GLN
1	E	45	HIS
1	E	224	ASN
1	E	319	ASN
1	E	325	GLN
1	E	471	HIS
2	F	437	ASN
2	F	517	GLN
2	F	531	GLN
2	F	612	GLN
2	F	624	GLN

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Mol	Chain	Res	Type
2	F	679	HIS
2	F	737	GLN
2	F	775	GLN
1	G	53	ASN
1	G	57	ASN
1	G	80	HIS
1	G	262	HIS
1	G	267	GLN
1	G	323	GLN
1	G	333	ASN
1	G	453	GLN
2	H	434	GLN
2	H	544	GLN
2	H	556	GLN
2	H	588	ASN
2	H	749	GLN
3	J	33	GLN
3	K	33	GLN
3	L	8	ASN
3	L	33	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	505/525 (96%)	-0.03	12 (2%) 59 40	67, 110, 249, 473	0
1	C	475/525 (90%)	0.07	18 (3%) 44 30	75, 145, 252, 431	0
1	E	486/525 (92%)	-0.09	12 (2%) 58 39	39, 104, 254, 314	1 (0%)
1	G	483/525 (92%)	0.10	14 (2%) 53 35	59, 139, 235, 370	0
2	B	374/417 (89%)	0.05	7 (1%) 66 48	69, 132, 176, 208	0
2	D	251/417 (60%)	0.11	3 (1%) 76 58	86, 145, 270, 299	0
2	F	371/417 (88%)	-0.05	5 (1%) 75 56	59, 121, 200, 247	0
2	H	233/417 (55%)	0.02	7 (3%) 52 35	58, 132, 263, 362	1 (0%)
3	I	47/65 (72%)	-0.35	1 (2%) 63 44	65, 106, 140, 149	0
3	J	57/65 (87%)	-0.01	2 (3%) 47 31	66, 108, 144, 153	0
3	K	55/65 (84%)	0.26	1 (1%) 67 49	136, 176, 205, 211	0
3	L	48/65 (73%)	0.42	1 (2%) 63 44	166, 194, 227, 283	0
All	All	3385/4028 (84%)	0.02	83 (2%) 58 39	39, 130, 246, 473	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	ALA	12.8
1	E	386	ALA	7.3
1	E	385	VAL	5.7
1	C	317	LEU	5.6
1	A	386	ALA	5.3
1	G	385	VAL	5.2
2	H	584	VAL	4.8
1	A	385	VAL	4.7
2	H	496	MET	4.6
1	C	385	VAL	4.5
1	A	383	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	31	GLY	4.3
1	C	318	ASN	4.3
1	E	466	LEU	3.9
2	D	719	PHE	3.4
1	E	384	ALA	3.3
3	L	40	TRP	3.2
2	B	473	ALA	3.2
1	A	393	ILE	3.2
1	C	194	CYS	3.1
1	G	312	VAL	3.1
1	E	81	GLY	3.1
1	C	381	GLU	3.1
3	J	63	PRO	3.0
1	G	386	ALA	3.0
1	A	379	ILE	3.0
1	C	389	ASN	3.0
2	B	470	LEU	2.9
2	B	445	PRO	2.9
1	A	389	ASN	2.9
1	C	313	GLY	2.9
1	A	19	SER	2.9
1	G	194	CYS	2.9
1	E	428	GLY	2.9
1	C	131	ALA	2.8
2	D	527	VAL	2.8
1	C	463	LEU	2.8
3	J	56	SER	2.7
3	K	51	GLY	2.7
1	E	458	ILE	2.7
1	C	246	ALA	2.7
2	H	400	LEU	2.7
1	G	393	ILE	2.6
2	F	677	LEU	2.6
1	G	422	ALA	2.6
1	G	417	LEU	2.6
1	G	198	ILE	2.5
2	B	719	PHE	2.5
1	C	320	LEU	2.4
2	B	474	LEU	2.4
1	E	504	GLU	2.4
1	E	424	LEU	2.4
1	E	393	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	384	ALA	2.4
1	C	363	THR	2.3
2	F	694	GLY	2.3
2	B	505	HIS	2.3
1	A	381	GLU	2.3
1	C	421	ALA	2.3
1	C	383	LEU	2.2
2	D	514	PHE	2.2
2	H	583	LEU	2.2
2	B	504	SER	2.2
1	A	223	ILE	2.2
1	C	247	GLU	2.2
1	A	446	GLY	2.2
2	H	726	LEU	2.2
1	A	443	VAL	2.2
2	F	735	SER	2.2
1	E	465	LYS	2.2
1	G	361	VAL	2.2
1	G	498	LEU	2.2
1	G	384	ALA	2.2
1	E	394	ILE	2.1
2	F	624	GLN	2.1
1	C	130	ILE	2.1
1	C	101	MET	2.1
2	F	404	PRO	2.1
2	H	513	PHE	2.1
1	G	155	ILE	2.0
3	I	51	GLY	2.0
1	G	481	LEU	2.0
2	H	580	LEU	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
4	ZN	B	1001	1/1	0.52	0.16	346,346,346,346	0
4	ZN	E	601	1/1	0.72	0.14	346,346,346,346	0
4	ZN	K	101	1/1	0.95	0.10	202,202,202,202	0
4	ZN	L	101	1/1	0.97	0.07	225,225,225,225	0
4	ZN	I	101	1/1	0.99	0.03	95,95,95,95	0
4	ZN	J	101	1/1	0.99	0.03	137,137,137,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.