



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:26 PM UTC

PDB ID : 4GAW / pdb_00004gaw
Title : Crystal structure of active human granzyme H
Authors : Wang, L.; Li, Q.; Wu, L.; Zhang, K.; Tong, L.; Sun, F.; Fan, Z.
Deposited on : 2012-07-25
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

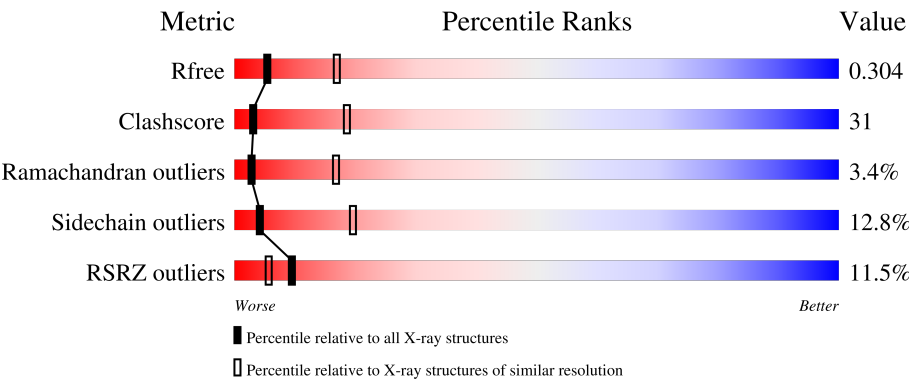
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	226	14% 30% 56% 10%
1	B	226	2% 42% 45% 12%
1	C	226	5% 41% 50% 9%
1	D	226	% 40% 50% 8%
1	E	226	2% 47% 43% 9%

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Mol	Chain	Length	Quality of chain
1	F	226	
1	G	226	
1	H	226	
1	I	226	
1	J	226	
1	K	226	
1	L	226	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	L	301	-	-	X	-

2 Entry composition

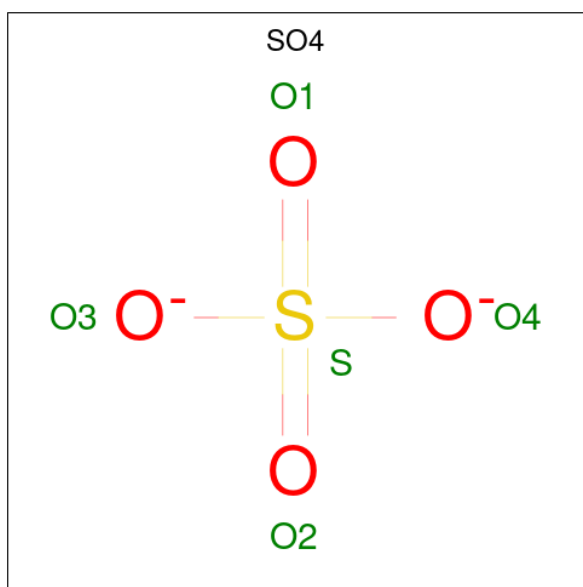
There are 4 unique types of molecules in this entry. The entry contains 21292 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Granzyme H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1754	1115	321	307	11			
1	B	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	C	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	D	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	E	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	F	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	G	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	H	221	Total	C	N	O	S	0	0	0
			1732	1101	317	303	11			
1	I	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	J	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	K	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			
1	L	226	Total	C	N	O	S	0	0	0
			1769	1124	324	310	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		

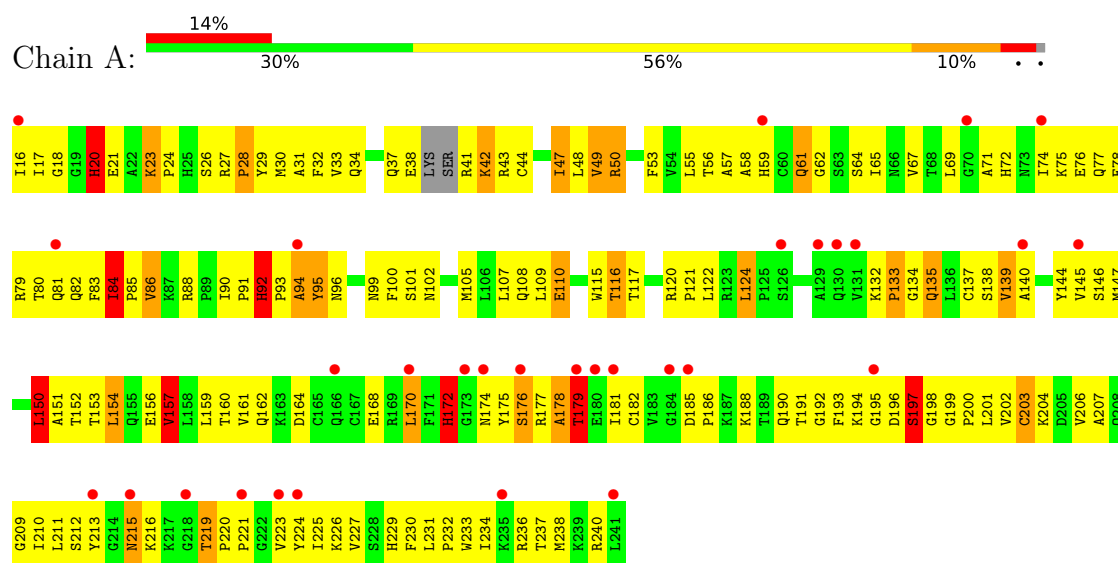
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	3	Total	O	0	0
			3	3		
4	D	6	Total	O	0	0
			6	6		
4	E	4	Total	O	0	0
			4	4		
4	F	4	Total	O	0	0
			4	4		
4	G	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		
4	I	8	Total	O	0	0
			8	8		
4	J	1	Total	O	0	0
			1	1		
4	K	2	Total	O	0	0
			2	2		
4	L	4	Total	O	0	0
			4	4		

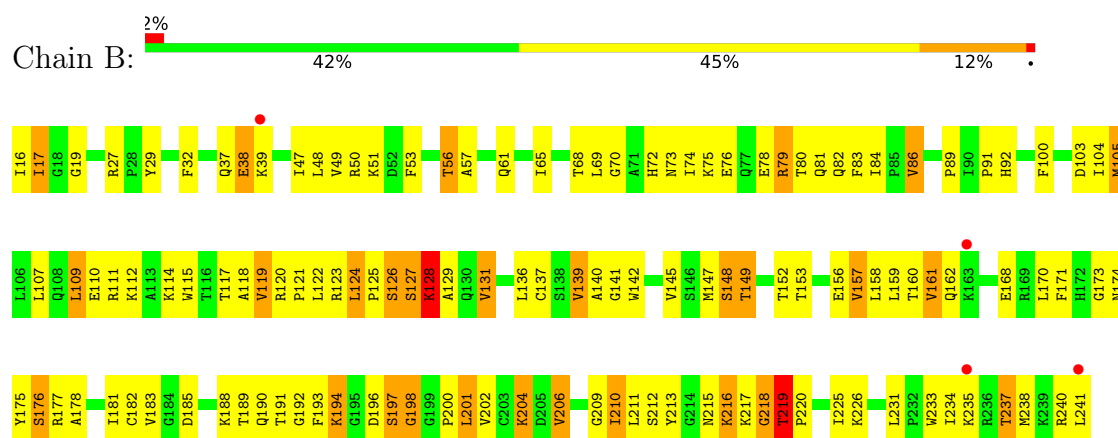
3 Residue-property plots

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.

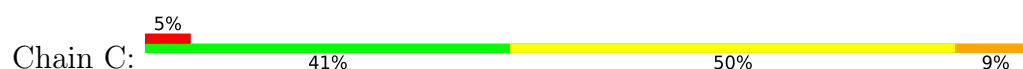
• Molecule 1: Granzyme H

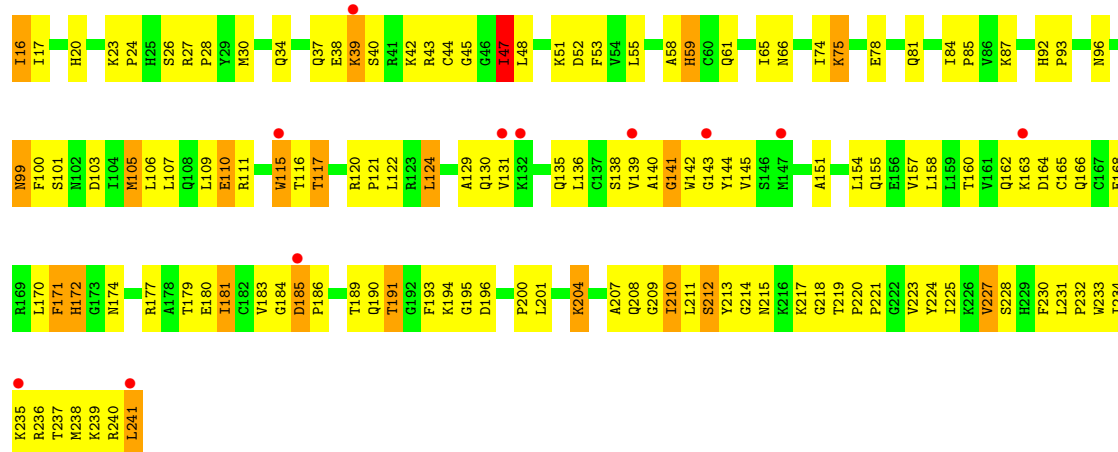


• Molecule 1: Granzyme H

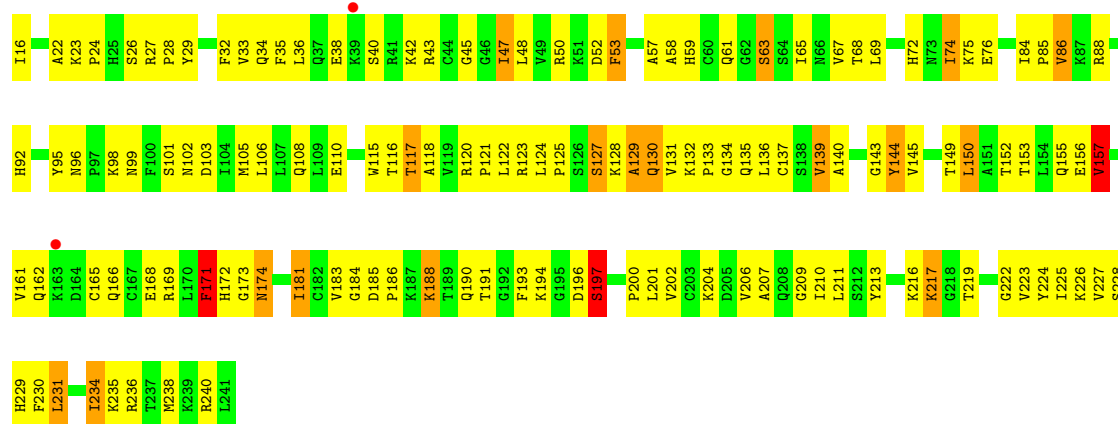


• Molecule 1: Granzyme H

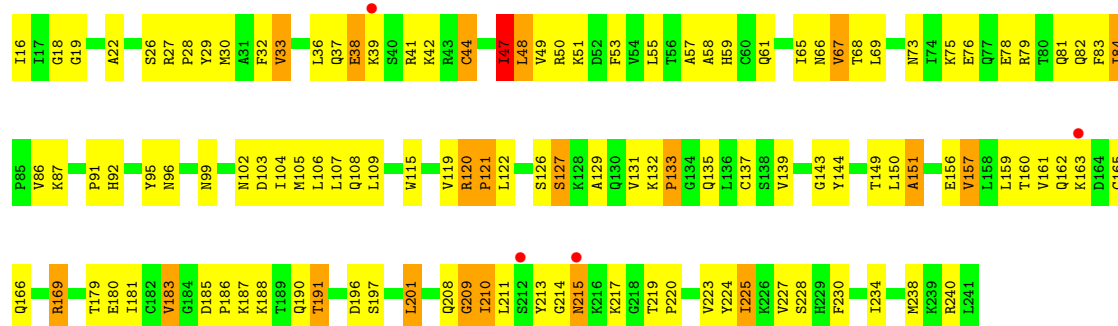




• Molecule 1: Granzyme H

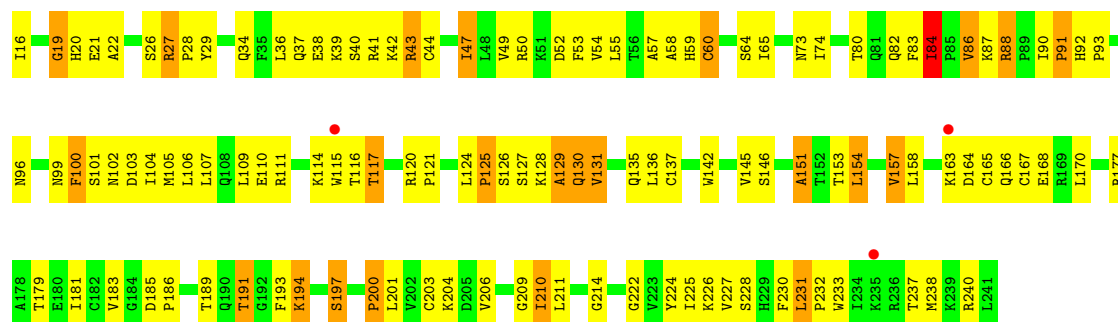


• Molecule 1: Granzyme H

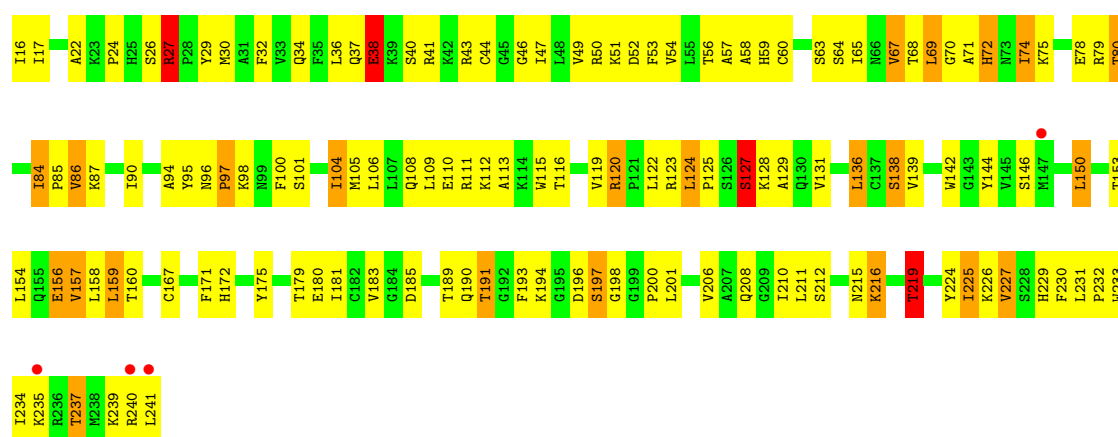


• Molecule 1: Granzyme H

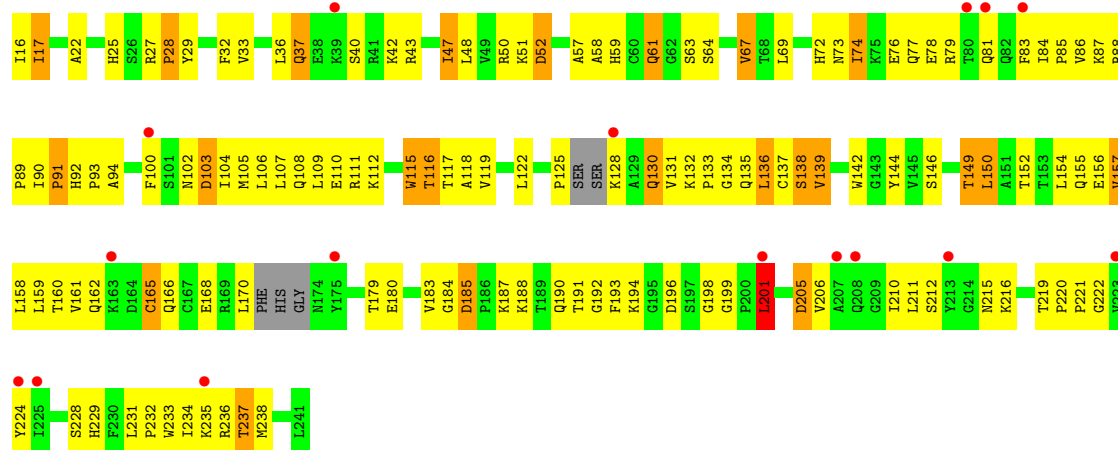




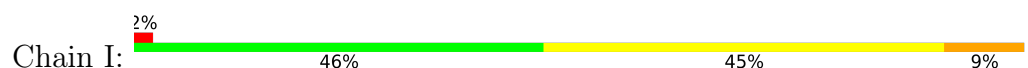
• Molecule 1: Granzyme H

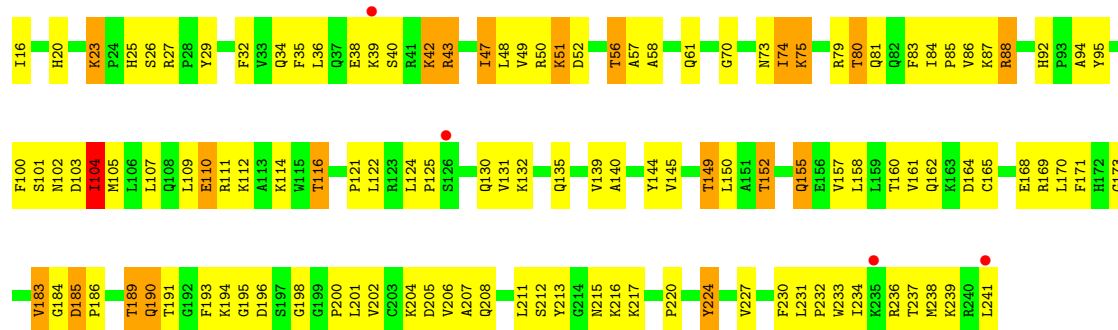


• Molecule 1: Granzyme H

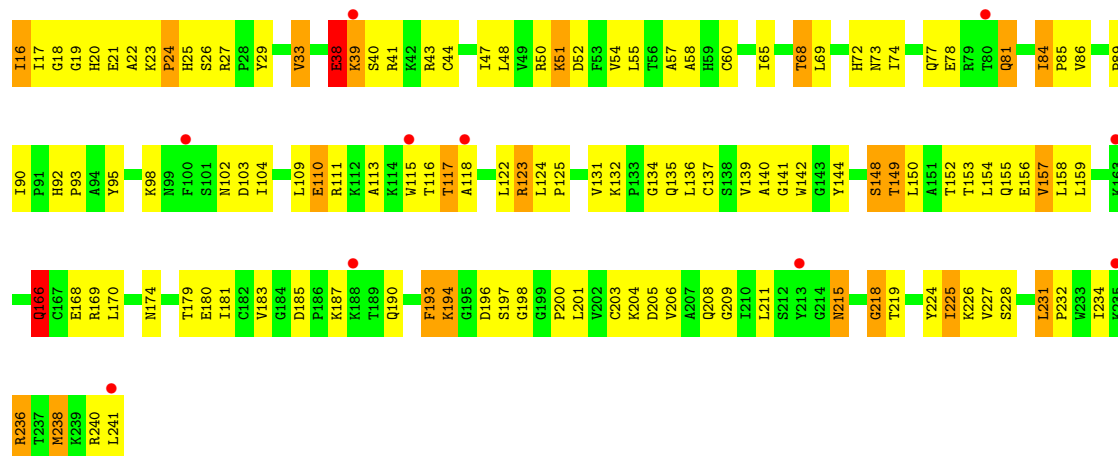
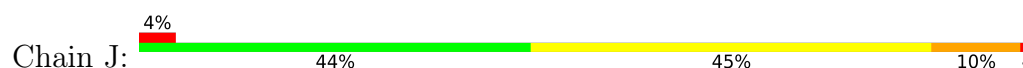


• Molecule 1: Granzyme H

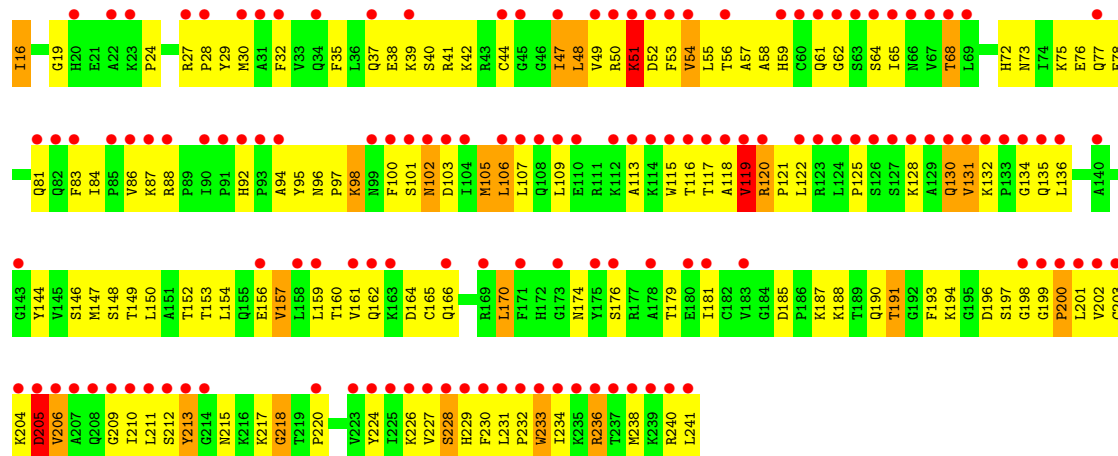




• Molecule 1: Granzyme H

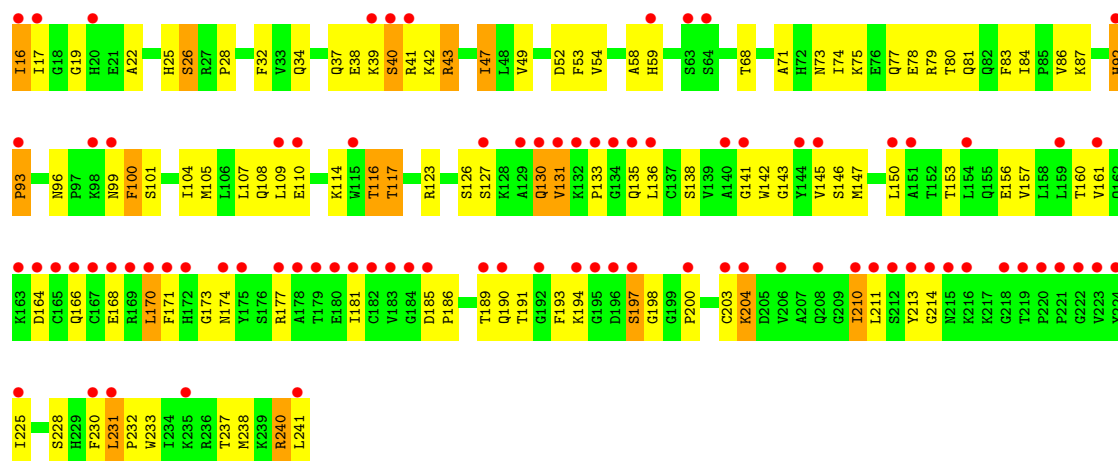


• Molecule 1: Granzyme H



• Molecule 1: Granzyme H





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.37Å 367.07Å 61.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 3.00 39.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.80-3.00) 99.8 (39.80-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.271 , 0.306 0.270 , 0.304	Depositor DCC
R_{free} test set	3935 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21292	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2609e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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	1.01	2/1794 (0.1%)	1.21	18/2420 (0.7%)
1	B	1.13	2/1810 (0.1%)	1.36	15/2442 (0.6%)
1	C	0.97	1/1810 (0.1%)	1.26	10/2442 (0.4%)
1	D	1.01	0/1810	1.23	12/2442 (0.5%)
1	E	0.94	0/1810	1.24	12/2442 (0.5%)
1	F	1.15	4/1810 (0.2%)	1.42	20/2442 (0.8%)
1	G	1.04	3/1810 (0.2%)	1.27	16/2442 (0.7%)
1	H	0.86	0/1769	1.19	16/2384 (0.7%)
1	I	1.00	0/1810	1.23	8/2442 (0.3%)
1	J	0.88	0/1810	1.14	11/2442 (0.5%)
1	K	0.76	0/1810	1.07	7/2442 (0.3%)
1	L	0.89	0/1810	1.07	8/2442 (0.3%)
All	All	0.98	12/21663 (0.1%)	1.23	153/29224 (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	A	0	1
1	B	0	2
1	G	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	LEU	CA-C	6.84	1.61	1.52
1	G	72	HIS	CA-C	-6.80	1.47	1.52
1	G	136	LEU	N-CA	-5.60	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	SER	N-CA	5.58	1.53	1.46
1	F	44	CYS	CA-C	-5.50	1.45	1.52
1	F	60	CYS	CA-C	-5.25	1.47	1.53
1	F	20	HIS	CG-CD2	5.17	1.41	1.35
1	A	20	HIS	CG-CD2	5.15	1.41	1.35
1	C	37	GLN	CA-C	-5.10	1.47	1.53
1	G	27	ARG	N-CA	-5.10	1.41	1.46
1	B	217	LYS	N-CA	-5.03	1.38	1.46
1	F	20	HIS	ND1-CE1	5.01	1.37	1.32

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	128	LYS	N-CA-C	-10.01	101.07	113.28
1	C	214	GLY	N-CA-C	-8.99	97.51	110.91
1	E	49	VAL	N-CA-C	-8.93	104.45	113.47
1	F	185	ASP	CA-C-N	-8.84	108.78	119.84
1	F	185	ASP	C-N-CA	-8.84	108.78	119.84
1	D	171	PHE	N-CA-C	8.56	121.32	108.31
1	F	84	ILE	CA-C-N	-8.46	112.15	120.52
1	F	84	ILE	C-N-CA	-8.46	112.15	120.52
1	G	127	SER	N-CA-C	8.42	122.88	107.73
1	H	185	ASP	CA-C-N	8.18	130.06	119.84
1	H	185	ASP	C-N-CA	8.18	130.06	119.84
1	I	185	ASP	CA-C-N	8.05	127.71	119.82
1	I	185	ASP	C-N-CA	8.05	127.71	119.82
1	H	132	LYS	CA-C-N	-7.87	112.59	120.31
1	H	132	LYS	C-N-CA	-7.87	112.59	120.31
1	B	141	GLY	N-CA-C	7.71	121.34	111.09
1	J	205	ASP	N-CA-C	7.59	119.55	110.44
1	B	127	SER	N-CA-C	7.38	121.73	112.87
1	D	102	ASN	N-CA-C	-7.36	101.35	111.28
1	I	43	ARG	N-CA-C	7.35	120.53	108.99
1	G	40	SER	N-CA-C	7.26	121.17	108.75
1	D	47	ILE	N-CA-C	7.24	118.54	108.12
1	F	191	THR	N-CA-C	7.21	119.11	108.14
1	H	152	THR	N-CA-C	-7.19	105.04	113.88
1	A	95	TYR	N-CA-C	7.16	120.13	111.40
1	C	110	GLU	N-CA-C	-7.12	104.46	113.01
1	F	214	GLY	N-CA-C	-7.10	100.33	110.63
1	K	120	ARG	CA-C-N	7.10	128.71	119.84
1	K	120	ARG	C-N-CA	7.10	128.71	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	GLY	N-CA-C	7.08	121.36	110.88
1	J	39	LYS	N-CA-C	-7.06	103.75	113.56
1	F	86	VAL	N-CA-C	6.98	117.55	106.32
1	B	17	ILE	CB-CA-C	-6.86	102.14	111.33
1	G	26	SER	N-CA-C	-6.85	106.81	114.62
1	J	38	GLU	N-CA-C	6.83	118.47	110.41
1	A	92	HIS	CA-C-N	6.82	128.36	119.84
1	A	92	HIS	C-N-CA	6.82	128.36	119.84
1	B	192	GLY	N-CA-C	-6.81	100.34	112.54
1	F	92	HIS	CA-C-N	6.73	128.25	119.84
1	F	92	HIS	C-N-CA	6.73	128.25	119.84
1	A	61	GLN	N-CA-C	6.57	118.44	109.11
1	A	23	LYS	N-CA-C	-6.57	101.29	109.64
1	A	159	LEU	N-CA-C	6.49	119.27	109.41
1	E	120	ARG	CA-C-N	-6.48	111.74	119.84
1	E	120	ARG	C-N-CA	-6.48	111.74	119.84
1	G	219	THR	CA-C-N	6.47	127.05	120.38
1	G	219	THR	C-N-CA	6.47	127.05	120.38
1	B	39	LYS	N-CA-C	-6.36	103.87	111.69
1	H	201	LEU	N-CA-C	-6.36	98.37	108.73
1	K	53	PHE	N-CA-C	6.35	119.86	109.06
1	H	61	GLN	N-CA-C	6.34	117.79	108.86
1	H	157	VAL	CB-CA-C	-6.33	101.20	110.62
1	A	154	LEU	N-CA-C	6.31	118.90	109.25
1	G	157	VAL	CB-CA-C	-6.24	101.07	110.55
1	D	86	VAL	N-CA-C	6.22	116.82	107.80
1	E	187	LYS	N-CA-C	-6.09	105.61	113.16
1	I	152	THR	N-CA-C	-6.09	105.89	113.38
1	D	222	GLY	N-CA-C	-6.05	101.87	111.18
1	B	198	GLY	N-CA-C	-6.04	95.77	113.30
1	L	92	HIS	CA-C-N	6.04	127.39	119.84
1	L	92	HIS	C-N-CA	6.04	127.39	119.84
1	B	217	LYS	N-CA-C	-6.01	100.58	109.11
1	E	61	GLN	N-CA-C	6.01	119.29	108.48
1	A	157	VAL	CB-CA-C	-5.98	101.61	110.82
1	G	49	VAL	N-CA-C	-5.97	106.43	113.42
1	I	116	THR	N-CA-C	-5.93	99.13	108.14
1	A	150	LEU	N-CA-C	5.93	118.90	109.24
1	D	174	ASN	N-CA-C	-5.91	104.96	111.82
1	F	88	ARG	N-CA-C	5.90	118.79	108.82
1	I	23	LYS	N-CA-C	-5.87	102.85	109.60
1	B	219	THR	CA-C-N	5.84	126.39	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	THR	C-N-CA	5.84	126.39	120.38
1	J	132	LYS	N-CA-C	5.83	118.73	109.64
1	D	117	THR	N-CA-C	-5.79	105.98	113.16
1	A	84	ILE	N-CA-C	5.75	113.56	107.76
1	B	65	ILE	N-CA-C	-5.75	101.39	109.21
1	I	149	THR	N-CA-C	5.74	119.04	110.14
1	J	84	ILE	N-CA-C	5.74	114.14	107.89
1	A	192	GLY	N-CA-C	-5.73	104.75	112.14
1	G	27	ARG	N-CA-C	-5.70	95.44	108.27
1	E	215	ASN	N-CA-C	5.67	117.85	110.43
1	G	71	ALA	CA-C-N	-5.64	114.80	121.90
1	G	71	ALA	C-N-CA	-5.64	114.80	121.90
1	G	225	ILE	N-CA-C	-5.63	101.92	109.30
1	H	137	CYS	N-CA-C	5.60	116.76	108.86
1	J	40	SER	N-CA-C	5.60	116.58	107.23
1	I	104	ILE	N-CA-C	-5.59	100.54	109.20
1	C	47	ILE	CA-C-N	-5.57	113.90	122.87
1	C	47	ILE	C-N-CA	-5.57	113.90	122.87
1	F	82	GLN	N-CA-C	-5.57	98.83	108.69
1	K	105	MET	N-CA-C	5.57	116.98	108.52
1	J	149	THR	N-CA-C	5.56	118.03	109.07
1	B	17	ILE	N-CA-C	5.56	116.17	108.84
1	D	171	PHE	CB-CA-C	-5.56	110.15	116.54
1	E	183	VAL	N-CA-C	5.55	120.88	109.34
1	E	67	VAL	N-CA-C	5.54	115.87	108.11
1	A	77	GLN	N-CA-C	5.54	118.05	107.75
1	C	105	MET	N-CA-C	5.50	117.45	108.55
1	F	222	GLY	N-CA-C	-5.49	103.09	112.64
1	A	216	LYS	N-CA-C	-5.48	99.80	108.73
1	F	206	VAL	N-CA-C	5.47	116.55	108.45
1	D	209	GLY	N-CA-C	5.47	119.27	111.12
1	D	53	PHE	N-CA-C	5.46	118.34	109.06
1	L	214	GLY	N-CA-C	-5.42	101.72	110.18
1	H	199	GLY	CA-C-N	5.42	125.89	120.14
1	H	199	GLY	C-N-CA	5.42	125.89	120.14
1	D	217	LYS	N-CA-C	-5.41	102.45	111.37
1	J	193	PHE	N-CA-C	5.41	115.38	108.24
1	H	52	ASP	N-CA-C	5.40	119.17	112.59
1	L	213	TYR	N-CA-C	5.38	115.23	108.45
1	L	141	GLY	N-CA-C	5.38	117.36	110.96
1	A	223	VAL	N-CA-C	5.36	116.49	109.58
1	C	45	GLY	N-CA-C	-5.36	104.42	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	189	THR	CB-CA-C	-5.36	100.39	110.67
1	J	166	GLN	N-CA-C	5.36	117.55	111.02
1	G	120	ARG	CA-C-N	-5.35	115.07	120.31
1	G	120	ARG	C-N-CA	-5.35	115.07	120.31
1	H	47	ILE	N-CA-C	5.34	116.28	108.53
1	E	127	SER	N-CA-C	-5.33	105.37	111.07
1	C	171	PHE	N-CA-C	-5.31	105.25	112.26
1	H	134	GLY	N-CA-C	-5.30	107.48	115.32
1	A	137	CYS	N-CA-C	5.29	117.86	109.50
1	B	190	GLN	N-CA-C	5.28	117.88	110.23
1	F	40	SER	N-CA-C	5.28	116.79	107.61
1	B	149	THR	N-CA-C	5.27	117.01	108.26
1	E	44	CYS	N-CA-C	5.24	117.04	109.07
1	A	42	LYS	N-CA-C	5.24	117.15	109.24
1	B	183	VAL	N-CA-C	5.22	116.23	108.46
1	A	49	VAL	N-CA-C	-5.21	108.76	113.71
1	L	47	ILE	N-CA-C	5.21	115.62	108.12
1	G	159	LEU	N-CA-C	-5.19	101.18	109.23
1	B	81	GLN	N-CA-C	5.18	118.00	109.76
1	H	180	GLU	N-CA-C	5.17	117.59	108.75
1	H	17	ILE	N-CA-C	5.16	115.90	108.93
1	L	185	ASP	CA-C-N	-5.16	114.30	119.56
1	L	185	ASP	C-N-CA	-5.16	114.30	119.56
1	C	181	ILE	CB-CA-C	-5.15	105.06	111.08
1	K	132	LYS	CA-C-N	-5.14	114.66	119.85
1	K	132	LYS	C-N-CA	-5.14	114.66	119.85
1	F	183	VAL	N-CA-C	5.11	116.01	108.45
1	F	19	GLY	N-CA-C	-5.07	101.16	113.18
1	K	130	GLN	N-CA-C	-5.07	100.01	110.80
1	J	183	VAL	N-CA-C	5.05	115.30	107.78
1	F	50	ARG	N-CA-C	-5.05	102.60	110.42
1	E	209	GLY	N-CA-C	5.02	118.41	112.33
1	A	50	ARG	N-CA-C	5.02	116.62	109.14
1	J	68	THR	N-CA-C	5.02	116.49	107.80
1	D	45	GLY	N-CA-C	-5.02	106.81	112.33
1	E	214	GLY	N-CA-C	-5.01	102.11	111.14
1	C	44	CYS	N-CA-C	5.01	116.69	109.07
1	F	120	ARG	CA-C-N	-5.01	115.44	120.85
1	F	120	ARG	C-N-CA	-5.01	115.44	120.85
1	G	227	VAL	N-CA-C	5.00	115.61	110.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASN	Peptide
1	B	126	SER	Peptide
1	B	197	SER	Peptide
1	G	127	SER	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	1754	0	1798	159	2
1	B	1769	0	1817	127	0
1	C	1769	0	1817	118	0
1	D	1769	0	1817	109	0
1	E	1769	0	1817	101	0
1	F	1769	0	1817	101	0
1	G	1769	0	1817	100	0
1	H	1732	0	1786	117	0
1	I	1769	0	1817	109	0
1	J	1769	0	1817	109	0
1	K	1769	0	1817	151	0
1	L	1769	0	1817	91	2
2	B	20	0	0	1	0
2	D	15	0	0	1	0
2	E	5	0	0	0	0
2	F	15	0	0	0	0
2	I	10	0	0	1	0
2	L	10	0	0	2	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	D	6	0	0	1	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	8	0	0	0	0
4	J	1	0	0	0	0
4	K	2	0	0	1	0
4	L	4	0	0	4	0
All	All	21292	0	21754	1350	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1350) 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)
1:B:233:TRP:O	1:B:237:THR:HG23	1.36	1.20
1:B:50:ARG:HD3	1:B:238:MET:HE2	1.24	1.18
1:H:61:GLN:HE22	1:H:91:PRO:HG3	1.07	1.17
1:B:19:GLY:HA3	1:B:157:VAL:HG12	1.21	1.15
1:L:37:GLN:HG3	1:L:42:LYS:HE2	1.20	1.13
1:H:16:ILE:HG21	1:H:155:GLN:HB2	1.20	1.12
1:F:16:ILE:HG21	1:F:157:VAL:HG13	1.31	1.12
1:B:91:PRO:HB3	1:B:105:MET:HE3	1.32	1.11
1:C:16:ILE:HG21	1:C:145:VAL:HA	1.29	1.09
1:B:19:GLY:HA3	1:B:157:VAL:CG1	1.83	1.09
1:B:50:ARG:HD3	1:B:238:MET:CE	1.84	1.06
1:G:84:ILE:HD13	1:G:111:ARG:HH21	0.93	1.05
1:G:38:GLU:O	1:G:38:GLU:HG2	1.53	1.04
1:E:183:VAL:HG21	1:E:224:TYR:CE2	1.92	1.03
1:B:19:GLY:CA	1:B:157:VAL:HG12	1.90	1.01
1:B:47:ILE:CG2	1:B:200:PRO:HG3	1.91	1.00
1:C:16:ILE:CG2	1:C:145:VAL:HA	1.92	1.00
1:D:134:GLY:O	1:H:83:PHE:HB3	1.61	1.00
1:G:84:ILE:HD13	1:G:111:ARG:NH2	1.78	0.98
1:B:47:ILE:HG23	1:B:200:PRO:HG3	1.45	0.98
1:A:17:ILE:HD11	1:A:193:PHE:CE2	1.98	0.98
1:B:117:THR:HA	1:B:120:ARG:HH21	1.30	0.96
1:E:143:GLY:HA3	1:E:196:ASP:OD1	1.65	0.95
1:D:36:LEU:HD12	1:D:40:SER:O	1.66	0.95
1:B:173:GLY:O	1:B:174:ASN:HB2	1.65	0.95
1:K:47:ILE:HG22	1:K:55:LEU:HB3	1.49	0.95
1:B:148:SER:HB2	1:J:168:GLU:OE2	1.67	0.94
1:C:58:ALA:O	1:C:61:GLN:HG3	1.68	0.94
1:H:16:ILE:HG21	1:H:155:GLN:CB	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HH22	1:A:138:SER:HB3	1.30	0.93
1:A:83:PHE:CD2	1:K:135:GLN:HA	2.04	0.93
1:E:96:ASN:HB3	1:E:99:ASN:OD1	1.69	0.93
1:G:84:ILE:CD1	1:G:111:ARG:HH21	1.81	0.91
1:F:19:GLY:HA3	1:F:157:VAL:HG12	1.49	0.91
1:D:134:GLY:C	1:H:83:PHE:HB3	1.94	0.91
1:A:72:HIS:O	1:A:153:THR:HA	1.69	0.91
1:D:115:TRP:HZ3	1:D:121:PRO:HD2	1.33	0.91
1:E:186:PRO:HA	1:E:220:PRO:HG2	1.53	0.90
1:A:138:SER:O	1:A:139:VAL:CG2	2.20	0.90
1:A:30:MET:HE1	1:A:200:PRO:CG	2.02	0.90
1:I:190:GLN:H	1:I:190:GLN:CD	1.79	0.90
1:L:19:GLY:HA3	1:L:157:VAL:HG12	1.51	0.90
1:B:91:PRO:HA	1:B:105:MET:HB2	1.55	0.89
1:D:143:GLY:HA3	1:D:196:ASP:OD1	1.72	0.89
1:K:50:ARG:HA	1:K:121:PRO:HB3	1.54	0.89
1:C:204:LYS:HD2	1:K:75:LYS:HZ2	1.36	0.89
1:L:19:GLY:CA	1:L:157:VAL:HG12	2.02	0.89
1:F:16:ILE:CG2	1:F:157:VAL:HG13	2.01	0.88
1:C:158:LEU:HD11	1:K:41:ARG:NH1	1.89	0.88
1:A:61:GLN:NE2	1:A:105:MET:SD	2.47	0.87
1:F:136:LEU:HD11	1:F:158:LEU:HB3	1.57	0.87
1:H:32:PHE:CE1	1:H:74:ILE:HD13	2.09	0.86
1:H:61:GLN:NE2	1:H:91:PRO:HG3	1.90	0.86
1:H:146:SER:HB3	1:H:149:THR:OG1	1.75	0.86
1:A:92:HIS:CG	1:A:93:PRO:HD2	2.11	0.86
1:A:17:ILE:HD11	1:A:193:PHE:HE2	1.38	0.85
1:D:172:HIS:C	1:D:174:ASN:H	1.81	0.85
1:K:28:PRO:HB3	1:K:120:ARG:H	1.42	0.84
1:J:20:HIS:CD2	1:L:39:LYS:HB2	2.12	0.84
1:H:25:HIS:O	1:H:28:PRO:HD3	1.78	0.84
1:C:158:LEU:HD11	1:K:41:ARG:HH11	1.42	0.83
1:A:59:HIS:HB3	1:A:95:TYR:OH	1.79	0.83
1:E:213:TYR:CE1	1:E:223:VAL:HG21	2.14	0.82
1:C:208:GLN:O	1:C:227:VAL:HG13	1.78	0.82
1:A:30:MET:HE1	1:A:200:PRO:HG3	1.61	0.82
1:A:49:VAL:HG23	1:A:50:ARG:HG3	1.62	0.82
1:H:16:ILE:CG2	1:H:155:GLN:HB2	2.07	0.82
1:D:115:TRP:CZ3	1:D:121:PRO:HD2	2.15	0.81
1:L:198:GLY:HA2	1:L:210:ILE:HG23	1.60	0.81
1:L:16:ILE:CG2	1:L:157:VAL:HG13	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:VAL:HG23	1:D:200:PRO:O	1.80	0.81
1:I:43:ARG:O	1:I:195:GLY:HA2	1.81	0.81
1:L:166:GLN:OE1	1:L:186:PRO:HG3	1.80	0.81
1:F:52:ASP:OD1	1:F:53:PHE:CD2	2.34	0.81
1:J:19:GLY:HA2	1:J:157:VAL:HG13	1.61	0.81
1:J:234:ILE:O	1:J:238:MET:HB2	1.81	0.81
1:L:225:ILE:HG23	1:L:230:PHE:HE2	1.45	0.81
1:D:58:ALA:HA	1:D:105:MET:HB2	1.64	0.80
1:B:124:LEU:HD12	1:B:124:LEU:N	1.97	0.80
1:E:183:VAL:HG21	1:E:224:TYR:CD2	2.17	0.80
1:B:125:PRO:HD3	1:B:206:VAL:HG13	1.62	0.80
1:E:55:LEU:HD12	1:E:106:LEU:CD2	2.12	0.80
1:C:16:ILE:HG21	1:C:145:VAL:CA	2.11	0.79
1:A:135:GLN:O	1:A:161:VAL:HG23	1.82	0.79
1:D:172:HIS:C	1:D:174:ASN:N	2.38	0.79
1:A:27:ARG:HB3	1:A:29:TYR:CE2	2.18	0.79
1:D:181:ILE:HD12	1:D:226:LYS:HG2	1.62	0.79
1:F:225:ILE:HG23	1:F:230:PHE:HE2	1.46	0.79
1:H:43:ARG:NH1	1:H:142:TRP:O	2.15	0.79
1:J:78:GLU:HB2	1:J:81:GLN:OE1	1.83	0.79
1:A:94:ALA:HB1	1:A:102:ASN:CB	2.13	0.78
1:B:48:LEU:HD22	1:B:69:LEU:HD13	1.65	0.78
1:G:67:VAL:HG12	1:G:84:ILE:O	1.83	0.78
1:A:23:LYS:O	1:A:26:SER:HB2	1.84	0.78
1:F:105:MET:HE3	1:F:107:LEU:HD21	1.64	0.78
1:A:47:ILE:HG21	1:A:200:PRO:HB3	1.65	0.78
1:I:155:GLN:HA	1:I:155:GLN:OE1	1.83	0.78
1:G:32:PHE:HB3	1:G:68:THR:HG23	1.66	0.77
1:C:204:LYS:HD2	1:K:75:LYS:NZ	1.98	0.77
1:E:50:ARG:HB3	1:E:53:PHE:HB2	1.67	0.77
1:K:47:ILE:CG2	1:K:55:LEU:HB3	2.13	0.77
1:C:30:MET:HE2	1:C:140:ALA:O	1.85	0.77
1:A:138:SER:O	1:A:139:VAL:HG23	1.84	0.77
1:J:21:GLU:HG3	1:J:153:THR:HG21	1.67	0.77
1:C:99:ASN:ND2	1:C:101:SER:OG	2.17	0.76
1:L:19:GLY:HA3	1:L:157:VAL:CG1	2.15	0.76
1:E:55:LEU:CD1	1:E:106:LEU:HD21	2.14	0.76
1:L:135:GLN:HE21	1:L:203:CYS:HB3	1.49	0.76
1:A:86:VAL:CG1	1:A:107:LEU:HD21	2.16	0.76
1:H:166:GLN:O	1:H:170:LEU:HD12	1.86	0.76
1:K:48:LEU:HD22	1:K:121:PRO:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:LEU:HD11	1:H:205:ASP:O	1.85	0.76
1:J:104:ILE:HD12	1:J:225:ILE:HG21	1.67	0.76
1:K:202:VAL:HG12	1:K:202:VAL:O	1.86	0.76
1:I:193:PHE:O	1:I:196:ASP:HB2	1.84	0.76
1:F:16:ILE:CG2	1:F:157:VAL:CG1	2.65	0.75
1:L:38:GLU:O	1:L:39:LYS:HG2	1.86	0.75
1:E:55:LEU:HD11	1:E:104:ILE:HD11	1.67	0.75
1:F:87:LYS:HB2	1:F:110:GLU:HA	1.67	0.75
1:F:26:SER:O	1:F:28:PRO:HD3	1.87	0.75
1:L:164:ASP:O	1:L:168:GLU:HG3	1.87	0.75
1:L:40:SER:CB	4:L:404:HOH:O	2.35	0.75
1:C:231:LEU:N	1:C:232:PRO:HD2	2.01	0.75
1:K:59:HIS:CE1	1:K:197:SER:HB3	2.22	0.75
1:B:127:SER:C	1:B:129:ALA:N	2.41	0.74
1:J:38:GLU:O	1:J:39:LYS:HB3	1.87	0.74
1:J:48:LEU:HD22	1:J:69:LEU:HD22	1.66	0.74
1:B:171:PHE:CD2	1:B:213:TYR:HE1	2.06	0.74
1:G:47:ILE:CG2	1:G:200:PRO:HG3	2.16	0.74
1:H:86:VAL:HG12	1:H:109:LEU:HD23	1.70	0.74
1:A:138:SER:O	1:A:139:VAL:HG22	1.87	0.74
1:B:117:THR:HA	1:B:120:ARG:NH2	2.03	0.74
1:D:116:THR:HG22	1:D:118:ALA:H	1.51	0.74
1:C:158:LEU:CD1	1:K:41:ARG:HH11	2.01	0.73
1:C:51:LYS:NZ	1:I:239:LYS:O	2.19	0.73
1:A:59:HIS:CB	1:A:95:TYR:OH	2.37	0.73
1:C:185:ASP:OD1	1:C:185:ASP:N	2.20	0.73
1:E:166:GLN:HA	1:E:169:ARG:HH12	1.53	0.73
1:B:19:GLY:CA	1:B:157:VAL:CG1	2.55	0.73
1:H:61:GLN:HE22	1:H:91:PRO:CG	1.96	0.73
1:L:135:GLN:NE2	1:L:203:CYS:HB3	2.03	0.73
1:A:164:ASP:HB3	1:A:175:TYR:HE2	1.54	0.73
1:I:27:ARG:NH1	1:I:29:TYR:OH	2.22	0.72
1:I:215:ASN:HD21	1:I:217:LYS:HB2	1.52	0.72
1:B:37:GLN:O	1:B:37:GLN:HG3	1.87	0.72
1:D:133:PRO:HA	1:D:161:VAL:CG1	2.18	0.72
1:F:37:GLN:HG3	1:F:42:LYS:HE2	1.70	0.72
1:H:16:ILE:CG2	1:H:155:GLN:CB	2.66	0.72
1:F:38:GLU:O	1:F:39:LYS:HG2	1.88	0.72
1:L:22:ALA:HB2	1:L:156:GLU:HG2	1.70	0.72
1:K:190:GLN:O	1:K:191:THR:HB	1.87	0.72
1:F:126:SER:HB3	1:F:130:GLN:NE2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:LYS:HB3	1:G:112:LYS:HB2	1.71	0.72
1:F:88:ARG:HH11	1:G:240:ARG:HH21	1.35	0.72
1:B:215:ASN:HB3	1:B:219:THR:OG1	1.90	0.71
1:J:19:GLY:CA	1:J:157:VAL:HG13	2.20	0.71
1:B:127:SER:C	1:B:129:ALA:H	1.95	0.71
1:J:38:GLU:O	1:J:39:LYS:CB	2.37	0.71
1:F:126:SER:HB3	1:F:130:GLN:HE22	1.55	0.71
1:C:47:ILE:HD11	1:C:122:LEU:HB3	1.73	0.71
1:G:17:ILE:HD11	1:G:193:PHE:CD2	2.26	0.71
1:G:47:ILE:HG21	1:G:200:PRO:HG3	1.73	0.71
1:L:16:ILE:HG21	1:L:157:VAL:HG13	1.73	0.71
1:H:84:ILE:HG21	1:H:109:LEU:HB3	1.73	0.71
1:C:23:LYS:O	1:C:24:PRO:C	2.31	0.71
1:J:169:ARG:HG2	1:J:170:LEU:HD23	1.73	0.71
1:H:188:LYS:HG2	1:H:190:GLN:HE22	1.55	0.70
1:I:47:ILE:HG12	1:I:49:VAL:HG12	1.72	0.70
1:B:198:GLY:HA3	1:B:210:ILE:HG23	1.72	0.70
1:B:128:LYS:HG2	1:G:79:ARG:NH1	2.07	0.70
1:I:211:LEU:HD13	1:I:224:TYR:CE2	2.26	0.70
1:E:55:LEU:HD12	1:E:106:LEU:HD23	1.72	0.70
1:H:201:LEU:HD23	1:H:224:TYR:CD1	2.27	0.70
1:J:19:GLY:HA2	1:J:157:VAL:CG1	2.21	0.70
1:A:84:ILE:N	1:A:84:ILE:HD12	2.07	0.70
1:D:162:GLN:NE2	1:D:185:ASP:HA	2.07	0.70
1:E:55:LEU:HD13	1:E:106:LEU:HD21	1.72	0.70
1:G:125:PRO:HB2	1:G:127:SER:HB2	1.73	0.70
1:C:209:GLY:O	1:C:210:ILE:HD12	1.91	0.70
1:J:38:GLU:OE1	1:J:38:GLU:HA	1.89	0.70
1:E:209:GLY:HA2	1:E:227:VAL:HG23	1.74	0.70
1:F:145:VAL:HG23	1:F:146:SER:H	1.57	0.70
1:C:96:ASN:HB3	1:C:99:ASN:O	1.92	0.69
1:C:208:GLN:C	1:C:227:VAL:HG13	2.16	0.69
1:J:95:TYR:HA	1:J:102:ASN:HB2	1.74	0.69
1:B:91:PRO:CB	1:B:105:MET:HE3	2.15	0.69
1:G:30:MET:HE2	1:G:154:LEU:HD11	1.73	0.69
1:A:61:GLN:HE22	1:A:91:PRO:HG3	1.56	0.69
1:K:229:HIS:O	1:K:229:HIS:ND1	2.25	0.69
1:C:209:GLY:HA2	1:C:225:ILE:O	1.92	0.69
1:C:99:ASN:C	1:C:99:ASN:HD22	2.00	0.69
1:K:51:LYS:HZ2	1:K:115:TRP:HB3	1.58	0.69
1:J:197:SER:HA	1:J:211:LEU:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:THR:HB	1:C:220:PRO:HD3	1.73	0.68
1:I:47:ILE:HG12	1:I:49:VAL:CG1	2.23	0.68
1:K:116:THR:HB	1:K:119:VAL:HG13	1.75	0.68
1:J:124:LEU:HB3	1:J:125:PRO:HD2	1.74	0.68
1:A:157:VAL:HG11	1:A:190:GLN:HB3	1.75	0.68
1:F:37:GLN:O	1:F:38:GLU:HG3	1.93	0.68
1:G:32:PHE:HB3	1:G:68:THR:CG2	2.23	0.68
1:B:136:LEU:HD13	1:B:158:LEU:HD23	1.74	0.68
1:K:146:SER:HB3	1:K:149:THR:OG1	1.93	0.68
1:C:30:MET:HE1	1:C:200:PRO:CD	2.23	0.68
1:H:57:ALA:H	1:H:198:GLY:HA2	1.59	0.68
1:H:184:GLY:H	1:H:222:GLY:H	1.38	0.68
1:B:37:GLN:HA	1:B:38:GLU:HG3	1.76	0.68
1:D:95:TYR:HA	1:D:101:SER:O	1.93	0.68
1:F:84:ILE:N	1:F:84:ILE:HD12	2.08	0.68
1:A:27:ARG:NH2	1:A:138:SER:HB3	2.07	0.67
1:J:84:ILE:HG22	1:J:85:PRO:O	1.94	0.67
1:E:115:TRP:CH2	1:E:121:PRO:HG3	2.29	0.67
1:L:40:SER:HB3	4:L:404:HOH:O	1.94	0.67
1:B:120:ARG:HB2	1:B:121:PRO:HD3	1.76	0.67
1:J:137:CYS:HB2	1:J:201:LEU:HD11	1.76	0.67
1:L:203:CYS:O	1:L:204:LYS:HB2	1.94	0.67
1:E:29:TYR:O	1:E:47:ILE:HA	1.95	0.67
1:B:32:PHE:CD2	1:B:74:ILE:HD11	2.29	0.67
1:E:183:VAL:HG21	1:E:224:TYR:HE2	1.59	0.67
1:L:40:SER:HB2	4:L:404:HOH:O	1.93	0.67
1:E:215:ASN:HB3	1:E:217:LYS:HG2	1.76	0.67
1:G:136:LEU:HD13	1:G:160:THR:HG22	1.75	0.67
1:J:144:TYR:CE2	1:J:150:LEU:HD13	2.29	0.67
1:B:53:PHE:CB	1:B:238:MET:HE3	2.25	0.66
1:K:134:GLY:HA2	1:K:160:THR:HG23	1.77	0.66
1:H:33:VAL:HG22	1:H:67:VAL:HG22	1.77	0.66
1:I:105:MET:HE3	1:I:107:LEU:CD2	2.25	0.66
1:B:80:THR:HB	1:B:118:ALA:CB	2.24	0.66
1:A:233:TRP:O	1:A:237:THR:HG22	1.94	0.66
1:C:38:GLU:O	1:C:39:LYS:HG2	1.96	0.66
1:E:166:GLN:HA	1:E:169:ARG:NH1	2.11	0.66
1:I:212:SER:HG	1:I:213:TYR:HD2	1.40	0.66
1:D:72:HIS:O	1:D:153:THR:HA	1.96	0.66
1:G:127:SER:HA	1:G:129:ALA:H	1.61	0.66
1:J:72:HIS:NE2	1:J:153:THR:HG23	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:LEU:HD12	1:K:209:GLY:HA3	1.77	0.66
1:F:124:LEU:HB3	1:F:125:PRO:CD	2.26	0.66
1:A:53:PHE:CE1	1:A:108:GLN:HB3	2.30	0.65
1:G:142:TRP:CZ2	1:G:154:LEU:HD13	2.31	0.65
1:J:215:ASN:OD1	1:J:219:THR:N	2.29	0.65
1:A:133:PRO:HG3	1:A:162:GLN:O	1.96	0.65
1:G:211:LEU:HD13	1:G:224:TYR:CZ	2.31	0.65
1:B:69:LEU:HB3	1:B:119:VAL:HG13	1.77	0.65
1:B:115:TRP:CZ3	1:B:121:PRO:HD3	2.30	0.65
1:E:55:LEU:CD1	1:E:106:LEU:CD2	2.74	0.65
1:H:184:GLY:H	1:H:222:GLY:N	1.94	0.65
1:C:38:GLU:C	1:C:40:SER:H	2.05	0.65
1:I:105:MET:HE3	1:I:107:LEU:HD21	1.79	0.65
1:B:53:PHE:HB2	1:B:238:MET:HE3	1.77	0.65
1:L:84:ILE:HG21	1:L:109:LEU:HB3	1.78	0.65
1:L:171:PHE:O	1:L:174:ASN:HB2	1.97	0.65
1:G:22:ALA:HB2	1:G:156:GLU:HG2	1.77	0.65
1:J:27:ARG:NE	1:J:156:GLU:OE1	2.27	0.65
1:I:155:GLN:OE1	1:I:155:GLN:CA	2.44	0.65
1:K:212:SER:O	1:K:213:TYR:HB3	1.96	0.65
1:F:19:GLY:CA	1:F:157:VAL:HG12	2.26	0.64
1:G:233:TRP:O	1:G:237:THR:HB	1.97	0.64
1:J:23:LYS:HB3	1:J:26:SER:OG	1.97	0.64
1:K:98:LYS:C	1:K:100:PHE:H	2.05	0.64
1:B:233:TRP:O	1:B:237:THR:CG2	2.30	0.64
1:G:87:LYS:HD2	1:G:108:GLN:OE1	1.97	0.64
1:J:103:ASP:H	1:J:225:ILE:HD11	1.61	0.64
1:C:168:GLU:O	1:C:172:HIS:HA	1.98	0.64
1:F:16:ILE:HG21	1:F:157:VAL:CG1	2.16	0.64
1:F:84:ILE:HG21	1:F:109:LEU:HB3	1.79	0.64
1:L:78:GLU:HB2	1:L:81:GLN:OE1	1.98	0.64
1:F:55:LEU:HG	1:F:210:ILE:HD11	1.79	0.64
1:C:53:PHE:HA	1:C:107:LEU:O	1.98	0.64
1:D:137:CYS:CB	1:D:201:LEU:HD11	2.27	0.64
1:C:204:LYS:CD	1:K:75:LYS:NZ	2.61	0.64
1:H:16:ILE:HB	1:H:196:ASP:OD2	1.98	0.64
1:B:191:THR:HB	1:B:220:PRO:HD3	1.79	0.64
1:K:19:GLY:HA3	1:K:157:VAL:HG22	1.80	0.64
1:A:30:MET:HE3	1:A:140:ALA:HB3	1.80	0.63
1:I:238:MET:O	1:I:241:LEU:HD23	1.98	0.63
1:A:93:PRO:C	1:A:95:TYR:H	2.05	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:50:ARG:HD2	1:J:52:ASP:OD1	1.98	0.63
1:A:85:PRO:HB2	1:A:110:GLU:HB2	1.80	0.63
1:A:226:LYS:HD3	1:A:229:HIS:CE1	2.34	0.63
1:B:231:LEU:HD21	1:B:235:LYS:NZ	2.13	0.63
1:C:136:LEU:HD12	1:C:160:THR:CG2	2.29	0.63
1:K:131:VAL:HG12	1:K:135:GLN:NE2	2.13	0.63
1:L:87:LYS:HB2	1:L:110:GLU:HA	1.79	0.63
1:I:131:VAL:HG12	1:J:77:GLN:HE22	1.64	0.63
1:I:190:GLN:CD	1:I:190:GLN:N	2.51	0.63
1:J:204:LYS:HB3	1:L:75:LYS:HD2	1.80	0.63
1:L:49:VAL:HG23	1:L:238:MET:HE1	1.81	0.63
1:C:20:HIS:O	1:C:155:GLN:HA	1.98	0.63
1:C:84:ILE:HG23	1:C:111:ARG:HG2	1.80	0.63
1:K:51:LYS:NZ	1:K:115:TRP:HB3	2.13	0.63
1:D:75:LYS:HG3	1:D:152:THR:HG22	1.78	0.63
1:K:73:ASN:ND2	1:K:152:THR:OG1	2.32	0.63
1:C:16:ILE:CD1	1:C:151:ALA:HB2	2.29	0.63
1:F:170:LEU:O	1:F:170:LEU:HD23	1.99	0.63
1:A:32:PHE:HE1	1:A:43:ARG:HD2	1.64	0.62
1:K:50:ARG:O	1:K:52:ASP:N	2.32	0.62
1:A:58:ALA:HA	1:A:105:MET:HB2	1.81	0.62
1:K:32:PHE:HD2	1:K:68:THR:CG2	2.12	0.62
1:K:44:CYS:HB3	1:K:197:SER:O	1.99	0.62
1:B:139:VAL:HG12	1:B:159:LEU:CD1	2.29	0.62
1:H:160:THR:O	1:H:183:VAL:O	2.17	0.62
1:A:27:ARG:HB3	1:A:29:TYR:CZ	2.34	0.62
1:C:20:HIS:ND1	1:K:39:LYS:HD2	2.15	0.62
1:G:51:LYS:HG3	1:G:115:TRP:CZ2	2.35	0.62
1:I:50:ARG:O	1:I:52:ASP:N	2.33	0.62
1:C:99:ASN:ND2	1:C:99:ASN:C	2.58	0.62
1:H:32:PHE:CE1	1:H:43:ARG:HD3	2.34	0.62
1:B:120:ARG:HB2	1:B:121:PRO:CD	2.30	0.62
1:L:17:ILE:O	1:L:190:GLN:HA	2.00	0.62
1:A:94:ALA:O	1:A:102:ASN:HB2	2.00	0.61
1:D:188:LYS:HG3	1:D:190:GLN:HG3	1.82	0.61
1:H:157:VAL:HG11	1:H:190:GLN:HB3	1.81	0.61
1:I:61:GLN:OE1	1:I:105:MET:SD	2.58	0.61
1:I:20:HIS:ND1	1:J:39:LYS:CG	2.63	0.61
1:E:84:ILE:HD13	1:E:109:LEU:HD23	1.81	0.61
1:D:33:VAL:O	1:D:43:ARG:HA	2.00	0.61
1:B:29:TYR:HA	1:B:120:ARG:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:HIS:HD2	1:C:103:ASP:OD2	1.84	0.61
1:E:165:CYS:O	1:E:169:ARG:HB2	2.01	0.61
1:I:208:GLN:O	1:I:227:VAL:HG13	2.01	0.61
1:J:104:ILE:HD12	1:J:225:ILE:CG2	2.30	0.61
1:K:231:LEU:N	1:K:232:PRO:HD2	2.16	0.61
1:A:122:LEU:HD21	1:A:207:ALA:HB2	1.83	0.61
1:C:59:HIS:CD2	1:C:100:PHE:CE2	2.89	0.61
1:H:89:PRO:O	1:H:91:PRO:HD3	2.00	0.61
1:D:103:ASP:HB3	1:D:225:ILE:HD11	1.82	0.61
1:F:34:GLN:OE1	1:F:41:ARG:NH2	2.34	0.61
1:G:175:TYR:HA	1:G:180:GLU:OE1	2.00	0.61
1:A:86:VAL:HB	1:A:107:LEU:HD21	1.82	0.60
1:B:139:VAL:HG12	1:B:159:LEU:HD12	1.83	0.60
1:I:36:LEU:HD21	1:I:39:LYS:HA	1.83	0.60
1:A:30:MET:CE	1:A:200:PRO:HG3	2.30	0.60
1:A:181:ILE:HB	1:A:224:TYR:HB2	1.82	0.60
1:I:95:TYR:HA	1:I:101:SER:O	2.01	0.60
1:L:126:SER:HB3	1:L:130:GLN:HE22	1.66	0.60
1:L:145:VAL:HG23	1:L:146:SER:H	1.66	0.60
1:G:144:TYR:CD2	1:G:150:LEU:HD13	2.36	0.60
1:K:28:PRO:CB	1:K:120:ARG:H	2.12	0.60
1:A:170:LEU:HD22	1:A:221:PRO:HD2	1.83	0.60
1:E:19:GLY:HA2	1:E:157:VAL:HG23	1.81	0.60
1:F:142:TRP:CZ2	1:F:154:LEU:HB2	2.35	0.60
1:F:231:LEU:N	1:F:232:PRO:HD2	2.17	0.60
1:C:47:ILE:HD12	1:C:207:ALA:HB2	1.82	0.60
1:H:52:ASP:HA	1:H:109:LEU:HD12	1.84	0.60
1:G:43:ARG:NH1	1:G:142:TRP:O	2.33	0.60
1:J:21:GLU:CG	1:J:153:THR:HG21	2.31	0.60
1:A:86:VAL:HG12	1:A:107:LEU:HD21	1.83	0.60
1:C:135:GLN:HG3	1:K:83:PHE:CZ	2.36	0.60
1:J:73:ASN:HA	1:J:152:THR:O	2.00	0.60
1:B:131:VAL:HG11	1:B:181:ILE:HD13	1.82	0.60
1:F:99:ASN:O	1:F:100:PHE:HB2	2.02	0.60
1:J:140:ALA:HB2	1:J:156:GLU:HB3	1.82	0.60
1:K:49:VAL:HG23	1:K:50:ARG:H	1.66	0.60
1:G:27:ARG:HB3	1:G:29:TYR:CZ	2.37	0.60
1:I:131:VAL:HG12	1:J:77:GLN:NE2	2.16	0.60
1:I:183:VAL:HG21	1:I:201:LEU:HD21	1.82	0.60
1:K:200:PRO:HA	1:K:209:GLY:O	2.00	0.59
1:C:43:ARG:O	1:C:195:GLY:HA2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:GLN:O	1:H:160:THR:HA	2.02	0.59
1:B:168:GLU:HG2	1:B:175:TYR:HD2	1.68	0.59
1:D:34:GLN:HA	1:D:42:LYS:O	2.01	0.59
1:K:57:ALA:HA	1:K:103:ASP:O	2.02	0.59
1:E:190:GLN:O	1:E:191:THR:HB	2.00	0.59
1:J:17:ILE:HG22	1:J:18:GLY:N	2.15	0.59
1:K:196:ASP:HB2	1:K:211:LEU:HD23	1.84	0.59
1:G:72:HIS:CE1	1:G:153:THR:HB	2.38	0.59
1:I:211:LEU:HD12	1:I:212:SER:N	2.17	0.59
1:C:30:MET:HE1	1:C:200:PRO:HD3	1.83	0.59
1:H:47:ILE:HD11	1:H:122:LEU:HB3	1.84	0.59
1:L:225:ILE:CG2	1:L:230:PHE:HE2	2.15	0.59
1:E:137:CYS:CB	1:E:201:LEU:CD1	2.81	0.59
1:E:209:GLY:CA	1:E:227:VAL:HG23	2.32	0.59
1:F:52:ASP:OD1	1:F:53:PHE:HD2	1.81	0.59
1:H:100:PHE:O	1:H:103:ASP:HB2	2.03	0.59
1:J:20:HIS:CG	1:L:39:LYS:HB2	2.37	0.59
1:K:59:HIS:NE2	1:K:197:SER:CB	2.66	0.59
1:L:59:HIS:NE2	1:L:197:SER:HB3	2.18	0.59
1:I:211:LEU:HD12	1:I:212:SER:H	1.66	0.59
1:J:48:LEU:HD22	1:J:69:LEU:CD2	2.32	0.59
1:E:102:ASN:HD22	1:E:230:PHE:HZ	1.51	0.58
1:F:73:ASN:HA	1:F:153:THR:HG22	1.85	0.58
1:J:110:GLU:OE2	1:J:111:ARG:HG3	2.03	0.58
1:F:179:THR:O	1:F:226:LYS:HB3	2.03	0.58
1:B:124:LEU:HB3	1:B:125:PRO:HD2	1.84	0.58
1:E:73:ASN:OD1	1:E:75:LYS:N	2.36	0.58
1:E:137:CYS:HB3	1:E:201:LEU:HD12	1.85	0.58
1:I:114:LYS:O	1:I:116:THR:HG23	2.03	0.58
1:J:134:GLY:HA3	1:L:83:PHE:O	2.02	0.58
1:K:130:GLN:HG2	1:K:131:VAL:N	2.17	0.58
1:K:185:ASP:OD1	1:K:187:LYS:HG2	2.03	0.58
1:L:19:GLY:HA2	1:L:157:VAL:HG12	1.82	0.58
1:L:233:TRP:O	1:L:237:THR:HG22	2.03	0.58
1:D:172:HIS:HB3	1:D:174:ASN:HB2	1.86	0.58
1:C:183:VAL:HG11	1:C:224:TYR:CD2	2.39	0.58
1:A:62:GLY:O	1:A:65:ILE:HG13	2.03	0.58
1:A:83:PHE:CD1	1:K:135:GLN:HG2	2.39	0.58
1:B:48:LEU:CD2	1:B:69:LEU:HD13	2.33	0.58
1:G:24:PRO:HB3	1:G:72:HIS:CD2	2.39	0.58
1:B:56:THR:HG23	1:B:57:ALA:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:SER:OG	1:C:213:TYR:HD2	1.86	0.58
1:E:22:ALA:HB2	1:E:156:GLU:HG2	1.85	0.58
1:I:86:VAL:HG12	1:I:88:ARG:H	1.68	0.58
1:C:26:SER:O	1:C:28:PRO:HD3	2.04	0.58
1:C:84:ILE:CG2	1:C:111:ARG:HG2	2.34	0.58
1:G:237:THR:HG23	1:G:237:THR:O	2.03	0.58
1:I:171:PHE:C	1:I:173:GLY:H	2.12	0.58
1:J:131:VAL:HA	1:L:77:GLN:NE2	2.18	0.58
1:D:132:LYS:NZ	1:H:79:ARG:O	2.32	0.57
1:F:142:TRP:CE2	1:F:154:LEU:HB2	2.39	0.57
1:I:215:ASN:ND2	1:I:217:LYS:H	2.02	0.57
1:K:16:ILE:N	1:K:144:TYR:O	2.37	0.57
1:A:88:ARG:NH1	1:A:90:ILE:HG12	2.19	0.57
1:H:17:ILE:HD11	1:H:193:PHE:CD2	2.39	0.57
1:G:138:SER:HB3	1:G:158:LEU:HD23	1.86	0.57
1:I:52:ASP:HA	1:I:109:LEU:HD12	1.87	0.57
1:K:29:TYR:HB3	1:K:122:LEU:HB2	1.86	0.57
1:F:16:ILE:HG22	1:F:157:VAL:CG1	2.34	0.57
1:K:76:GLU:HB2	1:K:78:GLU:OE1	2.04	0.57
1:C:124:LEU:N	1:C:124:LEU:HD22	2.20	0.57
1:H:211:LEU:HD12	1:H:212:SER:N	2.18	0.57
1:L:99:ASN:O	1:L:100:PHE:HB2	2.03	0.57
1:A:30:MET:HE1	1:A:200:PRO:CD	2.34	0.57
1:A:94:ALA:HB1	1:A:102:ASN:CG	2.30	0.57
1:A:212:SER:HB2	1:A:225:ILE:HD11	1.87	0.57
1:D:144:TYR:CD2	1:D:150:LEU:HD13	2.40	0.57
1:D:172:HIS:CB	1:D:174:ASN:HB2	2.34	0.57
1:I:171:PHE:C	1:I:173:GLY:N	2.61	0.57
1:B:136:LEU:HD22	1:B:158:LEU:HB3	1.86	0.57
1:B:170:LEU:O	1:B:170:LEU:HD23	2.04	0.57
1:E:181:ILE:HG22	1:E:183:VAL:CG1	2.34	0.57
1:K:32:PHE:HD2	1:K:68:THR:HG23	1.69	0.57
1:K:55:LEU:HD12	1:K:105:MET:O	2.05	0.57
1:D:36:LEU:HD12	1:D:40:SER:C	2.29	0.56
1:D:52:ASP:OD1	1:D:53:PHE:HD2	1.88	0.56
1:E:185:ASP:O	1:E:188:LYS:HB2	2.04	0.56
1:L:43:ARG:NH1	2:L:301:SO4:O4	2.38	0.56
1:C:162:GLN:HG3	1:C:184:GLY:O	2.06	0.56
1:E:137:CYS:CB	1:E:201:LEU:HD11	2.35	0.56
1:J:50:ARG:HG2	1:J:51:LYS:H	1.68	0.56
1:D:137:CYS:HB2	1:D:201:LEU:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:THR:O	1:G:237:THR:CG2	2.53	0.56
1:J:21:GLU:CD	1:J:153:THR:HG21	2.30	0.56
1:J:43:ARG:NH1	1:J:150:LEU:HG	2.21	0.56
1:L:240:ARG:O	1:L:241:LEU:HB2	2.05	0.56
1:A:86:VAL:CB	1:A:107:LEU:HD21	2.36	0.56
1:E:73:ASN:N	1:E:78:GLU:OE2	2.34	0.56
1:H:232:PRO:O	1:H:236:ARG:HB2	2.05	0.56
1:L:231:LEU:N	1:L:232:PRO:HD2	2.21	0.56
1:F:47:ILE:O	1:F:54:VAL:HG13	2.05	0.56
1:I:27:ARG:HB3	1:I:29:TYR:CZ	2.41	0.56
1:I:131:VAL:CG1	1:I:208:GLN:HG3	2.35	0.56
1:I:231:LEU:N	1:I:232:PRO:HD2	2.21	0.56
1:J:236:ARG:O	1:J:240:ARG:HB3	2.06	0.56
1:F:59:HIS:NE2	1:F:197:SER:HB3	2.20	0.56
1:I:95:TYR:HB2	1:I:102:ASN:O	2.05	0.56
1:J:116:THR:C	1:J:118:ALA:N	2.62	0.56
1:L:68:THR:HG22	1:L:71:ALA:HB2	1.87	0.56
1:F:16:ILE:HG22	1:F:157:VAL:HG11	1.88	0.56
1:J:23:LYS:O	1:J:24:PRO:C	2.48	0.56
1:A:31:ALA:HB1	1:A:67:VAL:CG1	2.36	0.56
1:A:47:ILE:CG2	1:A:200:PRO:HB3	2.36	0.56
1:L:193:PHE:O	1:L:194:LYS:C	2.48	0.56
1:A:83:PHE:CG	1:K:135:GLN:HG2	2.41	0.56
1:H:84:ILE:CG2	1:H:109:LEU:HB3	2.36	0.56
1:K:146:SER:C	1:K:148:SER:H	2.14	0.56
1:D:165:CYS:SG	1:D:166:GLN:N	2.79	0.55
1:D:204:LYS:HE3	1:H:81:GLN:HE22	1.71	0.55
1:G:104:ILE:HB	1:G:225:ILE:HG21	1.88	0.55
1:B:91:PRO:O	1:B:92:HIS:C	2.48	0.55
1:C:142:TRP:CH2	1:C:154:LEU:HD13	2.40	0.55
1:D:27:ARG:NH1	1:D:29:TYR:OH	2.38	0.55
1:D:29:TYR:HB2	1:D:47:ILE:HG13	1.89	0.55
1:D:65:ILE:O	1:D:86:VAL:HG22	2.05	0.55
1:E:27:ARG:HB3	1:E:30:MET:HG2	1.88	0.55
1:G:211:LEU:HD13	1:G:224:TYR:CE2	2.40	0.55
1:H:16:ILE:N	1:H:144:TYR:O	2.38	0.55
1:I:189:THR:O	1:I:191:THR:HG22	2.06	0.55
1:J:92:HIS:ND1	1:J:93:PRO:HD2	2.21	0.55
1:B:50:ARG:CD	1:B:238:MET:CE	2.72	0.55
1:D:216:LYS:O	1:D:217:LYS:C	2.49	0.55
1:D:135:GLN:HA	1:H:83:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LEU:HD11	1:E:69:LEU:HD22	1.88	0.55
1:D:115:TRP:HZ3	1:D:121:PRO:CD	2.15	0.55
1:E:137:CYS:HB2	1:E:201:LEU:HD11	1.88	0.55
1:H:184:GLY:HA3	1:H:221:PRO:HA	1.88	0.55
1:I:73:ASN:HA	1:I:152:THR:O	2.06	0.55
1:I:87:LYS:O	1:I:88:ARG:HB2	2.06	0.55
1:C:38:GLU:C	1:C:40:SER:N	2.63	0.55
1:F:91:PRO:HA	1:F:105:MET:HG3	1.88	0.55
1:I:20:HIS:ND1	1:J:39:LYS:HG2	2.21	0.55
1:J:57:ALA:H	1:J:198:GLY:HA2	1.71	0.55
1:F:225:ILE:HG23	1:F:230:PHE:CE2	2.35	0.55
1:I:20:HIS:ND1	1:J:39:LYS:HG3	2.22	0.55
1:K:215:ASN:O	1:K:218:GLY:HA2	2.06	0.55
1:E:129:ALA:HB1	1:E:208:GLN:HE22	1.72	0.55
1:I:183:VAL:HG21	1:I:201:LEU:CD2	2.36	0.55
1:B:107:LEU:O	1:B:109:LEU:HD13	2.07	0.55
1:C:38:GLU:O	1:C:40:SER:N	2.40	0.55
1:D:85:PRO:HG2	1:D:110:GLU:OE1	2.07	0.55
1:F:27:ARG:HB3	1:F:29:TYR:CE1	2.42	0.55
1:F:65:ILE:HG22	1:F:86:VAL:HG21	1.89	0.55
1:C:16:ILE:N	1:C:196:ASP:OD2	2.40	0.54
1:E:81:GLN:HE21	1:E:83:PHE:HE2	1.55	0.54
1:G:52:ASP:OD1	1:G:52:ASP:N	2.38	0.54
1:D:99:ASN:OD1	1:D:101:SER:HB2	2.07	0.54
1:A:20:HIS:CD2	1:A:156:GLU:HG3	2.42	0.54
1:E:86:VAL:HG11	1:E:107:LEU:HD13	1.90	0.54
1:E:179:THR:HG22	1:E:180:GLU:HG3	1.89	0.54
1:A:16:ILE:N	1:A:196:ASP:OD2	2.40	0.54
1:B:17:ILE:HG12	1:B:193:PHE:HB2	1.90	0.54
1:D:165:CYS:HA	1:D:168:GLU:OE2	2.08	0.54
1:F:55:LEU:HD13	1:F:106:LEU:HD21	1.89	0.54
1:F:137:CYS:HB2	1:F:201:LEU:HD11	1.88	0.54
1:I:85:PRO:HD2	1:I:110:GLU:OE2	2.07	0.54
1:I:158:LEU:HD21	1:J:41:ARG:HG2	1.90	0.54
1:B:136:LEU:HD13	1:B:158:LEU:CD2	2.37	0.54
1:G:29:TYR:CG	1:G:122:LEU:HB2	2.43	0.54
1:J:148:SER:HB2	1:J:149:THR:HG23	1.89	0.54
1:K:116:THR:HG22	1:K:117:THR:N	2.22	0.54
1:G:167:CYS:HB3	1:G:175:TYR:CD1	2.43	0.54
1:I:198:GLY:H	1:I:211:LEU:HB3	1.71	0.54
1:K:134:GLY:HA2	1:K:160:THR:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:126:SER:HB3	1:L:130:GLN:NE2	2.22	0.54
1:D:16:ILE:O	1:D:145:VAL:HA	2.08	0.54
1:F:166:GLN:OE1	1:F:186:PRO:HG3	2.06	0.54
1:J:18:GLY:HA3	1:J:190:GLN:HG3	1.89	0.54
1:K:51:LYS:O	1:K:113:ALA:HB3	2.07	0.54
1:K:196:ASP:HB2	1:K:211:LEU:CD2	2.36	0.54
1:K:202:VAL:O	1:K:202:VAL:CG1	2.56	0.54
1:F:55:LEU:HA	1:F:106:LEU:HD23	1.90	0.54
1:A:17:ILE:HD11	1:A:193:PHE:CD2	2.40	0.54
1:I:211:LEU:HD13	1:I:224:TYR:CZ	2.43	0.54
1:F:116:THR:HG22	1:F:117:THR:N	2.23	0.54
1:A:176:SER:O	1:A:178:ALA:N	2.42	0.53
1:E:215:ASN:HB3	1:E:217:LYS:CG	2.38	0.53
1:L:59:HIS:CE1	1:L:197:SER:HB3	2.43	0.53
1:L:133:PRO:HA	1:L:161:VAL:HG12	1.89	0.53
1:A:31:ALA:HB1	1:A:67:VAL:HG13	1.91	0.53
1:A:120:ARG:HG3	1:A:121:PRO:O	2.08	0.53
1:G:181:ILE:HG22	1:G:183:VAL:HG23	1.89	0.53
1:K:87:LYS:HG2	1:K:88:ARG:HG3	1.90	0.53
1:A:193:PHE:O	1:A:196:ASP:N	2.38	0.53
1:D:59:HIS:O	1:D:59:HIS:CD2	2.61	0.53
1:E:143:GLY:CA	1:E:196:ASP:OD1	2.47	0.53
1:G:136:LEU:CD1	1:G:160:THR:HG22	2.39	0.53
1:H:57:ALA:HB1	1:H:59:HIS:CE1	2.43	0.53
1:L:17:ILE:HG12	1:L:145:VAL:O	2.08	0.53
1:B:160:THR:O	1:B:161:VAL:C	2.52	0.53
1:F:52:ASP:C	1:F:109:LEU:HD12	2.34	0.53
1:L:16:ILE:CG2	1:L:157:VAL:CG1	2.85	0.53
1:A:84:ILE:CG2	1:A:109:LEU:HB3	2.38	0.53
1:G:189:THR:O	1:G:191:THR:HG22	2.08	0.53
1:H:191:THR:HB	1:H:220:PRO:HG3	1.90	0.53
1:J:17:ILE:CG2	1:J:18:GLY:N	2.71	0.53
1:J:116:THR:C	1:J:118:ALA:H	2.17	0.53
1:L:43:ARG:NH1	1:L:150:LEU:HD21	2.24	0.53
1:B:32:PHE:CD2	1:B:74:ILE:CD1	2.91	0.53
1:H:92:HIS:O	1:H:93:PRO:C	2.51	0.53
1:J:208:GLN:O	1:J:227:VAL:HG12	2.09	0.53
1:K:56:THR:HG22	1:K:57:ALA:O	2.09	0.53
1:K:227:VAL:O	1:K:230:PHE:N	2.38	0.53
1:A:55:LEU:HD22	1:A:234:ILE:HD11	1.89	0.53
1:A:138:SER:C	1:A:139:VAL:HG23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HB2	1:A:202:VAL:HG13	1.90	0.53
1:A:201:LEU:HB3	1:A:209:GLY:HA3	1.89	0.53
1:G:46:GLY:HA2	1:G:198:GLY:O	2.09	0.53
1:C:78:GLU:HB2	1:C:81:GLN:HG3	1.91	0.53
1:E:215:ASN:HD22	1:E:217:LYS:CE	2.22	0.53
1:K:204:LYS:O	1:K:206:VAL:HG22	2.09	0.53
1:A:16:ILE:HG13	1:A:157:VAL:CG2	2.39	0.53
1:A:193:PHE:HE1	1:A:194:LYS:HE2	1.74	0.53
1:E:18:GLY:HA3	1:E:190:GLN:HG3	1.91	0.53
1:I:212:SER:OG	1:I:213:TYR:HD2	1.91	0.53
1:J:190:GLN:CD	1:J:190:GLN:H	2.17	0.53
1:K:47:ILE:HG22	1:K:55:LEU:CB	2.32	0.53
1:L:78:GLU:C	1:L:80:THR:H	2.16	0.53
1:A:75:LYS:O	1:A:76:GLU:HG3	2.09	0.52
1:D:76:GLU:OE2	1:D:76:GLU:HA	2.08	0.52
1:D:193:PHE:CG	1:D:194:LYS:N	2.77	0.52
1:E:137:CYS:HB2	1:E:201:LEU:CD1	2.39	0.52
1:J:123:ARG:NH1	1:J:123:ARG:HB2	2.24	0.52
1:J:193:PHE:N	1:J:196:ASP:OD2	2.37	0.52
1:A:20:HIS:HD2	1:A:156:GLU:HG3	1.73	0.52
1:B:209:GLY:HA2	1:B:225:ILE:O	2.08	0.52
1:J:116:THR:HG22	1:J:117:THR:N	2.24	0.52
1:A:95:TYR:O	1:A:96:ASN:C	2.51	0.52
1:J:211:LEU:HB2	1:J:224:TYR:CE1	2.44	0.52
1:K:125:PRO:HG3	1:K:206:VAL:HB	1.92	0.52
1:D:88:ARG:HG2	1:D:108:GLN:HB3	1.90	0.52
1:E:227:VAL:O	1:E:228:SER:C	2.52	0.52
1:G:29:TYR:HA	1:G:120:ARG:O	2.09	0.52
1:G:37:GLN:O	1:G:38:GLU:OE2	2.27	0.52
1:A:225:ILE:HG22	1:A:230:PHE:CE2	2.44	0.52
1:B:50:ARG:NH1	1:B:238:MET:HB3	2.24	0.52
1:D:172:HIS:O	1:D:174:ASN:N	2.41	0.52
1:F:43:ARG:NH2	1:F:151:ALA:O	2.43	0.52
1:F:131:VAL:HG23	1:F:131:VAL:O	2.10	0.52
1:F:135:GLN:NE2	1:F:203:CYS:HB3	2.25	0.52
1:H:16:ILE:CG1	1:H:157:VAL:HG23	2.40	0.52
1:F:16:ILE:O	1:F:145:VAL:HA	2.10	0.52
1:H:131:VAL:HB	1:H:135:GLN:OE1	2.09	0.52
1:J:54:VAL:HG23	1:J:109:LEU:HD21	1.91	0.52
1:L:34:GLN:OE1	1:L:41:ARG:NH2	2.39	0.52
1:B:240:ARG:O	1:B:241:LEU:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:PHE:HB3	1:E:68:THR:HB	1.92	0.52
1:H:16:ILE:CG2	1:H:155:GLN:HG3	2.40	0.52
1:K:227:VAL:O	1:K:229:HIS:N	2.43	0.52
1:A:122:LEU:CD2	1:A:207:ALA:HB2	2.40	0.51
1:B:16:ILE:HD13	1:B:196:ASP:OD2	2.09	0.51
1:B:75:LYS:HE3	1:B:152:THR:HG22	1.92	0.51
1:B:79:ARG:H	1:B:79:ARG:NE	2.08	0.51
1:E:28:PRO:HB2	1:E:120:ARG:HB2	1.92	0.51
1:E:137:CYS:HB3	1:E:201:LEU:CD1	2.40	0.51
1:F:21:GLU:HG2	1:F:22:ALA:O	2.10	0.51
1:K:199:GLY:O	1:K:210:ILE:HA	2.09	0.51
1:A:96:ASN:O	1:A:96:ASN:CG	2.52	0.51
1:B:50:ARG:HH11	1:B:238:MET:HE2	1.75	0.51
1:C:183:VAL:CG1	1:C:224:TYR:CD2	2.94	0.51
1:C:231:LEU:N	1:C:232:PRO:CD	2.72	0.51
1:L:87:LYS:HB3	1:L:108:GLN:HG2	1.92	0.51
1:F:193:PHE:O	1:F:194:LYS:C	2.52	0.51
1:K:95:TYR:CE1	1:K:103:ASP:HB3	2.45	0.51
1:B:27:ARG:NE	1:B:156:GLU:OE1	2.44	0.51
1:C:124:LEU:HD22	1:C:124:LEU:H	1.76	0.51
1:D:230:PHE:O	1:D:234:ILE:HG13	2.10	0.51
1:F:88:ARG:NH1	1:G:240:ARG:HH21	2.07	0.51
1:G:171:PHE:O	1:G:172:HIS:C	2.52	0.51
1:B:19:GLY:HA2	1:B:157:VAL:HG12	1.87	0.51
1:F:59:HIS:ND1	1:F:103:ASP:OD2	2.36	0.51
1:A:94:ALA:HB1	1:A:102:ASN:HB2	1.89	0.51
1:H:50:ARG:HE	1:H:238:MET:HE3	1.76	0.51
1:A:93:PRO:C	1:A:95:TYR:N	2.66	0.51
1:B:91:PRO:HA	1:B:105:MET:CB	2.35	0.51
1:E:50:ARG:HD3	1:E:238:MET:HE3	1.92	0.51
1:K:51:LYS:HE2	1:K:121:PRO:HG3	1.93	0.51
1:B:139:VAL:HG22	1:B:140:ALA:N	2.26	0.51
1:A:43:ARG:NH1	1:A:150:LEU:HD23	2.26	0.51
1:B:61:GLN:CD	1:B:105:MET:HE1	2.36	0.51
1:H:29:TYR:HB2	1:H:47:ILE:HG13	1.93	0.51
1:J:193:PHE:HE1	1:J:218:GLY:HA3	1.75	0.51
1:D:133:PRO:HA	1:D:161:VAL:HG12	1.91	0.50
1:E:166:GLN:OE1	1:E:169:ARG:NH1	2.44	0.50
1:J:20:HIS:CG	1:L:39:LYS:CB	2.94	0.50
1:J:124:LEU:HB3	1:J:125:PRO:CD	2.42	0.50
1:K:73:ASN:HB3	1:K:76:GLU:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LYS:NZ	1:B:128:LYS:H	2.09	0.50
1:D:48:LEU:HD13	1:D:69:LEU:HD11	1.94	0.50
1:D:92:HIS:CD2	1:D:230:PHE:CE1	3.00	0.50
1:F:57:ALA:HB3	1:F:60:CYS:SG	2.51	0.50
1:L:73:ASN:HA	1:L:153:THR:HG22	1.92	0.50
1:B:117:THR:CA	1:B:120:ARG:HH21	2.13	0.50
1:C:30:MET:HE1	1:C:200:PRO:HD2	1.94	0.50
1:E:132:LYS:H	1:E:135:GLN:NE2	2.10	0.50
1:G:51:LYS:HE3	1:G:115:TRP:NE1	2.26	0.50
1:A:74:ILE:HG22	1:A:152:THR:O	2.11	0.50
1:A:93:PRO:O	1:A:95:TYR:N	2.45	0.50
1:B:131:VAL:CG1	1:B:181:ILE:HD13	2.41	0.50
1:C:171:PHE:O	1:C:172:HIS:C	2.55	0.50
1:D:171:PHE:CD1	1:D:172:HIS:N	2.80	0.50
1:E:211:LEU:HD13	1:E:224:TYR:CZ	2.46	0.50
1:H:83:PHE:O	1:H:111:ARG:NH1	2.43	0.50
1:J:16:ILE:CD1	1:J:141:GLY:N	2.75	0.50
1:J:29:TYR:CD2	1:J:122:LEU:HD13	2.46	0.50
1:K:28:PRO:HB3	1:K:120:ARG:N	2.20	0.50
1:K:58:ALA:H	1:K:103:ASP:HB2	1.76	0.50
1:L:78:GLU:O	1:L:80:THR:N	2.45	0.50
1:C:213:TYR:O	1:C:223:VAL:N	2.39	0.50
1:D:47:ILE:HD11	1:D:122:LEU:HB3	1.93	0.50
1:D:65:ILE:HB	1:D:86:VAL:CG2	2.41	0.50
1:G:124:LEU:HB3	1:G:125:PRO:HD2	1.92	0.50
1:K:84:ILE:HG21	1:K:109:LEU:HB3	1.93	0.50
1:A:32:PHE:CE1	1:A:43:ARG:HD2	2.45	0.50
1:A:88:ARG:HH11	1:A:90:ILE:HG12	1.75	0.50
1:C:17:ILE:O	1:C:190:GLN:HA	2.12	0.50
1:G:106:LEU:HD12	1:G:237:THR:HG22	1.93	0.50
1:J:22:ALA:HB2	1:J:156:GLU:HG2	1.94	0.50
1:F:104:ILE:HG12	1:F:105:MET:N	2.27	0.50
1:G:125:PRO:HB2	1:G:127:SER:CB	2.41	0.50
1:G:185:ASP:C	1:G:185:ASP:OD1	2.54	0.50
1:H:231:LEU:N	1:H:232:PRO:HD2	2.26	0.50
1:K:59:HIS:CE1	1:K:197:SER:CB	2.95	0.50
1:E:103:ASP:HB3	1:E:225:ILE:HD13	1.94	0.50
1:H:63:SER:O	1:H:64:SER:HB3	2.11	0.50
1:I:131:VAL:HB	1:I:135:GLN:NE2	2.27	0.50
1:K:38:GLU:C	1:K:40:SER:H	2.20	0.50
1:K:73:ASN:HB3	1:K:76:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:VAL:O	1:B:50:ARG:HG3	2.12	0.49
1:D:52:ASP:OD1	1:D:53:PHE:CD2	2.65	0.49
1:J:47:ILE:HG13	1:J:55:LEU:HB3	1.94	0.49
1:A:109:LEU:O	1:A:110:GLU:C	2.54	0.49
1:D:130:GLN:HA	4:D:405:HOH:O	2.12	0.49
1:E:16:ILE:HD13	1:E:196:ASP:CG	2.37	0.49
1:E:26:SER:O	1:E:28:PRO:HD3	2.11	0.49
1:F:105:MET:HE3	1:F:107:LEU:CD2	2.39	0.49
1:K:227:VAL:O	1:K:228:SER:C	2.55	0.49
1:A:145:VAL:HG13	1:A:151:ALA:HB2	1.94	0.49
1:C:61:GLN:HG2	1:C:105:MET:HE1	1.94	0.49
1:D:24:PRO:HA	1:D:72:HIS:ND1	2.28	0.49
1:E:215:ASN:ND2	1:E:217:LYS:HE3	2.27	0.49
1:J:231:LEU:N	1:J:232:PRO:HD2	2.27	0.49
1:K:48:LEU:HD22	1:K:121:PRO:CA	2.42	0.49
1:L:131:VAL:HG23	1:L:131:VAL:O	2.11	0.49
1:A:90:ILE:HG22	1:A:90:ILE:O	2.12	0.49
1:B:32:PHE:HB3	1:B:68:THR:HB	1.94	0.49
1:D:193:PHE:CE2	1:D:194:LYS:HG3	2.46	0.49
1:A:50:ARG:HB2	1:A:53:PHE:H	1.78	0.49
1:A:86:VAL:HG23	1:A:86:VAL:O	2.11	0.49
1:E:27:ARG:HG2	1:E:29:TYR:OH	2.12	0.49
1:E:133:PRO:HG3	1:E:162:GLN:O	2.12	0.49
1:J:140:ALA:HB1	1:J:155:GLN:O	2.13	0.49
1:H:22:ALA:HB2	1:H:156:GLU:HG2	1.94	0.49
1:H:90:ILE:O	1:H:105:MET:HG3	2.12	0.49
1:I:184:GLY:O	1:I:185:ASP:C	2.53	0.49
1:I:237:THR:O	1:I:241:LEU:N	2.41	0.49
1:K:56:THR:HG22	1:K:57:ALA:N	2.28	0.49
1:B:153:THR:HG23	1:B:153:THR:O	2.13	0.49
1:F:124:LEU:HB3	1:F:125:PRO:HD2	1.94	0.49
1:G:67:VAL:HG11	1:G:109:LEU:HD21	1.94	0.49
1:I:144:TYR:CE2	1:I:150:LEU:HD21	2.47	0.49
1:J:21:GLU:HG3	1:J:153:THR:CG2	2.41	0.49
1:J:201:LEU:HB3	1:J:209:GLY:HA3	1.95	0.49
1:A:57:ALA:HB1	1:A:59:HIS:HD1	1.76	0.49
1:A:225:ILE:HG22	1:A:230:PHE:HE2	1.78	0.49
1:C:144:TYR:HB3	1:C:193:PHE:HD2	1.77	0.49
1:G:56:THR:OG1	1:G:57:ALA:N	2.40	0.49
1:K:56:THR:HG23	1:K:198:GLY:HA3	1.95	0.49
1:A:57:ALA:HB1	1:A:59:HIS:ND1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:GLN:O	1:G:191:THR:HB	2.13	0.49
1:I:161:VAL:HG12	1:I:162:GLN:N	2.27	0.49
1:K:230:PHE:C	1:K:232:PRO:HD2	2.38	0.49
1:L:49:VAL:CG2	1:L:238:MET:HE1	2.42	0.49
1:B:177:ARG:O	1:B:226:LYS:NZ	2.41	0.48
1:D:162:GLN:NE2	1:D:184:GLY:O	2.45	0.48
1:E:157:VAL:CG1	1:E:159:LEU:HD21	2.43	0.48
1:J:51:LYS:HD3	1:J:115:TRP:CD1	2.47	0.48
1:J:65:ILE:HB	1:J:86:VAL:HG21	1.94	0.48
1:J:200:PRO:HA	1:J:209:GLY:O	2.13	0.48
1:K:54:VAL:O	1:K:106:LEU:HA	2.13	0.48
1:A:28:PRO:HG2	1:A:120:ARG:HG2	1.93	0.48
1:C:179:THR:HG22	1:C:180:GLU:HG3	1.95	0.48
1:H:50:ARG:O	1:H:51:LYS:C	2.54	0.48
1:I:131:VAL:HG13	1:I:208:GLN:HG3	1.94	0.48
1:K:233:TRP:HA	1:K:236:ARG:HG2	1.94	0.48
1:G:34:GLN:NE2	1:G:41:ARG:HH21	2.10	0.48
1:I:20:HIS:CD2	1:I:20:HIS:O	2.66	0.48
1:I:58:ALA:HB2	1:I:104:ILE:O	2.13	0.48
1:A:24:PRO:HA	1:A:72:HIS:CE1	2.48	0.48
1:B:49:VAL:HG23	1:B:238:MET:HE1	1.94	0.48
1:B:231:LEU:HD21	1:B:235:LYS:HZ1	1.77	0.48
1:A:83:PHE:CG	1:K:135:GLN:HA	2.48	0.48
1:D:84:ILE:HG22	1:D:85:PRO:O	2.13	0.48
1:I:110:GLU:O	1:I:110:GLU:HG2	2.12	0.48
1:A:84:ILE:N	1:A:84:ILE:CD1	2.76	0.48
1:E:82:GLN:HE21	1:E:119:VAL:HG21	1.78	0.48
1:G:211:LEU:HD12	1:G:212:SER:H	1.79	0.48
1:K:30:MET:HG3	1:K:154:LEU:HD21	1.95	0.48
1:K:35:PHE:CD1	1:K:35:PHE:N	2.81	0.48
1:D:171:PHE:HD1	1:D:172:HIS:N	2.12	0.48
1:E:131:VAL:HG13	1:E:135:GLN:OE1	2.13	0.48
1:H:16:ILE:HG12	1:H:157:VAL:HG23	1.95	0.48
1:I:50:ARG:HD2	1:I:50:ARG:HA	1.60	0.48
1:I:165:CYS:O	1:I:169:ARG:HB2	2.14	0.48
1:B:47:ILE:HG21	1:B:200:PRO:HG3	1.88	0.48
1:C:204:LYS:CD	1:K:75:LYS:HZ1	2.25	0.48
1:E:87:LYS:N	1:E:108:GLN:O	2.46	0.48
1:F:106:LEU:HD12	1:F:237:THR:HG21	1.95	0.48
1:G:50:ARG:HB3	1:G:53:PHE:HB2	1.95	0.48
1:G:85:PRO:O	1:G:110:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:TRP:CE2	1:G:154:LEU:HD13	2.49	0.48
1:I:75:LYS:HE2	1:I:75:LYS:HA	1.95	0.48
1:K:101:SER:HA	1:K:102:ASN:HA	1.63	0.48
1:K:105:MET:HE2	1:K:107:LEU:HD23	1.94	0.48
1:K:166:GLN:O	1:K:170:LEU:HD13	2.14	0.48
1:L:145:VAL:HG23	1:L:146:SER:N	2.28	0.48
1:B:204:LYS:N	2:B:301:SO4:O1	2.37	0.48
1:D:116:THR:O	1:D:120:ARG:HG3	2.14	0.48
1:E:68:THR:HG23	1:E:83:PHE:CE2	2.49	0.48
1:G:57:ALA:O	1:G:58:ALA:C	2.57	0.48
1:H:154:LEU:HG	1:H:155:GLN:N	2.29	0.48
1:L:84:ILE:HG21	1:L:109:LEU:HD22	1.96	0.48
1:L:198:GLY:N	1:L:211:LEU:O	2.47	0.48
1:B:124:LEU:HD12	1:B:124:LEU:H	1.75	0.47
1:D:229:HIS:HB3	1:D:230:PHE:CD2	2.48	0.47
1:F:55:LEU:HD11	1:F:104:ILE:HD11	1.96	0.47
1:H:179:THR:HG22	1:H:229:HIS:CG	2.49	0.47
1:J:208:GLN:C	1:J:227:VAL:HG12	2.39	0.47
1:L:170:LEU:HD23	1:L:170:LEU:O	2.14	0.47
1:D:38:GLU:O	1:D:38:GLU:HG2	2.13	0.47
1:H:16:ILE:HG12	1:H:157:VAL:CG2	2.44	0.47
1:H:162:GLN:OE1	1:H:185:ASP:HA	2.13	0.47
1:J:123:ARG:HB2	1:J:123:ARG:HH11	1.78	0.47
1:K:58:ALA:H	1:K:103:ASP:C	2.22	0.47
1:A:231:LEU:N	1:A:232:PRO:HD2	2.29	0.47
1:D:16:ILE:HG13	1:D:155:GLN:HB2	1.96	0.47
1:E:144:TYR:HD1	1:E:149:THR:O	1.96	0.47
1:K:27:ARG:NH1	1:K:29:TYR:OH	2.41	0.47
1:A:124:LEU:H	1:A:124:LEU:HG	1.40	0.47
1:C:183:VAL:HG11	1:C:224:TYR:CE2	2.49	0.47
1:C:183:VAL:HG22	1:C:184:GLY:N	2.29	0.47
1:E:209:GLY:HA2	1:E:225:ILE:O	2.14	0.47
1:E:209:GLY:H	1:E:227:VAL:HG23	1.80	0.47
1:G:90:ILE:C	1:G:105:MET:HG3	2.39	0.47
1:J:85:PRO:HB2	1:J:110:GLU:HG2	1.96	0.47
1:D:206:VAL:HG22	1:D:207:ALA:N	2.30	0.47
1:G:51:LYS:HG2	1:G:113:ALA:O	2.13	0.47
1:H:234:ILE:O	1:H:235:LYS:C	2.58	0.47
1:I:124:LEU:HD13	1:I:234:ILE:HG21	1.97	0.47
1:J:139:VAL:CG1	1:J:159:LEU:HD12	2.44	0.47
1:C:124:LEU:H	1:C:124:LEU:CD2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:TYR:CD2	1:D:122:LEU:HB2	2.50	0.47
1:E:26:SER:C	1:E:28:PRO:HD3	2.39	0.47
1:F:111:ARG:HG2	1:F:111:ARG:HH11	1.80	0.47
1:H:32:PHE:CD1	1:H:74:ILE:HD13	2.49	0.47
1:J:139:VAL:HG23	1:J:200:PRO:O	2.15	0.47
1:L:84:ILE:CG2	1:L:109:LEU:HD22	2.45	0.47
1:A:84:ILE:HG21	1:A:109:LEU:HB3	1.96	0.47
1:B:84:ILE:HG21	1:B:111:ARG:O	2.14	0.47
1:C:75:LYS:HA	1:C:75:LYS:HD2	1.56	0.47
1:E:104:ILE:HG12	1:E:105:MET:N	2.30	0.47
1:E:209:GLY:N	1:E:227:VAL:HG23	2.29	0.47
1:G:44:CYS:HB3	1:G:197:SER:O	2.14	0.47
1:H:58:ALA:HB2	1:H:104:ILE:C	2.40	0.47
1:H:73:ASN:CG	1:H:76:GLU:HG2	2.40	0.47
1:I:47:ILE:HB	1:I:200:PRO:HG3	1.97	0.47
1:I:50:ARG:C	1:I:52:ASP:N	2.72	0.47
1:I:81:GLN:HE21	1:I:83:PHE:HZ	1.58	0.47
1:I:161:VAL:O	1:I:162:GLN:NE2	2.40	0.47
1:A:134:GLY:O	1:A:135:GLN:C	2.57	0.47
1:D:231:LEU:HD12	1:D:231:LEU:HA	1.81	0.47
1:F:47:ILE:HG13	1:F:55:LEU:HB3	1.96	0.47
1:B:19:GLY:CA	1:B:157:VAL:HG11	2.41	0.47
1:C:16:ILE:HD11	1:C:151:ALA:CB	2.45	0.47
1:E:143:GLY:O	1:E:151:ALA:HB2	2.15	0.47
1:E:181:ILE:HG22	1:E:183:VAL:HG13	1.96	0.47
1:B:211:LEU:HD12	1:B:212:SER:N	2.29	0.47
1:C:59:HIS:CD2	1:C:103:ASP:OD2	2.67	0.47
1:E:230:PHE:O	1:E:234:ILE:HG13	2.15	0.47
1:F:102:ASN:ND2	1:F:230:PHE:CE1	2.79	0.47
1:G:208:GLN:C	1:G:227:VAL:HG12	2.40	0.47
1:H:94:ALA:O	1:H:102:ASN:HB3	2.14	0.47
1:I:139:VAL:HG22	1:I:140:ALA:N	2.29	0.47
1:L:32:PHE:HZ	2:L:301:SO4:O4	1.98	0.47
1:I:42:LYS:HE3	1:I:42:LYS:HB3	1.50	0.46
1:A:231:LEU:O	1:A:234:ILE:HG22	2.15	0.46
1:B:176:SER:C	1:B:178:ALA:N	2.73	0.46
1:C:16:ILE:HD13	1:C:155:GLN:HG3	1.97	0.46
1:D:32:PHE:CZ	1:D:74:ILE:HD13	2.50	0.46
1:K:27:ARG:NE	1:K:156:GLU:OE1	2.48	0.46
1:K:191:THR:HG21	1:K:220:PRO:HD3	1.98	0.46
1:A:16:ILE:HD11	1:A:140:ALA:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:PRO:CA	1:B:105:MET:HB2	2.36	0.46
1:F:165:CYS:HA	1:F:168:GLU:HG3	1.97	0.46
1:K:119:VAL:O	1:K:119:VAL:HG22	2.14	0.46
1:L:92:HIS:HB2	1:L:104:ILE:HG23	1.97	0.46
1:L:203:CYS:O	1:L:204:LYS:CB	2.62	0.46
1:B:193:PHE:CE1	1:B:218:GLY:CA	2.98	0.46
1:E:55:LEU:CD1	1:E:104:ILE:HD11	2.42	0.46
1:F:137:CYS:CB	1:F:201:LEU:HD11	2.45	0.46
1:H:43:ARG:NH1	1:H:150:LEU:HG	2.30	0.46
1:J:33:VAL:O	1:J:44:CYS:N	2.34	0.46
1:J:142:TRP:CE2	1:J:154:LEU:HD23	2.51	0.46
1:K:35:PHE:HB2	1:K:62:GLY:HA3	1.97	0.46
1:L:16:ILE:HG22	1:L:157:VAL:HG13	1.95	0.46
1:A:115:TRP:O	1:A:116:THR:HG23	2.15	0.46
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.83	0.46
1:C:141:GLY:HA2	1:C:154:LEU:HD12	1.98	0.46
1:D:124:LEU:HA	1:D:124:LEU:HD23	1.52	0.46
1:I:94:ALA:O	1:I:95:TYR:C	2.59	0.46
1:J:58:ALA:C	1:J:60:CYS:H	2.22	0.46
1:J:72:HIS:NE2	1:J:153:THR:CG2	2.78	0.46
1:A:146:SER:OG	1:A:147:MET:N	2.47	0.46
1:A:181:ILE:HG22	1:A:182:CYS:N	2.31	0.46
1:B:16:ILE:HG21	1:B:157:VAL:HG13	1.96	0.46
1:B:171:PHE:CD1	1:B:171:PHE:N	2.84	0.46
1:D:50:ARG:NH2	2:D:303:SO4:O4	2.48	0.46
1:I:102:ASN:HD22	1:I:230:PHE:HZ	1.63	0.46
1:I:125:PRO:HG3	1:I:208:GLN:NE2	2.30	0.46
1:K:59:HIS:HE1	1:K:197:SER:HB3	1.79	0.46
1:A:53:PHE:HA	1:A:107:LEU:O	2.14	0.46
1:B:139:VAL:HG12	1:B:159:LEU:HD11	1.98	0.46
1:C:233:TRP:O	1:C:237:THR:HG23	2.15	0.46
1:G:78:GLU:HB3	1:G:80:THR:HG23	1.97	0.46
1:H:17:ILE:HD11	1:H:193:PHE:HD2	1.79	0.46
1:H:92:HIS:CD2	1:H:93:PRO:HD2	2.50	0.46
1:J:136:LEU:HD13	1:J:158:LEU:HD13	1.97	0.46
1:K:131:VAL:HG21	1:K:181:ILE:HD12	1.98	0.46
1:K:159:LEU:HD21	1:K:191:THR:HA	1.97	0.46
1:A:50:ARG:C	1:A:115:TRP:HH2	2.24	0.46
1:A:232:PRO:O	1:A:236:ARG:HB2	2.16	0.46
1:B:82:GLN:HE22	1:B:114:LYS:N	2.12	0.46
1:C:215:ASN:OD1	1:C:217:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ILE:HB	1:D:86:VAL:HG21	1.98	0.46
1:D:197:SER:N	1:D:211:LEU:HD23	2.30	0.46
1:G:58:ALA:O	1:G:60:CYS:N	2.49	0.46
1:K:47:ILE:O	1:K:54:VAL:HA	2.16	0.46
1:B:32:PHE:CZ	1:B:74:ILE:HG12	2.51	0.46
1:B:100:PHE:O	1:B:103:ASP:HB2	2.16	0.46
1:D:137:CYS:HB3	1:D:201:LEU:HD11	1.96	0.46
1:G:179:THR:HG22	1:G:229:HIS:CG	2.51	0.46
1:I:145:VAL:HG11	1:I:155:GLN:HE21	1.81	0.46
1:J:193:PHE:CE1	1:J:218:GLY:HA3	2.51	0.46
1:B:86:VAL:HG11	1:B:107:LEU:HD13	1.98	0.46
1:C:240:ARG:HB2	1:C:241:LEU:HG	1.98	0.46
1:D:193:PHE:CZ	1:D:194:LYS:HE3	2.51	0.46
1:E:38:GLU:HB3	1:E:39:LYS:H	1.53	0.46
1:I:50:ARG:O	1:I:51:LYS:C	2.58	0.46
1:J:65:ILE:O	1:J:86:VAL:HG22	2.16	0.46
1:K:190:GLN:O	1:K:191:THR:CB	2.60	0.46
1:L:225:ILE:CG2	1:L:230:PHE:CE2	2.99	0.46
1:A:41:ARG:NH2	1:K:204:LYS:HD2	2.31	0.45
1:B:170:LEU:HD23	1:B:170:LEU:C	2.42	0.45
1:C:166:GLN:CD	1:C:186:PRO:HG2	2.42	0.45
1:D:28:PRO:CB	1:D:120:ARG:HB2	2.46	0.45
1:E:58:ALA:HB1	1:E:95:TYR:CD2	2.51	0.45
1:H:58:ALA:HA	1:H:105:MET:HB2	1.99	0.45
1:H:228:SER:O	1:H:231:LEU:HG	2.16	0.45
1:J:203:CYS:O	1:J:204:LYS:HB2	2.16	0.45
1:A:32:PHE:O	1:A:67:VAL:HA	2.15	0.45
1:A:67:VAL:HG12	1:A:69:LEU:CD1	2.46	0.45
1:A:79:ARG:HG2	1:K:130:GLN:HE22	1.80	0.45
1:A:82:GLN:HB3	1:A:84:ILE:HD11	1.97	0.45
1:A:86:VAL:O	1:A:86:VAL:CG2	2.65	0.45
1:B:50:ARG:HD3	1:B:238:MET:HE1	1.87	0.45
1:B:51:LYS:HB3	1:B:112:LYS:HG3	1.98	0.45
1:C:166:GLN:O	1:C:170:LEU:HD23	2.16	0.45
1:D:162:GLN:CG	1:D:184:GLY:O	2.65	0.45
1:E:209:GLY:H	1:E:227:VAL:CG2	2.29	0.45
1:H:37:GLN:HB2	1:H:42:LYS:HG3	1.98	0.45
1:H:106:LEU:HD23	1:H:106:LEU:HA	1.70	0.45
1:J:57:ALA:HB3	1:J:60:CYS:SG	2.56	0.45
1:K:193:PHE:O	1:K:196:ASP:OD2	2.34	0.45
1:K:227:VAL:HG23	1:K:228:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLN:HG3	1:B:119:VAL:HG21	1.99	0.45
1:B:193:PHE:CD1	1:B:218:GLY:CA	2.99	0.45
1:C:47:ILE:HG23	1:C:55:LEU:HB3	1.99	0.45
1:G:125:PRO:HG2	1:G:231:LEU:HD11	1.98	0.45
1:H:85:PRO:O	1:H:110:GLU:HB2	2.16	0.45
1:H:159:LEU:HD21	1:H:191:THR:HA	1.99	0.45
1:H:184:GLY:CA	1:H:221:PRO:HA	2.47	0.45
1:I:87:LYS:O	1:I:87:LYS:HG3	2.16	0.45
1:I:111:ARG:HG3	1:I:112:LYS:O	2.16	0.45
1:I:132:LYS:H	1:I:135:GLN:HE21	1.65	0.45
1:K:16:ILE:CG2	1:K:157:VAL:HG23	2.47	0.45
1:K:102:ASN:N	1:K:102:ASN:ND2	2.64	0.45
1:K:161:VAL:HG12	1:K:162:GLN:N	2.31	0.45
1:K:205:ASP:N	1:K:205:ASP:OD1	2.50	0.45
1:L:147:MET:SD	1:L:193:PHE:HZ	2.40	0.45
1:B:128:LYS:H	1:B:128:LYS:HZ3	1.64	0.45
1:B:162:GLN:NE2	1:B:185:ASP:HA	2.32	0.45
1:D:143:GLY:CA	1:D:196:ASP:OD1	2.55	0.45
1:F:126:SER:O	1:F:128:LYS:HG3	2.17	0.45
1:F:128:LYS:HD3	1:F:130:GLN:OE1	2.15	0.45
1:G:90:ILE:HD11	1:G:108:GLN:HB2	1.98	0.45
1:G:116:THR:O	1:G:120:ARG:NE	2.46	0.45
1:G:144:TYR:CG	1:G:150:LEU:HD13	2.51	0.45
1:H:116:THR:C	1:H:118:ALA:N	2.74	0.45
1:K:57:ALA:H	1:K:198:GLY:HA2	1.81	0.45
1:K:181:ILE:HG23	1:K:224:TYR:HB2	1.99	0.45
1:L:71:ALA:O	1:L:142:TRP:HZ2	2.00	0.45
1:D:156:GLU:C	1:D:157:VAL:HG22	2.42	0.45
1:F:47:ILE:HD13	1:F:200:PRO:HB3	1.98	0.45
1:F:58:ALA:HA	1:F:105:MET:HB2	1.98	0.45
1:J:166:GLN:O	1:J:170:LEU:HG	2.16	0.45
1:L:32:PHE:CE1	1:L:74:ILE:HG12	2.51	0.45
1:H:162:GLN:HE21	1:H:162:GLN:HA	1.81	0.45
1:H:233:TRP:O	1:H:237:THR:OG1	2.21	0.45
1:K:188:LYS:HB3	1:K:190:GLN:OE1	2.16	0.45
1:L:86:VAL:HG21	1:L:107:LEU:HD13	1.98	0.45
1:B:139:VAL:CG2	1:B:140:ALA:N	2.80	0.45
1:C:183:VAL:HG22	1:C:184:GLY:H	1.82	0.45
1:F:73:ASN:CB	1:F:153:THR:HG22	2.47	0.45
1:G:94:ALA:O	1:G:96:ASN:N	2.49	0.45
1:H:86:VAL:HG21	1:H:107:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ILE:HD12	1:K:47:ILE:HA	1.69	0.45
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.68	0.45
1:C:144:TYR:CB	1:C:193:PHE:HD2	2.29	0.45
1:G:16:ILE:HD13	1:G:196:ASP:OD2	2.17	0.45
1:H:72:HIS:HB3	1:H:78:GLU:OE2	2.16	0.45
1:L:54:VAL:HB	1:L:107:LEU:HB2	1.99	0.45
1:A:18:GLY:HA3	1:A:190:GLN:HG3	1.99	0.45
1:A:203:CYS:O	1:A:204:LYS:HB2	2.17	0.45
1:B:72:HIS:H	1:B:78:GLU:CD	2.24	0.45
1:C:142:TRP:CZ2	1:C:154:LEU:HD13	2.52	0.45
1:D:136:LEU:HA	1:D:136:LEU:HD12	1.60	0.45
1:D:139:VAL:HG22	1:D:140:ALA:H	1.82	0.45
1:F:83:PHE:N	1:F:83:PHE:CD1	2.85	0.45
1:H:165:CYS:HA	1:H:168:GLU:HG3	1.99	0.45
1:I:25:HIS:CE1	1:I:80:THR:HG21	2.52	0.45
1:I:47:ILE:HD13	1:I:207:ALA:HB2	1.99	0.45
1:I:58:ALA:HB3	1:I:95:TYR:CD1	2.51	0.45
1:K:236:ARG:NH1	4:K:301:HOH:O	2.45	0.45
1:A:71:ALA:HA	1:A:81:GLN:HG3	1.98	0.45
1:B:139:VAL:CG1	1:B:159:LEU:HD11	2.47	0.45
1:C:16:ILE:HD13	1:C:145:VAL:HG12	1.99	0.45
1:D:74:ILE:HD11	1:D:75:LYS:HZ3	1.81	0.45
1:D:92:HIS:CD2	1:D:230:PHE:HE1	2.34	0.45
1:E:59:HIS:ND1	1:E:103:ASP:OD2	2.50	0.45
1:G:65:ILE:O	1:G:86:VAL:HG13	2.16	0.45
1:G:69:LEU:HB3	1:G:119:VAL:HG22	1.98	0.45
1:I:16:ILE:HD12	1:I:155:GLN:HB2	1.99	0.45
1:K:37:GLN:HG2	1:K:42:LYS:CG	2.46	0.45
1:L:16:ILE:HG22	1:L:157:VAL:CG1	2.47	0.45
1:A:175:TYR:HE1	1:A:181:ILE:O	2.00	0.44
1:F:102:ASN:ND2	1:F:230:PHE:HE1	2.15	0.44
1:J:123:ARG:HH11	1:J:123:ARG:CB	2.30	0.44
1:A:193:PHE:CE1	1:A:194:LYS:HE2	2.52	0.44
1:C:120:ARG:HB3	1:C:121:PRO:CD	2.46	0.44
1:D:96:ASN:HD21	1:D:98:LYS:NZ	2.16	0.44
1:F:90:ILE:O	1:F:105:MET:HG3	2.17	0.44
1:K:29:TYR:CG	1:K:122:LEU:HD22	2.51	0.44
1:K:144:TYR:CZ	1:K:150:LEU:HD13	2.51	0.44
1:A:55:LEU:CD2	1:A:234:ILE:HD11	2.47	0.44
1:B:110:GLU:CD	1:B:111:ARG:H	2.25	0.44
1:C:231:LEU:CD2	1:C:235:LYS:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:PRO:O	1:C:236:ARG:HB2	2.17	0.44
1:D:35:PHE:HB3	1:D:65:ILE:HG12	1.99	0.44
1:F:233:TRP:O	1:F:237:THR:HG22	2.18	0.44
1:G:110:GLU:C	1:G:111:ARG:HG3	2.41	0.44
1:G:225:ILE:HG23	1:G:230:PHE:CE2	2.53	0.44
1:H:48:LEU:CD2	1:H:115:TRP:HZ3	2.30	0.44
1:H:150:LEU:HD12	1:H:150:LEU:HA	1.62	0.44
1:I:48:LEU:O	1:I:121:PRO:HA	2.17	0.44
1:I:49:VAL:HG23	1:I:238:MET:HE1	1.98	0.44
1:I:161:VAL:CG1	1:I:162:GLN:N	2.80	0.44
1:C:85:PRO:HD2	1:C:110:GLU:HB3	2.00	0.44
1:D:165:CYS:O	1:D:166:GLN:C	2.61	0.44
1:H:105:MET:HE3	1:H:107:LEU:HG	1.98	0.44
1:I:56:THR:HG23	1:I:57:ALA:N	2.31	0.44
1:I:124:LEU:CD1	1:I:234:ILE:HG21	2.48	0.44
1:K:29:TYR:HB2	1:K:47:ILE:HD11	1.98	0.44
1:A:59:HIS:CE1	1:A:197:SER:OG	2.70	0.44
1:A:88:ARG:HB3	1:A:108:GLN:HE21	1.83	0.44
1:A:100:PHE:O	1:A:101:SER:C	2.60	0.44
1:A:138:SER:C	1:A:139:VAL:CG2	2.85	0.44
1:C:144:TYR:CD2	1:C:194:LYS:HB2	2.52	0.44
1:A:179:THR:HG23	1:A:229:HIS:HB3	2.00	0.44
1:A:188:LYS:HB3	1:A:190:GLN:OE1	2.18	0.44
1:B:171:PHE:CD2	1:B:213:TYR:CE1	2.95	0.44
1:D:213:TYR:CE2	1:D:223:VAL:HG11	2.52	0.44
1:F:209:GLY:HA2	1:F:227:VAL:HG23	1.99	0.44
1:K:38:GLU:C	1:K:40:SER:N	2.75	0.44
1:A:226:LYS:O	1:A:229:HIS:HB2	2.16	0.44
1:A:227:VAL:O	1:A:227:VAL:CG1	2.65	0.44
1:D:204:LYS:HE3	1:H:81:GLN:NE2	2.32	0.44
1:I:124:LEU:HD23	1:I:125:PRO:HD2	1.99	0.44
1:I:164:ASP:O	1:I:165:CYS:C	2.61	0.44
1:K:174:ASN:HB3	1:K:213:TYR:OH	2.17	0.44
1:A:27:ARG:HH22	1:A:138:SER:CB	2.15	0.44
1:E:78:GLU:O	1:E:79:ARG:C	2.61	0.44
1:G:54:VAL:HG21	1:G:67:VAL:HG21	2.00	0.44
1:I:84:ILE:HG21	1:I:109:LEU:HB3	1.99	0.44
1:J:84:ILE:HG12	1:J:111:ARG:NH2	2.32	0.44
1:J:135:GLN:HG3	1:L:83:PHE:CD2	2.53	0.44
1:L:160:THR:O	1:L:161:VAL:C	2.60	0.44
1:C:179:THR:HG23	1:C:230:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LEU:HB2	1:C:224:TYR:CE1	2.53	0.44
1:E:33:VAL:O	1:E:44:CYS:N	2.34	0.44
1:E:133:PRO:HA	1:E:161:VAL:HG12	2.00	0.44
1:E:227:VAL:O	1:E:230:PHE:N	2.40	0.44
1:F:58:ALA:HB2	1:F:104:ILE:O	2.18	0.44
1:H:88:ARG:HA	1:H:89:PRO:HD3	1.78	0.44
1:J:194:LYS:HA	1:J:194:LYS:HD3	1.39	0.44
1:A:37:GLN:CG	1:A:42:LYS:HG3	2.48	0.43
1:A:231:LEU:HA	1:A:234:ILE:HG22	1.99	0.43
1:C:131:VAL:HA	1:K:77:GLN:NE2	2.33	0.43
1:G:70:GLY:O	1:G:80:THR:OG1	2.35	0.43
1:H:146:SER:CB	1:H:149:THR:OG1	2.56	0.43
1:A:78:GLU:HG2	1:A:79:ARG:H	1.83	0.43
1:A:107:LEU:HD23	1:A:107:LEU:C	2.43	0.43
1:E:210:ILE:O	1:E:224:TYR:HA	2.18	0.43
1:F:163:LYS:O	1:F:164:ASP:C	2.62	0.43
1:I:50:ARG:C	1:I:52:ASP:H	2.26	0.43
1:I:105:MET:CE	1:I:107:LEU:HD21	2.47	0.43
1:A:47:ILE:HD11	1:A:55:LEU:HB3	2.01	0.43
1:A:226:LYS:HB3	1:A:229:HIS:ND1	2.32	0.43
1:G:181:ILE:HG13	1:G:226:LYS:HB2	1.99	0.43
1:H:135:GLN:HG3	1:H:136:LEU:H	1.83	0.43
1:A:193:PHE:O	1:A:196:ASP:HB2	2.18	0.43
1:B:83:PHE:C	1:B:84:ILE:HG13	2.43	0.43
1:B:193:PHE:CD1	1:B:218:GLY:HA2	2.54	0.43
1:H:112:LYS:HB2	1:H:112:LYS:HE3	1.89	0.43
1:K:47:ILE:HD13	1:K:200:PRO:HG3	1.99	0.43
1:L:47:ILE:HD13	1:L:200:PRO:HB3	2.01	0.43
1:E:78:GLU:HB2	1:E:81:GLN:OE1	2.18	0.43
1:F:128:LYS:HB2	1:F:130:GLN:HG2	2.00	0.43
1:G:231:LEU:N	1:G:232:PRO:HD2	2.33	0.43
1:K:185:ASP:OD1	1:K:185:ASP:C	2.60	0.43
1:B:32:PHE:HD1	1:B:142:TRP:CE3	2.36	0.43
1:C:183:VAL:CG1	1:C:224:TYR:CE2	3.02	0.43
1:F:203:CYS:O	1:F:204:LYS:C	2.62	0.43
1:G:97:PRO:O	1:G:100:PHE:N	2.46	0.43
1:G:175:TYR:CD2	1:G:175:TYR:C	2.96	0.43
1:A:197:SER:HA	1:A:211:LEU:HG	2.00	0.43
1:C:115:TRP:HA	1:C:115:TRP:CE3	2.53	0.43
1:E:215:ASN:HD22	1:E:217:LYS:HE3	1.82	0.43
1:F:86:VAL:O	1:F:86:VAL:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:HIS:CD2	1:J:118:ALA:HB1	2.54	0.43
1:L:37:GLN:O	1:L:38:GLU:HG3	2.19	0.43
1:C:87:LYS:HB2	1:C:110:GLU:HA	2.01	0.43
1:C:139:VAL:HG12	1:C:201:LEU:HA	2.01	0.43
1:C:204:LYS:HA	1:C:204:LYS:HD3	1.46	0.43
1:C:237:THR:O	1:C:238:MET:C	2.61	0.43
1:E:115:TRP:CZ2	1:E:121:PRO:HG3	2.53	0.43
1:H:215:ASN:O	1:H:216:LYS:C	2.62	0.43
1:L:96:ASN:HB3	1:L:99:ASN:HB3	2.01	0.43
1:A:47:ILE:HG13	1:A:47:ILE:O	2.18	0.43
1:A:181:ILE:HG13	1:A:226:LYS:HG3	2.01	0.43
1:B:137:CYS:CB	1:B:201:LEU:HD22	2.49	0.43
1:D:162:GLN:NE2	1:D:186:PRO:HD3	2.34	0.43
1:E:37:GLN:HB3	1:E:42:LYS:HD2	2.01	0.43
1:E:144:TYR:HA	1:E:150:LEU:HA	2.01	0.43
1:F:115:TRP:NE1	1:F:121:PRO:HD3	2.33	0.43
1:F:124:LEU:HB3	1:F:125:PRO:HD3	2.01	0.43
1:F:129:ALA:HB1	1:F:226:LYS:HD2	1.99	0.43
1:H:27:ARG:HH22	1:H:138:SER:HB3	1.83	0.43
1:H:201:LEU:HD23	1:H:224:TYR:CE1	2.54	0.43
1:K:16:ILE:HG22	1:K:157:VAL:CG2	2.48	0.43
1:L:78:GLU:C	1:L:80:THR:N	2.77	0.43
1:A:179:THR:O	1:A:226:LYS:HB2	2.18	0.43
1:C:16:ILE:HD11	1:C:151:ALA:HB2	1.99	0.43
1:D:59:HIS:O	1:D:59:HIS:HD2	2.02	0.43
1:E:87:LYS:HD2	1:E:108:GLN:NE2	2.33	0.43
1:H:69:LEU:O	1:H:81:GLN:HA	2.19	0.43
1:I:194:LYS:C	1:I:196:ASP:H	2.27	0.43
1:J:51:LYS:HB3	1:J:113:ALA:HB3	2.01	0.43
1:K:61:GLN:HG3	1:K:105:MET:HE1	2.01	0.43
1:K:136:LEU:HD23	1:K:136:LEU:HA	1.69	0.43
1:L:105:MET:HE3	1:L:107:LEU:HD21	2.01	0.43
1:A:43:ARG:HB2	1:A:195:GLY:HA2	2.01	0.42
1:A:215:ASN:HB2	1:A:219:THR:O	2.19	0.42
1:B:123:ARG:HA	1:B:123:ARG:HD3	1.86	0.42
1:C:52:ASP:HA	1:C:109:LEU:HD12	2.01	0.42
1:C:105:MET:HE3	1:C:107:LEU:HD21	2.01	0.42
1:C:129:ALA:O	1:C:130:GLN:HG2	2.19	0.42
1:F:145:VAL:HG23	1:F:146:SER:N	2.29	0.42
1:H:144:TYR:CD2	1:H:194:LYS:HB3	2.54	0.42
1:K:37:GLN:HG2	1:K:42:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:56:THR:CG2	1:K:57:ALA:N	2.82	0.42
1:L:147:MET:SD	1:L:193:PHE:CZ	3.12	0.42
1:B:162:GLN:HB3	1:B:182:CYS:O	2.19	0.42
1:D:134:GLY:C	1:H:83:PHE:CB	2.81	0.42
1:E:68:THR:HG23	1:E:83:PHE:CD2	2.53	0.42
1:H:125:PRO:O	1:H:128:LYS:N	2.52	0.42
1:C:234:ILE:O	1:C:238:MET:HG3	2.20	0.42
1:G:119:VAL:O	1:G:119:VAL:HG12	2.19	0.42
1:G:196:ASP:O	1:G:197:SER:C	2.61	0.42
1:H:32:PHE:CE1	1:H:74:ILE:CD1	2.94	0.42
1:J:95:TYR:CA	1:J:102:ASN:HB2	2.47	0.42
1:K:73:ASN:OD1	1:K:76:GLU:HG2	2.18	0.42
1:K:130:GLN:HG2	1:K:131:VAL:H	1.84	0.42
1:D:227:VAL:O	1:D:228:SER:C	2.63	0.42
1:E:91:PRO:O	1:E:92:HIS:C	2.60	0.42
1:G:215:ASN:OD1	1:G:219:THR:O	2.36	0.42
1:H:84:ILE:HG22	1:H:110:GLU:H	1.84	0.42
1:H:92:HIS:HB3	1:H:94:ALA:O	2.19	0.42
1:J:136:LEU:HD23	1:J:136:LEU:HA	1.86	0.42
1:K:84:ILE:HB	1:K:109:LEU:HD22	2.00	0.42
1:K:135:GLN:NE2	1:K:203:CYS:SG	2.92	0.42
1:K:144:TYR:CD2	1:K:194:LYS:HG3	2.53	0.42
1:L:92:HIS:HA	1:L:93:PRO:HD2	1.79	0.42
1:A:185:ASP:OD2	1:A:188:LYS:HG2	2.19	0.42
1:B:70:GLY:O	1:B:80:THR:OG1	2.34	0.42
1:E:57:ALA:O	1:E:105:MET:HE2	2.19	0.42
1:F:224:TYR:N	1:F:224:TYR:CD2	2.88	0.42
1:K:96:ASN:ND2	1:K:98:LYS:O	2.52	0.42
1:A:33:VAL:HB	1:A:44:CYS:HB3	2.01	0.42
1:A:194:LYS:HE2	1:A:194:LYS:HB3	1.79	0.42
1:B:104:ILE:HD12	1:B:225:ILE:HG21	2.00	0.42
1:C:92:HIS:ND1	1:C:93:PRO:HD2	2.35	0.42
1:D:193:PHE:CD2	1:D:194:LYS:N	2.87	0.42
1:G:125:PRO:CB	1:G:127:SER:HB2	2.47	0.42
1:J:27:ARG:HB3	1:J:29:TYR:CZ	2.55	0.42
1:J:47:ILE:HD11	1:J:55:LEU:HD23	2.01	0.42
1:K:105:MET:HG2	1:K:106:LEU:O	2.20	0.42
1:L:116:THR:HG22	1:L:117:THR:H	1.85	0.42
1:D:48:LEU:HD13	1:D:69:LEU:HD21	2.01	0.42
1:D:169:ARG:C	1:D:171:PHE:N	2.78	0.42
1:D:211:LEU:HB2	1:D:224:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:ILE:HG22	1:H:85:PRO:O	2.20	0.42
1:I:233:TRP:O	1:I:236:ARG:HB3	2.20	0.42
1:K:24:PRO:HA	1:K:72:HIS:ND1	2.35	0.42
1:K:54:VAL:CG1	1:K:107:LEU:HB2	2.50	0.42
1:K:227:VAL:HG23	1:K:228:SER:H	1.85	0.42
1:L:74:ILE:HD12	1:L:74:ILE:HA	1.82	0.42
1:L:198:GLY:HA2	1:L:210:ILE:CG2	2.40	0.42
1:F:96:ASN:HB3	1:F:99:ASN:HB3	2.01	0.42
1:H:27:ARG:NH2	1:H:156:GLU:OE1	2.51	0.42
1:H:135:GLN:HG3	1:H:136:LEU:N	2.35	0.42
1:H:210:ILE:O	1:H:211:LEU:C	2.61	0.42
1:B:47:ILE:CG2	1:B:200:PRO:CG	2.80	0.42
1:B:73:ASN:HB3	1:B:76:GLU:OE1	2.20	0.42
1:C:52:ASP:OD1	1:C:52:ASP:N	2.51	0.42
1:E:132:LYS:HA	1:E:133:PRO:HD2	1.86	0.42
1:H:144:TYR:HD2	1:H:194:LYS:HB3	1.85	0.42
1:I:185:ASP:HA	1:I:186:PRO:HD2	1.76	0.42
1:J:139:VAL:HG11	1:J:159:LEU:HD12	2.02	0.42
1:J:215:ASN:OD1	1:J:219:THR:HB	2.20	0.42
1:K:116:THR:CG2	1:K:117:THR:N	2.82	0.42
1:A:27:ARG:HH12	1:A:202:VAL:HG11	1.84	0.42
1:A:50:ARG:HD3	1:A:53:PHE:HD2	1.84	0.42
1:A:92:HIS:ND1	1:A:93:PRO:HD2	2.34	0.42
1:B:153:THR:O	1:B:153:THR:CG2	2.68	0.42
1:B:160:THR:HG22	1:B:161:VAL:O	2.19	0.42
1:D:116:THR:HG22	1:D:117:THR:N	2.35	0.42
1:I:237:THR:O	1:I:238:MET:C	2.61	0.42
1:J:228:SER:O	1:J:231:LEU:HD12	2.20	0.42
1:K:146:SER:O	1:K:148:SER:N	2.52	0.42
1:L:114:LYS:HE3	1:L:114:LYS:HB2	1.87	0.42
1:A:27:ARG:NH1	1:A:202:VAL:HG11	2.34	0.41
1:A:50:ARG:HH11	1:A:238:MET:CG	2.33	0.41
1:B:83:PHE:O	1:B:111:ARG:NH2	2.53	0.41
1:D:127:SER:C	1:D:129:ALA:N	2.78	0.41
1:F:211:LEU:HB2	1:F:224:TYR:CE1	2.54	0.41
1:G:183:VAL:HG21	1:G:201:LEU:HD22	2.02	0.41
1:K:95:TYR:CZ	1:K:97:PRO:HA	2.55	0.41
1:K:144:TYR:HB2	1:K:193:PHE:HD2	1.85	0.41
1:K:229:HIS:O	1:K:229:HIS:CG	2.73	0.41
1:A:23:LYS:O	1:A:26:SER:CB	2.64	0.41
1:A:200:PRO:HA	1:A:209:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TRP:O	1:A:234:ILE:C	2.63	0.41
1:E:143:GLY:HA3	1:E:196:ASP:CG	2.43	0.41
1:E:217:LYS:HG3	1:E:219:THR:OG1	2.21	0.41
1:F:49:VAL:HG23	1:F:238:MET:HE1	2.02	0.41
1:H:61:GLN:CD	1:H:105:MET:SD	3.03	0.41
1:H:111:ARG:HG3	1:H:112:LYS:O	2.20	0.41
1:I:49:VAL:CG2	1:I:238:MET:HE1	2.50	0.41
1:K:86:VAL:HG11	1:K:107:LEU:HD13	2.02	0.41
1:K:240:ARG:O	1:K:241:LEU:HB2	2.20	0.41
1:A:65:ILE:O	1:A:86:VAL:HG13	2.21	0.41
1:F:86:VAL:O	1:F:87:LYS:C	2.63	0.41
1:F:111:ARG:HG2	1:F:111:ARG:NH1	2.35	0.41
1:G:127:SER:CA	1:G:129:ALA:H	2.30	0.41
1:I:144:TYR:CE1	1:I:150:LEU:HG	2.55	0.41
1:I:202:VAL:CG1	1:I:205:ASP:HA	2.51	0.41
1:J:227:VAL:O	1:J:228:SER:C	2.63	0.41
1:C:193:PHE:H	1:C:196:ASP:HB2	1.85	0.41
1:E:186:PRO:HA	1:E:220:PRO:CG	2.37	0.41
1:F:209:GLY:HA2	1:F:225:ILE:O	2.20	0.41
1:H:16:ILE:CG2	1:H:155:GLN:CG	2.98	0.41
1:K:157:VAL:HG11	1:K:190:GLN:HB3	2.01	0.41
1:B:168:GLU:HG2	1:B:175:TYR:CD2	2.53	0.41
1:B:216:LYS:HA	1:B:216:LYS:HD2	1.72	0.41
1:C:215:ASN:OD1	1:C:218:GLY:N	2.54	0.41
1:D:23:LYS:HB3	1:D:26:SER:HB3	2.01	0.41
1:D:57:ALA:HA	1:D:103:ASP:O	2.21	0.41
1:E:37:GLN:O	1:E:38:GLU:C	2.63	0.41
1:F:55:LEU:CD2	1:F:210:ILE:HD11	2.51	0.41
1:H:188:LYS:HG2	1:H:190:GLN:NE2	2.31	0.41
1:I:23:LYS:HB3	1:I:26:SER:CB	2.51	0.41
1:I:34:GLN:O	1:I:35:PHE:HB3	2.20	0.41
1:I:100:PHE:HB3	1:I:103:ASP:HB2	2.02	0.41
1:J:181:ILE:HD11	1:J:226:LYS:HA	2.01	0.41
1:L:52:ASP:OD1	1:L:53:PHE:CD2	2.73	0.41
1:A:32:PHE:CE1	1:A:43:ARG:CD	3.04	0.41
1:F:165:CYS:C	1:F:167:CYS:N	2.79	0.41
1:G:74:ILE:HG22	1:G:75:LYS:HG2	2.03	0.41
1:G:105:MET:HG2	1:G:106:LEU:O	2.21	0.41
1:K:234:ILE:O	1:K:238:MET:HB2	2.21	0.41
1:B:120:ARG:CB	1:B:121:PRO:HD3	2.50	0.41
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:HIS:CD2	1:D:59:HIS:C	2.99	0.41
1:D:144:TYR:CZ	1:D:150:LEU:HD22	2.55	0.41
1:G:69:LEU:N	1:G:69:LEU:CD1	2.83	0.41
1:K:73:ASN:HA	1:K:152:THR:O	2.21	0.41
1:K:95:TYR:HE1	1:K:103:ASP:HB3	1.83	0.41
1:A:164:ASP:HB3	1:A:175:TYR:CE2	2.45	0.41
1:A:199:GLY:O	1:A:210:ILE:HA	2.20	0.41
1:B:193:PHE:CG	1:B:194:LYS:N	2.87	0.41
1:B:231:LEU:HA	1:B:234:ILE:HD12	2.03	0.41
1:C:34:GLN:HB2	1:C:66:ASN:HD22	1.86	0.41
1:D:234:ILE:HG22	1:D:238:MET:HE2	2.01	0.41
1:F:52:ASP:OD1	1:F:52:ASP:C	2.63	0.41
1:L:225:ILE:HG23	1:L:230:PHE:CE2	2.37	0.41
1:A:56:THR:OG1	1:A:57:ALA:N	2.54	0.41
1:A:198:GLY:H	1:A:211:LEU:HB3	1.85	0.41
1:C:74:ILE:HD12	1:C:74:ILE:C	2.46	0.41
1:D:58:ALA:CA	1:D:105:MET:HB2	2.42	0.41
1:D:92:HIS:HD2	1:D:230:PHE:CD1	2.39	0.41
1:D:106:LEU:HA	1:D:106:LEU:HD23	1.86	0.41
1:D:135:GLN:HB3	1:D:161:VAL:HG21	2.02	0.41
1:D:162:GLN:CD	1:D:186:PRO:HD3	2.46	0.41
1:F:84:ILE:N	1:F:84:ILE:CD1	2.77	0.41
1:G:17:ILE:HG12	1:G:193:PHE:HB2	2.02	0.41
1:G:74:ILE:HA	1:G:74:ILE:HD13	1.76	0.41
1:H:130:GLN:CD	1:H:130:GLN:H	2.29	0.41
1:H:139:VAL:CG1	1:H:159:LEU:HD12	2.51	0.41
1:H:184:GLY:HA3	1:H:220:PRO:HB3	2.03	0.41
1:H:191:THR:OG1	1:H:192:GLY:N	2.53	0.41
1:I:32:PHE:O	1:I:32:PHE:CD2	2.74	0.41
1:I:204:LYS:HG3	1:J:77:GLN:HG2	2.02	0.41
1:I:208:GLN:C	1:I:227:VAL:HG13	2.46	0.41
1:J:215:ASN:OD1	1:J:219:THR:CB	2.69	0.41
1:K:116:THR:C	1:K:118:ALA:H	2.29	0.41
1:K:131:VAL:HG12	1:K:135:GLN:HE22	1.84	0.41
1:C:34:GLN:O	1:C:65:ILE:HG23	2.20	0.41
1:C:124:LEU:N	1:C:124:LEU:CD2	2.82	0.41
1:C:235:LYS:O	1:C:239:LYS:HB2	2.21	0.41
1:E:69:LEU:O	1:E:81:GLN:HA	2.20	0.41
1:F:74:ILE:HD12	1:F:74:ILE:HA	1.76	0.41
1:F:142:TRP:NE1	1:F:154:LEU:N	2.69	0.41
1:G:32:PHE:HD1	1:G:142:TRP:CE3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:GLU:O	1:G:38:GLU:CG	2.39	0.41
1:G:179:THR:O	1:G:180:GLU:HG2	2.21	0.41
1:L:73:ASN:CB	1:L:153:THR:HG22	2.51	0.41
1:C:163:LYS:C	1:C:165:CYS:N	2.79	0.40
1:I:208:GLN:HA	1:I:227:VAL:HG22	2.02	0.40
1:L:53:PHE:HB3	1:L:238:MET:HE2	2.03	0.40
1:A:94:ALA:HB1	1:A:102:ASN:HB3	2.01	0.40
1:C:27:ARG:HH22	1:C:138:SER:HB2	1.85	0.40
1:C:30:MET:CE	1:C:140:ALA:O	2.63	0.40
1:C:116:THR:HG22	1:C:117:THR:N	2.36	0.40
1:C:136:LEU:HD21	1:C:158:LEU:HD11	2.03	0.40
1:C:177:ARG:H	1:C:177:ARG:HG3	1.59	0.40
1:E:86:VAL:O	1:E:86:VAL:HG23	2.20	0.40
1:F:106:LEU:HD12	1:F:237:THR:CG2	2.50	0.40
1:G:234:ILE:O	1:G:235:LYS:C	2.62	0.40
1:H:58:ALA:HA	1:H:105:MET:CB	2.51	0.40
1:H:116:THR:C	1:H:118:ALA:H	2.29	0.40
1:H:133:PRO:HA	1:H:161:VAL:HG12	2.03	0.40
1:I:204:LYS:N	2:I:302:SO4:O2	2.51	0.40
1:K:61:GLN:HA	1:K:65:ILE:HD11	2.03	0.40
1:K:179:THR:O	1:K:226:LYS:HB3	2.21	0.40
1:D:16:ILE:HG23	1:D:157:VAL:CG2	2.51	0.40
1:E:215:ASN:HD22	1:E:217:LYS:CD	2.35	0.40
1:F:84:ILE:HD12	1:F:84:ILE:H	1.85	0.40
1:G:96:ASN:HA	1:G:97:PRO:HD3	1.85	0.40
1:G:97:PRO:O	1:G:98:LYS:C	2.64	0.40
1:G:144:TYR:CD2	1:G:194:LYS:HB2	2.56	0.40
1:I:32:PHE:CD1	1:I:74:ILE:HG21	2.57	0.40
1:I:70:GLY:O	1:I:80:THR:OG1	2.36	0.40
1:I:161:VAL:C	1:I:162:GLN:HE21	2.28	0.40
1:I:186:PRO:HA	1:I:220:PRO:HG2	2.03	0.40
1:J:201:LEU:N	1:J:209:GLY:O	2.43	0.40
1:L:58:ALA:HB2	1:L:104:ILE:O	2.21	0.40
1:A:178:ALA:O	1:A:229:HIS:CD2	2.74	0.40
1:B:139:VAL:CG2	1:B:140:ALA:H	2.34	0.40
1:C:183:VAL:O	1:C:221:PRO:CB	2.70	0.40
1:F:114:LYS:HE3	1:F:114:LYS:HB2	1.71	0.40
1:H:185:ASP:OD1	1:H:185:ASP:C	2.64	0.40
1:I:139:VAL:CG2	1:I:140:ALA:N	2.85	0.40
1:K:92:HIS:ND1	1:K:94:ALA:HB3	2.36	0.40
1:A:50:ARG:HD3	1:A:53:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PRO:HA	1:A:220:PRO:HG2	2.03	0.40
1:B:69:LEU:HB3	1:B:119:VAL:CG1	2.49	0.40
1:C:92:HIS:NE2	1:C:230:PHE:HD1	2.19	0.40
1:D:123:ARG:O	1:D:206:VAL:HG23	2.21	0.40
1:F:38:GLU:O	1:F:39:LYS:C	2.64	0.40
1:H:187:LYS:HE3	1:H:187:LYS:HB2	1.60	0.40
1:K:29:TYR:CB	1:K:122:LEU:HB2	2.51	0.40
1:L:26:SER:C	1:L:28:PRO:HD3	2.47	0.40
1:L:37:GLN:HB2	4:L:404:HOH:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:HIS:CE1	1:L:173:GLY:O[1_554]	1.68	0.52
1:A:172:HIS:ND1	1:L:173:GLY:O[1_554]	2.06	0.14

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	220/226 (97%)	167 (76%)	39 (18%)	14 (6%)	1	6
1	B	224/226 (99%)	196 (88%)	24 (11%)	4 (2%)	6	31
1	C	224/226 (99%)	185 (83%)	35 (16%)	4 (2%)	6	31
1	D	224/226 (99%)	183 (82%)	31 (14%)	10 (4%)	2	12
1	E	224/226 (99%)	193 (86%)	23 (10%)	8 (4%)	2	16
1	F	224/226 (99%)	190 (85%)	23 (10%)	11 (5%)	1	10
1	G	224/226 (99%)	187 (84%)	30 (13%)	7 (3%)	3	19
1	H	215/226 (95%)	181 (84%)	27 (13%)	7 (3%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	224/226 (99%)	192 (86%)	28 (12%)	4 (2%)	6	31
1	J	224/226 (99%)	187 (84%)	31 (14%)	6 (3%)	4	22
1	K	224/226 (99%)	183 (82%)	31 (14%)	10 (4%)	2	12
1	L	224/226 (99%)	192 (86%)	25 (11%)	7 (3%)	3	19
All	All	2675/2712 (99%)	2236 (84%)	347 (13%)	92 (3%)	3	17

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ALA
1	A	172	HIS
1	A	177	ARG
1	D	240	ARG
1	E	191	THR
1	K	51	LYS
1	L	131	VAL
1	B	128	LYS
1	C	39	LYS
1	C	164	ASP
1	C	172	HIS
1	D	144	TYR
1	D	197	SER
1	F	125	PRO
1	G	59	HIS
1	G	95	TYR
1	G	191	THR
1	H	117	THR
1	I	51	LYS
1	K	191	THR
1	K	200	PRO
1	K	213	TYR
1	K	218	GLY
1	L	100	PHE
1	L	143	GLY
1	L	240	ARG
1	A	28	PRO
1	A	144	TYR
1	C	143	GLY
1	D	63	SER
1	E	151	ALA
1	E	169	ARG

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Mol	Chain	Res	Type
1	G	97	PRO
1	G	216	LYS
1	H	91	PRO
1	J	218	GLY
1	J	238	MET
1	K	147	MET
1	K	205	ASP
1	K	228	SER
1	L	79	ARG
1	L	93	PRO
1	L	197	SER
1	A	34	GLN
1	A	110	GLU
1	A	179	THR
1	A	197	SER
1	A	240	ARG
1	D	125	PRO
1	F	129	ALA
1	F	131	VAL
1	F	151	ALA
1	F	194	LYS
1	F	240	ARG
1	G	239	LYS
1	H	28	PRO
1	H	77	GLN
1	H	103	ASP
1	H	115	TRP
1	I	168	GLU
1	J	24	PRO
1	J	117	THR
1	A	133	PRO
1	A	139	VAL
1	A	168	GLU
1	A	178	ALA
1	B	161	VAL
1	D	22	ALA
1	D	129	ALA
1	E	51	LYS
1	E	121	PRO
1	E	133	PRO
1	E	197	SER
1	H	165	CYS

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Mol	Chain	Res	Type
1	J	98	LYS
1	K	119	VAL
1	K	164	ASP
1	F	93	PRO
1	F	100	PHE
1	F	197	SER
1	G	38	GLU
1	I	88	ARG
1	I	92	HIS
1	D	157	VAL
1	J	89	PRO
1	D	234	ILE
1	E	47	ILE
1	F	27	ARG
1	F	200	PRO
1	B	89	PRO
1	B	218	GLY
1	D	173	GLY

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	192/194 (99%)	161 (84%)	31 (16%)	2	12
1	B	194/194 (100%)	165 (85%)	29 (15%)	3	15
1	C	194/194 (100%)	170 (88%)	24 (12%)	4	20
1	D	194/194 (100%)	169 (87%)	25 (13%)	4	19
1	E	194/194 (100%)	172 (89%)	22 (11%)	5	24
1	F	194/194 (100%)	175 (90%)	19 (10%)	7	30
1	G	194/194 (100%)	163 (84%)	31 (16%)	2	12
1	H	190/194 (98%)	169 (89%)	21 (11%)	6	25
1	I	194/194 (100%)	170 (88%)	24 (12%)	4	20
1	J	194/194 (100%)	169 (87%)	25 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	194/194 (100%)	170 (88%)	24 (12%)	4	20
1	L	194/194 (100%)	172 (89%)	22 (11%)	5	24
All	All	2322/2328 (100%)	2025 (87%)	297 (13%)	4	19

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	21	GLU
1	A	38	GLU
1	A	47	ILE
1	A	48	LEU
1	A	64	SER
1	A	80	THR
1	A	84	ILE
1	A	86	VAL
1	A	92	HIS
1	A	99	ASN
1	A	116	THR
1	A	117	THR
1	A	124	LEU
1	A	132	LYS
1	A	135	GLN
1	A	150	LEU
1	A	154	LEU
1	A	157	VAL
1	A	160	THR
1	A	170	LEU
1	A	172	HIS
1	A	174	ASN
1	A	176	SER
1	A	179	THR
1	A	191	THR
1	A	197	SER
1	A	203	CYS
1	A	206	VAL
1	A	213	TYR
1	A	219	THR
1	B	38	GLU
1	B	56	THR
1	B	79	ARG

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Mol	Chain	Res	Type
1	B	86	VAL
1	B	105	MET
1	B	109	LEU
1	B	119	VAL
1	B	124	LEU
1	B	128	LYS
1	B	131	VAL
1	B	139	VAL
1	B	145	VAL
1	B	147	MET
1	B	148	SER
1	B	149	THR
1	B	157	VAL
1	B	176	SER
1	B	188	LYS
1	B	189	THR
1	B	194	LYS
1	B	197	SER
1	B	201	LEU
1	B	202	VAL
1	B	204	LYS
1	B	206	VAL
1	B	210	ILE
1	B	216	LYS
1	B	219	THR
1	B	237	THR
1	C	16	ILE
1	C	42	LYS
1	C	47	ILE
1	C	48	LEU
1	C	59	HIS
1	C	75	LYS
1	C	99	ASN
1	C	106	LEU
1	C	115	TRP
1	C	117	THR
1	C	124	LEU
1	C	157	VAL
1	C	174	ASN
1	C	181	ILE
1	C	185	ASP
1	C	189	THR

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Mol	Chain	Res	Type
1	C	191	THR
1	C	204	LYS
1	C	210	ILE
1	C	212	SER
1	C	219	THR
1	C	227	VAL
1	C	228	SER
1	C	241	LEU
1	D	61	GLN
1	D	63	SER
1	D	67	VAL
1	D	68	THR
1	D	74	ILE
1	D	127	SER
1	D	128	LYS
1	D	130	GLN
1	D	131	VAL
1	D	139	VAL
1	D	149	THR
1	D	150	LEU
1	D	157	VAL
1	D	171	PHE
1	D	181	ILE
1	D	183	VAL
1	D	188	LYS
1	D	191	THR
1	D	197	SER
1	D	202	VAL
1	D	210	ILE
1	D	219	THR
1	D	231	LEU
1	D	235	LYS
1	D	236	ARG
1	E	33	VAL
1	E	36	LEU
1	E	38	GLU
1	E	41	ARG
1	E	47	ILE
1	E	48	LEU
1	E	65	ILE
1	E	66	ASN
1	E	67	VAL

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Mol	Chain	Res	Type
1	E	76	GLU
1	E	84	ILE
1	E	122	LEU
1	E	126	SER
1	E	127	SER
1	E	139	VAL
1	E	157	VAL
1	E	160	THR
1	E	163	LYS
1	E	201	LEU
1	E	210	ILE
1	E	225	ILE
1	E	240	ARG
1	F	36	LEU
1	F	43	ARG
1	F	47	ILE
1	F	64	SER
1	F	80	THR
1	F	84	ILE
1	F	91	PRO
1	F	101	SER
1	F	117	THR
1	F	127	SER
1	F	130	GLN
1	F	154	LEU
1	F	157	VAL
1	F	177	ARG
1	F	181	ILE
1	F	191	THR
1	F	210	ILE
1	F	228	SER
1	F	231	LEU
1	G	27	ARG
1	G	36	LEU
1	G	38	GLU
1	G	63	SER
1	G	64	SER
1	G	67	VAL
1	G	69	LEU
1	G	74	ILE
1	G	80	THR
1	G	84	ILE

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Mol	Chain	Res	Type
1	G	86	VAL
1	G	101	SER
1	G	104	ILE
1	G	123	ARG
1	G	124	LEU
1	G	127	SER
1	G	131	VAL
1	G	138	SER
1	G	139	VAL
1	G	146	SER
1	G	150	LEU
1	G	156	GLU
1	G	157	VAL
1	G	159	LEU
1	G	197	SER
1	G	206	VAL
1	G	210	ILE
1	G	216	LYS
1	G	219	THR
1	G	237	THR
1	G	241	LEU
1	H	36	LEU
1	H	37	GLN
1	H	40	SER
1	H	67	VAL
1	H	74	ILE
1	H	87	LYS
1	H	108	GLN
1	H	116	THR
1	H	119	VAL
1	H	130	GLN
1	H	136	LEU
1	H	138	SER
1	H	139	VAL
1	H	149	THR
1	H	150	LEU
1	H	158	LEU
1	H	201	LEU
1	H	205	ASP
1	H	206	VAL
1	H	219	THR
1	H	237	THR

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Mol	Chain	Res	Type
1	I	38	GLU
1	I	40	SER
1	I	42	LYS
1	I	47	ILE
1	I	56	THR
1	I	74	ILE
1	I	75	LYS
1	I	79	ARG
1	I	80	THR
1	I	104	ILE
1	I	110	GLU
1	I	122	LEU
1	I	130	GLN
1	I	149	THR
1	I	155	GLN
1	I	157	VAL
1	I	160	THR
1	I	170	LEU
1	I	183	VAL
1	I	189	THR
1	I	190	GLN
1	I	206	VAL
1	I	216	LYS
1	I	224	TYR
1	J	16	ILE
1	J	33	VAL
1	J	38	GLU
1	J	51	LYS
1	J	68	THR
1	J	74	ILE
1	J	81	GLN
1	J	90	ILE
1	J	110	GLU
1	J	123	ARG
1	J	148	SER
1	J	157	VAL
1	J	166	GLN
1	J	174	ASN
1	J	179	THR
1	J	180	GLU
1	J	185	ASP
1	J	187	LYS

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Mol	Chain	Res	Type
1	J	194	LYS
1	J	206	VAL
1	J	215	ASN
1	J	225	ILE
1	J	231	LEU
1	J	236	ARG
1	J	241	LEU
1	K	16	ILE
1	K	47	ILE
1	K	48	LEU
1	K	51	LYS
1	K	54	VAL
1	K	64	SER
1	K	68	THR
1	K	81	GLN
1	K	98	LYS
1	K	102	ASN
1	K	106	LEU
1	K	119	VAL
1	K	128	LYS
1	K	131	VAL
1	K	153	THR
1	K	157	VAL
1	K	165	CYS
1	K	170	LEU
1	K	176	SER
1	K	205	ASP
1	K	206	VAL
1	K	217	LYS
1	K	233	TRP
1	K	236	ARG
1	L	16	ILE
1	L	25	HIS
1	L	26	SER
1	L	40	SER
1	L	43	ARG
1	L	101	SER
1	L	116	THR
1	L	117	THR
1	L	123	ARG
1	L	127	SER
1	L	130	GLN

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Mol	Chain	Res	Type
1	L	136	LEU
1	L	138	SER
1	L	170	LEU
1	L	177	ARG
1	L	181	ILE
1	L	189	THR
1	L	191	THR
1	L	204	LYS
1	L	210	ILE
1	L	228	SER
1	L	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	59	HIS
1	A	108	GLN
1	A	215	ASN
1	B	82	GLN
1	B	108	GLN
1	B	130	GLN
1	B	135	GLN
1	B	155	GLN
1	B	162	GLN
1	C	59	HIS
1	C	96	ASN
1	C	99	ASN
1	C	108	GLN
1	C	130	GLN
1	C	190	GLN
1	D	34	GLN
1	D	77	GLN
1	D	96	ASN
1	D	99	ASN
1	D	108	GLN
1	D	130	GLN
1	D	135	GLN
1	D	162	GLN
1	D	208	GLN
1	E	81	GLN
1	E	102	ASN

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Mol	Chain	Res	Type
1	E	108	GLN
1	E	135	GLN
1	E	190	GLN
1	E	215	ASN
1	F	99	ASN
1	F	130	GLN
1	F	162	GLN
1	F	190	GLN
1	F	229	HIS
1	G	66	ASN
1	G	72	HIS
1	G	174	ASN
1	H	20	HIS
1	H	25	HIS
1	H	61	GLN
1	H	77	GLN
1	H	92	HIS
1	H	96	ASN
1	H	174	ASN
1	H	190	GLN
1	I	25	HIS
1	I	66	ASN
1	I	135	GLN
1	I	208	GLN
1	I	215	ASN
1	J	25	HIS
1	J	61	GLN
1	J	96	ASN
1	J	155	GLN
1	K	73	ASN
1	K	81	GLN
1	K	102	ASN
1	K	162	GLN
1	K	208	GLN
1	L	77	GLN
1	L	99	ASN
1	L	130	GLN
1	L	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	E	301	-	4,4,4	0.55	0	6,6,6	0.45	0
2	SO4	B	304	-	4,4,4	0.52	0	6,6,6	0.48	0
2	SO4	F	302	-	4,4,4	0.70	0	6,6,6	0.52	0
2	SO4	I	302	-	4,4,4	0.46	0	6,6,6	0.25	0
2	SO4	B	302	-	4,4,4	0.94	0	6,6,6	0.74	0
2	SO4	D	303	-	4,4,4	0.52	0	6,6,6	0.44	0
2	SO4	L	302	-	4,4,4	0.46	0	6,6,6	0.26	0
2	SO4	L	301	-	4,4,4	0.54	0	6,6,6	0.45	0
2	SO4	B	301	-	4,4,4	0.74	0	6,6,6	0.85	0
2	SO4	D	302	-	4,4,4	0.60	0	6,6,6	0.59	0
2	SO4	F	303	-	4,4,4	0.50	0	6,6,6	0.45	0
2	SO4	I	301	-	4,4,4	0.47	0	6,6,6	0.51	0
2	SO4	B	303	-	4,4,4	0.46	0	6,6,6	0.43	0
2	SO4	D	301	-	4,4,4	0.55	0	6,6,6	0.63	0
2	SO4	F	301	-	4,4,4	0.85	0	6,6,6	0.58	0

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	302	SO4	1	0
2	D	303	SO4	1	0
2	L	301	SO4	2	0
2	B	301	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	224/226 (99%)	1.22	31 (13%) 6 4	35, 79, 114, 155	2 (0%)
1	B	226/226 (100%)	-0.11	4 (1%) 67 44	26, 38, 61, 91	3 (1%)
1	C	226/226 (100%)	0.60	11 (4%) 35 18	43, 62, 91, 127	3 (1%)
1	D	226/226 (100%)	0.20	2 (0%) 81 61	31, 49, 73, 97	3 (1%)
1	E	226/226 (100%)	0.26	4 (1%) 67 44	35, 54, 76, 101	3 (1%)
1	F	226/226 (100%)	-0.15	3 (1%) 75 53	28, 39, 65, 120	3 (1%)
1	G	226/226 (100%)	-0.13	4 (1%) 67 44	27, 44, 79, 149	3 (1%)
1	H	221/226 (97%)	0.78	16 (7%) 21 11	49, 74, 114, 173	3 (1%)
1	I	226/226 (100%)	-0.02	4 (1%) 67 44	34, 45, 77, 117	3 (1%)
1	J	226/226 (100%)	0.46	10 (4%) 39 21	40, 69, 103, 151	3 (1%)
1	K	226/226 (100%)	2.23	135 (59%) 0 0	70, 115, 197, 314	3 (1%)
1	L	226/226 (100%)	1.90	86 (38%) 1 1	71, 102, 152, 183	3 (1%)
All	All	2705/2712 (99%)	0.60	310 (11%) 9 6	26, 61, 129, 314	35 (1%)

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	163	LYS	9.3
1	A	185	ASP	6.4
1	K	235	LYS	5.9
1	K	31	ALA	5.3
1	A	218	GLY	5.1
1	L	189	THR	5.0
1	K	115	TRP	4.9
1	K	210	ILE	4.8
1	L	132	LYS	4.7
1	K	131	VAL	4.7
1	L	166	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	4.6
1	K	207	ALA	4.6
1	K	114	LYS	4.6
1	L	195	GLY	4.6
1	K	81	GLN	4.5
1	K	83	PHE	4.5
1	E	163	LYS	4.4
1	L	39	LYS	4.4
1	K	237	THR	4.3
1	L	183	VAL	4.3
1	L	235	LYS	4.2
1	L	131	VAL	4.2
1	H	235	LYS	4.2
1	L	141	GLY	4.2
1	A	235	LYS	4.2
1	K	213	TYR	4.2
1	K	82	GLN	4.1
1	K	212	SER	4.1
1	K	203	CYS	4.0
1	E	39	LYS	4.0
1	L	223	VAL	4.0
1	K	113	ALA	4.0
1	H	163	LYS	4.0
1	K	45	GLY	3.9
1	J	100	PHE	3.9
1	L	213	TYR	3.9
1	L	241	LEU	3.9
1	K	91	PRO	3.9
1	A	170	LEU	3.8
1	K	228	SER	3.8
1	D	39	LYS	3.8
1	K	107	LEU	3.7
1	J	235	LYS	3.7
1	K	90	ILE	3.7
1	K	176	SER	3.7
1	K	112	LYS	3.7
1	L	140	ALA	3.7
1	K	223	VAL	3.7
1	K	238	MET	3.7
1	L	181	ILE	3.6
1	L	129	ALA	3.6
1	L	144	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	211	LEU	3.6
1	K	34	GLN	3.6
1	K	224	TYR	3.6
1	L	170	LEU	3.5
1	L	230	PHE	3.5
1	L	214	GLY	3.5
1	K	240	ARG	3.5
1	K	117	THR	3.5
1	L	182	CYS	3.5
1	L	136	LEU	3.5
1	K	93	PRO	3.5
1	K	101	SER	3.4
1	K	128	LYS	3.4
1	L	16	ILE	3.4
1	L	167	CYS	3.4
1	K	239	LYS	3.4
1	H	39	LYS	3.4
1	A	173	GLY	3.4
1	H	223	VAL	3.4
1	L	145	VAL	3.4
1	L	184	GLY	3.4
1	A	16	ILE	3.4
1	K	104	ILE	3.4
1	L	159	LEU	3.3
1	K	163	LYS	3.3
1	L	190	GLN	3.3
1	K	102	ASN	3.3
1	K	124	LEU	3.3
1	L	161	VAL	3.3
1	L	133	PRO	3.3
1	K	94	ALA	3.3
1	L	165	CYS	3.3
1	C	131	VAL	3.3
1	K	161	VAL	3.3
1	K	125	PRO	3.2
1	L	110	GLU	3.2
1	K	201	LEU	3.2
1	L	216	LYS	3.2
1	K	44	CYS	3.2
1	A	241	LEU	3.2
1	H	81	GLN	3.2
1	K	135	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	39	LYS	3.2
1	B	163	LYS	3.2
1	L	185	ASP	3.1
1	L	222	GLY	3.1
1	A	174	ASN	3.1
1	L	215	ASN	3.1
1	K	37	GLN	3.1
1	L	169	ARG	3.1
1	K	199	GLY	3.1
1	K	202	VAL	3.1
1	K	130	GLN	3.1
1	L	208	GLN	3.1
1	K	56	THR	3.1
1	A	131	VAL	3.0
1	K	64	SER	3.0
1	K	234	ILE	3.0
1	K	205	ASP	3.0
1	K	109	LEU	3.0
1	K	51	LYS	3.0
1	K	204	LYS	3.0
1	K	126	SER	3.0
1	C	39	LYS	3.0
1	K	39	LYS	3.0
1	K	226	LYS	3.0
1	K	241	LEU	3.0
1	L	127	SER	3.0
1	K	158	LEU	2.9
1	A	140	ALA	2.9
1	I	235	LYS	2.9
1	C	147	MET	2.9
1	A	94	ALA	2.9
1	A	129	ALA	2.9
1	K	54	VAL	2.9
1	K	166	GLN	2.9
1	K	133	PRO	2.9
1	L	200	PRO	2.9
1	L	224	TYR	2.9
1	K	62	GLY	2.9
1	K	230	PHE	2.9
1	L	135	GLN	2.9
1	L	221	PRO	2.9
1	K	53	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	235	LYS	2.9
1	K	116	THR	2.9
1	K	232	PRO	2.9
1	K	50	ARG	2.9
1	G	147	MET	2.9
1	K	127	SER	2.8
1	A	224	TYR	2.8
1	A	145	VAL	2.8
1	K	92	HIS	2.8
1	C	163	LYS	2.8
1	G	235	LYS	2.8
1	K	206	VAL	2.8
1	K	214	GLY	2.8
1	K	99	ASN	2.8
1	K	85	PRO	2.8
1	K	200	PRO	2.8
1	J	241	LEU	2.8
1	A	223	VAL	2.7
1	H	100	PHE	2.7
1	J	163	LYS	2.7
1	A	81	GLN	2.7
1	L	17	ILE	2.7
1	G	241	LEU	2.7
1	L	204	LYS	2.7
1	K	68	THR	2.7
1	A	126	SER	2.7
1	K	227	VAL	2.7
1	L	109	LEU	2.7
1	L	150	LEU	2.7
1	L	196	ASP	2.7
1	K	120	ARG	2.6
1	K	156	GLU	2.6
1	L	197	SER	2.6
1	L	171	PHE	2.6
1	K	225	ILE	2.6
1	K	100	PHE	2.6
1	L	218	GLY	2.6
1	K	118	ALA	2.6
1	E	212	SER	2.6
1	K	209	GLY	2.6
1	F	163	LYS	2.6
1	L	115	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	134	GLY	2.6
1	B	241	LEU	2.6
1	K	30	MET	2.5
1	L	92	HIS	2.5
1	L	172	HIS	2.5
1	C	139	VAL	2.5
1	J	39	LYS	2.5
1	L	219	THR	2.5
1	K	178	ALA	2.5
1	A	179	THR	2.5
1	L	154	LEU	2.5
1	K	173	GLY	2.5
1	A	221	PRO	2.5
1	K	20	HIS	2.5
1	K	136	LEU	2.5
1	K	108	GLN	2.5
1	A	176	SER	2.5
1	J	118	ALA	2.5
1	L	210	ILE	2.5
1	E	215	ASN	2.5
1	K	231	LEU	2.5
1	K	129	ALA	2.4
1	K	63	SER	2.4
1	K	27	ARG	2.4
1	K	132	LYS	2.4
1	L	220	PRO	2.4
1	K	77	GLN	2.4
1	L	130	GLN	2.4
1	D	163	LYS	2.4
1	K	122	LEU	2.4
1	C	185	ASP	2.4
1	K	220	PRO	2.4
1	A	184	GLY	2.4
1	K	208	GLN	2.4
1	C	235	LYS	2.4
1	K	119	VAL	2.4
1	L	20	HIS	2.4
1	K	181	ILE	2.4
1	K	236	ARG	2.4
1	J	115	TRP	2.4
1	C	143	GLY	2.4
1	H	224	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	140	ALA	2.3
1	H	80	THR	2.3
1	K	66	ASN	2.3
1	K	32	PHE	2.3
1	H	213	TYR	2.3
1	K	61	GLN	2.3
1	K	110	GLU	2.3
1	L	98	LYS	2.3
1	L	211	LEU	2.3
1	K	67	VAL	2.3
1	K	123	ARG	2.3
1	K	233	TRP	2.3
1	K	65	ILE	2.2
1	K	198	GLY	2.2
1	L	40	SER	2.2
1	L	175	TYR	2.2
1	L	212	SER	2.2
1	A	215	ASN	2.2
1	K	60	CYS	2.2
1	I	241	LEU	2.2
1	C	241	LEU	2.2
1	K	103	ASP	2.2
1	L	178	ALA	2.2
1	H	128	LYS	2.2
1	K	87	LYS	2.2
1	K	229	HIS	2.2
1	I	126	SER	2.2
1	K	159	LEU	2.2
1	L	177	ARG	2.2
1	K	86	VAL	2.2
1	K	183	VAL	2.2
1	A	181	ILE	2.2
1	H	207	ALA	2.2
1	L	151	ALA	2.2
1	L	203	CYS	2.2
1	J	213	TYR	2.1
1	A	130	GLN	2.1
1	H	208	GLN	2.1
1	K	28	PRO	2.1
1	L	93	PRO	2.1
1	L	225	ILE	2.1
1	B	235	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	41	ARG	2.1
1	A	70	GLY	2.1
1	L	64	SER	2.1
1	L	180	GLU	2.1
1	L	192	GLY	2.1
1	L	99	ASN	2.1
1	F	115	TRP	2.1
1	K	49	VAL	2.1
1	A	59	HIS	2.1
1	K	23	LYS	2.1
1	A	180	GLU	2.1
1	L	134	GLY	2.1
1	L	174	ASN	2.1
1	C	132	LYS	2.1
1	A	74	ILE	2.1
1	L	164	ASP	2.1
1	H	175	TYR	2.1
1	K	22	ALA	2.1
1	K	162	GLN	2.1
1	H	83	PHE	2.1
1	H	225	ILE	2.1
1	K	69	LEU	2.1
1	L	59	HIS	2.1
1	A	213	TYR	2.1
1	K	175	TYR	2.1
1	A	166	GLN	2.1
1	K	143	GLY	2.1
1	I	39	LYS	2.0
1	J	188	LYS	2.0
1	L	63	SER	2.0
1	K	88	ARG	2.0
1	K	169	ARG	2.0
1	C	115	TRP	2.0
1	K	59	HIS	2.0
1	L	179	THR	2.0
1	L	168	GLU	2.0
1	L	194	LYS	2.0
1	J	80	THR	2.0
1	K	52	ASP	2.0
1	K	171	PHE	2.0
1	K	180	GLU	2.0
1	G	240	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	206	VAL	2.0
1	H	201	LEU	2.0
1	K	106	LEU	2.0
1	L	231	LEU	2.0
1	K	47	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	L	302	5/5	0.61	0.15	132,140,145,147	0
2	SO4	B	303	5/5	0.85	0.14	82,83,87,88	0
2	SO4	I	301	5/5	0.88	0.12	67,69,70,73	0
2	SO4	B	304	5/5	0.88	0.11	69,71,75,78	0
2	SO4	F	303	5/5	0.89	0.12	77,81,82,85	0
2	SO4	L	301	5/5	0.90	0.18	87,87,88,92	0
2	SO4	I	302	5/5	0.90	0.10	68,69,71,75	0
2	SO4	E	301	5/5	0.92	0.10	65,66,68,71	0
2	SO4	D	302	5/5	0.92	0.11	72,76,79,80	0
3	CL	C	301	1/1	0.94	0.20	54,54,54,54	0
3	CL	D	304	1/1	0.94	0.14	48,48,48,48	0
2	SO4	D	303	5/5	0.95	0.12	66,67,67,68	0
3	CL	I	303	1/1	0.95	0.08	44,44,44,44	0
2	SO4	B	301	5/5	0.97	0.07	34,34,36,37	0
2	SO4	B	302	5/5	0.97	0.11	32,33,35,36	0
2	SO4	D	301	5/5	0.97	0.11	46,48,49,50	0
2	SO4	F	302	5/5	0.97	0.07	43,44,46,47	0
2	SO4	F	301	5/5	0.98	0.07	35,36,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.