



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:22 PM UTC

PDB ID : 2EHO / pdb_00002eho
Title : Crystal structure of human GINS complex
Authors : Choi, J.M.; Lim, H.S.; Kim, J.J.; Song, O.K.; Cho, Y.
Deposited on : 2007-03-07
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

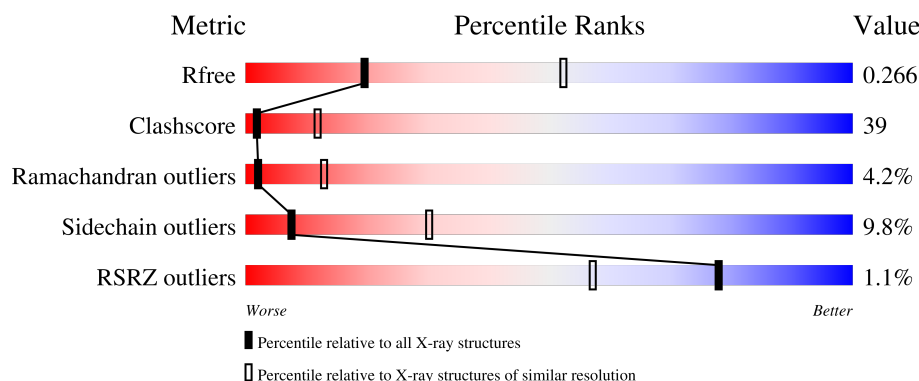
1 Overall quality at a glance

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.



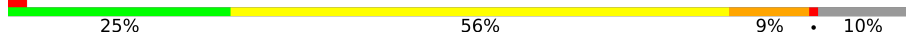
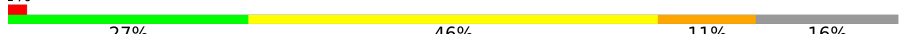
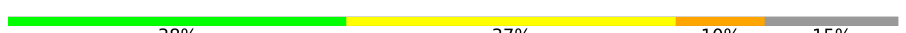
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	203	2% 25% 48% 5% • 21%
1	E	203	% 41% 45% 7% • 6%
1	I	203	% 39% 43% 10% • 5%
2	B	152	% 35% 50% 10% • 5%
2	F	152	43% 45% 8% •

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Mol	Chain	Length	Quality of chain
2	J	152	
3	C	186	
3	G	186	
3	K	186	
4	D	216	
4	H	216	
4	L	216	

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
5	SO4	B	1016	-	-	X	-
5	SO4	F	1010	-	-	X	-
5	SO4	K	1007	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16937 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 GINS complex subunit 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	Se	0	0	0
			1340	857	227	246	2	8			
1	E	190	Total	C	N	O	S	Se	0	0	0
			1583	1005	269	299	2	8			
1	I	192	Total	C	N	O	S	Se	0	0	0
			1604	1016	278	300	2	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MSE	MET	modified residue	UNP Q9BRT9
A	55	MSE	MET	modified residue	UNP Q9BRT9
A	61	MSE	MET	modified residue	UNP Q9BRT9
A	80	MSE	MET	modified residue	UNP Q9BRT9
A	82	MSE	MET	modified residue	UNP Q9BRT9
A	98	MSE	MET	modified residue	UNP Q9BRT9
A	134	MSE	MET	modified residue	UNP Q9BRT9
A	149	MSE	MET	modified residue	UNP Q9BRT9
E	35	MSE	MET	modified residue	UNP Q9BRT9
E	55	MSE	MET	modified residue	UNP Q9BRT9
E	61	MSE	MET	modified residue	UNP Q9BRT9
E	80	MSE	MET	modified residue	UNP Q9BRT9
E	82	MSE	MET	modified residue	UNP Q9BRT9
E	98	MSE	MET	modified residue	UNP Q9BRT9
E	134	MSE	MET	modified residue	UNP Q9BRT9
E	149	MSE	MET	modified residue	UNP Q9BRT9
I	35	MSE	MET	modified residue	UNP Q9BRT9
I	55	MSE	MET	modified residue	UNP Q9BRT9
I	61	MSE	MET	modified residue	UNP Q9BRT9
I	80	MSE	MET	modified residue	UNP Q9BRT9
I	82	MSE	MET	modified residue	UNP Q9BRT9
I	98	MSE	MET	modified residue	UNP Q9BRT9
I	134	MSE	MET	modified residue	UNP Q9BRT9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	149	MSE	MET	modified residue	UNP Q9BRT9

- Molecule 2 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	Se	0	0	0
			1188	744	217	217	3	7			
2	F	146	Total	C	N	O	S	Se	0	0	0
			1196	749	218	218	3	8			
2	J	145	Total	C	N	O	S	Se	0	0	0
			1188	744	217	217	3	7			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MSE	-	cloning artifact	UNP Q14691
B	1	MSE	MET	modified residue	UNP Q14691
B	7	MSE	MET	modified residue	UNP Q14691
B	36	MSE	MET	modified residue	UNP Q14691
B	97	ILE	VAL	SEE REMARK 999	UNP Q14691
B	106	MSE	MET	modified residue	UNP Q14691
B	111	MSE	MET	modified residue	UNP Q14691
B	125	MSE	MET	modified residue	UNP Q14691
B	140	MSE	MET	modified residue	UNP Q14691
F	0	MSE	-	cloning artifact	UNP Q14691
F	1	MSE	MET	modified residue	UNP Q14691
F	7	MSE	MET	modified residue	UNP Q14691
F	36	MSE	MET	modified residue	UNP Q14691
F	97	ILE	VAL	SEE REMARK 999	UNP Q14691
F	106	MSE	MET	modified residue	UNP Q14691
F	111	MSE	MET	modified residue	UNP Q14691
F	125	MSE	MET	modified residue	UNP Q14691
F	140	MSE	MET	modified residue	UNP Q14691
J	0	MSE	-	cloning artifact	UNP Q14691
J	1	MSE	MET	modified residue	UNP Q14691
J	7	MSE	MET	modified residue	UNP Q14691
J	36	MSE	MET	modified residue	UNP Q14691
J	97	ILE	VAL	SEE REMARK 999	UNP Q14691
J	106	MSE	MET	modified residue	UNP Q14691
J	111	MSE	MET	modified residue	UNP Q14691
J	125	MSE	MET	modified residue	UNP Q14691
J	140	MSE	MET	modified residue	UNP Q14691

- Molecule 3 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	168	Total	C	N	O	S	Se	0	0	0
			1369	876	230	253	1	9			
3	G	176	Total	C	N	O	S	Se	0	0	0
			1432	916	242	264	1	9			
3	K	175	Total	C	N	O	S	Se	0	0	0
			1423	911	240	262	1	9			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MSE	-	cloning artifact	UNP Q9Y248
C	1	MSE	MET	modified residue	UNP Q9Y248
C	66	MSE	MET	modified residue	UNP Q9Y248
C	74	MSE	MET	modified residue	UNP Q9Y248
C	87	MSE	MET	modified residue	UNP Q9Y248
C	93	MSE	MET	modified residue	UNP Q9Y248
C	120	MSE	MET	modified residue	UNP Q9Y248
C	151	MSE	MET	modified residue	UNP Q9Y248
C	167	MSE	MET	modified residue	UNP Q9Y248
G	0	MSE	-	cloning artifact	UNP Q9Y248
G	1	MSE	MET	modified residue	UNP Q9Y248
G	66	MSE	MET	modified residue	UNP Q9Y248
G	74	MSE	MET	modified residue	UNP Q9Y248
G	87	MSE	MET	modified residue	UNP Q9Y248
G	93	MSE	MET	modified residue	UNP Q9Y248
G	120	MSE	MET	modified residue	UNP Q9Y248
G	151	MSE	MET	modified residue	UNP Q9Y248
G	167	MSE	MET	modified residue	UNP Q9Y248
K	0	MSE	-	cloning artifact	UNP Q9Y248
K	1	MSE	MET	modified residue	UNP Q9Y248
K	66	MSE	MET	modified residue	UNP Q9Y248
K	74	MSE	MET	modified residue	UNP Q9Y248
K	87	MSE	MET	modified residue	UNP Q9Y248
K	93	MSE	MET	modified residue	UNP Q9Y248
K	120	MSE	MET	modified residue	UNP Q9Y248
K	151	MSE	MET	modified residue	UNP Q9Y248
K	167	MSE	MET	modified residue	UNP Q9Y248

- Molecule 4 is a protein called GINS complex subunit 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	182	Total	C	N	O	S	Se	0	0	0
			1462	931	251	274	1	5			
4	H	183	Total	C	N	O	S	Se	0	0	0
			1470	935	253	276	1	5			
4	L	182	Total	C	N	O	S	Se	0	0	0
			1462	931	252	273	1	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	modified residue	UNP Q9BRX5
D	27	MSE	MET	modified residue	UNP Q9BRX5
D	40	MSE	MET	modified residue	UNP Q9BRX5
D	112	MSE	MET	modified residue	UNP Q9BRX5
D	150	MSE	MET	modified residue	UNP Q9BRX5
D	171	MSE	MET	modified residue	UNP Q9BRX5
H	1	MSE	MET	modified residue	UNP Q9BRX5
H	27	MSE	MET	modified residue	UNP Q9BRX5
H	40	MSE	MET	modified residue	UNP Q9BRX5
H	112	MSE	MET	modified residue	UNP Q9BRX5
H	150	MSE	MET	modified residue	UNP Q9BRX5
H	171	MSE	MET	modified residue	UNP Q9BRX5
L	1	MSE	MET	modified residue	UNP Q9BRX5
L	27	MSE	MET	modified residue	UNP Q9BRX5
L	40	MSE	MET	modified residue	UNP Q9BRX5
L	112	MSE	MET	modified residue	UNP Q9BRX5
L	150	MSE	MET	modified residue	UNP Q9BRX5
L	171	MSE	MET	modified residue	UNP Q9BRX5

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		

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

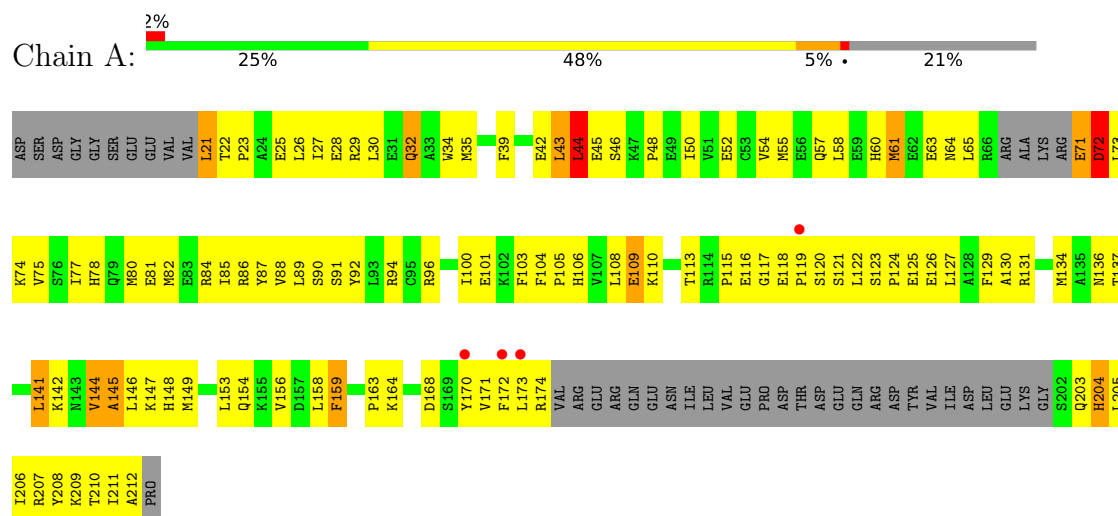
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	5	Total	O	0	0
			5	5		
6	C	2	Total	O	0	0
			2	2		
6	D	1	Total	O	0	0
			1	1		
6	E	22	Total	O	0	0
			22	22		
6	F	11	Total	O	0	0
			11	11		
6	G	6	Total	O	0	0
			6	6		
6	H	7	Total	O	0	0
			7	7		
6	I	18	Total	O	0	0
			18	18		
6	J	23	Total	O	0	0
			23	23		
6	K	13	Total	O	0	0
			13	13		
6	L	19	Total	O	0	0
			19	19		

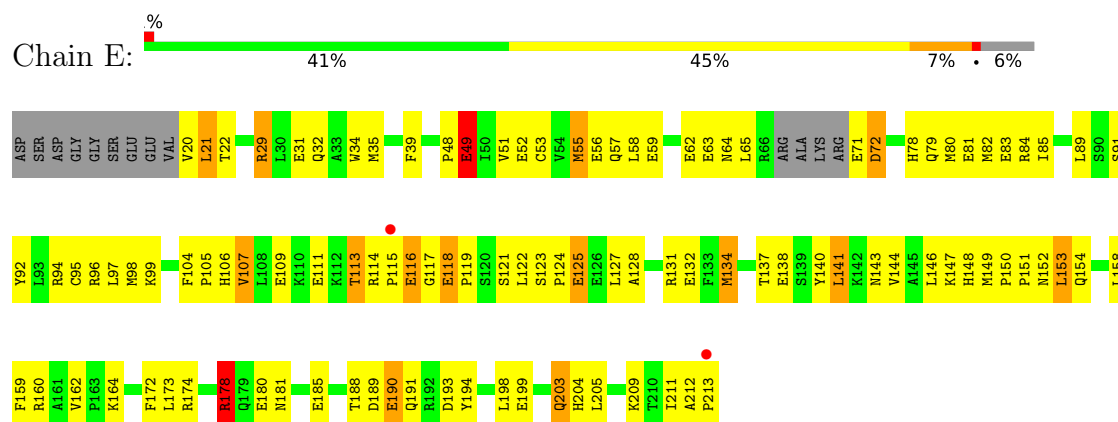
3 Residue-property plots [i](#)

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

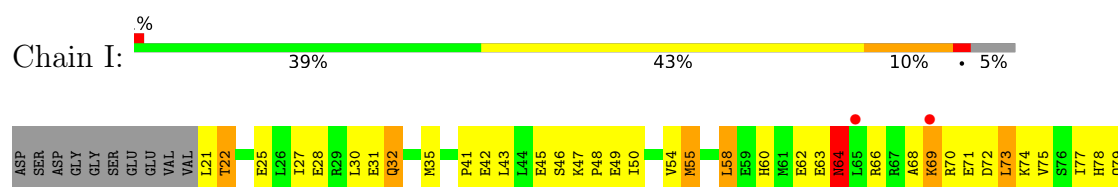
• Molecule 1: GINS complex subunit 4

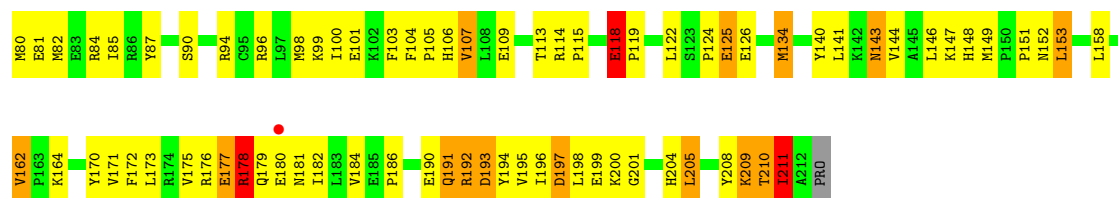


• Molecule 1: GINS complex subunit 4

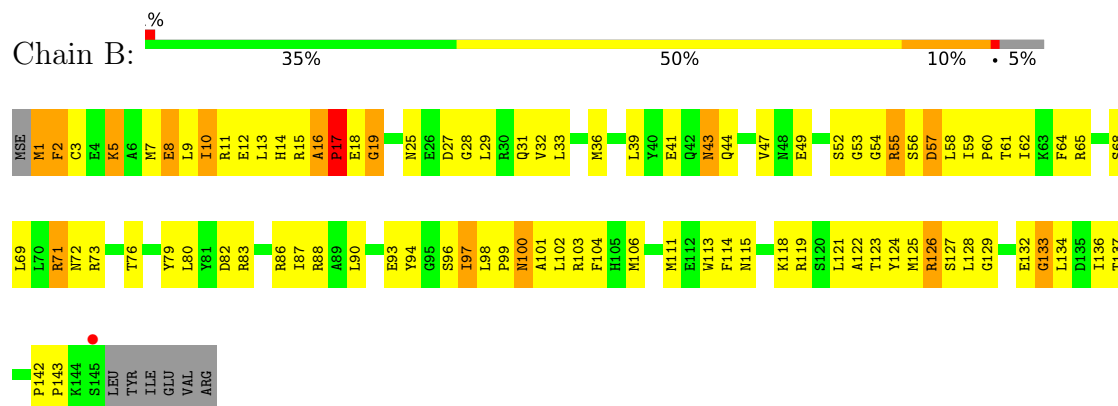


• Molecule 1: GINS complex subunit 4

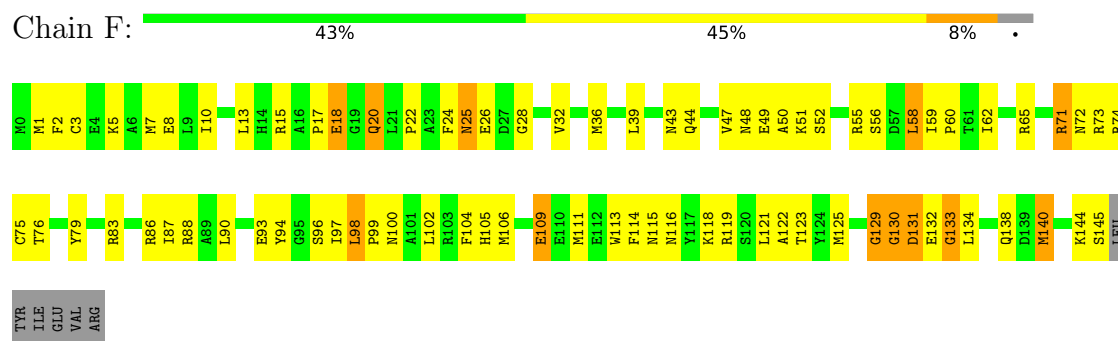




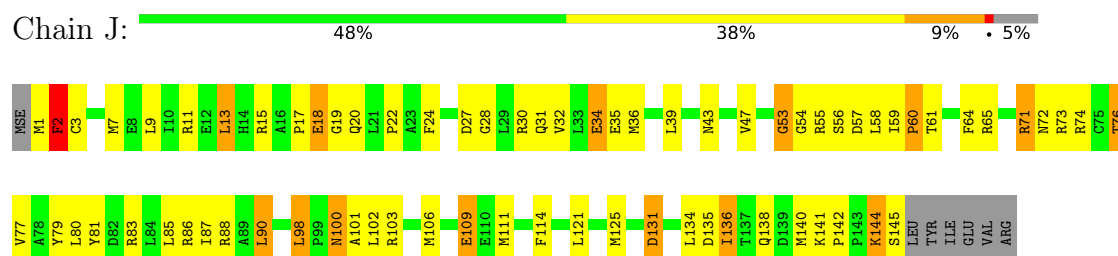
• Molecule 2: DNA replication complex GINS protein PSF1



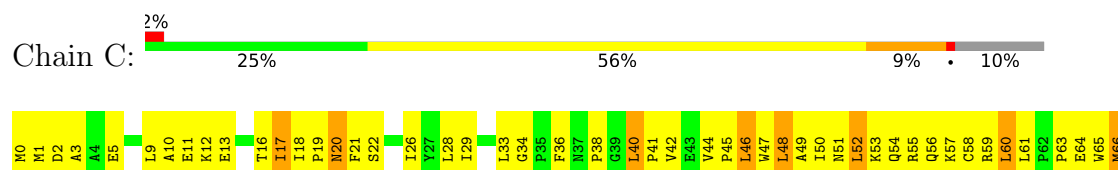
• Molecule 2: DNA replication complex GINS protein PSF1

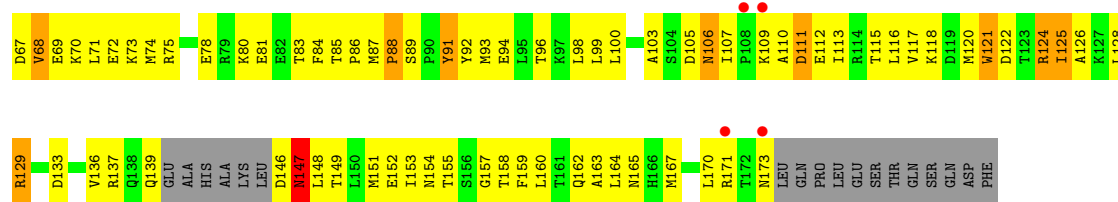


• Molecule 2: DNA replication complex GINS protein PSF1

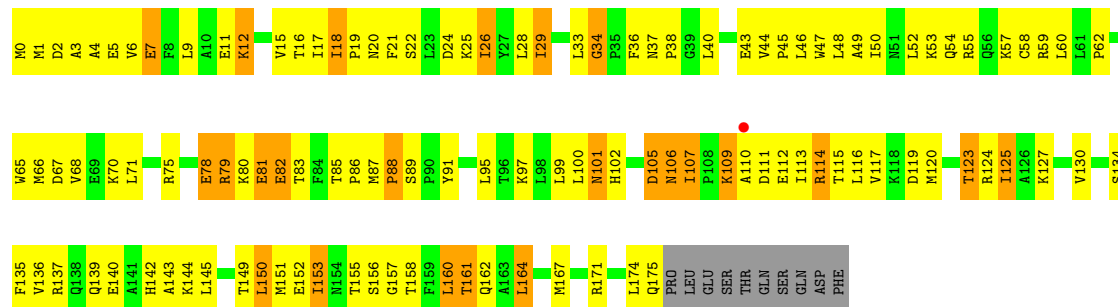


• Molecule 3: DNA replication complex GINS protein PSF2

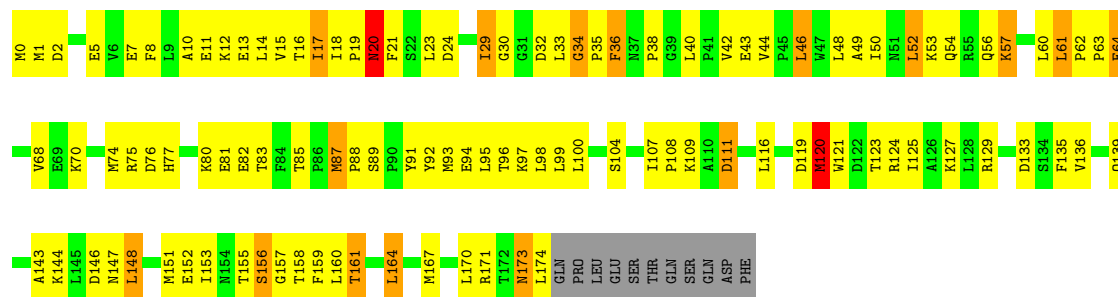




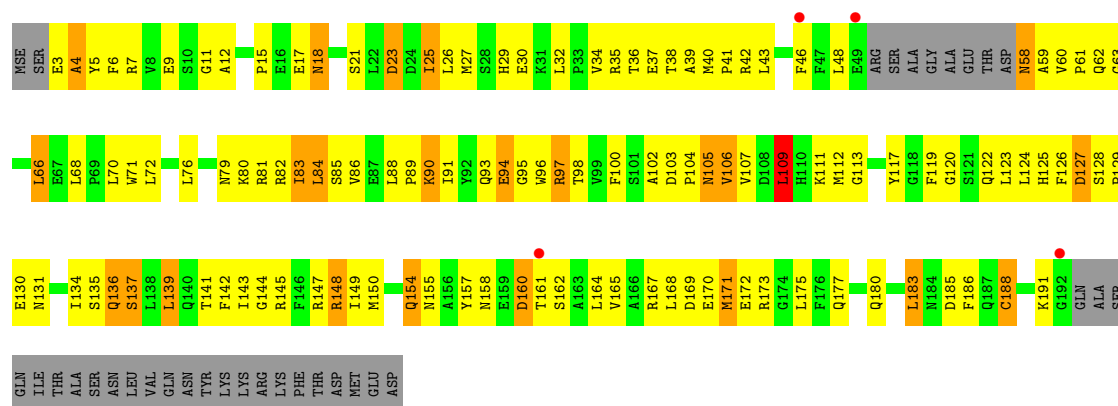
• Molecule 3: DNA replication complex GINS protein PSF2



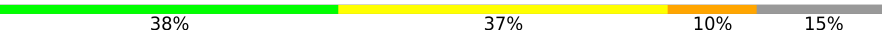
• Molecule 3: DNA replication complex GINS protein PSF2

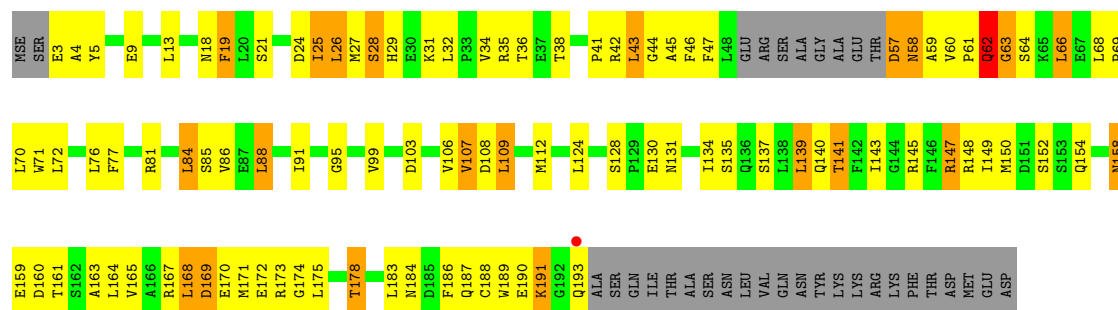


• Molecule 4: GINS complex subunit 3

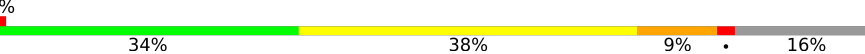


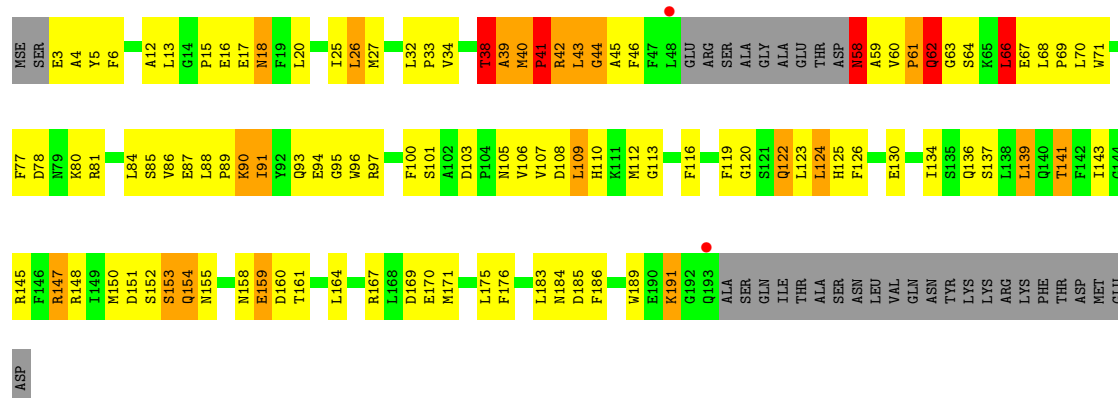
• Molecule 4: GINS complex subunit 3

Chain H:  38% 37% 10% 15%



• Molecule 4: GINS complex subunit 3

Chain L:  34% 38% 9% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.94Å 177.00Å 126.51Å 90.00° 105.91° 90.00°	Depositor
Resolution (Å)	29.90 – 3.00 29.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.90-3.00) 97.5 (29.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.274 0.216 , 0.266	Depositor DCC
R_{free} test set	4073 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16937	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/1359	0.86	1/1814 (0.1%)
1	E	0.50	0/1606	1.02	8/2150 (0.4%)
1	I	0.53	0/1627	1.23	21/2177 (1.0%)
2	B	0.46	0/1205	0.94	4/1608 (0.2%)
2	F	0.53	0/1212	1.02	7/1615 (0.4%)
2	J	0.53	0/1205	0.99	5/1608 (0.3%)
3	C	0.42	0/1389	0.95	7/1866 (0.4%)
3	G	0.46	0/1454	1.04	14/1955 (0.7%)
3	K	0.53	0/1445	1.00	9/1943 (0.5%)
4	D	0.39	0/1491	0.95	11/2003 (0.5%)
4	H	0.53	0/1499	1.06	5/2014 (0.2%)
4	L	0.86	4/1491 (0.3%)	1.87	23/2003 (1.1%)
All	All	0.53	4/16983 (0.0%)	1.12	115/22756 (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
4	L	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	58	ASN	C-O	17.88	1.59	1.23
4	L	60	VAL	C-O	14.66	1.43	1.24
4	L	38	THR	C-O	-10.31	1.10	1.24
4	L	41	PRO	N-CD	8.07	1.59	1.47

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	60	VAL	CA-C-O	-45.17	93.82	119.12
4	L	60	VAL	O-C-N	36.80	147.68	121.55
4	L	38	THR	O-C-N	-19.15	97.13	122.59
4	L	38	THR	CA-C-O	17.14	145.02	120.51
1	I	211	ILE	CB-CA-C	-14.83	86.97	111.29
1	I	211	ILE	N-CA-CB	-12.37	90.82	111.23
4	L	40	MSE	CB-CA-C	12.35	125.68	108.76
4	L	58	ASN	O-C-N	-11.84	104.05	123.00
1	I	209	LYS	N-CA-C	-11.81	94.29	110.35
1	I	192	ARG	N-CA-C	-9.74	87.35	107.70
1	I	193	ASP	N-CA-C	-9.59	91.22	108.48
4	L	39	ALA	N-CA-C	-9.41	90.75	110.80
4	L	38	THR	CB-CA-C	9.24	128.81	110.42
1	I	193	ASP	N-CA-CB	9.11	125.83	110.71
4	L	38	THR	N-CA-C	-8.77	92.11	110.80
2	F	96	SER	N-CA-C	-8.43	102.70	113.16
1	I	179	GLN	N-CA-CB	8.43	124.74	110.49
1	E	118	GLU	CA-C-N	-8.25	110.06	120.79
1	E	118	GLU	C-N-CA	-8.25	110.06	120.79
3	G	107	ILE	N-CA-C	8.18	117.70	108.05
2	B	16	ALA	CA-C-N	8.10	129.97	119.84
2	B	16	ALA	C-N-CA	8.10	129.97	119.84
3	G	34	GLY	CA-C-N	7.95	127.71	119.76
3	G	34	GLY	C-N-CA	7.95	127.71	119.76
4	L	40	MSE	N-CA-C	-7.78	98.57	110.32
4	H	107	VAL	N-CA-C	7.60	118.80	109.30
1	E	181	ASN	N-CA-C	7.59	119.79	110.91
1	E	123	SER	N-CA-C	-7.27	99.62	110.24
1	I	178	ARG	CB-CA-C	7.20	124.75	110.42
3	G	55	ARG	N-CA-C	-7.15	103.71	113.30
4	L	41	PRO	CB-CA-C	-6.99	100.02	111.56
1	E	64	ASN	N-CA-C	-6.96	104.91	113.19
4	L	61	PRO	CB-CA-C	-6.90	100.17	111.56
2	J	2	PHE	N-CA-C	-6.89	103.98	113.56
3	K	87	MSE	CA-C-N	6.89	126.70	119.05
3	K	87	MSE	C-N-CA	6.89	126.70	119.05
3	C	12	LYS	N-CA-C	-6.79	105.14	113.50
4	L	113	GLY	N-CA-C	-6.75	98.57	112.34
3	C	125	ILE	N-CA-C	-6.71	104.22	110.53
1	I	107	VAL	N-CA-C	-6.70	103.99	110.42
4	L	61	PRO	N-CA-C	6.64	126.16	112.47
4	D	137	SER	N-CA-C	-6.62	107.07	114.62
1	E	119	PRO	N-CA-C	-6.59	99.80	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	159	GLU	N-CA-C	-6.55	104.77	112.89
1	I	22	THR	CA-C-N	6.52	126.02	119.24
1	I	22	THR	C-N-CA	6.52	126.02	119.24
3	C	124	ARG	N-CA-C	-6.44	105.96	113.88
3	G	101	ASN	N-CA-C	-6.44	104.91	112.89
1	I	205	LEU	N-CA-C	-6.36	98.05	108.41
2	J	144	LYS	N-CA-C	-6.30	99.38	109.96
4	H	26	LEU	N-CA-C	-6.29	103.71	112.45
4	D	160	ASP	N-CA-C	-6.26	105.77	113.41
2	B	43	ASN	N-CA-C	-6.22	106.32	114.04
3	G	81	GLU	N-CA-C	6.18	119.66	111.75
1	A	144	VAL	N-CA-C	6.14	118.77	111.09
3	G	18	ILE	CA-C-N	6.14	126.33	120.31
3	G	18	ILE	C-N-CA	6.14	126.33	120.31
4	L	66	LEU	N-CA-C	6.11	118.07	108.96
1	I	71	GLU	N-CA-C	6.10	118.40	110.53
1	I	68	ALA	N-CA-C	-6.09	104.05	112.03
4	L	43	LEU	N-CA-C	5.95	117.84	111.36
3	G	40	LEU	CA-C-N	5.92	126.22	119.83
3	G	40	LEU	C-N-CA	5.92	126.22	119.83
3	K	20	ASN	N-CA-C	-5.91	105.25	112.88
2	F	24	PHE	CA-C-N	-5.88	115.19	122.84
2	F	24	PHE	C-N-CA	-5.88	115.19	122.84
4	L	116	PHE	N-CA-C	5.86	118.17	111.02
2	F	98	LEU	N-CA-C	5.85	117.18	109.93
3	K	139	GLN	N-CA-C	5.83	119.39	111.17
1	E	117	GLY	N-CA-C	-5.77	99.51	113.18
4	D	4	ALA	N-CA-C	-5.74	106.32	113.38
4	H	60	VAL	CA-C-N	5.74	126.07	119.93
4	H	60	VAL	C-N-CA	5.74	126.07	119.93
4	D	185	ASP	N-CA-C	-5.73	105.96	113.12
1	I	118	GLU	CA-C-N	5.65	127.19	120.23
1	I	118	GLU	C-N-CA	5.65	127.19	120.23
1	E	180	GLU	N-CA-C	5.60	119.37	109.96
4	D	111	LYS	N-CA-C	-5.58	105.10	111.07
2	J	24	PHE	CA-C-N	-5.55	115.14	122.85
2	J	24	PHE	C-N-CA	-5.55	115.14	122.85
3	C	91	TYR	N-CA-C	-5.54	104.08	112.99
3	K	120	MSE	N-CA-C	-5.52	105.16	111.07
1	I	143	ASN	N-CA-C	5.51	119.62	113.01
4	L	20	LEU	N-CA-C	5.50	119.69	112.92
2	J	34	GLU	N-CA-C	-5.49	104.94	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	40	LEU	CA-C-N	5.48	125.24	119.76
3	K	40	LEU	C-N-CA	5.48	125.24	119.76
1	I	46	SER	N-CA-C	5.42	116.88	110.97
4	D	170	GLU	N-CA-C	5.36	117.88	111.71
1	I	28	GLU	N-CA-C	-5.35	105.11	111.69
3	C	40	LEU	CA-C-N	5.35	126.52	119.84
3	C	40	LEU	C-N-CA	5.35	126.52	119.84
2	F	140	MSE	N-CA-C	5.28	117.78	111.71
4	L	41	PRO	CA-N-CD	-5.28	104.61	112.00
4	D	175	LEU	N-CA-C	-5.27	105.43	111.07
4	D	188	CYS	N-CA-C	-5.23	106.74	113.02
3	G	107	ILE	CA-C-N	5.21	125.37	119.90
3	G	107	ILE	C-N-CA	5.21	125.37	119.90
4	H	4	ALA	N-CA-C	-5.20	106.97	113.15
4	D	106	VAL	N-CA-C	-5.19	108.78	113.71
2	F	49	GLU	N-CA-C	-5.19	106.78	113.01
4	D	66	LEU	N-CA-C	5.16	117.53	109.52
3	G	7	GLU	N-CA-C	-5.16	105.57	111.14
3	G	156	SER	N-CA-C	-5.15	105.75	113.89
3	K	156	SER	N-CA-C	-5.14	105.90	113.61
1	I	162	VAL	CA-C-N	5.09	124.85	119.76
1	I	162	VAL	C-N-CA	5.09	124.85	119.76
3	C	121	TRP	N-CA-C	-5.09	106.23	112.90
4	D	161	THR	N-CA-C	-5.07	106.26	112.90
2	F	56	SER	N-CA-C	-5.06	106.69	112.92
4	L	62	GLN	N-CA-C	5.05	121.56	110.80
4	L	91	ILE	N-CA-C	5.05	119.17	111.89
2	B	121	LEU	N-CA-C	-5.04	105.24	111.33
4	L	12	ALA	N-CA-C	5.02	117.49	111.71
3	K	82	GLU	N-CA-C	-5.01	105.49	112.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	58	ASN	Mainchain

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	1340	0	1353	138	0
1	E	1583	0	1587	120	0
1	I	1604	0	1616	137	0
2	B	1188	0	1180	123	0
2	F	1196	0	1189	88	0
2	J	1188	0	1180	85	0
3	C	1369	0	1391	165	0
3	G	1432	0	1458	119	0
3	K	1423	0	1450	124	0
4	D	1462	0	1418	135	0
4	H	1470	0	1424	122	0
4	L	1462	0	1420	124	0
5	A	5	0	0	0	0
5	B	5	0	0	5	0
5	E	20	0	0	0	0
5	F	20	0	0	5	0
5	I	15	0	0	1	0
5	J	5	0	0	0	0
5	K	5	0	0	0	0
5	L	10	0	0	0	0
6	A	8	0	0	2	0
6	B	5	0	0	3	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	22	0	0	5	0
6	F	11	0	0	1	0
6	G	6	0	0	0	0
6	H	7	0	0	0	0
6	I	18	0	0	6	0
6	J	23	0	0	1	0
6	K	13	0	0	2	0
6	L	19	0	0	5	0
All	All	16937	0	16666	1318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1318) 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:I:211:ILE:CG2	1:I:211:ILE:O	1.92	1.18
1:I:144:VAL:HG22	2:J:109:GLU:HG3	1.29	1.13
4:L:13:LEU:HD21	4:L:171:MSE:HE2	1.27	1.11
1:I:149:MSE:HE3	2:J:36:MSE:HE1	1.15	1.10
4:L:90:LYS:HE3	4:L:90:LYS:H	1.12	1.09
3:G:16:THR:HG22	3:G:43:GLU:HG2	1.37	1.07
4:D:80:LYS:HG2	4:D:82:ARG:HE	1.21	1.04
1:E:35:MSE:HG2	6:E:1028:HOH:O	1.61	1.01
1:I:211:ILE:O	1:I:211:ILE:HG22	1.55	1.00
3:K:93:MSE:HE1	3:K:121:TRP:HB2	1.43	1.00
3:K:87:MSE:HE2	3:K:124:ARG:HD2	1.40	1.00
1:I:80:MSE:HE3	2:J:145:SER:HB2	1.40	1.00
4:D:90:LYS:HE3	4:D:90:LYS:H	1.24	1.00
1:I:101:GLU:OE2	2:J:88:ARG:HD3	1.62	0.99
1:A:171:VAL:HG12	1:A:172:PHE:H	1.25	0.99
1:E:144:VAL:HG22	2:F:109:GLU:HG3	1.44	0.99
3:G:66:MSE:HE1	3:G:100:LEU:HD11	1.44	0.99
1:I:186:PRO:HD2	1:I:192:ARG:O	1.61	0.98
4:L:38:THR:O	4:L:62:GLN:HA	1.61	0.98
3:K:75:ARG:NH2	3:K:119:ASP:HB3	1.80	0.97
3:G:44:VAL:HG21	3:G:48:LEU:HD22	1.43	0.97
3:K:57:LYS:HA	3:K:57:LYS:HE2	1.44	0.97
2:J:17:PRO:HB2	2:J:20:GLN:HG3	1.44	0.96
4:D:35:ARG:HB3	4:D:85:SER:HB2	1.47	0.95
3:K:75:ARG:HH22	3:K:119:ASP:HB3	1.28	0.95
3:K:87:MSE:HE3	3:K:92:TYR:CZ	2.01	0.95
4:H:91:ILE:HD13	4:H:112:MSE:HE2	1.48	0.93
1:I:27:ILE:HD13	3:K:29:ILE:HD11	1.50	0.91
2:B:12:GLU:HG3	2:F:17:PRO:HG3	1.54	0.90
4:H:88:LEU:HD12	4:H:88:LEU:H	1.35	0.90
4:H:34:VAL:HG21	4:H:84:LEU:HD12	1.55	0.89
4:H:109:LEU:HD22	4:H:145:ARG:NH2	1.88	0.89
3:K:20:ASN:C	3:K:20:ASN:HD22	1.80	0.89
2:B:98:LEU:HD21	2:B:114:PHE:CE2	2.08	0.88
1:I:211:ILE:O	1:I:211:ILE:HG23	1.74	0.88
2:J:98:LEU:HD23	2:J:106:MSE:HE1	1.54	0.88
3:G:1:MSE:HE3	3:G:6:VAL:HG22	1.56	0.88
3:C:66:MSE:HE1	3:C:99:LEU:HD12	1.56	0.87
1:A:149:MSE:HE1	2:B:73:ARG:HG3	1.55	0.86
1:I:149:MSE:HE2	1:I:153:LEU:O	1.75	0.86
1:E:212:ALA:HB3	1:E:213:PRO:HD3	1.57	0.86
3:K:93:MSE:CE	3:K:121:TRP:HB2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:MSE:HE3	2:F:36:MSE:HE1	1.58	0.85
3:K:87:MSE:HE3	3:K:92:TYR:CE1	2.11	0.85
1:E:209:LYS:O	1:E:213:PRO:HD2	1.76	0.85
1:A:23:PRO:HG3	1:A:57:GLN:NE2	1.90	0.85
3:C:75:ARG:HH11	3:C:75:ARG:HB3	1.42	0.85
3:K:17:ILE:HG22	3:K:60:LEU:HD13	1.60	0.84
4:L:41:PRO:O	4:L:42:ARG:HG2	1.77	0.83
1:E:109:GLU:HG3	1:E:159:PHE:CE1	2.13	0.83
2:J:17:PRO:HB2	2:J:20:GLN:CG	2.09	0.83
2:B:28:GLY:O	2:B:32:VAL:HG23	1.77	0.83
2:J:121:LEU:HG	2:J:125:MSE:HE2	1.60	0.83
3:G:18:ILE:HG23	3:G:59:ARG:HB3	1.59	0.83
3:K:133:ASP:OD2	4:L:147:ARG:HG2	1.79	0.82
3:C:71:LEU:HD12	3:C:113:ILE:HD11	1.61	0.82
2:J:71:ARG:HG3	2:J:71:ARG:HH11	1.45	0.82
3:G:1:MSE:HE1	3:G:150:LEU:HD13	1.61	0.81
4:L:90:LYS:HE3	4:L:90:LYS:N	1.94	0.81
1:A:163:PRO:HB3	4:D:18:ASN:HD21	1.46	0.81
4:D:90:LYS:H	4:D:90:LYS:CE	1.92	0.81
3:K:92:TYR:CE2	3:K:93:MSE:HE2	2.15	0.81
3:C:75:ARG:HB3	3:C:75:ARG:NH1	1.97	0.80
3:G:136:VAL:HG12	4:H:143:ILE:HG23	1.62	0.80
3:K:87:MSE:CE	3:K:124:ARG:HD2	2.10	0.80
1:I:104:PHE:CG	1:I:105:PRO:HD3	2.17	0.80
1:I:32:GLN:HE21	1:I:176:ARG:HE	1.31	0.80
4:L:91:ILE:HD12	4:L:112:MSE:HB3	1.64	0.80
1:I:80:MSE:HE3	2:J:145:SER:CB	2.12	0.79
4:H:34:VAL:HG11	4:H:68:LEU:HG	1.62	0.79
2:J:73:ARG:O	2:J:77:VAL:HG23	1.82	0.79
3:C:139:GLN:NE2	3:C:171:ARG:HD3	1.98	0.79
1:I:73:LEU:HD12	1:I:74:LYS:N	1.98	0.79
1:E:55:MSE:HE3	1:E:89:LEU:HD23	1.65	0.78
4:L:105:ASN:HD21	4:L:145:ARG:HA	1.48	0.78
4:H:158:ASN:C	4:H:158:ASN:HD22	1.92	0.78
4:H:109:LEU:HD22	4:H:145:ARG:HH21	1.46	0.77
1:A:27:ILE:HD12	1:A:85:ILE:HD12	1.65	0.77
2:B:98:LEU:HD21	2:B:114:PHE:HE2	1.48	0.77
3:C:20:ASN:C	3:C:20:ASN:HD22	1.92	0.77
2:J:30:ARG:O	2:J:34:GLU:HG2	1.83	0.77
4:H:193:GLN:HE21	4:H:193:GLN:HA	1.49	0.77
4:D:34:VAL:CG2	4:D:84:LEU:HG	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:VAL:HG21	4:D:84:LEU:HG	1.66	0.77
2:J:72:ASN:O	2:J:76:THR:HG23	1.83	0.77
4:L:90:LYS:H	4:L:90:LYS:CE	1.95	0.77
1:I:200:LYS:HD3	1:I:200:LYS:C	2.09	0.77
1:E:134:MSE:HE3	1:E:158:LEU:HD12	1.67	0.77
1:E:173:LEU:HD22	1:E:211:ILE:HD13	1.66	0.77
2:J:88:ARG:HH22	4:L:6:PHE:HZ	1.32	0.77
3:C:49:ALA:HB1	3:C:60:LEU:HD21	1.67	0.76
2:J:43:ASN:O	2:J:47:VAL:HG23	1.84	0.76
2:F:59:ILE:HB	2:F:60:PRO:HD3	1.67	0.76
3:G:123:THR:O	3:G:127:LYS:HG3	1.86	0.76
3:K:87:MSE:HE2	3:K:124:ARG:CD	2.14	0.76
3:K:29:ILE:HD12	3:K:29:ILE:C	2.10	0.76
1:E:149:MSE:HE1	2:F:73:ARG:CD	2.16	0.76
1:A:149:MSE:HE1	2:B:73:ARG:CG	2.15	0.75
1:I:204:HIS:HE1	3:K:144:LYS:HE3	1.51	0.75
1:A:35:MSE:HE3	3:C:1:MSE:SE	2.36	0.75
3:C:106:ASN:N	3:C:106:ASN:HD22	1.85	0.75
2:J:71:ARG:HH11	2:J:71:ARG:CG	2.00	0.75
3:K:93:MSE:HE3	3:K:121:TRP:CE3	2.21	0.75
1:E:134:MSE:CE	1:E:158:LEU:HD12	2.17	0.75
2:J:59:ILE:HB	2:J:60:PRO:HD3	1.68	0.75
3:G:66:MSE:HE3	3:G:113:ILE:HG21	1.69	0.75
1:I:81:GLU:OE2	3:K:29:ILE:HG13	1.87	0.74
4:D:94:GLU:HB3	4:D:97:ARG:HH21	1.50	0.74
4:H:38:THR:HA	4:H:62:GLN:HG3	1.69	0.74
1:I:180:GLU:O	1:I:197:ASP:HA	1.87	0.74
3:K:93:MSE:HE3	3:K:121:TRP:HE3	1.51	0.74
3:G:60:LEU:O	3:G:62:PRO:HD3	1.87	0.74
1:A:118:GLU:HB2	1:A:119:PRO:HD2	1.69	0.74
3:C:160:LEU:O	3:C:164:LEU:HD23	1.88	0.74
2:B:61:THR:HG23	4:D:43:LEU:HD13	1.70	0.73
3:G:44:VAL:HG22	3:G:45:PRO:HD2	1.68	0.73
3:C:48:LEU:HD22	3:C:52:LEU:HD22	1.70	0.73
2:B:99:PRO:HB2	2:B:102:LEU:HD23	1.69	0.73
4:D:141:THR:O	4:D:145:ARG:HG3	1.87	0.73
3:C:67:ASP:HB3	3:C:70:LYS:HB2	1.70	0.72
1:I:73:LEU:O	1:I:77:ILE:HG12	1.88	0.72
1:A:163:PRO:HB3	4:D:18:ASN:ND2	2.02	0.72
1:I:124:PRO:HG2	1:I:125:GLU:OE1	1.88	0.72
1:A:108:LEU:HD11	1:A:130:ALA:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD11	1:A:127:LEU:HA	1.70	0.72
2:F:1:MSE:HB2	5:F:1004:SO4:S	2.30	0.72
3:G:97:LYS:O	3:G:101:ASN:HB2	1.90	0.72
2:B:8:GLU:HG3	6:F:1015:HOH:O	1.89	0.72
2:J:22:PRO:O	2:J:83:ARG:NH2	2.22	0.72
3:C:72:GLU:HA	3:C:116:LEU:HD11	1.70	0.71
1:I:172:PHE:HB3	3:K:0:MSE:HE1	1.72	0.71
4:D:27:MSE:HE1	4:D:122:GLN:HG3	1.72	0.71
1:E:128:ALA:O	1:E:132:GLU:HG3	1.89	0.71
2:F:7:MSE:HE3	2:F:71:ARG:NH1	2.05	0.71
3:G:100:LEU:HD23	3:G:114:ARG:HB2	1.72	0.71
1:E:71:GLU:O	1:E:72:ASP:HB2	1.90	0.71
1:E:149:MSE:HE2	1:E:153:LEU:HB3	1.73	0.71
1:E:124:PRO:HG2	1:E:125:GLU:OE2	1.90	0.71
1:I:204:HIS:CE1	3:K:144:LYS:HE3	2.24	0.71
2:F:74:ARG:CZ	4:H:25:ILE:HG22	2.20	0.71
1:I:149:MSE:CE	2:J:36:MSE:HE1	2.09	0.71
1:A:81:GLU:O	1:A:85:ILE:HG12	1.91	0.71
1:E:211:ILE:HG13	1:E:212:ALA:N	2.06	0.71
2:J:55:ARG:HG2	2:J:57:ASP:OD2	1.91	0.71
4:D:157:TYR:HE2	4:D:162:SER:HB2	1.56	0.70
4:D:79:ASN:HA	4:D:81:ARG:NH1	2.06	0.70
1:I:109:GLU:O	1:I:113:THR:HG22	1.91	0.70
1:I:80:MSE:CE	2:J:145:SER:HB2	2.17	0.70
1:E:55:MSE:HE2	1:E:55:MSE:HA	1.72	0.70
1:I:77:ILE:HA	6:I:1009:HOH:O	1.91	0.70
1:I:74:LYS:HD2	3:K:23:LEU:HD11	1.71	0.70
3:G:71:LEU:HB2	3:G:116:LEU:HD23	1.74	0.70
3:C:93:MSE:HG3	3:C:121:TRP:CE3	2.26	0.70
1:I:177:GLU:O	1:I:178:ARG:HB2	1.92	0.70
4:L:91:ILE:CD1	4:L:112:MSE:HB3	2.22	0.70
3:K:70:LYS:O	3:K:74:MSE:HG3	1.91	0.69
2:J:55:ARG:NH2	4:L:42:ARG:HH21	1.90	0.69
4:L:38:THR:O	4:L:62:GLN:CA	2.37	0.69
1:E:134:MSE:HE2	1:E:138:GLU:CD	2.17	0.69
1:A:106:HIS:ND1	1:A:164:LYS:HB3	2.07	0.69
4:D:128:SER:HB3	4:D:131:ASN:ND2	2.07	0.69
1:E:188:THR:HG22	1:E:189:ASP:H	1.58	0.69
3:C:120:MSE:O	3:C:124:ARG:HB2	1.92	0.69
3:K:18:ILE:CD1	3:K:61:LEU:HD13	2.23	0.69
3:K:48:LEU:HD22	3:K:52:LEU:HD22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:GLU:HG3	4:D:81:ARG:O	1.93	0.69
1:I:35:MSE:HG2	3:K:1:MSE:HE1	1.75	0.69
2:F:71:ARG:NH2	4:H:28:SER:HB3	2.07	0.69
2:J:103:ARG:HA	2:J:106:MSE:HE3	1.74	0.68
3:K:68:VAL:HG13	3:K:116:LEU:HD11	1.73	0.68
4:H:158:ASN:HD22	4:H:159:GLU:N	1.91	0.68
1:I:77:ILE:HD13	6:I:1009:HOH:O	1.92	0.68
1:A:108:LEU:HD21	1:A:131:ARG:N	2.09	0.68
3:K:20:ASN:C	3:K:20:ASN:ND2	2.51	0.68
2:F:115:ASN:HA	2:F:118:LYS:HG2	1.74	0.68
1:I:90:SER:HB3	1:I:94:ARG:HH21	1.58	0.68
4:H:148:ARG:HG3	4:H:148:ARG:HH11	1.59	0.68
4:D:94:GLU:HA	4:D:97:ARG:HE	1.58	0.68
1:E:91:SER:HA	1:E:94:ARG:NH1	2.09	0.68
4:H:34:VAL:HG23	4:H:85:SER:O	1.93	0.68
4:H:175:LEU:O	4:H:178:THR:HG23	1.93	0.67
1:A:210:THR:HG21	6:A:1022:HOH:O	1.94	0.67
1:E:115:PRO:O	1:E:118:GLU:HB3	1.95	0.67
3:G:33:LEU:HD21	3:G:45:PRO:HD3	1.76	0.67
4:H:88:LEU:H	4:H:88:LEU:CD1	2.07	0.67
4:H:145:ARG:O	4:H:149:ILE:HG12	1.95	0.67
4:H:149:ILE:CD1	4:H:168:LEU:HD11	2.25	0.67
2:J:144:LYS:C	2:J:144:LYS:HD3	2.19	0.67
3:C:68:VAL:HG11	3:C:112:GLU:OE2	1.93	0.67
2:F:88:ARG:NH2	5:F:1010:SO4:O4	2.24	0.67
4:H:68:LEU:HD13	4:H:72:LEU:HD12	1.77	0.67
1:I:32:GLN:HE21	1:I:176:ARG:NE	1.93	0.67
1:A:105:PRO:HG2	1:A:106:HIS:CD2	2.29	0.67
1:E:21:LEU:N	1:E:21:LEU:HD23	2.10	0.67
1:E:143:ASN:HA	1:E:147:LYS:HE2	1.76	0.67
1:E:198:LEU:HD22	1:E:204:HIS:CD2	2.29	0.67
1:A:106:HIS:CE1	1:A:164:LYS:HB3	2.30	0.67
2:B:118:LYS:HG3	2:B:119:ARG:N	2.10	0.67
4:H:41:PRO:HA	4:H:59:ALA:HB2	1.77	0.67
4:L:183:LEU:C	4:L:183:LEU:HD13	2.20	0.67
4:D:94:GLU:HA	4:D:97:ARG:HB3	1.75	0.66
1:A:171:VAL:HG12	1:A:172:PHE:N	2.05	0.66
3:C:78:GLU:OE1	3:C:85:THR:HB	1.96	0.66
3:K:74:MSE:SE	3:K:88:PRO:HG3	2.45	0.66
2:J:27:ASP:O	2:J:31:GLN:HG3	1.95	0.66
2:B:8:GLU:HB3	6:B:1021:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:19:PRO:O	3:G:38:PRO:HA	1.95	0.66
2:F:39:LEU:HD23	2:F:65:ARG:HD3	1.75	0.66
2:J:19:GLY:HA2	4:L:5:TYR:CD2	2.31	0.66
1:A:149:MSE:CE	2:B:73:ARG:HG3	2.25	0.66
1:I:209:LYS:HE3	5:I:1001:SO4:O3	1.96	0.66
2:B:83:ARG:O	2:B:87:ILE:HG13	1.96	0.66
4:D:58:ASN:N	4:D:58:ASN:HD22	1.94	0.65
3:C:153:ILE:C	3:C:154:ASN:HD22	2.03	0.65
1:E:134:MSE:O	1:E:138:GLU:HB2	1.97	0.65
4:H:91:ILE:CD1	4:H:112:MSE:HE2	2.26	0.65
4:L:41:PRO:O	4:L:42:ARG:CG	2.45	0.65
4:L:148:ARG:HH11	4:L:148:ARG:HG3	1.61	0.65
1:I:27:ILE:O	1:I:31:GLU:HG3	1.96	0.65
2:B:10:ILE:HG13	4:D:25:ILE:HD11	1.78	0.65
4:D:80:LYS:CG	4:D:82:ARG:HE	2.03	0.65
3:C:44:VAL:HG22	3:C:45:PRO:HD2	1.79	0.65
3:G:21:PHE:O	3:G:38:PRO:HD3	1.97	0.65
4:L:3:GLU:HG3	4:L:5:TYR:H	1.62	0.65
4:L:58:ASN:ND2	4:L:59:ALA:H	1.95	0.65
1:E:140:TYR:CE1	1:E:144:VAL:HG21	2.31	0.65
1:E:173:LEU:HD22	1:E:211:ILE:CD1	2.26	0.65
1:I:31:GLU:OE2	3:K:12:LYS:HE3	1.96	0.65
1:A:104:PHE:CD1	1:A:105:PRO:HD3	2.32	0.65
2:B:17:PRO:HG2	2:F:94:TYR:OH	1.97	0.65
3:C:75:ARG:HH11	3:C:75:ARG:CB	2.10	0.65
4:D:38:THR:HA	4:D:62:GLN:NE2	2.11	0.65
3:C:33:LEU:HD22	3:C:44:VAL:HG23	1.79	0.65
3:C:151:MSE:HE3	4:D:186:PHE:HD2	1.62	0.65
3:K:18:ILE:HD13	3:K:61:LEU:HD13	1.77	0.64
1:A:23:PRO:HG3	1:A:57:GLN:HE22	1.63	0.64
3:C:18:ILE:HG13	3:C:18:ILE:O	1.97	0.64
1:E:21:LEU:HD23	1:E:21:LEU:H	1.61	0.64
1:I:149:MSE:HE1	2:J:73:ARG:HD2	1.79	0.64
3:C:137:ARG:HH11	3:C:137:ARG:HB2	1.62	0.64
6:E:1028:HOH:O	3:G:1:MSE:SE	2.64	0.64
3:G:119:ASP:O	3:G:123:THR:HG23	1.97	0.64
4:H:21:SER:HB3	4:H:24:ASP:HB2	1.79	0.64
4:H:68:LEU:HD13	4:H:72:LEU:CD1	2.28	0.64
1:A:29:ARG:HG2	1:A:50:ILE:CD1	2.27	0.64
2:B:98:LEU:N	2:B:98:LEU:HD22	2.12	0.64
1:E:85:ILE:HG13	3:G:29:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:VAL:CG2	3:G:48:LEU:HD22	2.21	0.64
1:I:180:GLU:HG2	1:I:181:ASN:H	1.60	0.64
4:L:109:LEU:HD22	4:L:145:ARG:CZ	2.27	0.64
4:D:43:LEU:O	4:D:60:VAL:HG13	1.98	0.64
1:E:172:PHE:CD2	3:G:0:MSE:HE1	2.33	0.64
4:H:21:SER:O	4:H:25:ILE:HG23	1.98	0.64
4:H:193:GLN:HA	4:H:193:GLN:NE2	2.13	0.64
1:A:61:MSE:HE2	1:A:61:MSE:HA	1.80	0.64
3:C:54:GLN:C	3:C:56:GLN:H	2.05	0.64
4:D:105:ASN:HB3	4:D:148:ARG:HD2	1.79	0.64
3:G:26:ILE:HG13	3:G:33:LEU:HB2	1.80	0.64
2:B:7:MSE:O	2:B:10:ILE:HD13	1.98	0.63
3:C:74:MSE:HE1	3:C:88:PRO:HG3	1.80	0.63
1:E:56:GLU:O	1:E:59:GLU:HG2	1.97	0.63
4:D:90:LYS:HE3	4:D:90:LYS:N	2.06	0.63
1:E:48:PRO:O	1:E:52:GLU:HG2	1.98	0.63
3:G:67:ASP:HB3	3:G:70:LYS:HD3	1.79	0.63
1:I:45:GLU:OE2	1:I:119:PRO:HB2	1.98	0.63
6:I:1015:HOH:O	2:J:88:ARG:HD2	1.98	0.63
1:A:77:ILE:HD12	3:C:48:LEU:HD21	1.80	0.63
1:E:149:MSE:HE1	2:F:73:ARG:HD3	1.81	0.63
4:H:41:PRO:HA	4:H:59:ALA:CB	2.29	0.63
4:H:88:LEU:HD12	4:H:88:LEU:N	2.12	0.63
2:B:43:ASN:O	2:B:47:VAL:HG23	1.98	0.63
3:C:20:ASN:C	3:C:20:ASN:ND2	2.56	0.63
3:C:153:ILE:HG13	3:C:154:ASN:ND2	2.13	0.63
4:H:158:ASN:C	4:H:158:ASN:ND2	2.57	0.63
3:K:173:ASN:HD22	3:K:174:LEU:N	1.97	0.63
4:D:25:ILE:C	4:D:25:ILE:HD12	2.23	0.63
1:I:149:MSE:HE1	2:J:73:ARG:CG	2.29	0.63
1:I:196:ILE:HG22	1:I:197:ASP:N	2.14	0.63
1:A:48:PRO:O	1:A:52:GLU:HG2	1.98	0.62
2:B:64:PHE:CE1	4:D:72:LEU:HD21	2.34	0.62
4:D:36:THR:HB	4:D:63:GLY:H	1.64	0.62
3:C:18:ILE:CG1	3:C:59:ARG:HB3	2.29	0.62
1:E:104:PHE:CG	1:E:105:PRO:HD3	2.34	0.62
3:G:109:LYS:HB3	3:G:112:GLU:HB3	1.81	0.62
2:F:74:ARG:NH2	4:H:25:ILE:HG22	2.15	0.62
1:I:58:LEU:O	1:I:62:GLU:HB2	1.98	0.62
1:I:96:ARG:O	1:I:100:ILE:HG13	1.99	0.62
1:I:140:TYR:CE1	1:I:144:VAL:HG21	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:NH1	1:A:126:GLU:OE1	2.33	0.62
2:F:144:LYS:O	2:F:145:SER:HB3	1.99	0.62
2:F:28:GLY:O	2:F:32:VAL:HG23	2.00	0.62
4:H:61:PRO:HG2	4:H:64:SER:OG	2.00	0.62
3:K:2:ASP:HB3	3:K:5:GLU:HG3	1.81	0.62
4:L:137:SER:O	4:L:141:THR:HG22	1.99	0.62
1:A:106:HIS:O	1:A:110:LYS:HB2	2.00	0.62
3:C:50:ILE:O	3:C:54:GLN:HG2	2.00	0.62
3:C:64:GLU:OE1	3:C:70:LYS:HE2	2.00	0.62
3:C:106:ASN:N	3:C:106:ASN:ND2	2.46	0.62
4:D:125:HIS:C	4:D:127:ASP:H	2.07	0.61
1:I:134:MSE:HE1	1:I:158:LEU:HB2	1.81	0.61
3:C:10:ALA:O	3:C:13:GLU:HB2	2.00	0.61
2:J:87:ILE:O	2:J:90:LEU:HB2	1.99	0.61
3:K:151:MSE:HE3	3:K:155:THR:OG1	2.00	0.61
3:C:0:MSE:HE3	3:C:158:THR:N	2.16	0.61
1:E:53:CYS:O	1:E:57:GLN:HG2	2.00	0.61
2:F:102:LEU:HD12	2:F:102:LEU:H	1.63	0.61
1:E:118:GLU:O	1:E:118:GLU:HG3	2.00	0.61
2:J:61:THR:HG23	4:L:43:LEU:HD21	1.82	0.61
1:A:123:SER:HB2	1:A:124:PRO:HD2	1.83	0.61
1:E:137:THR:CG2	2:F:113:TRP:HE1	2.14	0.61
4:H:168:LEU:HG	4:H:172:GLU:HB3	1.83	0.61
4:L:191:LYS:HD2	4:L:191:LYS:O	2.01	0.61
1:E:149:MSE:CE	1:E:153:LEU:HB3	2.30	0.61
3:G:120:MSE:O	3:G:124:ARG:HG3	2.01	0.60
4:H:3:GLU:HG3	4:H:5:TYR:HB3	1.82	0.60
4:L:34:VAL:HG11	4:L:68:LEU:HD12	1.82	0.60
4:D:100:PHE:HB3	4:D:141:THR:HG22	1.81	0.60
3:G:88:PRO:HG2	3:G:89:SER:H	1.66	0.60
3:G:134:SER:HA	3:G:137:ARG:HH21	1.65	0.60
1:A:110:LYS:HA	1:A:113:THR:HG22	1.82	0.60
1:A:149:MSE:HE1	2:B:73:ARG:CD	2.31	0.60
4:D:167:ARG:HG3	4:D:167:ARG:HH11	1.66	0.60
3:G:75:ARG:HD2	3:G:119:ASP:OD2	2.02	0.60
3:G:162:GLN:OE1	4:H:178:THR:HG21	2.01	0.60
4:H:108:ASP:OD2	4:H:108:ASP:C	2.45	0.60
1:A:30:LEU:HD22	1:A:54:VAL:HG11	1.83	0.60
4:D:180:GLN:HG2	2:F:100:ASN:HD21	1.66	0.60
2:B:73:ARG:HA	2:B:76:THR:HG22	1.82	0.60
4:L:34:VAL:HG21	4:L:84:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MSE:HE3	2:B:36:MSE:HE1	1.83	0.60
2:B:18:GLU:CD	2:B:19:GLY:N	2.59	0.60
3:C:139:GLN:HB3	3:C:171:ARG:NH2	2.17	0.60
3:C:173:ASN:ND2	4:D:135:SER:HB3	2.16	0.60
3:G:144:LYS:O	3:G:145:LEU:HD23	2.02	0.60
3:G:174:LEU:H	3:G:174:LEU:HD23	1.67	0.60
1:E:52:GLU:HA	1:E:55:MSE:HB2	1.84	0.59
1:E:55:MSE:HE3	1:E:89:LEU:CD2	2.31	0.59
3:G:49:ALA:HB1	3:G:60:LEU:HD11	1.83	0.59
1:I:209:LYS:O	1:I:210:THR:CB	2.48	0.59
4:L:122:GLN:HG3	6:L:1020:HOH:O	2.01	0.59
2:B:44:GLN:O	2:B:47:VAL:HB	2.03	0.59
4:L:41:PRO:O	4:L:42:ARG:CB	2.49	0.59
4:L:137:SER:O	4:L:141:THR:CG2	2.49	0.59
3:C:19:PRO:O	3:C:38:PRO:HA	2.03	0.59
4:H:34:VAL:CG1	4:H:68:LEU:HG	2.31	0.59
1:I:104:PHE:HE1	1:I:134:MSE:HE3	1.66	0.59
2:J:11:ARG:HB3	2:J:15:ARG:NH2	2.17	0.59
2:B:16:ALA:HB3	2:B:86:ARG:HH12	1.67	0.59
2:F:7:MSE:HE3	2:F:71:ARG:HH11	1.68	0.59
2:B:61:THR:HG22	2:B:65:ARG:NH1	2.18	0.59
2:F:10:ILE:HG13	4:H:25:ILE:HD11	1.83	0.59
4:L:34:VAL:CG2	4:L:84:LEU:HG	2.33	0.59
4:L:16:GLU:CD	6:L:1013:HOH:O	2.46	0.59
3:C:129:ARG:HH11	3:C:129:ARG:HB2	1.68	0.59
3:G:46:LEU:O	3:G:50:ILE:HG12	2.03	0.59
1:I:170:TYR:CD1	3:K:164:LEU:HB3	2.38	0.59
2:J:88:ARG:NH2	4:L:6:PHE:CZ	2.71	0.59
3:G:66:MSE:CE	3:G:113:ILE:HG21	2.33	0.59
1:I:177:GLU:CD	1:I:178:ARG:H	2.11	0.59
1:I:196:ILE:HG22	1:I:197:ASP:H	1.68	0.59
4:D:39:ALA:H	4:D:62:GLN:HE21	1.49	0.59
4:D:39:ALA:N	4:D:62:GLN:HG2	2.17	0.58
2:J:56:SER:C	2:J:58:LEU:H	2.11	0.58
1:A:173:LEU:C	1:A:173:LEU:HD23	2.29	0.58
3:C:33:LEU:HD21	3:C:45:PRO:HD3	1.85	0.58
4:D:103:ASP:O	4:D:106:VAL:HG12	2.03	0.58
4:D:112:MSE:O	4:D:113:GLY:C	2.46	0.58
4:D:117:TYR:CE1	4:D:142:PHE:HB2	2.37	0.58
4:D:164:LEU:HD13	4:D:164:LEU:C	2.29	0.58
4:L:38:THR:HA	4:L:62:GLN:HE21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:ILE:O	3:K:54:GLN:HG3	2.03	0.58
3:K:119:ASP:O	3:K:123:THR:HG23	2.03	0.58
4:L:183:LEU:HD13	4:L:183:LEU:O	2.03	0.58
4:D:68:LEU:HD22	4:D:72:LEU:HD23	1.85	0.58
4:D:135:SER:C	4:D:137:SER:H	2.11	0.58
3:G:17:ILE:O	3:G:17:ILE:HD12	2.04	0.58
1:A:203:GLN:O	3:C:146:ASP:HB3	2.04	0.58
3:C:22:SER:HA	3:C:36:PHE:O	2.02	0.58
3:C:129:ARG:HH11	3:C:129:ARG:CB	2.16	0.58
4:D:88:LEU:HD22	4:D:130:GLU:OE1	2.03	0.58
4:H:13:LEU:HD11	4:H:171:MSE:HG3	1.86	0.58
2:J:1:MSE:C	2:J:3:CYS:H	2.12	0.58
2:J:61:THR:HG23	4:L:43:LEU:CD2	2.34	0.58
1:A:205:LEU:HD12	1:A:205:LEU:O	2.03	0.58
1:E:63:GLU:C	1:E:65:LEU:H	2.10	0.58
1:E:194:TYR:OH	3:G:142:HIS:HD2	1.87	0.58
1:A:122:LEU:HD11	1:A:127:LEU:CA	2.33	0.57
1:E:107:VAL:HG13	1:E:122:LEU:HD11	1.86	0.57
1:E:20:VAL:HG12	1:E:21:LEU:N	2.19	0.57
1:E:172:PHE:HD2	3:G:0:MSE:HE1	1.68	0.57
2:F:10:ILE:CD1	4:H:25:ILE:HD11	2.33	0.57
3:G:22:SER:HA	3:G:36:PHE:O	2.04	0.57
3:K:64:GLU:CD	3:K:64:GLU:C	2.70	0.57
1:A:43:LEU:HD22	1:A:100:ILE:HG22	1.86	0.57
3:C:84:PHE:CE1	3:C:148:LEU:HD11	2.40	0.57
1:E:188:THR:HG22	6:E:1037:HOH:O	2.03	0.57
3:C:137:ARG:HB2	3:C:137:ARG:NH1	2.19	0.57
2:F:55:ARG:NH1	4:H:57:ASP:OD2	2.29	0.57
2:F:102:LEU:O	2:F:106:MSE:HG3	2.05	0.57
3:G:99:LEU:C	3:G:100:LEU:HD12	2.30	0.57
1:A:29:ARG:HG2	1:A:50:ILE:HD13	1.85	0.57
2:B:99:PRO:C	2:B:101:ALA:H	2.11	0.57
3:C:139:GLN:CD	3:C:171:ARG:HH21	2.12	0.57
3:K:57:LYS:HE2	3:K:57:LYS:CA	2.27	0.57
3:K:124:ARG:HD3	3:K:152:GLU:OE2	2.04	0.57
4:D:48:LEU:H	4:D:48:LEU:HD22	1.69	0.57
1:E:106:HIS:CD2	1:E:164:LYS:HG2	2.40	0.57
1:I:125:GLU:OE1	1:I:125:GLU:N	2.38	0.57
1:A:64:ASN:N	1:A:64:ASN:HD22	2.02	0.57
2:B:3:CYS:SG	2:B:71:ARG:HB3	2.45	0.57
3:C:71:LEU:HD12	3:C:113:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:GLN:CD	3:C:171:ARG:HD3	2.29	0.57
3:G:151:MSE:O	3:G:155:THR:HG23	2.05	0.57
2:F:99:PRO:HD2	2:F:102:LEU:HD13	1.86	0.57
2:F:129:GLY:O	2:F:131:ASP:N	2.38	0.57
1:I:143:ASN:HA	1:I:147:LYS:HE3	1.85	0.57
4:L:153:SER:O	4:L:155:ASN:N	2.37	0.57
2:B:87:ILE:HD13	2:B:106:MSE:HE3	1.87	0.56
1:E:35:MSE:O	1:E:39:PHE:HD1	1.88	0.56
1:E:137:THR:HG22	2:F:113:TRP:NE1	2.19	0.56
1:A:65:LEU:HG	1:A:75:VAL:HG13	1.87	0.56
6:B:1020:HOH:O	2:F:15:ARG:HD2	2.04	0.56
1:I:22:THR:OG1	1:I:25:GLU:HG3	2.05	0.56
1:I:94:ARG:O	1:I:98:MSE:HG2	2.05	0.56
3:C:86:PRO:HB3	3:C:147:ASN:HD21	1.70	0.56
3:C:94:GLU:OE1	3:C:94:GLU:N	2.38	0.56
2:F:7:MSE:HE1	4:H:25:ILE:HG13	1.87	0.56
2:F:71:ARG:HG3	4:H:71:TRP:CD2	2.40	0.56
2:F:71:ARG:HG3	4:H:71:TRP:CE2	2.40	0.56
3:G:11:GLU:HB3	3:G:47:TRP:HB3	1.87	0.56
3:G:87:MSE:HE2	3:G:87:MSE:HA	1.87	0.56
1:I:106:HIS:HE1	1:I:162:VAL:O	1.89	0.56
2:J:100:ASN:HD22	2:J:101:ALA:N	2.03	0.56
3:K:18:ILE:HD12	3:K:18:ILE:N	2.20	0.56
4:L:41:PRO:C	4:L:42:ARG:HG2	2.30	0.56
2:B:56:SER:C	2:B:58:LEU:H	2.12	0.56
1:E:144:VAL:CG2	2:F:109:GLU:HG3	2.27	0.56
4:H:109:LEU:HB2	4:H:145:ARG:HH22	1.69	0.56
1:I:144:VAL:HG22	2:J:109:GLU:CG	2.18	0.56
3:K:158:THR:HB	6:K:1020:HOH:O	2.05	0.56
3:C:92:TYR:CE1	3:C:93:MSE:HG2	2.41	0.56
1:E:211:ILE:HG13	1:E:212:ALA:H	1.70	0.56
1:A:146:LEU:HD12	1:A:149:MSE:SE	2.56	0.56
2:B:58:LEU:HD23	4:D:41:PRO:HG3	1.87	0.56
1:I:149:MSE:HE1	2:J:73:ARG:HG3	1.86	0.56
3:K:20:ASN:HD22	3:K:21:PHE:N	2.03	0.56
1:E:137:THR:HG22	2:F:113:TRP:HE1	1.69	0.56
4:H:158:ASN:ND2	4:H:160:ASP:N	2.54	0.56
3:G:174:LEU:HD22	4:H:135:SER:OG	2.06	0.56
2:J:136:ILE:HG12	2:J:136:ILE:O	2.06	0.56
1:E:127:LEU:O	1:E:131:ARG:HG3	2.06	0.56
2:F:48:ASN:HA	2:F:51:LYS:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:67:ASP:OD2	3:G:70:LYS:HG3	2.06	0.56
1:A:106:HIS:CD2	1:A:106:HIS:N	2.74	0.55
3:G:2:ASP:HB3	3:G:5:GLU:HG3	1.88	0.55
3:G:44:VAL:HG22	3:G:45:PRO:CD	2.34	0.55
3:G:71:LEU:HD22	3:G:120:MSE:HE1	1.88	0.55
1:I:62:GLU:O	1:I:66:ARG:NE	2.39	0.55
1:I:30:LEU:HD22	1:I:54:VAL:HG21	1.87	0.55
1:I:42:GLU:C	1:I:99:LYS:HD3	2.31	0.55
1:I:104:PHE:CD1	1:I:105:PRO:HD3	2.41	0.55
3:C:63:PRO:HD2	3:C:66:MSE:HE3	1.87	0.55
1:I:181:ASN:N	1:I:181:ASN:HD22	2.04	0.55
3:K:160:LEU:O	3:K:164:LEU:HD22	2.06	0.55
4:L:27:MSE:HE1	4:L:122:GLN:HG2	1.87	0.55
4:L:167:ARG:HG2	4:L:167:ARG:HH11	1.71	0.55
2:B:15:ARG:HD3	2:F:22:PRO:HA	1.87	0.55
2:B:14:HIS:NE2	5:B:1016:SO4:S	2.80	0.55
2:B:55:ARG:HG2	2:B:57:ASP:OD2	2.06	0.55
2:B:115:ASN:HA	2:B:118:LYS:HG2	1.87	0.55
4:H:167:ARG:HH11	4:H:167:ARG:HG2	1.71	0.55
1:I:70:ARG:NH2	3:K:24:ASP:OD2	2.39	0.55
1:A:110:LYS:O	1:A:110:LYS:HD3	2.07	0.55
2:B:122:ALA:O	2:B:126:ARG:HG3	2.07	0.55
3:C:78:GLU:C	3:C:80:LYS:H	2.13	0.55
3:C:136:VAL:HG22	3:C:167:MSE:HE3	1.88	0.55
3:C:67:ASP:HB3	3:C:70:LYS:HD2	1.89	0.55
4:D:91:ILE:HD12	4:D:112:MSE:HE3	1.88	0.55
4:D:149:ILE:HG12	4:D:168:LEU:HD21	1.88	0.55
3:G:85:THR:HG23	3:G:86:PRO:HD2	1.87	0.55
4:L:34:VAL:HG11	4:L:68:LEU:CD1	2.37	0.55
2:B:14:HIS:NE2	5:B:1016:SO4:O2	2.35	0.55
3:C:136:VAL:HG13	3:C:167:MSE:CE	2.36	0.55
1:I:63:GLU:O	1:I:64:ASN:C	2.50	0.55
1:I:104:PHE:CD2	1:I:105:PRO:HD3	2.41	0.55
2:B:9:LEU:HG	2:B:79:TYR:CD1	2.42	0.55
1:E:56:GLU:HA	1:E:59:GLU:HG2	1.88	0.55
4:H:183:LEU:O	4:H:187:GLN:HG3	2.06	0.55
1:A:57:GLN:O	1:A:60:HIS:HB3	2.07	0.55
2:F:73:ARG:O	2:F:76:THR:HG22	2.07	0.55
3:G:157:GLY:O	3:G:161:THR:HB	2.07	0.55
3:C:115:THR:HG23	3:C:116:LEU:N	2.23	0.54
2:F:129:GLY:O	2:F:130:GLY:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:HZ2	3:C:26:ILE:HG22	1.73	0.54
4:D:38:THR:HA	4:D:62:GLN:HE21	1.72	0.54
1:E:80:MSE:C	1:E:82:MSE:H	2.15	0.54
1:A:30:LEU:HD13	1:A:50:ILE:HG22	1.89	0.54
2:B:99:PRO:C	2:B:101:ALA:N	2.65	0.54
3:C:87:MSE:HA	3:C:87:MSE:HE2	1.89	0.54
4:D:183:LEU:HD13	4:D:183:LEU:O	2.06	0.54
4:H:106:VAL:O	4:H:167:ARG:NH2	2.40	0.54
1:A:110:LYS:HA	1:A:113:THR:CG2	2.37	0.54
4:D:70:LEU:HD22	4:D:119:PHE:CE1	2.41	0.54
3:K:94:GLU:N	3:K:94:GLU:OE1	2.40	0.54
4:L:89:PRO:HD2	4:L:123:LEU:HD21	1.89	0.54
1:A:120:SER:C	1:A:122:LEU:H	2.15	0.54
2:B:98:LEU:HD11	2:B:114:PHE:CZ	2.43	0.54
4:D:94:GLU:CB	4:D:97:ARG:HH21	2.21	0.54
3:G:15:VAL:HG13	3:G:15:VAL:O	2.08	0.54
3:G:158:THR:O	3:G:162:GLN:HG3	2.07	0.54
1:I:106:HIS:CD2	1:I:164:LYS:HG2	2.41	0.54
1:A:103:PHE:C	1:A:105:PRO:HD2	2.32	0.54
2:B:87:ILE:CG2	2:B:106:MSE:HE3	2.37	0.54
2:F:25:ASN:H	2:F:25:ASN:HD22	1.55	0.54
4:H:103:ASP:O	4:H:106:VAL:HG12	2.08	0.54
2:J:1:MSE:HE3	2:J:39:LEU:HD21	1.90	0.54
1:E:104:PHE:CE1	1:E:105:PRO:HG3	2.43	0.54
3:G:109:LYS:HB3	3:G:112:GLU:CB	2.38	0.54
4:D:105:ASN:HD22	4:D:148:ARG:HD2	1.73	0.54
2:F:144:LYS:O	2:F:145:SER:CB	2.56	0.54
1:A:23:PRO:HG3	1:A:57:GLN:HE21	1.70	0.53
2:B:9:LEU:HG	2:B:79:TYR:CE1	2.44	0.53
1:E:63:GLU:C	1:E:65:LEU:N	2.65	0.53
1:E:92:TYR:O	1:E:96:ARG:HG3	2.08	0.53
3:G:19:PRO:HA	3:G:58:CYS:HA	1.90	0.53
1:I:170:TYR:O	3:K:161:THR:CG2	2.56	0.53
2:J:28:GLY:O	2:J:32:VAL:HG23	2.08	0.53
1:A:39:PHE:CE2	1:A:172:PHE:HD2	2.24	0.53
3:C:50:ILE:HD11	3:C:98:LEU:HB3	1.91	0.53
1:E:147:LYS:HG3	1:E:148:HIS:CD2	2.42	0.53
3:G:134:SER:CA	3:G:137:ARG:HH21	2.21	0.53
1:A:100:ILE:HG13	1:A:101:GLU:N	2.22	0.53
3:C:113:ILE:O	3:C:117:VAL:HG23	2.09	0.53
4:H:158:ASN:ND2	4:H:161:THR:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ASN:HB3	4:H:188:CYS:SG	2.48	0.53
3:C:17:ILE:HD13	3:C:42:VAL:O	2.09	0.53
4:L:58:ASN:CG	4:L:59:ALA:H	2.16	0.53
1:A:42:GLU:O	1:A:44:LEU:HD13	2.09	0.53
1:I:180:GLU:HG2	1:I:181:ASN:ND2	2.24	0.53
2:B:87:ILE:O	2:B:90:LEU:HB2	2.09	0.53
3:C:139:GLN:HE22	3:C:171:ARG:HD3	1.72	0.53
1:I:85:ILE:HD11	3:K:29:ILE:HG12	1.90	0.53
3:K:75:ARG:HG3	3:K:76:ASP:N	2.24	0.53
4:L:90:LYS:O	4:L:93:GLN:HB2	2.09	0.53
1:A:22:THR:HG23	1:A:25:GLU:OE1	2.09	0.53
4:D:21:SER:O	4:D:25:ILE:HG23	2.09	0.53
1:E:56:GLU:HA	1:E:59:GLU:CD	2.34	0.53
1:A:168:ASP:OD1	1:A:209:LYS:HD2	2.09	0.53
2:B:9:LEU:HD11	2:B:25:ASN:HB3	1.91	0.53
2:B:99:PRO:O	2:B:101:ALA:N	2.42	0.53
4:D:80:LYS:HG2	4:D:82:ARG:NE	2.05	0.53
4:H:169:ASP:OD1	4:H:169:ASP:C	2.51	0.53
1:A:100:ILE:O	1:A:104:PHE:N	2.42	0.53
2:B:33:LEU:O	2:B:36:MSE:N	2.41	0.53
3:C:103:ALA:O	3:C:107:ILE:HD13	2.09	0.53
2:B:82:ASP:O	2:B:86:ARG:HG3	2.09	0.53
3:C:85:THR:O	3:C:87:MSE:HE3	2.08	0.53
3:G:113:ILE:C	3:G:115:THR:H	2.16	0.53
1:I:184:VAL:O	1:I:186:PRO:HD3	2.09	0.53
2:J:74:ARG:CZ	4:L:25:ILE:HD13	2.39	0.53
3:K:29:ILE:HD12	3:K:30:GLY:N	2.22	0.53
4:L:105:ASN:HD21	4:L:145:ARG:CA	2.21	0.53
1:A:145:ALA:HB2	2:B:29:LEU:HD21	1.92	0.52
3:C:170:LEU:O	4:D:139:LEU:HD21	2.08	0.52
4:D:3:GLU:HG3	4:D:5:TYR:H	1.74	0.52
1:I:107:VAL:HG12	1:I:122:LEU:HD11	1.90	0.52
3:K:77:HIS:O	3:K:80:LYS:HB3	2.09	0.52
2:B:5:LYS:HE3	2:B:31:GLN:OE1	2.09	0.52
1:E:81:GLU:CD	3:G:28:LEU:HB3	2.33	0.52
4:H:3:GLU:CG	4:H:5:TYR:HB3	2.39	0.52
2:F:25:ASN:HD22	2:F:25:ASN:N	2.07	0.52
4:H:137:SER:O	4:H:141:THR:CG2	2.57	0.52
1:E:109:GLU:HG3	1:E:159:PHE:CD1	2.43	0.52
1:I:98:MSE:HE3	4:L:4:ALA:HB1	1.90	0.52
1:I:149:MSE:HE1	2:J:73:ARG:CD	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1:MSE:C	2:J:3:CYS:N	2.66	0.52
2:J:20:GLN:O	2:J:86:ARG:HD3	2.09	0.52
4:D:9:GLU:CD	4:D:9:GLU:H	2.18	0.52
2:F:22:PRO:O	2:F:83:ARG:NH2	2.43	0.52
3:G:17:ILE:HD12	3:G:17:ILE:C	2.34	0.52
3:K:92:TYR:CE2	3:K:93:MSE:CE	2.91	0.52
1:A:22:THR:OG1	1:A:25:GLU:HG3	2.09	0.52
2:B:58:LEU:O	2:B:62:ILE:HG12	2.10	0.52
4:D:34:VAL:HG13	4:D:66:LEU:HB2	1.91	0.52
4:D:100:PHE:HB3	4:D:141:THR:CG2	2.39	0.52
1:E:49:GLU:HB2	6:E:1032:HOH:O	2.10	0.52
2:F:13:LEU:HD22	2:F:79:TYR:CD1	2.44	0.52
2:F:86:ARG:O	2:F:90:LEU:HD13	2.10	0.52
3:G:150:LEU:O	3:G:151:MSE:C	2.52	0.52
3:C:153:ILE:HG13	3:C:154:ASN:HD22	1.74	0.52
3:G:171:ARG:O	3:G:171:ARG:HG2	2.10	0.52
1:I:81:GLU:CD	3:K:29:ILE:HG13	2.34	0.52
1:I:176:ARG:HG3	1:I:176:ARG:HH11	1.74	0.52
1:A:149:MSE:HE1	2:B:73:ARG:HD3	1.91	0.52
1:A:206:ILE:CG2	1:A:211:ILE:HD11	2.40	0.52
1:E:204:HIS:ND1	3:G:142:HIS:HE1	2.08	0.52
4:H:36:THR:HG23	4:H:66:LEU:CD2	2.40	0.52
2:J:144:LYS:HD3	2:J:145:SER:N	2.24	0.52
1:A:32:GLN:NE2	6:A:1023:HOH:O	2.42	0.52
4:D:89:PRO:HD2	4:D:123:LEU:HD21	1.91	0.52
1:E:146:LEU:HB3	1:E:154:GLN:O	2.09	0.52
4:L:122:GLN:NE2	4:L:125:HIS:NE2	2.58	0.52
2:B:2:PHE:HB2	4:D:46:PHE:CE2	2.44	0.52
3:C:89:SER:C	3:C:91:TYR:H	2.18	0.52
1:E:199:GLU:OE1	1:E:199:GLU:HA	2.10	0.52
3:G:16:THR:HA	3:G:43:GLU:HA	1.91	0.52
4:H:103:ASP:OD2	4:H:106:VAL:HB	2.09	0.52
1:I:180:GLU:HG2	1:I:181:ASN:N	2.25	0.52
2:B:32:VAL:O	2:B:36:MSE:HG3	2.10	0.51
3:C:110:ALA:HA	3:C:113:ILE:HG22	1.91	0.51
3:C:125:ILE:O	3:C:128:LEU:N	2.41	0.51
4:D:40:MSE:HE3	4:D:60:VAL:HG21	1.92	0.51
2:J:98:LEU:HD11	2:J:114:PHE:CZ	2.45	0.51
3:K:173:ASN:HD22	3:K:173:ASN:C	2.18	0.51
1:A:149:MSE:HE3	2:B:36:MSE:CE	2.40	0.51
4:H:148:ARG:HG3	4:H:148:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD21	1:A:156:VAL:HG23	1.93	0.51
4:D:17:GLU:HG3	4:D:122:GLN:NE2	2.24	0.51
1:E:149:MSE:HE3	2:F:36:MSE:CE	2.37	0.51
1:I:103:PHE:O	1:I:107:VAL:HG23	2.10	0.51
1:I:175:VAL:HG21	1:I:198:LEU:HB3	1.91	0.51
3:K:75:ARG:CZ	3:K:119:ASP:HB3	2.39	0.51
1:A:74:LYS:NZ	3:C:26:ILE:HG22	2.25	0.51
1:A:115:PRO:O	1:A:117:GLY:N	2.43	0.51
1:A:55:MSE:HE2	2:B:128:LEU:O	2.11	0.51
1:A:148:HIS:HB2	2:B:33:LEU:HD13	1.92	0.51
1:I:177:GLU:O	1:I:178:ARG:CB	2.58	0.51
3:K:36:PHE:N	3:K:36:PHE:CD2	2.78	0.51
4:D:96:TRP:C	4:D:98:THR:H	2.19	0.51
1:I:49:GLU:O	1:I:50:ILE:C	2.54	0.51
1:I:190:GLU:N	1:I:190:GLU:OE1	2.44	0.51
2:J:53:GLY:C	2:J:55:ARG:H	2.18	0.51
3:K:48:LEU:CD2	3:K:52:LEU:HD22	2.40	0.51
4:D:109:LEU:HD22	4:D:145:ARG:NH2	2.25	0.51
4:D:145:ARG:HH21	4:D:172:GLU:CD	2.18	0.51
4:H:147:ARG:HG3	4:H:147:ARG:HH11	1.75	0.51
1:E:20:VAL:CG1	1:E:21:LEU:N	2.74	0.51
1:E:34:TRP:HZ3	3:G:9:LEU:HD11	1.75	0.51
1:E:48:PRO:HG2	1:E:49:GLU:H	1.75	0.51
3:G:53:LYS:HD2	3:G:60:LEU:HD23	1.93	0.51
4:H:32:LEU:HD21	4:H:86:VAL:HG11	1.93	0.51
1:I:147:LYS:HD2	1:I:148:HIS:NE2	2.26	0.51
1:I:209:LYS:O	1:I:210:THR:HB	2.10	0.51
2:J:17:PRO:O	2:J:20:GLN:HG2	2.10	0.51
2:J:111:MSE:HE3	2:J:111:MSE:O	2.11	0.51
1:A:21:LEU:HD23	1:A:21:LEU:N	2.25	0.51
1:A:89:LEU:O	1:A:92:TYR:HB3	2.11	0.51
2:B:103:ARG:HH11	2:B:111:MSE:HE3	1.76	0.51
2:B:129:GLY:N	2:B:133:GLY:HA2	2.26	0.51
4:D:100:PHE:CD1	4:D:141:THR:HG21	2.46	0.51
3:G:89:SER:OG	3:G:95:LEU:HD12	2.11	0.51
1:A:147:LYS:HG2	1:A:148:HIS:HD2	1.76	0.50
3:C:18:ILE:HG13	3:C:59:ARG:HB3	1.94	0.50
4:D:40:MSE:CE	4:D:60:VAL:HG21	2.41	0.50
2:F:47:VAL:HG22	2:F:62:ILE:HD13	1.93	0.50
4:H:31:LYS:HE3	4:H:69:PRO:HG3	1.91	0.50
1:I:27:ILE:HG21	3:K:29:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:PHE:CD1	3:C:148:LEU:HD21	2.46	0.50
1:E:78:HIS:O	1:E:82:MSE:HB2	2.11	0.50
2:F:17:PRO:HG2	2:F:20:GLN:HG3	1.93	0.50
4:L:108:ASP:O	4:L:112:MSE:HG2	2.11	0.50
1:E:56:GLU:HA	1:E:59:GLU:CG	2.41	0.50
1:I:22:THR:O	1:I:25:GLU:HB2	2.11	0.50
1:A:77:ILE:CD1	3:C:48:LEU:HD21	2.42	0.50
1:A:86:ARG:HG3	1:A:86:ARG:HH11	1.77	0.50
2:B:18:GLU:CG	2:B:19:GLY:H	2.24	0.50
3:G:87:MSE:HB3	3:G:88:PRO:HD2	1.92	0.50
1:I:85:ILE:CD1	3:K:29:ILE:HG12	2.41	0.50
3:K:10:ALA:O	3:K:13:GLU:HB2	2.11	0.50
3:C:129:ARG:HB3	4:D:150:MSE:HE3	1.94	0.50
3:K:170:LEU:HD21	4:L:13:LEU:HG	1.93	0.50
4:L:167:ARG:HG2	4:L:167:ARG:NH1	2.25	0.50
2:B:11:ARG:C	2:B:13:LEU:N	2.69	0.50
1:E:80:MSE:C	1:E:82:MSE:N	2.70	0.50
2:J:81:TYR:O	2:J:85:LEU:HG	2.11	0.50
2:J:100:ASN:HD22	2:J:101:ALA:H	1.58	0.50
1:A:74:LYS:HG3	3:C:26:ILE:HG22	1.93	0.50
3:C:44:VAL:HG22	3:C:45:PRO:CD	2.42	0.50
4:D:37:GLU:O	4:D:62:GLN:HB3	2.11	0.50
1:E:140:TYR:O	1:E:144:VAL:HG23	2.11	0.50
2:B:71:ARG:HH11	2:B:71:ARG:HG2	1.77	0.50
4:D:165:VAL:C	4:D:167:ARG:H	2.18	0.50
2:F:93:GLU:HG2	2:F:94:TYR:CD1	2.46	0.50
4:H:108:ASP:HB2	4:H:167:ARG:NH1	2.27	0.50
4:H:174:GLY:O	4:H:178:THR:HG22	2.12	0.50
1:I:147:LYS:HD2	1:I:148:HIS:CD2	2.47	0.50
5:B:1016:SO4:S	2:F:105:HIS:NE2	2.84	0.50
3:K:53:LYS:HB2	3:K:60:LEU:HD21	1.94	0.50
3:C:136:VAL:HG13	3:C:167:MSE:HE3	1.94	0.49
1:E:114:ARG:HH12	1:E:121:SER:H	1.59	0.49
1:E:114:ARG:HH12	1:E:121:SER:N	2.09	0.49
1:E:134:MSE:HE1	1:E:158:LEU:HD12	1.94	0.49
2:B:125:MSE:SE	2:B:137:THR:HG23	2.62	0.49
1:E:149:MSE:HE1	2:F:73:ARG:CG	2.41	0.49
2:B:1:MSE:SE	2:B:64:PHE:HE2	2.45	0.49
2:F:47:VAL:O	2:F:50:ALA:HB3	2.11	0.49
4:H:103:ASP:HB2	3:K:64:GLU:HB2	1.94	0.49
3:K:159:PHE:CE2	4:L:175:LEU:HG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLU:CB	6:B:1021:HOH:O	2.58	0.49
3:C:57:LYS:O	3:C:58:CYS:HB3	2.12	0.49
3:C:67:ASP:HB3	3:C:70:LYS:CB	2.42	0.49
3:C:80:LYS:O	3:C:81:GLU:C	2.55	0.49
1:E:146:LEU:N	1:E:146:LEU:HD12	2.27	0.49
1:E:172:PHE:CE1	1:E:205:LEU:HD13	2.47	0.49
2:F:111:MSE:HE1	2:F:114:PHE:HD2	1.75	0.49
4:H:137:SER:O	4:H:141:THR:HG22	2.11	0.49
3:K:136:VAL:HG12	4:L:143:ILE:HG23	1.94	0.49
1:A:124:PRO:HG2	1:A:125:GLU:OE2	2.13	0.49
4:D:129:PRO:HG2	4:D:130:GLU:H	1.77	0.49
2:F:10:ILE:CG1	4:H:25:ILE:HD11	2.42	0.49
3:G:52:LEU:HB2	3:G:58:CYS:SG	2.53	0.49
3:G:109:LYS:HB3	3:G:109:LYS:HZ2	1.77	0.49
3:K:74:MSE:HE1	3:K:88:PRO:HG3	1.93	0.49
4:L:94:GLU:O	4:L:95:GLY:C	2.55	0.49
3:C:173:ASN:HD21	4:D:135:SER:HB3	1.76	0.49
1:E:212:ALA:HB3	1:E:213:PRO:CD	2.37	0.49
2:B:1:MSE:HE3	2:B:65:ARG:HG2	1.95	0.49
2:B:59:ILE:HB	2:B:60:PRO:HD3	1.94	0.49
3:C:17:ILE:HD12	3:C:44:VAL:HG12	1.93	0.49
3:C:71:LEU:HD23	3:C:74:MSE:SE	2.63	0.49
4:D:40:MSE:HB2	4:D:60:VAL:CG2	2.43	0.49
1:E:149:MSE:SE	2:F:73:ARG:HG3	2.62	0.49
4:H:186:PHE:O	4:H:190:GLU:HG2	2.11	0.49
3:K:133:ASP:OD2	4:L:147:ARG:CG	2.54	0.49
4:L:153:SER:C	4:L:155:ASN:H	2.20	0.49
2:F:5:LYS:O	2:F:8:GLU:HG2	2.13	0.49
3:G:70:LYS:NZ	3:G:70:LYS:HB3	2.27	0.49
4:H:41:PRO:O	4:H:42:ARG:HB2	2.12	0.49
4:H:189:TRP:C	4:H:191:LYS:H	2.20	0.49
1:I:41:PRO:HD2	1:I:208:TYR:CD2	2.48	0.49
4:L:70:LEU:HD23	4:L:70:LEU:O	2.12	0.49
6:I:1015:HOH:O	2:J:88:ARG:CD	2.58	0.49
3:K:144:LYS:HG2	3:K:146:ASP:OD1	2.13	0.49
4:L:158:ASN:H	4:L:161:THR:HG23	1.78	0.49
2:B:104:PHE:CE2	4:H:184:ASN:HB2	2.47	0.48
3:C:54:GLN:C	3:C:56:GLN:N	2.70	0.48
2:J:9:LEU:HG	2:J:79:TYR:CD1	2.47	0.48
4:L:43:LEU:O	4:L:44:GLY:C	2.55	0.48
3:C:154:ASN:HD22	3:C:154:ASN:N	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:ALA:HB1	4:D:27:MSE:HE2	1.94	0.48
1:E:79:GLN:O	1:E:83:GLU:HG3	2.12	0.48
3:G:36:PHE:C	3:G:37:ASN:HD22	2.21	0.48
3:K:91:TYR:O	3:K:95:LEU:HD23	2.13	0.48
4:L:42:ARG:N	4:L:58:ASN:O	2.43	0.48
1:E:174:ARG:HG2	1:E:174:ARG:HH11	1.78	0.48
3:K:19:PRO:O	3:K:38:PRO:HA	2.13	0.48
4:L:40:MSE:O	4:L:59:ALA:HB1	2.13	0.48
2:B:58:LEU:HD23	4:D:41:PRO:CG	2.43	0.48
2:B:98:LEU:N	2:B:98:LEU:CD2	2.75	0.48
2:B:100:ASN:H	4:H:191:LYS:NZ	2.10	0.48
2:B:100:ASN:HB2	4:H:191:LYS:HZ3	1.78	0.48
4:D:136:GLN:O	4:D:136:GLN:HG2	2.14	0.48
3:G:130:VAL:HG22	4:H:147:ARG:HH22	1.77	0.48
1:I:173:LEU:HD22	1:I:211:ILE:HD11	1.96	0.48
1:I:177:GLU:O	1:I:200:LYS:HB2	2.12	0.48
2:B:18:GLU:CG	2:B:19:GLY:N	2.77	0.48
2:B:96:SER:O	2:B:118:LYS:NZ	2.42	0.48
1:E:98:MSE:HB2	5:F:1010:SO4:O1	2.12	0.48
6:E:1030:HOH:O	3:G:0:MSE:HE2	2.13	0.48
3:G:142:HIS:CG	3:G:143:ALA:N	2.81	0.48
2:F:79:TYR:O	2:F:83:ARG:HG3	2.13	0.48
2:F:88:ARG:NH2	5:F:1010:SO4:O2	2.47	0.48
1:A:108:LEU:HD11	1:A:131:ARG:HA	1.95	0.48
1:A:137:THR:O	1:A:141:LEU:HD22	2.14	0.48
3:C:51:ASN:HD21	3:C:55:ARG:NE	2.12	0.48
4:H:149:ILE:HD13	4:H:168:LEU:HD11	1.96	0.48
2:J:111:MSE:HE1	2:J:114:PHE:HD2	1.78	0.48
2:J:125:MSE:SE	2:J:136:ILE:HD13	2.64	0.48
1:A:71:GLU:O	1:A:72:ASP:C	2.57	0.48
1:A:73:LEU:O	1:A:77:ILE:HG12	2.14	0.48
1:A:94:ARG:HD3	2:B:136:ILE:O	2.14	0.48
3:C:146:ASP:O	3:C:147:ASN:HB2	2.14	0.48
1:E:134:MSE:HE2	1:E:138:GLU:OE1	2.13	0.48
4:H:160:ASP:O	4:H:163:ALA:HB3	2.13	0.48
4:L:34:VAL:HG12	4:L:66:LEU:O	2.14	0.48
3:C:136:VAL:HG13	3:C:167:MSE:SE	2.64	0.48
3:G:149:THR:OG1	3:G:152:GLU:HG3	2.14	0.48
4:H:91:ILE:HB	4:H:112:MSE:HE2	1.95	0.48
2:J:111:MSE:HG2	6:J:1029:HOH:O	2.14	0.48
2:J:121:LEU:O	2:J:125:MSE:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:87:MSE:SE	3:K:120:MSE:HE3	2.64	0.48
4:D:76:LEU:CB	4:D:84:LEU:HD22	2.44	0.47
4:D:109:LEU:HB2	4:D:145:ARG:HH22	1.79	0.47
1:E:185:GLU:HG2	1:E:193:ASP:OD2	2.14	0.47
1:E:188:THR:HG22	1:E:190:GLU:OE2	2.14	0.47
2:F:7:MSE:HG3	4:H:29:HIS:CE1	2.49	0.47
2:F:32:VAL:O	2:F:36:MSE:HG3	2.13	0.47
4:H:169:ASP:OD1	4:H:171:MSE:N	2.47	0.47
2:J:1:MSE:HE3	2:J:39:LEU:CD2	2.44	0.47
2:J:56:SER:C	2:J:58:LEU:N	2.68	0.47
3:K:17:ILE:HG22	3:K:60:LEU:CD1	2.38	0.47
3:K:21:PHE:HE2	3:K:23:LEU:HB2	1.79	0.47
4:L:32:LEU:HD12	4:L:33:PRO:CD	2.44	0.47
1:A:81:GLU:O	1:A:81:GLU:HG2	2.15	0.47
2:B:88:ARG:NH1	4:D:6:PHE:HE1	2.11	0.47
2:B:100:ASN:H	4:H:191:LYS:HZ3	1.61	0.47
2:F:97:ILE:HG23	2:F:97:ILE:O	2.14	0.47
3:G:70:LYS:HB3	3:G:70:LYS:HZ3	1.78	0.47
3:K:91:TYR:HD1	3:K:94:GLU:OE2	1.96	0.47
3:K:167:MSE:HE2	3:K:171:ARG:NH1	2.29	0.47
4:L:89:PRO:CD	4:L:123:LEU:HD21	2.44	0.47
2:B:58:LEU:O	2:B:59:ILE:C	2.56	0.47
2:B:102:LEU:N	2:B:102:LEU:HD22	2.29	0.47
3:C:44:VAL:HG21	3:C:48:LEU:HD13	1.96	0.47
4:D:96:TRP:C	4:D:98:THR:N	2.72	0.47
3:G:85:THR:O	3:G:124:ARG:NH1	2.47	0.47
2:J:87:ILE:HA	2:J:90:LEU:HD22	1.96	0.47
1:E:71:GLU:O	1:E:72:ASP:CB	2.62	0.47
3:G:139:GLN:NE2	3:G:171:ARG:HH21	2.13	0.47
1:A:108:LEU:HD21	1:A:131:ARG:CA	2.44	0.47
3:C:121:TRP:CZ3	3:C:152:GLU:HG2	2.50	0.47
1:E:80:MSE:O	1:E:84:ARG:HG3	2.14	0.47
1:I:90:SER:CB	1:I:94:ARG:HH21	2.24	0.47
4:L:70:LEU:HD23	4:L:70:LEU:C	2.39	0.47
3:C:105:ASP:C	3:C:106:ASN:HD22	2.22	0.47
3:G:99:LEU:HB3	3:G:107:ILE:HD11	1.97	0.47
3:K:148:LEU:HD12	3:K:148:LEU:HA	1.76	0.47
4:L:158:ASN:H	4:L:161:THR:CG2	2.28	0.47
2:B:39:LEU:HD13	2:B:68:SER:HB3	1.96	0.47
2:B:88:ARG:NH1	4:D:4:ALA:O	2.47	0.47
3:C:18:ILE:HG12	3:C:59:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:ALA:HA	3:C:113:ILE:CG2	2.43	0.47
3:C:137:ARG:HA	4:D:143:ILE:CG2	2.44	0.47
1:I:80:MSE:O	1:I:84:ARG:HG3	2.15	0.47
1:I:178:ARG:O	1:I:198:LEU:O	2.32	0.47
1:I:194:TYR:C	1:I:194:TYR:CD1	2.93	0.47
1:A:78:HIS:CE1	3:C:28:LEU:HD23	2.50	0.47
1:A:146:LEU:HG	1:A:154:GLN:O	2.15	0.47
2:B:10:ILE:HD13	2:B:11:ARG:N	2.29	0.47
3:C:146:ASP:O	3:C:147:ASN:CB	2.62	0.47
4:D:76:LEU:O	4:D:83:ILE:HG21	2.15	0.47
1:I:75:VAL:O	1:I:79:GLN:HG3	2.15	0.47
2:J:34:GLU:O	2:J:35:GLU:C	2.57	0.47
4:L:152:SER:CB	4:L:164:LEU:HD23	2.45	0.47
1:A:58:LEU:HD21	1:A:85:ILE:HB	1.96	0.47
4:D:125:HIS:O	4:D:127:ASP:N	2.48	0.47
3:G:2:ASP:OD1	3:G:3:ALA:N	2.48	0.47
4:H:34:VAL:HG11	4:H:68:LEU:CG	2.38	0.47
1:A:208:TYR:CE1	1:A:212:ALA:HB2	2.50	0.46
1:E:178:ARG:HE	1:E:178:ARG:HB3	1.54	0.46
3:K:29:ILE:C	3:K:29:ILE:CD1	2.82	0.46
4:L:153:SER:C	4:L:155:ASN:N	2.74	0.46
4:L:183:LEU:C	4:L:183:LEU:CD1	2.88	0.46
1:A:173:LEU:HD23	1:A:174:ARG:N	2.29	0.46
4:D:29:HIS:O	4:D:29:HIS:ND1	2.48	0.46
4:D:145:ARG:NH2	4:D:172:GLU:OE2	2.48	0.46
2:F:121:LEU:O	2:F:125:MSE:HG3	2.15	0.46
1:I:54:VAL:O	1:I:58:LEU:HD23	2.16	0.46
4:L:100:PHE:CE1	4:L:107:VAL:HG21	2.50	0.46
1:A:27:ILE:CD1	1:A:85:ILE:HD12	2.42	0.46
4:D:70:LEU:HD22	4:D:119:PHE:CD1	2.50	0.46
1:E:31:GLU:OE2	3:G:12:LYS:HE2	2.15	0.46
2:F:55:ARG:HH12	4:H:57:ASP:CG	2.19	0.46
2:J:111:MSE:HE1	2:J:114:PHE:CD2	2.51	0.46
3:K:151:MSE:HE3	3:K:155:THR:HG1	1.80	0.46
3:K:167:MSE:HE2	3:K:171:ARG:HH12	1.79	0.46
1:A:87:TYR:OH	3:C:5:GLU:HG2	2.15	0.46
3:C:75:ARG:N	3:C:120:MSE:HE2	2.30	0.46
3:C:92:TYR:CD1	3:C:92:TYR:C	2.93	0.46
1:I:21:LEU:HD12	1:I:25:GLU:HB3	1.97	0.46
4:L:41:PRO:HA	4:L:59:ALA:CB	2.45	0.46
1:A:134:MSE:HE2	1:A:158:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ARG:O	2:B:69:LEU:HD22	2.16	0.46
2:B:115:ASN:O	2:B:119:ARG:HB2	2.15	0.46
4:D:76:LEU:HB2	4:D:84:LEU:HD22	1.97	0.46
4:D:158:ASN:OD1	4:D:160:ASP:HB2	2.15	0.46
2:J:141:LYS:O	2:J:142:PRO:C	2.59	0.46
3:K:85:THR:O	3:K:124:ARG:NH1	2.48	0.46
4:L:88:LEU:HD21	4:L:134:ILE:HD11	1.97	0.46
1:A:171:VAL:CG1	1:A:172:PHE:H	2.04	0.46
2:B:87:ILE:HG21	2:B:106:MSE:HE3	1.97	0.46
3:G:125:ILE:HD13	3:G:125:ILE:O	2.16	0.46
1:I:151:PRO:O	1:I:152:ASN:HB2	2.16	0.46
4:L:68:LEU:HD12	4:L:84:LEU:HD21	1.96	0.46
4:D:142:PHE:C	4:D:144:GLY:N	2.70	0.46
2:J:31:GLN:HA	2:J:34:GLU:CG	2.46	0.46
3:C:91:TYR:HD1	3:C:94:GLU:OE2	1.99	0.46
4:D:27:MSE:O	4:D:30:GLU:HG2	2.15	0.46
2:F:111:MSE:HE1	2:F:114:PHE:CD2	2.51	0.46
4:H:150:MSE:HE2	4:H:154:GLN:HE22	1.81	0.46
2:B:65:ARG:O	2:B:69:LEU:CD2	2.64	0.46
1:E:78:HIS:CE1	3:G:28:LEU:HD23	2.50	0.46
1:I:55:MSE:HE3	2:J:134:LEU:HD12	1.97	0.46
4:L:34:VAL:HG23	4:L:86:VAL:HA	1.96	0.46
2:B:14:HIS:HE2	2:F:105:HIS:HE2	1.64	0.46
3:G:139:GLN:HE21	3:G:171:ARG:NH2	2.14	0.46
1:I:200:LYS:HD3	1:I:201:GLY:N	2.32	0.46
2:J:141:LYS:HG2	2:J:142:PRO:HD2	1.97	0.46
1:A:34:TRP:CD2	1:A:88:VAL:HG13	2.51	0.45
2:B:71:ARG:HG3	4:D:71:TRP:CE2	2.51	0.45
4:D:104:PRO:C	4:D:106:VAL:H	2.24	0.45
3:G:82:GLU:OE1	3:G:82:GLU:C	2.59	0.45
1:I:60:HIS:O	1:I:64:ASN:N	2.43	0.45
3:K:21:PHE:CD2	3:K:21:PHE:C	2.94	0.45
4:L:109:LEU:HD22	4:L:145:ARG:NH1	2.30	0.45
2:B:56:SER:C	2:B:58:LEU:N	2.73	0.45
3:C:149:THR:OG1	3:C:152:GLU:HG3	2.16	0.45
3:G:1:MSE:CE	3:G:6:VAL:HG22	2.39	0.45
3:G:75:ARG:HG2	3:G:75:ARG:HH11	1.82	0.45
4:H:43:LEU:O	4:H:44:GLY:C	2.59	0.45
1:I:172:PHE:CE1	3:K:153:ILE:HD13	2.51	0.45
2:J:71:ARG:CG	2:J:71:ARG:NH1	2.68	0.45
3:K:48:LEU:HD23	3:K:48:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:ALA:HB2	3:C:151:MSE:HE1	1.98	0.45
4:D:143:ILE:HD12	4:D:143:ILE:H	1.82	0.45
2:F:51:LYS:HE3	2:F:51:LYS:HB2	1.82	0.45
3:G:81:GLU:O	3:G:82:GLU:HB3	2.16	0.45
3:G:135:PHE:CE2	3:G:140:GLU:HB2	2.51	0.45
4:H:145:ARG:NH2	4:H:172:GLU:OE2	2.49	0.45
1:I:199:GLU:O	1:I:200:LYS:C	2.59	0.45
4:L:139:LEU:O	4:L:143:ILE:HG12	2.14	0.45
2:B:11:ARG:HD3	2:B:15:ARG:NH2	2.31	0.45
3:C:122:ASP:C	3:C:124:ARG:H	2.24	0.45
3:C:159:PHE:CD1	3:C:159:PHE:C	2.93	0.45
4:D:48:LEU:HD22	4:D:48:LEU:N	2.29	0.45
3:G:50:ILE:O	3:G:54:GLN:HB2	2.16	0.45
4:L:38:THR:O	4:L:39:ALA:HB2	2.16	0.45
1:A:54:VAL:HG21	1:A:89:LEU:HD13	1.97	0.45
3:C:1:MSE:HE2	3:C:5:GLU:HB3	1.98	0.45
3:C:78:GLU:HA	3:C:85:THR:OG1	2.17	0.45
1:E:151:PRO:O	1:E:152:ASN:HB2	2.17	0.45
3:G:71:LEU:HD13	3:G:117:VAL:HG22	1.98	0.45
3:G:78:GLU:OE2	3:G:85:THR:HB	2.16	0.45
3:G:112:GLU:O	3:G:115:THR:HG22	2.15	0.45
4:H:34:VAL:HG22	4:H:35:ARG:N	2.32	0.45
1:I:182:ILE:O	1:I:195:VAL:HG23	2.16	0.45
3:K:108:PRO:C	3:K:109:LYS:HG2	2.40	0.45
1:A:204:HIS:N	1:A:204:HIS:CD2	2.85	0.45
3:C:50:ILE:HD13	3:C:98:LEU:HD22	1.98	0.45
3:C:137:ARG:C	3:C:139:GLN:N	2.74	0.45
2:F:2:PHE:O	2:F:3:CYS:C	2.59	0.45
3:K:15:VAL:CG1	3:K:16:THR:N	2.80	0.45
3:K:156:SER:OG	4:L:154:GLN:NE2	2.49	0.45
3:C:46:LEU:HD22	3:C:50:ILE:CD1	2.47	0.45
3:C:137:ARG:C	3:C:139:GLN:H	2.24	0.45
4:H:88:LEU:HD23	4:H:134:ILE:HD11	1.98	0.45
3:K:109:LYS:HA	6:K:1017:HOH:O	2.17	0.45
4:L:17:GLU:HG3	6:L:1013:HOH:O	2.16	0.45
4:L:33:PRO:HA	4:L:67:GLU:OE1	2.17	0.45
4:L:110:HIS:CD2	6:L:1012:HOH:O	2.69	0.45
3:C:17:ILE:HD13	3:C:17:ILE:H	1.81	0.45
4:D:100:PHE:CD2	4:D:107:VAL:HG21	2.52	0.45
4:D:177:GLN:NE2	2:F:104:PHE:HE2	2.13	0.45
1:E:114:ARG:NH1	1:E:121:SER:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:148:ARG:HG3	4:L:148:ARG:NH1	2.31	0.45
1:A:82:MSE:HE3	1:A:86:ARG:NH1	2.32	0.45
4:H:167:ARG:HG2	4:H:167:ARG:NH1	2.32	0.45
1:I:200:LYS:C	1:I:200:LYS:CD	2.85	0.45
2:J:13:LEU:HD22	2:J:79:TYR:CD1	2.52	0.45
4:L:158:ASN:HB2	4:L:160:ASP:OD1	2.16	0.45
3:C:65:TRP:C	3:C:67:ASP:H	2.25	0.45
4:D:100:PHE:HD1	4:D:141:THR:HG21	1.81	0.45
4:H:109:LEU:HB2	4:H:145:ARG:NH2	2.31	0.45
3:K:49:ALA:HB1	3:K:60:LEU:HD11	1.98	0.45
1:A:90:SER:O	1:A:91:SER:C	2.59	0.44
2:B:132:GLU:O	2:B:133:GLY:C	2.60	0.44
3:C:64:GLU:OE2	3:C:64:GLU:C	2.61	0.44
4:D:135:SER:O	4:D:139:LEU:HD23	2.17	0.44
1:I:101:GLU:HB3	2:J:88:ARG:CZ	2.47	0.44
2:J:1:MSE:O	2:J:2:PHE:HB2	2.16	0.44
2:J:1:MSE:HE1	2:J:65:ARG:HG2	1.98	0.44
1:A:42:GLU:O	1:A:44:LEU:N	2.50	0.44
2:B:2:PHE:HB2	4:D:46:PHE:CZ	2.52	0.44
3:C:51:ASN:CG	3:C:55:ARG:HD2	2.42	0.44
3:C:72:GLU:N	3:C:116:LEU:HD21	2.32	0.44
3:G:20:ASN:HD21	3:G:57:LYS:HA	1.81	0.44
3:G:151:MSE:HE1	4:H:186:PHE:HD1	1.83	0.44
4:H:158:ASN:HD22	4:H:160:ASP:N	2.15	0.44
4:H:191:LYS:HE2	4:H:193:GLN:O	2.18	0.44
1:I:173:LEU:HD22	1:I:211:ILE:CD1	2.47	0.44
3:K:7:GLU:O	3:K:8:PHE:C	2.60	0.44
3:K:89:SER:C	3:K:91:TYR:H	2.25	0.44
4:L:6:PHE:O	4:L:6:PHE:CD2	2.70	0.44
1:A:29:ARG:O	1:A:32:GLN:HB2	2.18	0.44
1:A:147:LYS:CG	1:A:148:HIS:HD2	2.29	0.44
2:B:103:ARG:HD3	2:B:111:MSE:HE3	1.99	0.44
3:C:125:ILE:O	3:C:126:ALA:C	2.60	0.44
4:H:191:LYS:O	4:H:191:LYS:HG2	2.17	0.44
3:K:99:LEU:HB3	3:K:107:ILE:HD11	1.99	0.44
4:L:123:LEU:HD12	4:L:126:PHE:CD2	2.53	0.44
1:A:149:MSE:SE	2:B:73:ARG:HG3	2.68	0.44
2:B:36:MSE:HE3	2:B:69:LEU:O	2.17	0.44
1:E:191:GLN:NE2	1:E:193:ASP:HB2	2.32	0.44
3:G:124:ARG:NH2	3:G:152:GLU:OE1	2.50	0.44
4:H:27:MSE:SE	4:H:27:MSE:C	3.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:7:MSE:HE1	4:L:26:LEU:HD12	2.00	0.44
1:A:100:ILE:HD11	1:A:129:PHE:CD2	2.52	0.44
1:A:136:ASN:ND2	2:B:113:TRP:CD1	2.85	0.44
3:C:78:GLU:C	3:C:80:LYS:N	2.74	0.44
4:D:188:CYS:HA	4:D:191:LYS:HD3	1.98	0.44
3:G:53:LYS:HE2	3:G:106:ASN:ND2	2.32	0.44
4:H:106:VAL:HG13	4:H:107:VAL:N	2.32	0.44
2:J:135:ASP:OD2	2:J:138:GLN:HG2	2.17	0.44
3:K:53:LYS:HD3	3:K:60:LEU:CD2	2.47	0.44
3:K:121:TRP:O	3:K:125:ILE:HG12	2.18	0.44
4:L:16:GLU:HG3	4:L:17:GLU:N	2.32	0.44
4:L:86:VAL:HG12	4:L:87:GLU:N	2.32	0.44
3:C:124:ARG:NH2	3:C:152:GLU:OE1	2.51	0.44
3:C:146:ASP:C	3:C:146:ASP:OD2	2.60	0.44
1:E:51:VAL:O	1:E:55:MSE:HB2	2.18	0.44
3:G:53:LYS:CD	3:G:60:LEU:HD23	2.47	0.44
3:K:15:VAL:HG12	3:K:16:THR:N	2.32	0.44
4:L:101:SER:HA	6:L:1027:HOH:O	2.18	0.44
4:D:41:PRO:HA	4:D:59:ALA:HB2	1.99	0.44
4:D:93:GLN:C	4:D:95:GLY:N	2.76	0.44
2:F:72:ASN:O	2:F:76:THR:HG22	2.16	0.44
4:H:109:LEU:CD2	4:H:145:ARG:NH2	2.72	0.44
4:H:139:LEU:O	4:H:143:ILE:HG12	2.18	0.44
1:A:106:HIS:ND1	1:A:164:LYS:CB	2.80	0.44
1:A:206:ILE:O	1:A:207:ARG:C	2.61	0.44
2:B:18:GLU:CD	2:B:19:GLY:H	2.25	0.44
2:B:123:THR:O	2:B:124:TYR:C	2.61	0.44
3:C:3:ALA:CB	3:C:151:MSE:HE1	2.47	0.44
4:H:81:ARG:HD2	4:H:81:ARG:N	2.32	0.44
3:K:87:MSE:CE	3:K:92:TYR:CZ	2.89	0.44
3:K:96:THR:O	3:K:100:LEU:HB2	2.18	0.44
1:A:25:GLU:O	1:A:28:GLU:HB3	2.17	0.43
4:D:41:PRO:C	4:D:42:ARG:HG2	2.43	0.43
1:E:141:LEU:O	1:E:146:LEU:HD13	2.17	0.43
2:F:87:ILE:HA	2:F:90:LEU:HD22	1.99	0.43
1:I:32:GLN:NE2	1:I:176:ARG:NE	2.65	0.43
4:L:191:LYS:HD2	4:L:191:LYS:C	2.42	0.43
1:A:170:TYR:CE1	1:A:207:ARG:HG2	2.53	0.43
2:B:18:GLU:HG3	2:B:19:GLY:H	1.84	0.43
2:B:18:GLU:OE2	2:B:19:GLY:N	2.51	0.43
3:C:53:LYS:NZ	3:C:106:ASN:HD21	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:ILE:HD12	4:D:143:ILE:N	2.33	0.43
1:E:58:LEU:O	1:E:62:GLU:HB2	2.18	0.43
4:H:3:GLU:C	4:H:5:TYR:H	2.24	0.43
4:L:109:LEU:HD12	4:L:109:LEU:HA	1.82	0.43
1:A:110:LYS:CA	1:A:113:THR:HG22	2.48	0.43
2:B:15:ARG:O	2:B:17:PRO:HD3	2.19	0.43
4:D:58:ASN:N	4:D:58:ASN:ND2	2.63	0.43
1:E:160:ARG:HG2	1:E:160:ARG:HH11	1.83	0.43
3:G:67:ASP:O	3:G:70:LYS:N	2.49	0.43
1:I:171:VAL:CG1	1:I:172:PHE:N	2.81	0.43
3:K:33:LEU:O	3:K:34:GLY:C	2.61	0.43
4:L:32:LEU:HD12	4:L:89:PRO:HG3	2.00	0.43
2:B:97:ILE:HD13	2:B:97:ILE:H	1.82	0.43
3:C:75:ARG:HA	3:C:120:MSE:HE2	2.00	0.43
3:C:137:ARG:HA	4:D:143:ILE:HG21	2.00	0.43
1:I:62:GLU:HG3	1:I:66:ARG:CZ	2.48	0.43
1:I:134:MSE:CE	1:I:158:LEU:HD12	2.47	0.43
1:I:146:LEU:N	1:I:146:LEU:CD1	2.81	0.43
2:J:64:PHE:C	2:J:64:PHE:CD2	2.95	0.43
2:J:71:ARG:HG2	4:L:71:TRP:CE2	2.53	0.43
2:B:64:PHE:HA	4:D:76:LEU:HD11	2.01	0.43
2:B:94:TYR:CD2	2:B:99:PRO:HG2	2.53	0.43
5:B:1016:SO4:O3	2:F:105:HIS:NE2	2.51	0.43
2:F:58:LEU:HD12	4:H:41:PRO:CG	2.48	0.43
2:F:88:ARG:HD3	2:F:88:ARG:C	2.43	0.43
4:H:145:ARG:NH2	4:H:172:GLU:OE1	2.51	0.43
3:C:0:MSE:HG3	3:C:1:MSE:H	1.84	0.43
3:C:1:MSE:HB2	3:C:154:ASN:OD1	2.18	0.43
3:C:18:ILE:HG22	3:C:41:PRO:HG3	2.00	0.43
3:C:110:ALA:O	3:C:111:ASP:C	2.61	0.43
3:C:151:MSE:O	3:C:155:THR:HG23	2.19	0.43
4:D:157:TYR:CG	4:D:158:ASN:N	2.85	0.43
1:E:116:GLU:C	1:E:118:GLU:N	2.74	0.43
1:E:140:TYR:CZ	1:E:144:VAL:HG21	2.53	0.43
1:E:144:VAL:HG13	5:F:1014:SO4:O4	2.19	0.43
3:G:81:GLU:C	3:G:83:THR:H	2.26	0.43
3:K:33:LEU:HD23	3:K:33:LEU:HA	1.85	0.43
3:K:74:MSE:CE	3:K:88:PRO:HG3	2.48	0.43
4:L:67:GLU:OE1	4:L:67:GLU:HA	2.18	0.43
4:L:151:ASP:O	4:L:155:ASN:HB2	2.18	0.43
1:A:34:TRP:CG	1:A:88:VAL:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD13	1:A:123:SER:O	2.19	0.43
1:A:173:LEU:CD1	1:A:211:ILE:HG21	2.49	0.43
2:B:142:PRO:HA	2:B:143:PRO:HD3	1.87	0.43
5:B:1016:SO4:O2	2:F:105:HIS:NE2	2.27	0.43
3:C:75:ARG:CA	3:C:120:MSE:HE2	2.48	0.43
3:C:137:ARG:NH1	3:C:137:ARG:CB	2.81	0.43
3:C:139:GLN:NE2	3:C:171:ARG:HH21	2.16	0.43
2:F:132:GLU:O	2:F:133:GLY:C	2.61	0.43
1:I:35:MSE:HE3	3:K:1:MSE:HE1	2.01	0.43
1:I:80:MSE:SE	6:I:1009:HOH:O	2.87	0.43
2:J:17:PRO:O	2:J:18:GLU:C	2.61	0.43
2:J:102:LEU:HD12	2:J:102:LEU:HA	1.87	0.43
3:K:64:GLU:HG2	3:K:70:LYS:NZ	2.33	0.43
3:K:167:MSE:CE	3:K:171:ARG:HH12	2.31	0.43
4:L:91:ILE:HG13	4:L:112:MSE:HE3	2.00	0.43
4:L:130:GLU:O	4:L:134:ILE:HG13	2.18	0.43
1:E:146:LEU:N	1:E:146:LEU:CD1	2.81	0.43
4:H:44:GLY:O	4:H:45:ALA:C	2.61	0.43
1:I:47:LYS:N	1:I:48:PRO:CD	2.82	0.43
3:K:50:ILE:HD11	3:K:98:LEU:HD13	2.01	0.43
3:C:16:THR:O	3:C:61:LEU:HB2	2.19	0.43
4:D:171:MSE:HE3	4:D:171:MSE:O	2.19	0.43
2:F:10:ILE:HD12	4:H:25:ILE:HD11	2.01	0.43
1:I:43:LEU:HA	1:I:99:LYS:HD2	2.01	0.43
1:I:79:GLN:HA	1:I:82:MSE:HE2	2.01	0.43
3:K:11:GLU:HA	3:K:46:LEU:HB3	2.00	0.43
4:L:119:PHE:O	4:L:123:LEU:N	2.51	0.43
1:A:58:LEU:HD21	1:A:85:ILE:CG2	2.49	0.43
1:A:109:GLU:HB3	1:A:159:PHE:HZ	1.84	0.43
1:A:205:LEU:HD12	1:A:205:LEU:C	2.43	0.43
2:B:1:MSE:CE	2:B:65:ARG:HG2	2.48	0.43
4:D:79:ASN:C	4:D:81:ARG:HH11	2.27	0.43
4:H:95:GLY:O	4:H:99:VAL:HG23	2.18	0.43
1:I:180:GLU:CG	1:I:181:ASN:H	2.24	0.43
1:A:74:LYS:HZ2	3:C:26:ILE:HA	1.84	0.42
1:A:211:ILE:O	1:A:212:ALA:C	2.61	0.42
2:B:71:ARG:O	2:B:72:ASN:C	2.63	0.42
1:E:109:GLU:O	1:E:113:THR:HB	2.19	0.42
1:I:180:GLU:C	1:I:197:ASP:HA	2.44	0.42
3:K:83:THR:O	3:K:127:LYS:NZ	2.43	0.42
4:L:38:THR:C	4:L:62:GLN:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:ASP:O	3:C:70:LYS:HB2	2.19	0.42
3:C:71:LEU:C	3:C:73:LYS:N	2.75	0.42
3:C:133:ASP:O	3:C:137:ARG:HD3	2.19	0.42
3:G:54:GLN:HE22	3:G:102:HIS:CE1	2.36	0.42
3:G:62:PRO:HG3	3:G:107:ILE:HG12	2.01	0.42
3:G:79:ARG:O	3:G:80:LYS:C	2.61	0.42
4:H:193:GLN:HE21	4:H:193:GLN:CA	2.18	0.42
3:K:157:GLY:O	3:K:158:THR:C	2.63	0.42
2:B:52:SER:C	2:B:54:GLY:H	2.28	0.42
4:D:27:MSE:SE	4:D:27:MSE:C	3.12	0.42
4:D:157:TYR:CE2	4:D:162:SER:HB2	2.46	0.42
1:E:80:MSE:HE2	3:G:47:TRP:CE3	2.54	0.42
1:E:106:HIS:HE1	1:E:162:VAL:O	2.02	0.42
1:E:173:LEU:O	1:E:203:GLN:HA	2.20	0.42
4:H:189:TRP:C	4:H:191:LYS:N	2.78	0.42
4:L:42:ARG:CA	4:L:58:ASN:O	2.67	0.42
1:A:61:MSE:C	1:A:63:GLU:N	2.76	0.42
1:A:104:PHE:CE2	1:A:134:MSE:HE3	2.54	0.42
3:C:69:GLU:HA	3:C:72:GLU:HB3	2.00	0.42
3:C:151:MSE:HE3	4:D:186:PHE:CD2	2.50	0.42
4:D:93:GLN:C	4:D:95:GLY:H	2.27	0.42
4:D:168:LEU:HD22	4:D:172:GLU:HB3	2.00	0.42
1:E:94:ARG:NH2	2:F:140:MSE:HA	2.35	0.42
2:F:138:GLN:C	2:F:140:MSE:H	2.27	0.42
3:K:146:ASP:O	3:K:147:ASN:HB2	2.19	0.42
4:L:77:PHE:CG	4:L:78:ASP:N	2.88	0.42
1:A:80:MSE:O	1:A:84:ARG:HG3	2.19	0.42
1:E:55:MSE:HG2	1:E:89:LEU:HD21	2.00	0.42
3:G:136:VAL:HG13	3:G:167:MSE:SE	2.70	0.42
1:I:49:GLU:HB2	6:I:1014:HOH:O	2.20	0.42
3:K:33:LEU:O	3:K:34:GLY:O	2.36	0.42
3:K:76:ASP:O	3:K:77:HIS:C	2.62	0.42
3:K:135:PHE:CE2	3:K:143:ALA:HB2	2.54	0.42
1:A:64:ASN:N	1:A:64:ASN:ND2	2.67	0.42
1:A:144:VAL:CG1	2:B:80:LEU:HD13	2.50	0.42
3:C:83:THR:OG1	3:C:84:PHE:N	2.52	0.42
3:C:91:TYR:O	3:C:92:TYR:C	2.63	0.42
4:H:152:SER:CB	4:H:164:LEU:HD22	2.49	0.42
1:I:73:LEU:HD12	1:I:74:LYS:H	1.82	0.42
3:K:62:PRO:HA	3:K:63:PRO:HD3	1.98	0.42
2:B:125:MSE:C	2:B:127:SER:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ILE:HG22	3:C:60:LEU:HD23	2.00	0.42
3:C:59:ARG:HE	3:C:59:ARG:HB2	1.54	0.42
3:C:129:ARG:HD3	4:D:154:GLN:HG3	2.01	0.42
2:F:18:GLU:OE2	2:F:18:GLU:N	2.47	0.42
1:I:27:ILE:HG21	3:K:29:ILE:HD11	2.02	0.42
1:I:27:ILE:HG21	3:K:29:ILE:HD13	2.02	0.42
1:I:87:TYR:OH	2:J:142:PRO:HG3	2.19	0.42
2:J:138:GLN:C	2:J:140:MSE:H	2.27	0.42
2:B:11:ARG:C	2:B:13:LEU:H	2.27	0.42
3:G:17:ILE:HG22	3:G:60:LEU:HA	2.00	0.42
4:H:34:VAL:CG2	4:H:84:LEU:HB2	2.49	0.42
1:I:118:GLU:HA	1:I:119:PRO:HD3	1.76	0.42
4:L:16:GLU:HG3	4:L:17:GLU:H	1.84	0.42
4:L:61:PRO:O	4:L:62:GLN:C	2.63	0.42
3:G:24:ASP:O	3:G:25:LYS:C	2.63	0.42
3:G:105:ASP:O	3:G:107:ILE:N	2.53	0.42
1:I:114:ARG:HA	1:I:115:PRO:HD2	1.87	0.42
2:J:53:GLY:C	2:J:55:ARG:N	2.78	0.42
2:J:100:ASN:HD22	2:J:100:ASN:N	2.17	0.42
1:A:65:LEU:HD11	1:A:78:HIS:HB2	2.02	0.42
1:A:144:VAL:HG11	2:B:80:LEU:HD13	2.01	0.42
2:B:61:THR:HG22	2:B:65:ARG:HH12	1.83	0.42
4:D:48:LEU:H	4:D:48:LEU:CD2	2.33	0.42
4:H:141:THR:O	4:H:145:ARG:HG3	2.20	0.42
4:L:103:ASP:O	4:L:106:VAL:HG12	2.20	0.42
1:A:45:GLU:OE2	1:A:119:PRO:HG3	2.20	0.41
3:C:46:LEU:CD2	3:C:50:ILE:HG13	2.50	0.41
1:I:176:ARG:O	1:I:200:LYS:HG2	2.19	0.41
1:A:90:SER:C	1:A:92:TYR:N	2.76	0.41
2:B:7:MSE:C	2:B:9:LEU:H	2.28	0.41
2:B:7:MSE:C	2:B:9:LEU:N	2.77	0.41
3:C:162:GLN:O	3:C:163:ALA:C	2.64	0.41
2:F:58:LEU:HD12	4:H:41:PRO:HG2	2.03	0.41
3:G:89:SER:C	3:G:91:TYR:H	2.27	0.41
3:G:89:SER:C	3:G:91:TYR:N	2.78	0.41
4:H:165:VAL:HA	4:H:168:LEU:HD22	2.01	0.41
4:L:41:PRO:C	4:L:42:ARG:CG	2.92	0.41
4:L:62:GLN:C	4:L:64:SER:H	2.28	0.41
4:L:137:SER:O	4:L:141:THR:HG23	2.19	0.41
1:A:147:LYS:HG2	1:A:148:HIS:CD2	2.54	0.41
3:C:74:MSE:SE	3:C:88:PRO:HG3	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:THR:O	3:C:100:LEU:HB2	2.19	0.41
4:D:7:ARG:NH1	4:D:23:ASP:OD1	2.53	0.41
4:D:120:GLY:O	4:D:124:LEU:HD13	2.19	0.41
1:E:95:CYS:O	1:E:99:LYS:HG3	2.20	0.41
2:F:13:LEU:HD12	2:F:13:LEU:HA	1.84	0.41
2:F:116:ASN:OD1	2:F:119:ARG:NH2	2.53	0.41
4:H:128:SER:OG	4:H:130:GLU:HG2	2.20	0.41
4:H:168:LEU:HD12	4:H:168:LEU:HA	1.86	0.41
4:L:120:GLY:O	4:L:124:LEU:HD13	2.20	0.41
3:C:2:ASP:O	3:C:3:ALA:C	2.63	0.41
3:C:60:LEU:N	3:C:106:ASN:OD1	2.51	0.41
4:D:39:ALA:N	4:D:62:GLN:HE21	2.17	0.41
2:F:48:ASN:C	2:F:50:ALA:N	2.78	0.41
2:F:74:ARG:HG3	4:H:19:PHE:CE1	2.55	0.41
4:H:169:ASP:O	4:H:173:ARG:HG3	2.21	0.41
4:L:27:MSE:SE	4:L:27:MSE:C	3.13	0.41
4:L:69:PRO:O	4:L:70:LEU:C	2.61	0.41
4:L:96:TRP:O	4:L:97:ARG:C	2.61	0.41
4:L:100:PHE:CD1	4:L:107:VAL:HG21	2.54	0.41
1:A:46:SER:OG	1:A:48:PRO:HD3	2.21	0.41
1:A:123:SER:CB	1:A:124:PRO:HD2	2.50	0.41
2:B:56:SER:O	2:B:58:LEU:N	2.53	0.41
3:C:74:MSE:CE	3:C:88:PRO:HG3	2.49	0.41
4:D:41:PRO:C	4:D:43:LEU:H	2.26	0.41
4:D:125:HIS:C	4:D:127:ASP:N	2.76	0.41
4:D:147:ARG:O	4:D:149:ILE:N	2.54	0.41
3:G:139:GLN:NE2	3:G:171:ARG:NH2	2.68	0.41
3:K:23:LEU:HD13	3:K:24:ASP:N	2.35	0.41
4:L:123:LEU:HD12	4:L:126:PHE:HD2	1.85	0.41
3:C:48:LEU:HD22	3:C:52:LEU:CD2	2.44	0.41
3:C:110:ALA:O	3:C:113:ILE:HG22	2.21	0.41
3:C:129:ARG:HB2	3:C:129:ARG:NH1	2.33	0.41
1:E:29:ARG:HE	1:E:29:ARG:CA	2.33	0.41
2:F:25:ASN:H	2:F:25:ASN:ND2	2.17	0.41
2:F:125:MSE:HB3	2:F:134:LEU:O	2.21	0.41
3:G:113:ILE:C	3:G:115:THR:N	2.79	0.41
1:I:54:VAL:HG12	1:I:58:LEU:HD23	2.03	0.41
3:K:97:LYS:HD3	4:L:189:TRP:CZ2	2.56	0.41
1:A:50:ILE:O	1:A:54:VAL:HG22	2.20	0.41
4:D:94:GLU:N	4:D:97:ARG:HH21	2.19	0.41
4:D:96:TRP:O	4:D:98:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ARG:HE	1:E:29:ARG:HA	1.86	0.41
3:G:68:VAL:HG11	3:G:109:LYS:HG3	2.02	0.41
4:L:176:PHE:CD1	4:L:176:PHE:C	2.98	0.41
1:A:209:LYS:O	1:A:212:ALA:HB3	2.20	0.41
3:C:71:LEU:C	3:C:73:LYS:H	2.28	0.41
4:D:158:ASN:C	4:D:160:ASP:H	2.29	0.41
3:G:2:ASP:OD1	3:G:4:ALA:N	2.44	0.41
4:H:193:GLN:NE2	4:H:193:GLN:CA	2.76	0.41
1:I:205:LEU:HD12	1:I:205:LEU:HA	1.85	0.41
4:L:41:PRO:HA	4:L:59:ALA:HB2	2.03	0.41
4:L:58:ASN:ND2	4:L:59:ALA:N	2.67	0.41
1:A:74:LYS:NZ	3:C:26:ILE:HA	2.36	0.41
1:A:173:LEU:HD12	1:A:211:ILE:HG21	2.02	0.41
2:B:39:LEU:CD1	2:B:68:SER:HB3	2.51	0.41
3:C:162:GLN:O	3:C:165:ASN:N	2.53	0.41
4:D:25:ILE:HG13	4:D:26:LEU:N	2.36	0.41
1:E:55:MSE:HA	1:E:55:MSE:CE	2.45	0.41
1:E:116:GLU:C	1:E:118:GLU:H	2.28	0.41
2:F:122:ALA:O	2:F:123:THR:C	2.62	0.41
1:I:50:ILE:HD12	1:I:50:ILE:H	1.86	0.41
1:I:73:LEU:HD11	3:K:23:LEU:CD2	2.50	0.41
1:I:77:ILE:O	1:I:78:HIS:C	2.64	0.41
1:I:176:ARG:HG3	1:I:176:ARG:NH1	2.36	0.41
1:I:181:ASN:N	1:I:181:ASN:ND2	2.68	0.41
2:J:76:THR:O	2:J:80:LEU:HG	2.20	0.41
3:K:17:ILE:C	3:K:18:ILE:HD12	2.45	0.41
3:K:21:PHE:CD1	3:K:57:LYS:HB3	2.55	0.41
4:L:18:ASN:HD22	4:L:18:ASN:HA	1.61	0.41
4:L:43:LEU:O	4:L:45:ALA:N	2.54	0.41
4:L:184:ASN:O	4:L:185:ASP:C	2.64	0.41
1:A:48:PRO:O	1:A:52:GLU:CG	2.67	0.41
1:E:55:MSE:HE2	1:E:58:LEU:HD12	2.03	0.41
2:F:87:ILE:O	2:F:90:LEU:HB2	2.21	0.41
3:G:149:THR:O	3:G:153:ILE:HG23	2.21	0.41
4:H:32:LEU:HD21	4:H:86:VAL:CG1	2.51	0.41
4:H:61:PRO:O	4:H:63:GLY:N	2.52	0.41
4:H:69:PRO:O	4:H:70:LEU:C	2.64	0.41
4:D:94:GLU:N	4:D:94:GLU:OE1	2.54	0.40
3:G:111:ASP:HA	3:G:114:ARG:HB3	2.02	0.40
1:A:100:ILE:CG1	1:A:101:GLU:N	2.84	0.40
1:A:108:LEU:HD21	1:A:130:ALA:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MSE:HE3	2:B:39:LEU:CD2	2.50	0.40
2:B:43:ASN:OD1	2:B:65:ARG:HB2	2.21	0.40
2:B:134:LEU:HD13	2:B:134:LEU:C	2.46	0.40
3:C:118:LYS:C	3:C:120:MSE:N	2.77	0.40
4:D:142:PHE:C	4:D:144:GLY:H	2.28	0.40
1:E:81:GLU:CD	3:G:29:ILE:HG12	2.47	0.40
1:E:97:LEU:HD23	1:E:97:LEU:HA	1.95	0.40
3:G:124:ARG:HD3	3:G:152:GLU:OE2	2.21	0.40
4:H:18:ASN:O	4:H:19:PHE:C	2.63	0.40
1:I:21:LEU:HB2	1:I:25:GLU:OE1	2.21	0.40
1:I:140:TYR:CZ	1:I:144:VAL:HG21	2.55	0.40
2:J:100:ASN:ND2	2:J:101:ALA:N	2.67	0.40
3:K:21:PHE:CE2	3:K:23:LEU:HB2	2.56	0.40
4:L:68:LEU:HA	4:L:69:PRO:HD3	1.95	0.40
4:L:141:THR:O	4:L:145:ARG:HG3	2.21	0.40
1:A:25:GLU:O	1:A:26:LEU:C	2.63	0.40
4:D:97:ARG:NH1	4:D:134:ILE:HG13	2.36	0.40
1:E:31:GLU:O	1:E:35:MSE:HG3	2.20	0.40
4:H:91:ILE:CG1	4:H:112:MSE:HE2	2.50	0.40
1:I:85:ILE:HD11	3:K:29:ILE:CG1	2.50	0.40
4:L:33:PRO:HD2	4:L:87:GLU:O	2.22	0.40
1:A:23:PRO:HB3	3:C:29:ILE:HG23	2.03	0.40
1:A:104:PHE:N	1:A:105:PRO:HD2	2.37	0.40
1:A:149:MSE:HE3	2:B:36:MSE:SE	2.72	0.40
2:B:41:GLU:C	2:B:43:ASN:H	2.29	0.40
3:C:11:GLU:O	3:C:47:TRP:HD1	2.05	0.40
3:C:33:LEU:CD1	3:C:48:LEU:HD12	2.52	0.40
3:C:51:ASN:ND2	3:C:55:ARG:CD	2.85	0.40
3:C:118:LYS:HB2	3:C:118:LYS:HE3	1.88	0.40
3:C:133:ASP:OD1	4:D:147:ARG:HB2	2.22	0.40
4:D:32:LEU:HD21	4:D:86:VAL:HG11	2.03	0.40
3:G:65:TRP:HA	3:G:70:LYS:NZ	2.37	0.40
3:G:160:LEU:O	3:G:164:LEU:HD13	2.21	0.40
4:H:77:PHE:N	4:H:84:LEU:HD21	2.36	0.40
4:H:140:GLN:HE21	4:H:140:GLN:HB2	1.66	0.40
1:I:196:ILE:CG2	1:I:197:ASP:H	2.35	0.40
3:K:64:GLU:HG2	3:K:70:LYS:HZ2	1.86	0.40
3:K:129:ARG:HB3	4:L:150:MSE:HE3	2.02	0.40
3:K:151:MSE:HE2	4:L:186:PHE:HD1	1.86	0.40
4:L:147:ARG:HG3	4:L:147:ARG:HH11	1.86	0.40
1:A:172:PHE:HE1	1:A:203:GLN:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LEU:O	2:B:43:ASN:HB2	2.21	0.40
3:C:20:ASN:ND2	3:C:21:PHE:HD1	2.20	0.40
4:D:168:LEU:HB3	4:D:172:GLU:HB2	2.04	0.40
1:E:150:PRO:HA	1:E:151:PRO:HD3	1.99	0.40
2:F:7:MSE:HE2	2:F:75:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/203 (76%)	119 (77%)	28 (18%)	8 (5%)	1	9
1	E	186/203 (92%)	162 (87%)	20 (11%)	4 (2%)	5	26
1	I	190/203 (94%)	159 (84%)	25 (13%)	6 (3%)	3	18
2	B	143/152 (94%)	117 (82%)	18 (13%)	8 (6%)	1	8
2	F	144/152 (95%)	127 (88%)	10 (7%)	7 (5%)	1	10
2	J	143/152 (94%)	125 (87%)	14 (10%)	4 (3%)	4	21
3	C	164/186 (88%)	126 (77%)	30 (18%)	8 (5%)	1	10
3	G	174/186 (94%)	148 (85%)	19 (11%)	7 (4%)	2	14
3	K	173/186 (93%)	152 (88%)	17 (10%)	4 (2%)	5	25
4	D	178/216 (82%)	136 (76%)	29 (16%)	13 (7%)	1	4
4	H	179/216 (83%)	160 (89%)	14 (8%)	5 (3%)	4	21
4	L	178/216 (82%)	150 (84%)	18 (10%)	10 (6%)	1	8
All	All	2007/2271 (88%)	1681 (84%)	242 (12%)	84 (4%)	2	13

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	72	ASP
1	A	116	GLU
2	B	17	PRO
3	C	68	VAL
4	D	15	PRO
4	D	127	ASP
1	E	72	ASP
2	F	131	ASP
3	G	110	ALA
4	H	62	GLN
1	I	64	ASN
4	L	62	GLN
4	L	153	SER
1	A	44	LEU
1	A	121	SER
1	A	153	LEU
2	B	53	GLY
2	B	57	ASP
2	B	133	GLY
3	C	34	GLY
4	D	105	ASN
4	D	109	LEU
4	D	126	PHE
4	D	148	ARG
1	E	116	GLU
2	F	18	GLU
2	F	130	GLY
3	G	34	GLY
3	G	106	ASN
3	G	114	ARG
1	I	210	THR
2	J	18	GLU
3	K	34	GLY
3	K	81	GLU
3	K	111	ASP
4	L	42	ARG
4	L	44	GLY
4	L	80	LYS
4	L	154	GLN
2	B	55	ARG
2	B	100	ASN
2	B	126	ARG

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Mol	Chain	Res	Type
1	E	178	ARG
2	F	52	SER
4	H	19	PHE
4	H	47	PHE
4	H	58	ASN
1	I	178	ARG
1	I	191	GLN
4	L	63	GLY
3	C	88	PRO
3	C	109	LYS
3	C	111	ASP
4	D	102	ALA
2	F	20	GLN
3	G	150	LEU
4	H	63	GLY
1	I	72	ASP
2	J	53	GLY
2	J	131	ASP
1	A	145	ALA
3	C	66	MSE
3	C	147	ASN
4	D	154	GLN
1	E	49	GLU
3	G	79	ARG
1	I	69	LYS
4	L	41	PRO
4	L	46	PHE
1	A	142	LYS
4	D	97	ARG
4	D	136	GLN
2	F	129	GLY
2	F	133	GLY
3	C	157	GLY
2	B	19	GLY
4	D	11	GLY
3	K	35	PRO
4	L	15	PRO
2	J	54	GLY
3	G	88	PRO
4	D	61	PRO
4	D	83	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/181 (83%)	141 (93%)	10 (7%)	15	46
1	E	179/181 (99%)	163 (91%)	16 (9%)	9	34
1	I	180/181 (99%)	163 (91%)	17 (9%)	8	32
2	B	126/125 (101%)	115 (91%)	11 (9%)	9	35
2	F	127/125 (102%)	119 (94%)	8 (6%)	16	48
2	J	126/125 (101%)	115 (91%)	11 (9%)	9	35
3	C	154/161 (96%)	143 (93%)	11 (7%)	13	43
3	G	160/161 (99%)	145 (91%)	15 (9%)	8	32
3	K	159/161 (99%)	137 (86%)	22 (14%)	3	17
4	D	157/180 (87%)	143 (91%)	14 (9%)	9	34
4	H	158/180 (88%)	133 (84%)	25 (16%)	2	13
4	L	157/180 (87%)	138 (88%)	19 (12%)	5	21
All	All	1834/1941 (94%)	1655 (90%)	179 (10%)	7	30

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	32	GLN
1	A	44	LEU
1	A	61	MSE
1	A	71	GLU
1	A	72	ASP
1	A	109	GLU
1	A	141	LEU
1	A	159	PHE
1	A	204	HIS
2	B	1	MSE
2	B	2	PHE
2	B	5	LYS
2	B	8	GLU

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Mol	Chain	Res	Type
2	B	10	ILE
2	B	17	PRO
2	B	27	ASP
2	B	49	GLU
2	B	71	ARG
2	B	93	GLU
2	B	97	ILE
3	C	9	LEU
3	C	17	ILE
3	C	20	ASN
3	C	40	LEU
3	C	46	LEU
3	C	48	LEU
3	C	52	LEU
3	C	60	LEU
3	C	106	ASN
3	C	129	ARG
3	C	147	ASN
4	D	18	ASN
4	D	23	ASP
4	D	25	ILE
4	D	58	ASN
4	D	84	LEU
4	D	90	LYS
4	D	94	GLU
4	D	109	LEU
4	D	139	LEU
4	D	155	ASN
4	D	169	ASP
4	D	171	MSE
4	D	173	ARG
4	D	183	LEU
1	E	21	LEU
1	E	22	THR
1	E	29	ARG
1	E	32	GLN
1	E	49	GLU
1	E	55	MSE
1	E	107	VAL
1	E	111	GLU
1	E	113	THR
1	E	125	GLU

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Mol	Chain	Res	Type
1	E	134	MSE
1	E	141	LEU
1	E	153	LEU
1	E	178	ARG
1	E	190	GLU
1	E	203	GLN
2	F	25	ASN
2	F	26	GLU
2	F	43	ASN
2	F	44	GLN
2	F	58	LEU
2	F	71	ARG
2	F	98	LEU
2	F	109	GLU
3	G	7	GLU
3	G	12	LYS
3	G	26	ILE
3	G	29	ILE
3	G	78	GLU
3	G	82	GLU
3	G	105	ASP
3	G	109	LYS
3	G	123	THR
3	G	125	ILE
3	G	153	ILE
3	G	160	LEU
3	G	161	THR
3	G	164	LEU
3	G	175	GLN
4	H	9	GLU
4	H	25	ILE
4	H	26	LEU
4	H	28	SER
4	H	43	LEU
4	H	46	PHE
4	H	57	ASP
4	H	58	ASN
4	H	62	GLN
4	H	66	LEU
4	H	76	LEU
4	H	84	LEU
4	H	88	LEU

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Mol	Chain	Res	Type
4	H	109	LEU
4	H	124	LEU
4	H	131	ASN
4	H	139	LEU
4	H	141	THR
4	H	147	ARG
4	H	158	ASN
4	H	168	LEU
4	H	169	ASP
4	H	170	GLU
4	H	178	THR
4	H	191	LYS
1	I	32	GLN
1	I	55	MSE
1	I	58	LEU
1	I	64	ASN
1	I	69	LYS
1	I	73	LEU
1	I	118	GLU
1	I	125	GLU
1	I	126	GLU
1	I	134	MSE
1	I	141	LEU
1	I	153	LEU
1	I	177	GLU
1	I	191	GLN
1	I	193	ASP
1	I	197	ASP
1	I	211	ILE
2	J	2	PHE
2	J	13	LEU
2	J	60	PRO
2	J	71	ARG
2	J	76	THR
2	J	90	LEU
2	J	98	LEU
2	J	100	ASN
2	J	109	GLU
2	J	131	ASP
2	J	136	ILE
3	K	14	LEU
3	K	17	ILE

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Mol	Chain	Res	Type
3	K	20	ASN
3	K	29	ILE
3	K	32	ASP
3	K	36	PHE
3	K	42	VAL
3	K	43	GLU
3	K	44	VAL
3	K	46	LEU
3	K	52	LEU
3	K	56	GLN
3	K	57	LYS
3	K	61	LEU
3	K	64	GLU
3	K	104	SER
3	K	111	ASP
3	K	120	MSE
3	K	148	LEU
3	K	161	THR
3	K	164	LEU
3	K	173	ASN
4	L	18	ASN
4	L	26	LEU
4	L	38	THR
4	L	41	PRO
4	L	66	LEU
4	L	81	ARG
4	L	85	SER
4	L	90	LYS
4	L	109	LEU
4	L	122	GLN
4	L	124	LEU
4	L	136	GLN
4	L	139	LEU
4	L	141	THR
4	L	147	ARG
4	L	159	GLU
4	L	169	ASP
4	L	170	GLU
4	L	191	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	64	ASN
1	A	78	HIS
1	A	79	GLN
1	A	143	ASN
1	A	148	HIS
1	A	154	GLN
1	A	203	GLN
1	A	204	HIS
2	B	20	GLN
2	B	25	ASN
2	B	72	ASN
2	B	100	ASN
2	B	138	GLN
3	C	20	ASN
3	C	51	ASN
3	C	101	ASN
3	C	106	ASN
3	C	138	GLN
3	C	139	GLN
3	C	147	ASN
3	C	154	ASN
3	C	162	GLN
4	D	18	ASN
4	D	62	GLN
4	D	93	GLN
4	D	115	HIS
4	D	122	GLN
4	D	131	ASN
4	D	177	GLN
4	D	180	GLN
1	E	36	ASN
1	E	60	HIS
1	E	78	HIS
1	E	106	HIS
1	E	154	GLN
1	E	179	GLN
1	E	181	ASN
1	E	203	GLN
2	F	14	HIS
2	F	25	ASN
2	F	100	ASN
2	F	115	ASN

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Mol	Chain	Res	Type
3	G	37	ASN
3	G	54	GLN
3	G	101	ASN
3	G	139	GLN
3	G	142	HIS
3	G	147	ASN
4	H	18	ASN
4	H	29	HIS
4	H	58	ASN
4	H	62	GLN
4	H	93	GLN
4	H	110	HIS
4	H	122	GLN
4	H	125	HIS
4	H	131	ASN
4	H	136	GLN
4	H	140	GLN
4	H	154	GLN
4	H	158	ASN
4	H	177	GLN
4	H	184	ASN
4	H	193	GLN
1	I	32	GLN
1	I	36	ASN
1	I	64	ASN
1	I	106	HIS
1	I	136	ASN
1	I	181	ASN
1	I	191	GLN
2	J	20	GLN
2	J	31	GLN
2	J	100	ASN
3	K	20	ASN
3	K	102	HIS
3	K	138	GLN
3	K	139	GLN
3	K	147	ASN
3	K	162	GLN
3	K	173	ASN
4	L	18	ASN
4	L	58	ASN
4	L	62	GLN

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Mol	Chain	Res	Type
4	L	110	HIS
4	L	122	GLN
4	L	131	ASN
4	L	136	GLN
4	L	154	GLN
4	L	180	GLN
4	L	184	ASN
4	L	193	GLN

5.3.3 RNA [i](#)

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](#)

17 ligands are modelled in this entry.

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	$\# Z > 2$
5	SO4	F	1005	-	4,4,4	0.40	0	6,6,6	0.06	0
5	SO4	I	1003	-	4,4,4	0.39	0	6,6,6	0.11	0
5	SO4	J	1006	-	4,4,4	0.44	0	6,6,6	0.06	0
5	SO4	L	1008	-	4,4,4	0.45	0	6,6,6	0.09	0
5	SO4	E	1011	-	4,4,4	0.42	0	6,6,6	0.09	0
5	SO4	F	1010	-	4,4,4	0.38	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	L	1009	-	4,4,4	0.42	0	6,6,6	0.13	0
5	SO4	A	1017	-	4,4,4	0.44	0	6,6,6	0.10	0
5	SO4	E	1012	-	4,4,4	0.44	0	6,6,6	0.12	0
5	SO4	K	1007	-	4,4,4	0.45	0	6,6,6	0.19	0
5	SO4	F	1014	-	4,4,4	0.43	0	6,6,6	0.07	0
5	SO4	I	1001	-	4,4,4	0.38	0	6,6,6	0.13	0
5	SO4	E	1013	-	4,4,4	0.43	0	6,6,6	0.12	0
5	SO4	E	1015	-	4,4,4	0.44	0	6,6,6	0.06	0
5	SO4	B	1016	-	4,4,4	0.41	0	6,6,6	0.19	0
5	SO4	F	1004	-	4,4,4	0.39	0	6,6,6	0.13	0
5	SO4	I	1002	-	4,4,4	0.38	0	6,6,6	0.12	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.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1010	SO4	3	0
5	F	1014	SO4	1	0
5	I	1001	SO4	1	0
5	B	1016	SO4	5	0
5	F	1004	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	153/203 (75%)	0.49	4 (2%) 57 34	48, 77, 108, 115	0
1	E	182/203 (89%)	-0.30	2 (1%) 78 57	21, 47, 79, 108	0
1	I	184/203 (90%)	-0.12	3 (1%) 70 47	21, 44, 87, 97	0
2	B	138/152 (90%)	0.09	1 (0%) 84 66	33, 65, 92, 106	0
2	F	138/152 (90%)	-0.29	0 100 100	18, 44, 77, 98	0
2	J	138/152 (90%)	-0.37	0 100 100	19, 40, 69, 86	0
3	C	159/186 (85%)	0.40	4 (2%) 58 35	43, 78, 115, 123	0
3	G	167/186 (89%)	0.14	1 (0%) 85 69	22, 65, 103, 112	0
3	K	166/186 (89%)	-0.42	0 100 100	22, 41, 63, 72	0
4	D	177/216 (81%)	0.47	4 (2%) 61 38	40, 83, 104, 113	0
4	H	178/216 (82%)	-0.35	1 (0%) 85 69	18, 40, 76, 88	0
4	L	177/216 (81%)	-0.24	2 (1%) 78 57	19, 43, 85, 97	0
All	All	1957/2271 (86%)	-0.04	22 (1%) 78 57	18, 54, 101, 123	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	65	LEU	4.3
3	C	108	PRO	3.0
4	D	192	GLY	3.0
1	A	173	LEU	2.9
1	I	69	LYS	2.8
4	L	193	GLN	2.8
1	I	180	GLU	2.7
3	C	171	ARG	2.6
4	D	49	GLU	2.6
4	D	161	THR	2.6
1	A	172	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
4	H	193	GLN	2.5
3	C	173	ASN	2.3
1	E	115	PRO	2.2
1	A	170	TYR	2.1
2	B	145	SER	2.1
3	G	110	ALA	2.1
1	A	119	PRO	2.1
4	L	48	LEU	2.1
3	C	109	LYS	2.1
1	E	213	PRO	2.0
4	D	46	PHE	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
5	SO4	I	1001	5/5	0.60	0.14	124,124,125,125	0
5	SO4	E	1015	5/5	0.64	0.19	125,125,126,126	0
5	SO4	F	1004	5/5	0.67	0.23	137,138,138,138	0
5	SO4	F	1005	5/5	0.76	0.19	111,112,112,112	0
5	SO4	E	1011	5/5	0.78	0.23	107,107,108,108	0
5	SO4	K	1007	5/5	0.80	0.44	114,114,115,116	0
5	SO4	E	1012	5/5	0.81	0.13	107,107,108,108	0
5	SO4	L	1008	5/5	0.83	0.24	118,118,118,119	0
5	SO4	E	1013	5/5	0.84	0.16	117,118,118,118	0
5	SO4	B	1016	5/5	0.86	0.14	95,97,98,98	0
5	SO4	J	1006	5/5	0.86	0.33	96,96,96,97	0
5	SO4	A	1017	5/5	0.87	0.19	115,115,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	F	1010	5/5	0.90	0.27	106,107,107,107	0
5	SO4	I	1002	5/5	0.90	0.13	95,96,96,97	0
5	SO4	I	1003	5/5	0.90	0.15	137,137,138,138	0
5	SO4	F	1014	5/5	0.91	0.15	115,116,116,116	0
5	SO4	L	1009	5/5	0.91	0.22	102,102,102,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.