



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:56 PM UTC

PDB ID : 4OC9 / pdb_00004oc9
Title : 2.35 Angstrom resolution crystal structure of putative O-acetylhomoserine (thiol)-lyase (metY) from Campylobacter jejuni subsp. jejuni NCTC 11168 with N⁵-Pyridoxyl-Lysine-5'-Monophosphate at position 205
Authors : Halavaty, A.S.; Brunzelle, J.S.; Wawrzak, Z.; Onopriyenko, O.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2014-01-08
Resolution : 2.35 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)

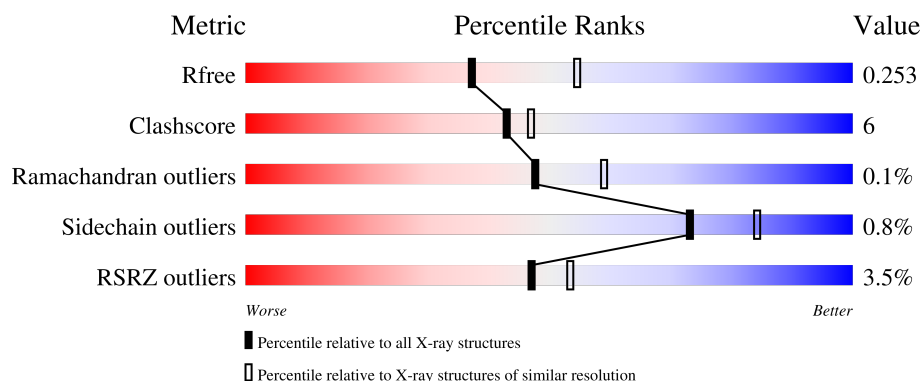
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

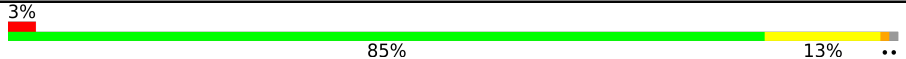
The reported resolution of this entry is 2.35 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

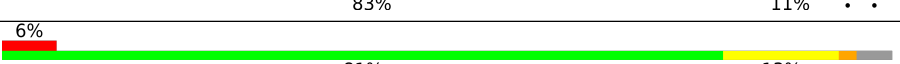
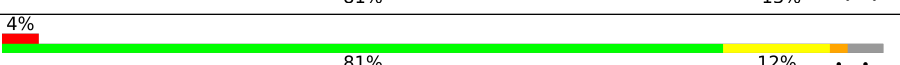
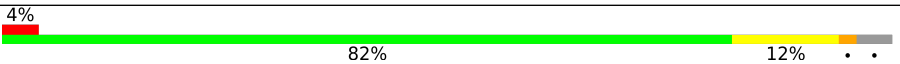
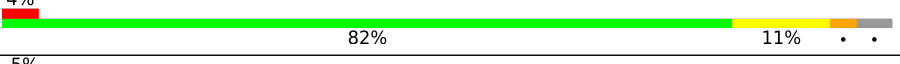
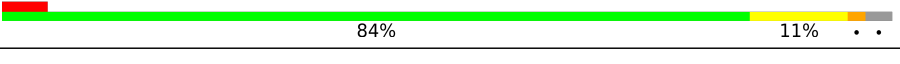
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	424	 3% 85% 13% ..
1	B	424	 3% 83% 14% ..
1	C	424	 2% 87% 11% ..
1	D	424	 2% 87% 11% .

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	424	 4% 88% 10% ••
1	F	424	 2% 86% 12% •
1	G	424	 2% 85% 13% •
1	H	424	 3% 84% 14% •
1	I	424	 4% 82% 11% • 5%
1	J	424	 3% 83% 11% • •
1	K	424	 6% 81% 13% • •
1	L	424	 4% 81% 12% • •
1	M	424	 4% 82% 12% • •
1	N	424	 4% 82% 11% • •
1	O	424	 4% 82% 11% • •
1	P	424	 5% 84% 11% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 55287 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.

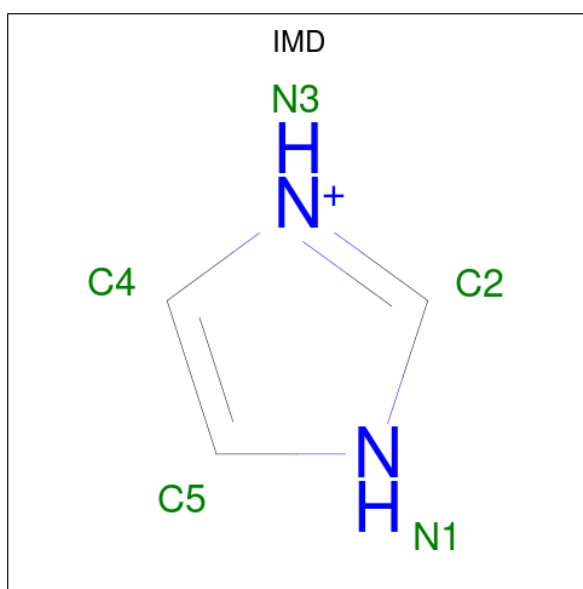
- Molecule 1 is a protein called Putative O-acetylhomoserine (Thiol)-lyase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	P	S	Se	0	5	0
			3335	2112	570	648	1	3	1			
1	B	421	Total	C	N	O	P	S	Se	0	4	0
			3329	2108	571	645	1	3	1			
1	C	421	Total	C	N	O	P	S	Se	0	3	0
			3311	2097	566	643	1	3	1			
1	D	422	Total	C	N	O	P	S	Se	0	3	0
			3327	2107	570	645	1	3	1			
1	E	421	Total	C	N	O	P	S	Se	0	3	0
			3320	2102	568	645	1	3	1			
1	F	422	Total	C	N	O	P	S	Se	0	2	0
			3318	2101	568	644	1	3	1			
1	G	422	Total	C	N	O	P	S	Se	0	3	0
			3326	2105	570	646	1	3	1			
1	H	422	Total	C	N	O	P	S	Se	0	3	0
			3326	2107	569	645	1	3	1			
1	I	403	Total	C	N	O	P	S	Se	0	1	0
			3166	2012	541	608	1	3	1			
1	J	407	Total	C	N	O	P	S	Se	0	1	0
			3195	2029	547	614	1	3	1			
1	K	406	Total	C	N	O	P	S	Se	0	0	0
			3184	2023	545	611	1	3	1			
1	L	407	Total	C	N	O	P	S	Se	0	3	0
			3211	2039	549	618	1	3	1			
1	M	407	Total	C	N	O	P	S	Se	0	1	0
			3197	2032	547	613	1	3	1			
1	N	405	Total	C	N	O	P	S	Se	0	1	0
			3188	2025	545	613	1	3	1			
1	O	405	Total	C	N	O	P	S	Se	0	1	0
			3189	2026	545	613	1	3	1			
1	P	412	Total	C	N	O	P	S	Se	0	2	0
			3252	2063	559	625	1	3	1			

There are 16 discrepancies between the modelled and reference sequences:

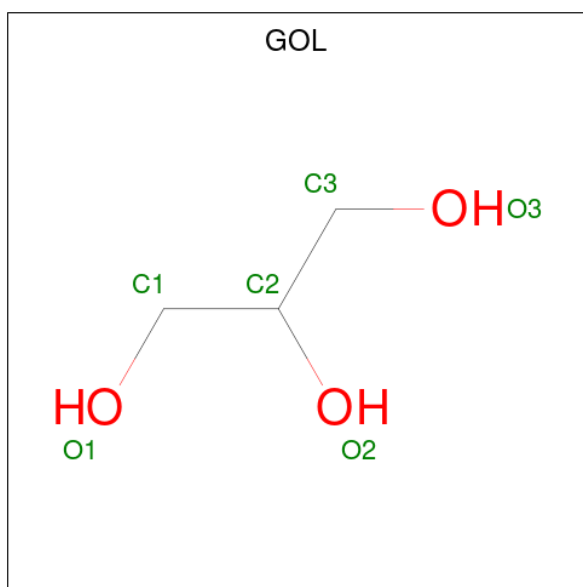
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q0P7Q4
B	0	GLY	-	expression tag	UNP Q0P7Q4
C	0	GLY	-	expression tag	UNP Q0P7Q4
D	0	GLY	-	expression tag	UNP Q0P7Q4
E	0	GLY	-	expression tag	UNP Q0P7Q4
F	0	GLY	-	expression tag	UNP Q0P7Q4
G	0	GLY	-	expression tag	UNP Q0P7Q4
H	0	GLY	-	expression tag	UNP Q0P7Q4
I	0	GLY	-	expression tag	UNP Q0P7Q4
J	0	GLY	-	expression tag	UNP Q0P7Q4
K	0	GLY	-	expression tag	UNP Q0P7Q4
L	0	GLY	-	expression tag	UNP Q0P7Q4
M	0	GLY	-	expression tag	UNP Q0P7Q4
N	0	GLY	-	expression tag	UNP Q0P7Q4
O	0	GLY	-	expression tag	UNP Q0P7Q4
P	0	GLY	-	expression tag	UNP Q0P7Q4

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



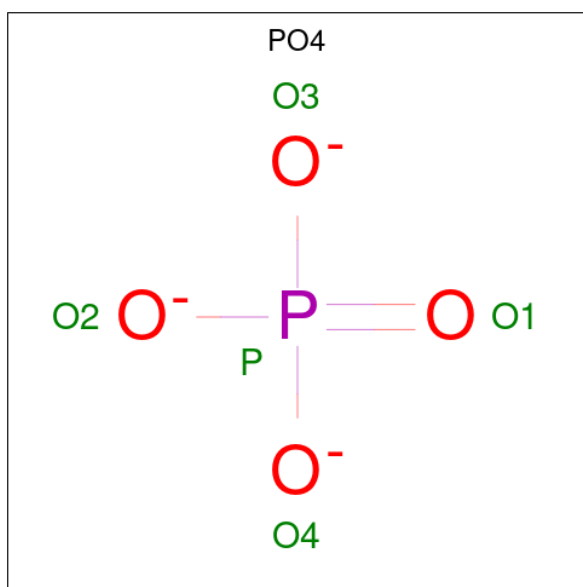
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

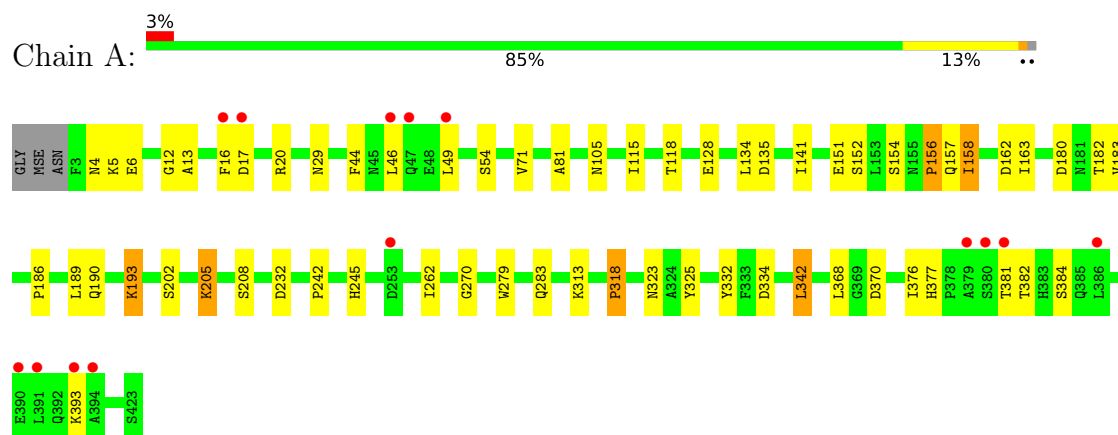
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total 194	O 194	0	7
5	B	214	Total 220	O 220	0	6
5	C	206	Total 212	O 212	0	6
5	D	186	Total 195	O 195	0	9
5	E	210	Total 217	O 217	0	8
5	F	195	Total 197	O 197	0	2
5	G	199	Total 207	O 207	0	8
5	H	187	Total 191	O 191	0	4
5	I	192	Total 195	O 195	0	3
5	J	185	Total 192	O 192	0	7
5	K	177	Total 181	O 181	0	5
5	L	154	Total 159	O 159	0	6
5	M	161	Total 166	O 166	0	5
5	N	162	Total 168	O 168	0	6
5	O	188	Total 193	O 193	0	5
5	P	180	Total 187	O 187	0	7

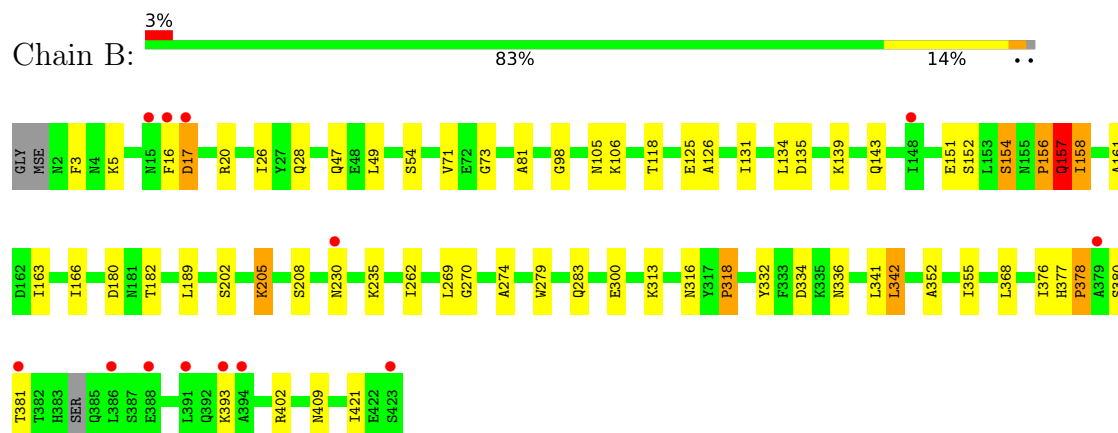
3 Residue-property plots [i](#)

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.

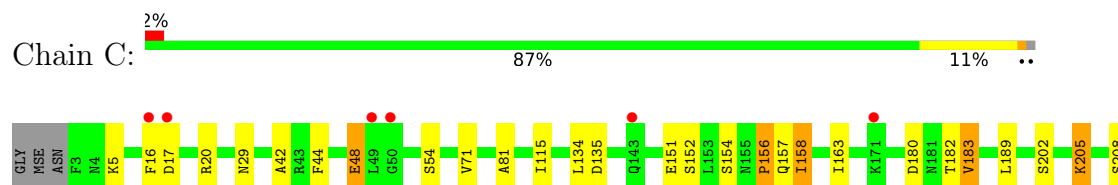
- Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase



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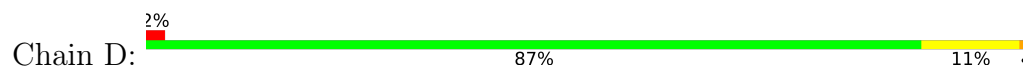


- Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase

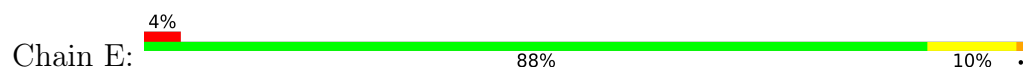




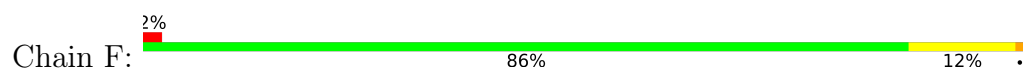
- Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase



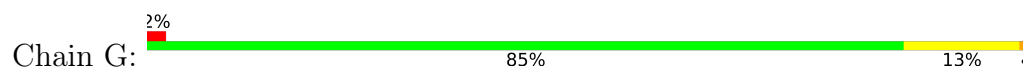
- Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase



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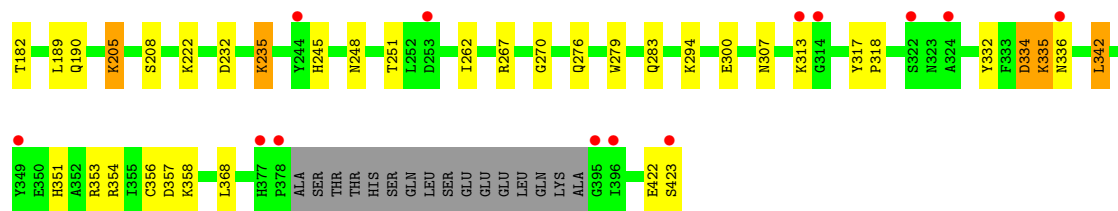


- Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase

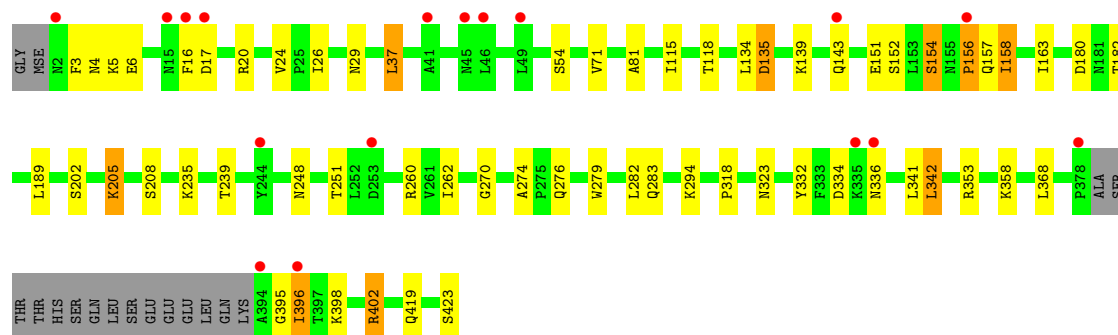
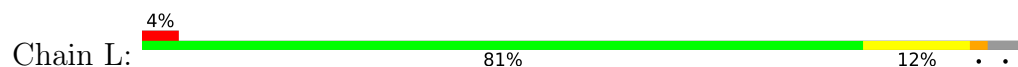


- Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase

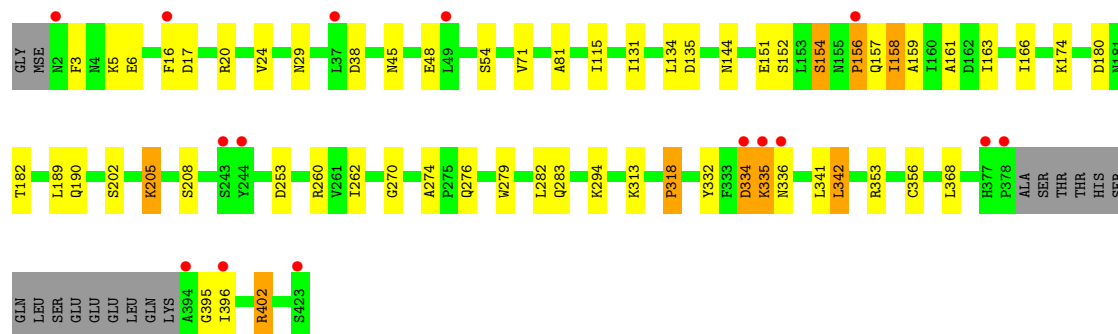
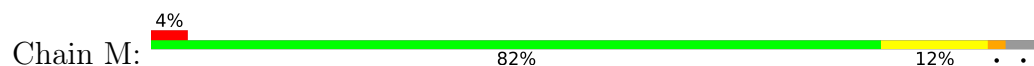




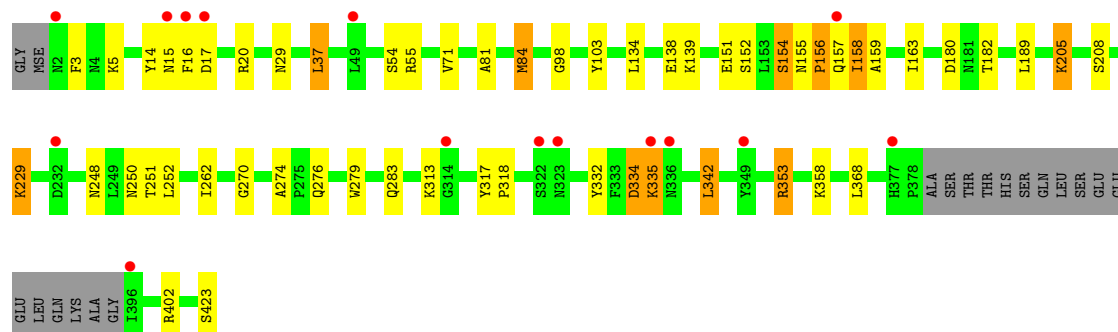
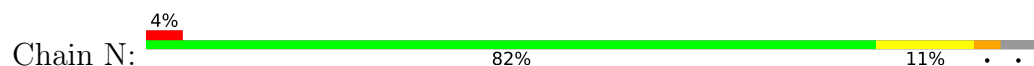
• Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase



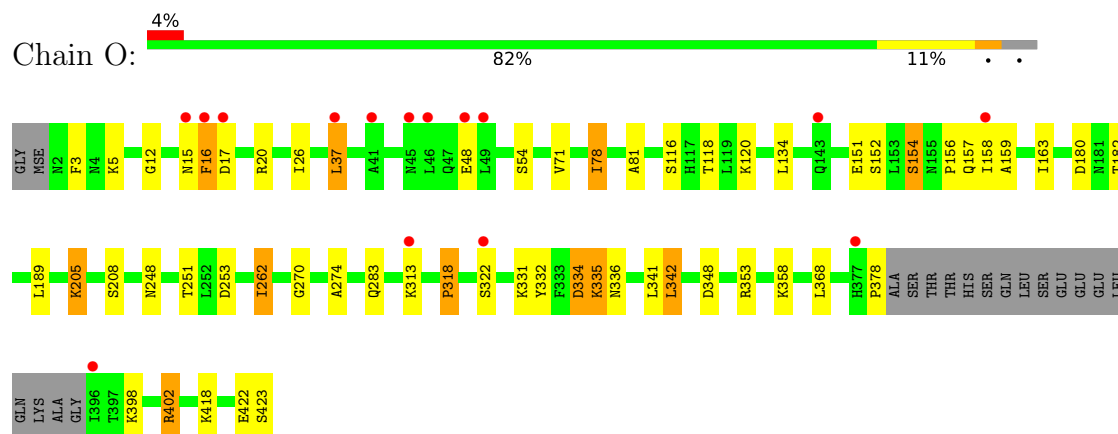
• Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase



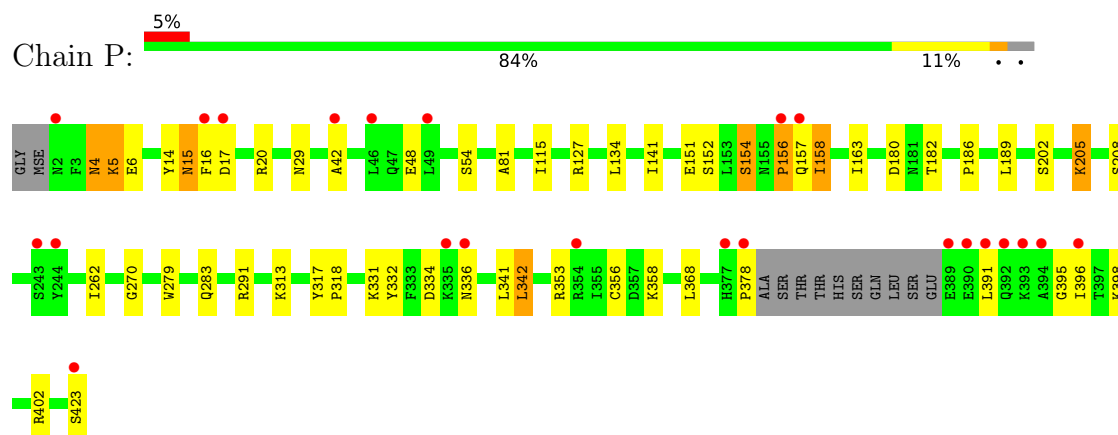
• Molecule 1: Putative O-acetylhomoserine (Thiol)-lyase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.43Å 149.79Å 186.59Å 100.58° 92.47° 90.10°	Depositor
Resolution (Å)	29.65 – 2.35 29.65 – 2.35	Depositor EDS
% Data completeness (in resolution range)	73.4 (29.65-2.35) 73.4 (29.65-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.249 0.209 , 0.253	Depositor DCC
R_{free} test set	9880 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55287	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0867e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, PO4, IMD, GOL

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	0.81	0/3370	1.17	26/4564 (0.6%)
1	B	0.83	2/3363 (0.1%)	1.17	23/4552 (0.5%)
1	C	0.84	1/3353 (0.0%)	1.18	24/4541 (0.5%)
1	D	0.84	1/3362 (0.0%)	1.19	27/4552 (0.6%)
1	E	0.83	2/3355 (0.1%)	1.16	20/4544 (0.4%)
1	F	0.86	1/3353 (0.0%)	1.19	22/4541 (0.5%)
1	G	0.79	0/3361	1.18	23/4552 (0.5%)
1	H	0.81	0/3361	1.18	23/4552 (0.5%)
1	I	0.82	0/3197	1.19	26/4329 (0.6%)
1	J	0.78	0/3228	1.20	24/4371 (0.5%)
1	K	0.81	0/3218	1.21	20/4359 (0.5%)
1	L	0.81	2/3244 (0.1%)	1.30	29/4393 (0.7%)
1	M	0.82	3/3231 (0.1%)	1.32	31/4377 (0.7%)
1	N	0.82	2/3222 (0.1%)	1.24	30/4365 (0.7%)
1	O	0.83	3/3223 (0.1%)	1.23	30/4366 (0.7%)
1	P	0.83	2/3286 (0.1%)	1.20	22/4449 (0.5%)
All	All	0.82	19/52727 (0.0%)	1.21	400/71407 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	260	ARG	CZ-NH1	-8.07	1.21	1.32
1	B	157	GLN	CA-CB	7.91	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	260	ARG	CZ-NH1	-7.85	1.21	1.32
1	F	308	SER	CA-CB	7.50	1.66	1.53
1	O	402	ARG	CD-NE	-6.95	1.36	1.46
1	O	422	GLU	CA-C	6.87	1.61	1.52
1	L	260	ARG	CZ-NH2	6.72	1.42	1.33
1	E	421	ILE	CA-CB	6.66	1.62	1.54
1	N	138	GLU	CA-CB	6.25	1.63	1.53
1	M	395	GLY	N-CA	6.12	1.54	1.45
1	M	260	ARG	CZ-NH2	6.08	1.41	1.33
1	C	48	GLU	CA-C	5.95	1.59	1.52
1	D	15	ASN	CA-C	-5.47	1.45	1.52
1	P	14	TYR	CA-C	-5.36	1.48	1.52
1	B	157	GLN	CA-C	5.25	1.59	1.52
1	N	15	ASN	N-CA	5.24	1.53	1.46
1	P	395	GLY	N-CA	5.18	1.52	1.45
1	O	78	ILE	CB-CG1	5.17	1.63	1.53
1	E	421	ILE	N-CA	5.02	1.52	1.46

All (400) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	260	ARG	NE-CZ-NH2	24.27	141.04	119.20
1	L	260	ARG	NE-CZ-NH2	24.10	140.89	119.20
1	L	260	ARG	NE-CZ-NH1	-23.65	97.85	121.50
1	M	260	ARG	NE-CZ-NH1	-23.41	98.09	121.50
1	J	335	LYS	N-CA-C	-16.97	86.93	110.35
1	K	335	LYS	N-CA-C	-16.38	87.74	110.35
1	N	335	LYS	N-CA-C	-16.14	88.08	110.35
1	O	335	LYS	N-CA-C	-16.12	88.10	110.35
1	M	335	LYS	N-CA-C	-15.87	88.46	110.35
1	N	15	ASN	N-CA-C	11.29	126.45	112.23
1	L	402	ARG	CG-CD-NE	10.58	135.28	112.00
1	P	395	GLY	CA-C-N	9.95	136.81	122.69
1	P	395	GLY	C-N-CA	9.95	136.81	122.69
1	H	3	PHE	N-CA-C	9.68	123.02	110.53
1	K	158	ILE	CB-CA-C	9.44	126.77	111.29
1	L	235	LYS	CB-CA-C	-9.34	95.28	110.79
1	G	3	PHE	N-CA-C	9.16	122.35	110.53
1	M	3	PHE	N-CA-C	9.02	122.72	110.55
1	D	402	ARG	CG-CD-NE	8.93	131.64	112.00
1	D	3	PHE	N-CA-C	8.63	122.20	110.55
1	M	402	ARG	CG-CD-NE	8.58	130.87	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	3	PHE	N-CA-C	8.45	121.96	110.55
1	K	3	PHE	N-CA-C	8.11	121.49	110.55
1	N	3	PHE	N-CA-C	7.94	121.27	110.55
1	O	48	GLU	CG-CD-OE2	7.85	136.45	118.40
1	M	48	GLU	CG-CD-OE2	7.84	136.44	118.40
1	M	335	LYS	CA-C-O	-7.76	113.11	121.88
1	N	335	LYS	CA-C-O	-7.64	113.24	121.88
1	B	270	GLY	N-CA-C	7.63	127.50	113.76
1	E	270	GLY	N-CA-C	7.52	127.30	113.76
1	I	283	GLN	CG-CD-NE2	-7.49	105.16	116.40
1	K	335	LYS	CA-C-O	-7.46	113.45	121.88
1	M	48	GLU	CG-CD-OE1	-7.46	101.24	118.40
1	O	283	GLN	CG-CD-NE2	-7.40	105.30	116.40
1	O	48	GLU	CG-CD-OE1	-7.36	101.47	118.40
1	N	229	LYS	CG-CD-CE	7.36	128.22	111.30
1	L	235	LYS	N-CA-C	7.34	119.29	111.28
1	O	335	LYS	CA-C-O	-7.30	113.63	121.88
1	G	270	GLY	N-CA-C	7.26	126.82	113.76
1	E	81	ALA	N-CA-C	7.25	120.05	111.71
1	O	402	ARG	CG-CD-NE	7.25	127.94	112.00
1	N	15	ASN	CB-CA-C	-7.24	95.61	110.38
1	D	270	GLY	N-CA-C	7.23	126.77	113.76
1	C	48	GLU	CB-CA-C	7.22	122.93	109.71
1	A	270	GLY	N-CA-C	7.21	126.73	113.76
1	F	270	GLY	N-CA-C	7.12	126.57	113.76
1	N	154	SER	N-CA-C	7.10	119.90	110.53
1	O	154	SER	N-CA-C	7.09	119.88	110.53
1	M	270	GLY	N-CA-C	7.08	126.51	113.76
1	P	270	GLY	N-CA-C	7.08	126.51	113.76
1	L	270	GLY	N-CA-C	7.08	126.50	113.76
1	O	270	GLY	N-CA-C	7.07	126.48	113.76
1	A	128	GLU	CG-CD-OE2	7.01	134.52	118.40
1	I	270	GLY	N-CA-C	6.99	126.35	113.76
1	J	335	LYS	CA-C-O	-6.97	114.00	121.88
1	I	154	SER	N-CA-C	6.94	119.70	110.53
1	N	55	ARG	NE-CZ-NH1	-6.94	114.56	121.50
1	I	81	ALA	N-CA-C	6.93	119.68	111.71
1	C	270	GLY	N-CA-C	6.89	126.16	113.76
1	O	398	LYS	CG-CD-CE	-6.88	95.47	111.30
1	M	81	ALA	N-CA-C	6.88	119.62	111.71
1	K	154	SER	N-CA-C	6.86	119.59	110.53
1	K	270	GLY	N-CA-C	6.86	126.10	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	253	ASP	N-CA-CB	6.85	118.02	110.35
1	N	270	GLY	N-CA-C	6.84	126.07	113.76
1	C	377	HIS	CA-C-N	6.83	126.34	119.24
1	C	377	HIS	C-N-CA	6.83	126.34	119.24
1	A	128	GLU	CG-CD-OE1	-6.83	102.70	118.40
1	F	377	HIS	CA-C-N	6.80	126.31	119.24
1	F	377	HIS	C-N-CA	6.80	126.31	119.24
1	L	154	SER	N-CA-C	6.80	119.50	110.53
1	J	270	GLY	N-CA-C	6.78	125.96	113.76
1	H	270	GLY	N-CA-C	6.76	125.93	113.76
1	N	81	ALA	N-CA-C	6.76	119.48	111.71
1	G	377	HIS	CA-C-N	6.75	126.26	119.24
1	G	377	HIS	C-N-CA	6.75	126.26	119.24
1	N	55	ARG	NE-CZ-NH2	6.75	125.28	119.20
1	C	81	ALA	N-CA-C	6.74	119.46	111.71
1	A	377	HIS	CA-C-N	6.68	126.19	119.24
1	A	377	HIS	C-N-CA	6.68	126.19	119.24
1	B	154	SER	N-CA-C	6.65	119.88	110.50
1	F	154	SER	N-CA-C	6.65	119.88	110.50
1	K	262	ILE	N-CA-C	6.63	116.65	110.42
1	H	377	HIS	CA-C-N	6.62	126.12	119.24
1	H	377	HIS	C-N-CA	6.62	126.12	119.24
1	G	154	SER	N-CA-C	6.61	119.83	110.50
1	O	81	ALA	N-CA-C	6.61	119.31	111.71
1	P	15	ASN	N-CA-C	6.60	123.64	113.28
1	M	154	SER	N-CA-C	6.57	119.20	110.53
1	H	81	ALA	N-CA-C	6.57	119.26	111.71
1	G	81	ALA	N-CA-C	6.55	119.25	111.71
1	P	81	ALA	N-CA-C	6.52	119.21	111.71
1	B	81	ALA	N-CA-C	6.52	119.21	111.71
1	K	81	ALA	N-CA-C	6.44	119.12	111.71
1	N	208	SER	N-CA-C	-6.44	104.19	111.14
1	C	154	SER	N-CA-C	6.42	119.56	110.50
1	D	154	SER	N-CA-C	6.42	119.55	110.50
1	E	377	HIS	CA-C-N	6.42	125.92	119.24
1	E	377	HIS	C-N-CA	6.42	125.92	119.24
1	I	334	ASP	N-CA-C	6.42	118.27	111.28
1	M	336	ASN	N-CA-C	-6.40	100.77	109.54
1	F	334	ASP	N-CA-C	6.40	118.25	111.28
1	P	154	SER	N-CA-C	6.38	118.95	110.53
1	E	154	SER	N-CA-C	6.36	119.47	110.50
1	E	208	SER	N-CA-C	-6.36	104.27	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	154	SER	N-CA-C	6.35	119.46	110.50
1	M	253	ASP	N-CA-CB	6.35	117.46	110.35
1	F	3	PHE	N-CA-C	6.35	118.72	110.53
1	J	81	ALA	N-CA-C	6.33	118.99	111.71
1	E	334	ASP	N-CA-C	6.31	118.15	111.28
1	G	208	SER	N-CA-C	-6.29	104.35	111.14
1	G	391	LEU	N-CA-CB	-6.26	100.92	110.12
1	D	208	SER	N-CA-C	-6.25	104.39	111.14
1	O	422	GLU	CB-CA-C	6.25	122.86	110.42
1	L	334	ASP	N-CA-C	6.25	118.09	111.28
1	H	274	ALA	CA-C-N	6.25	125.98	119.05
1	H	274	ALA	C-N-CA	6.25	125.98	119.05
1	D	81	ALA	N-CA-C	6.25	118.89	111.71
1	O	334	ASP	N-CA-C	6.23	118.07	111.28
1	J	154	SER	N-CA-C	6.22	119.28	110.50
1	K	307	ASN	CB-CG-ND2	6.22	125.72	116.40
1	M	208	SER	N-CA-C	-6.21	104.14	111.03
1	F	208	SER	N-CA-C	-6.20	104.15	111.03
1	L	81	ALA	N-CA-C	6.19	118.83	111.71
1	F	81	ALA	N-CA-C	6.18	118.82	111.71
1	G	262	ILE	N-CA-C	6.16	116.35	110.74
1	J	208	SER	N-CA-C	-6.13	104.52	111.14
1	C	262	ILE	N-CA-C	6.12	116.18	110.42
1	A	81	ALA	N-CA-C	6.11	118.74	111.71
1	B	208	SER	N-CA-C	-6.11	104.25	111.03
1	B	3	PHE	N-CA-C	6.10	118.40	110.53
1	K	334	ASP	N-CA-C	6.09	117.92	111.28
1	A	154	SER	N-CA-C	6.09	119.08	110.50
1	B	334	ASP	N-CA-C	6.09	117.91	111.28
1	F	262	ILE	N-CA-C	6.09	116.14	110.42
1	O	15	ASN	CA-C-N	6.08	133.16	121.54
1	O	15	ASN	C-N-CA	6.08	133.16	121.54
1	P	334	ASP	N-CA-C	6.08	117.91	111.28
1	O	262	ILE	N-CA-C	6.08	116.27	110.74
1	B	274	ALA	CA-C-N	6.05	125.76	119.05
1	B	274	ALA	C-N-CA	6.05	125.76	119.05
1	G	334	ASP	N-CA-C	6.05	117.87	111.28
1	C	208	SER	N-CA-C	-6.04	104.32	111.03
1	C	334	ASP	N-CA-C	6.03	117.85	111.28
1	J	262	ILE	N-CA-C	6.02	116.22	110.74
1	I	15	ASN	CA-C-N	6.01	133.01	121.54
1	I	15	ASN	C-N-CA	6.01	133.01	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	262	ILE	N-CA-C	6.00	116.20	110.74
1	J	334	ASP	N-CA-C	6.00	117.81	111.28
1	E	262	ILE	N-CA-C	5.99	116.05	110.42
1	H	334	ASP	N-CA-C	5.99	117.81	111.28
1	H	208	SER	N-CA-C	-5.98	104.39	111.03
1	B	377	HIS	CA-C-N	5.98	125.46	119.24
1	B	377	HIS	C-N-CA	5.98	125.46	119.24
1	P	14	TYR	CB-CA-C	5.97	121.44	112.31
1	D	377	HIS	CA-C-N	5.95	125.43	119.24
1	D	377	HIS	C-N-CA	5.95	125.43	119.24
1	L	262	ILE	N-CA-C	5.95	116.15	110.74
1	D	334	ASP	N-CA-C	5.94	117.75	111.28
1	K	208	SER	N-CA-C	-5.93	104.45	111.03
1	M	274	ALA	CA-C-N	5.92	125.63	119.05
1	M	274	ALA	C-N-CA	5.92	125.63	119.05
1	L	208	SER	N-CA-C	-5.92	104.46	111.03
1	N	262	ILE	N-CA-C	5.91	116.12	110.74
1	B	262	ILE	N-CA-C	5.91	116.12	110.74
1	H	182	THR	N-CA-C	5.90	118.19	111.11
1	M	334	ASP	N-CA-C	5.90	117.71	111.28
1	N	139	LYS	N-CA-C	5.89	117.70	111.28
1	A	262	ILE	N-CA-C	5.88	116.09	110.74
1	L	274	ALA	CA-C-N	5.87	125.57	119.05
1	L	274	ALA	C-N-CA	5.87	125.57	119.05
1	J	37	LEU	N-CA-C	5.84	118.40	111.33
1	O	37	LEU	N-CA-C	5.83	118.38	111.33
1	A	208	SER	N-CA-C	-5.83	104.56	111.03
1	O	182	THR	N-CA-C	5.83	118.10	111.11
1	L	402	ARG	CD-NE-CZ	-5.82	116.25	124.40
1	P	262	ILE	N-CA-C	5.80	116.02	110.74
1	B	134	LEU	N-CA-C	5.80	119.46	112.38
1	O	283	GLN	CG-CD-OE1	5.79	132.39	120.80
1	I	398	LYS	CG-CD-CE	5.78	124.59	111.30
1	L	37	LEU	N-CA-C	5.78	118.32	111.33
1	O	208	SER	N-CA-C	-5.77	104.62	111.03
1	K	134	LEU	N-CA-C	5.76	119.41	112.38
1	N	37	LEU	N-CA-C	5.76	118.30	111.33
1	O	163	ILE	N-CA-C	5.76	116.41	110.36
1	I	283	GLN	CG-CD-OE1	5.76	132.31	120.80
1	N	334	ASP	N-CA-C	5.75	117.55	111.28
1	H	134	LEU	N-CA-C	5.73	119.37	112.38
1	I	262	ILE	N-CA-C	5.72	115.94	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	274	ALA	CA-C-N	5.71	125.39	119.05
1	J	274	ALA	C-N-CA	5.71	125.39	119.05
1	I	163	ILE	N-CA-C	5.71	116.36	110.36
1	M	332	TYR	N-CA-C	5.70	120.51	113.50
1	N	182	THR	N-CA-C	5.69	117.93	111.11
1	K	54	SER	N-CA-C	5.68	119.31	112.38
1	P	163	ILE	N-CA-C	5.68	116.33	110.36
1	O	78	ILE	CA-CB-CG1	5.68	120.05	110.40
1	J	3	PHE	N-CA-C	5.67	117.84	110.53
1	J	134	LEU	N-CA-C	5.66	119.28	112.38
1	K	163	ILE	N-CA-C	5.64	116.29	110.36
1	I	332	TYR	N-CA-C	5.63	120.43	113.50
1	P	182	THR	N-CA-C	5.63	117.86	111.11
1	L	115	ILE	N-CA-C	5.63	115.82	110.53
1	N	163	ILE	N-CA-C	5.63	116.27	110.36
1	P	208	SER	N-CA-C	-5.62	105.07	111.14
1	D	134	LEU	N-CA-C	5.62	119.23	112.38
1	L	54	SER	N-CA-C	5.59	119.20	112.38
1	G	134	LEU	N-CA-C	5.59	119.20	112.38
1	C	54	SER	N-CA-C	5.58	119.19	112.38
1	C	182	THR	N-CA-C	5.58	117.81	111.11
1	N	15	ASN	CA-C-O	5.58	126.37	119.79
1	P	134	LEU	N-CA-C	5.57	119.18	112.38
1	C	163	ILE	N-CA-C	5.57	116.21	110.36
1	J	163	ILE	N-CA-C	5.57	116.21	110.36
1	E	157	GLN	CB-CG-CD	5.56	122.05	112.60
1	A	134	LEU	N-CA-C	5.56	119.16	112.38
1	E	182	THR	N-CA-C	5.54	117.76	111.11
1	O	54	SER	N-CA-C	5.54	119.13	112.38
1	P	54	SER	N-CA-C	5.54	119.13	112.38
1	N	274	ALA	CA-C-N	5.53	125.19	119.05
1	N	274	ALA	C-N-CA	5.53	125.19	119.05
1	O	134	LEU	N-CA-C	5.53	119.13	112.38
1	C	398	LYS	CA-CB-CG	-5.53	103.03	114.10
1	A	54	SER	N-CA-C	5.53	119.12	112.38
1	O	332	TYR	N-CA-C	5.53	120.30	113.50
1	L	134	LEU	N-CA-C	5.53	119.12	112.38
1	G	165	LYS	CG-CD-CE	5.52	124.00	111.30
1	D	15	ASN	N-CA-C	5.52	119.86	113.18
1	D	183	VAL	N-CA-C	5.51	116.29	110.72
1	A	318	PRO	N-CA-C	5.51	121.00	113.84
1	H	262	ILE	N-CA-C	5.51	115.75	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	194	HIS	N-CA-C	5.50	118.79	112.57
1	I	274	ALA	CA-C-N	5.50	125.15	119.05
1	I	274	ALA	C-N-CA	5.50	125.15	119.05
1	A	202	SER	N-CA-C	-5.47	97.57	107.75
1	B	318	PRO	N-CA-C	5.47	120.95	113.84
1	O	274	ALA	CA-C-N	5.47	125.12	119.05
1	O	274	ALA	C-N-CA	5.47	125.12	119.05
1	M	134	LEU	N-CA-C	5.46	119.05	112.38
1	A	183	VAL	N-CA-C	5.46	115.66	110.53
1	A	182	THR	N-CA-C	5.46	117.66	111.11
1	F	54	SER	N-CA-C	5.45	119.43	112.34
1	L	3	PHE	N-CA-C	5.45	117.91	110.55
1	F	183	VAL	N-CA-C	5.44	116.22	110.72
1	C	134	LEU	N-CA-C	5.44	119.02	112.38
1	P	29	ASN	N-CA-CB	-5.44	101.86	111.39
1	F	308	SER	CB-CA-C	5.44	119.18	110.09
1	M	402	ARG	CD-NE-CZ	5.44	132.01	124.40
1	N	332	TYR	N-CA-C	5.44	120.19	113.50
1	A	193	LYS	CA-CB-CG	5.43	124.97	114.10
1	J	115	ILE	N-CA-C	5.43	115.64	110.53
1	A	313	LYS	N-CA-C	5.43	120.01	113.17
1	L	182	THR	N-CA-C	5.42	117.62	111.11
1	E	332	TYR	N-CA-C	5.42	120.17	113.50
1	H	29	ASN	N-CA-CB	-5.42	101.90	111.39
1	G	318	PRO	N-CA-C	5.42	120.89	113.84
1	G	202	SER	N-CA-C	-5.41	97.69	107.75
1	M	163	ILE	N-CA-C	5.41	116.04	110.36
1	L	202	SER	N-CA-C	-5.40	97.70	107.75
1	H	193	LYS	CA-CB-CG	5.40	124.90	114.10
1	A	334	ASP	N-CA-C	5.39	117.91	111.71
1	B	202	SER	N-CA-C	-5.39	97.72	107.75
1	F	163	ILE	N-CA-C	5.39	116.02	110.36
1	J	182	THR	N-CA-C	5.39	117.58	111.11
1	D	14	TYR	CA-C-N	5.38	132.08	121.58
1	D	14	TYR	C-N-CA	5.38	132.08	121.58
1	E	313	LYS	N-CA-C	5.38	119.95	113.17
1	I	115	ILE	N-CA-C	5.38	115.59	110.53
1	D	182	THR	N-CA-C	5.38	117.56	111.11
1	E	134	LEU	N-CA-C	5.38	118.94	112.38
1	G	193	LYS	CA-CB-CG	5.38	124.85	114.10
1	K	182	THR	N-CA-C	5.37	117.55	111.11
1	L	235	LYS	N-CA-CB	-5.36	102.23	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	332	TYR	N-CA-C	5.36	120.09	113.50
1	M	54	SER	N-CA-C	5.36	118.92	112.38
1	N	54	SER	N-CA-C	5.36	118.92	112.38
1	L	163	ILE	N-CA-C	5.36	115.98	110.36
1	I	134	LEU	N-CA-C	5.35	118.91	112.38
1	C	332	TYR	N-CA-C	5.35	120.08	113.50
1	A	115	ILE	N-CA-C	5.34	115.55	110.53
1	H	163	ILE	N-CA-C	5.34	115.97	110.36
1	B	378	PRO	N-CA-C	5.34	122.43	113.78
1	D	274	ALA	CA-C-N	5.33	124.97	119.05
1	D	274	ALA	C-N-CA	5.33	124.97	119.05
1	G	54	SER	N-CA-C	5.33	118.89	112.38
1	B	313	LYS	N-CA-C	5.33	119.89	113.17
1	P	115	ILE	N-CA-C	5.33	115.54	110.53
1	H	183	VAL	N-CA-C	5.31	115.52	110.53
1	I	118	THR	N-CA-C	5.30	117.06	111.28
1	M	182	THR	N-CA-C	5.29	117.45	111.11
1	N	14	TYR	CA-C-N	5.29	129.67	120.68
1	N	14	TYR	C-N-CA	5.29	129.67	120.68
1	B	135	ASP	N-CA-C	-5.28	105.63	111.71
1	H	115	ILE	N-CA-C	5.28	115.49	110.53
1	J	332	TYR	N-CA-C	5.28	119.99	113.50
1	N	252	LEU	N-CA-C	5.28	118.82	109.96
1	C	183	VAL	N-CA-C	5.27	115.49	110.53
1	I	208	SER	N-CA-C	-5.27	105.17	111.03
1	K	29	ASN	N-CA-CB	-5.27	102.16	111.39
1	M	202	SER	N-CA-C	-5.27	97.95	107.75
1	H	54	SER	N-CA-C	5.26	118.80	112.38
1	F	274	ALA	CA-C-N	5.26	124.89	119.05
1	F	274	ALA	C-N-CA	5.26	124.89	119.05
1	A	163	ILE	N-CA-C	5.26	115.89	110.36
1	M	318	PRO	N-CA-C	5.26	120.68	113.84
1	D	115	ILE	N-CA-C	5.26	115.47	110.53
1	I	29	ASN	N-CA-CB	-5.25	102.19	111.39
1	E	29	ASN	N-CA-CB	-5.25	102.20	111.39
1	I	54	SER	N-CA-C	5.24	118.78	112.38
1	N	134	LEU	N-CA-C	5.24	118.78	112.38
1	O	3	PHE	N-CA-C	5.24	117.62	110.55
1	A	135	ASP	N-CA-C	-5.24	105.69	111.71
1	M	115	ILE	N-CA-C	5.23	115.45	110.53
1	L	332	TYR	N-CA-C	5.23	119.93	113.50
1	C	115	ILE	N-CA-C	5.22	115.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	THR	N-CA-C	5.22	116.97	111.28
1	C	29	ASN	N-CA-CB	-5.21	102.27	111.39
1	J	395	GLY	N-CA-C	5.21	125.54	113.18
1	F	134	LEU	N-CA-C	5.21	118.73	112.38
1	N	29	ASN	N-CA-CB	-5.21	102.28	111.39
1	E	318	PRO	N-CA-C	5.20	120.61	113.84
1	D	28	GLN	N-CA-C	-5.20	99.47	108.52
1	G	332	TYR	N-CA-C	5.20	119.89	113.50
1	O	118	THR	N-CA-C	5.19	116.94	111.28
1	N	313	LYS	N-CA-C	5.19	119.71	113.17
1	D	313	LYS	N-CA-C	5.18	119.70	113.17
1	C	135	ASP	N-CA-C	-5.18	105.75	111.71
1	J	313	LYS	N-CA-C	5.18	119.69	113.17
1	G	182	THR	N-CA-C	5.17	117.31	111.11
1	K	332	TYR	N-CA-C	5.17	119.86	113.50
1	F	182	THR	N-CA-C	5.17	117.31	111.11
1	G	400	THR	N-CA-C	5.16	117.70	109.96
1	F	332	TYR	N-CA-C	5.16	119.85	113.50
1	G	362	PHE	N-CA-C	-5.16	102.00	109.59
1	E	54	SER	N-CA-C	5.16	118.67	112.38
1	M	396	ILE	N-CA-CB	-5.15	103.78	112.44
1	A	29	ASN	N-CA-CB	-5.15	102.38	111.39
1	B	54	SER	N-CA-C	5.14	118.66	112.38
1	E	163	ILE	N-CA-C	5.14	115.75	110.36
1	F	202	SER	N-CA-C	-5.14	98.20	107.75
1	D	262	ILE	N-CA-C	5.13	115.41	110.74
1	J	183	VAL	N-CA-C	5.12	115.34	110.53
1	H	118	THR	N-CA-C	5.12	116.86	111.28
1	C	398	LYS	CG-CD-CE	5.11	123.06	111.30
1	O	313	LYS	N-CA-C	5.11	119.61	113.17
1	E	141	ILE	N-CA-C	5.11	116.16	109.21
1	L	135	ASP	N-CA-C	-5.11	105.83	111.71
1	J	135	ASP	N-CA-C	-5.11	105.84	111.71
1	A	118	THR	N-CA-C	5.10	116.84	111.28
1	C	202	SER	N-CA-C	-5.10	98.26	107.75
1	I	47	GLN	N-CA-C	-5.10	105.63	111.14
1	H	135	ASP	N-CA-C	-5.10	105.85	111.71
1	P	313	LYS	N-CA-C	5.10	119.59	113.17
1	I	313	LYS	N-CA-C	5.10	119.59	113.17
1	D	402	ARG	CD-NE-CZ	5.09	131.53	124.40
1	B	118	THR	N-CA-C	5.09	116.83	111.28
1	F	378	PRO	N-CA-C	5.09	122.03	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	54	SER	N-CA-C	5.09	118.59	112.38
1	D	202	SER	N-CA-C	-5.08	98.29	107.75
1	M	29	ASN	N-CA-CB	-5.08	102.49	111.39
1	D	163	ILE	N-CA-C	5.08	115.70	110.36
1	F	313	LYS	N-CA-C	5.08	119.58	113.17
1	O	318	PRO	N-CA-C	5.08	120.45	113.84
1	P	332	TYR	N-CA-C	5.08	119.75	113.50
1	C	362	PHE	N-CA-C	-5.08	102.13	109.59
1	K	115	ILE	N-CA-C	5.07	115.30	110.53
1	D	378	PRO	N-CA-C	5.07	122.00	113.78
1	G	378	PRO	N-CA-C	5.07	121.99	113.78
1	H	313	LYS	N-CA-C	5.07	119.56	113.17
1	P	202	SER	N-CA-C	-5.06	98.34	107.75
1	C	274	ALA	CA-C-N	5.06	124.67	119.05
1	C	274	ALA	C-N-CA	5.06	124.67	119.05
1	L	398	LYS	CD-CE-NZ	5.06	128.09	111.90
1	N	15	ASN	N-CA-CB	-5.06	102.51	110.30
1	A	332	TYR	N-CA-C	5.05	119.72	113.50
1	B	182	THR	N-CA-C	5.05	117.17	111.11
1	J	29	ASN	N-CA-CB	-5.05	102.55	111.39
1	L	118	THR	N-CA-C	5.05	116.78	111.28
1	B	28	GLN	N-CA-C	-5.04	99.75	108.52
1	K	313	LYS	N-CA-C	5.04	119.52	113.17
1	I	135	ASP	N-CA-C	-5.04	105.92	111.71
1	B	163	ILE	N-CA-C	5.03	115.65	110.36
1	L	29	ASN	N-CA-CB	-5.03	102.58	111.39
1	D	135	ASP	N-CA-C	-5.03	105.92	111.71
1	P	4	ASN	CB-CG-ND2	5.03	123.95	116.40
1	M	135	ASP	N-CA-C	-5.03	105.92	111.71
1	M	313	LYS	N-CA-C	5.03	119.51	113.17
1	G	183	VAL	N-CA-C	5.03	115.80	110.72
1	A	4	ASN	CB-CG-ND2	5.03	123.94	116.40
1	P	291	ARG	N-CA-C	5.02	116.44	111.07
1	I	291	ARG	N-CA-C	5.02	116.44	111.07
1	E	378	PRO	N-CA-C	5.02	121.91	113.78
1	D	118	THR	N-CA-C	5.01	116.74	111.28
1	F	400	THR	N-CA-C	5.01	117.47	109.96
1	P	141	ILE	N-CA-C	5.01	116.02	109.21
1	K	235	LYS	CD-CE-NZ	-5.01	95.88	111.90
1	I	182	THR	N-CA-C	5.00	117.11	111.11
1	L	4	ASN	CB-CG-ND2	5.00	123.91	116.40
1	A	141	ILE	N-CA-C	5.00	116.01	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	TYR	N-CA-C	5.00	119.65	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	353	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	3335	0	3298	37	0
1	B	3329	0	3295	54	0
1	C	3311	0	3278	30	0
1	D	3327	0	3296	41	0
1	E	3320	0	3282	34	0
1	F	3318	0	3284	39	0
1	G	3326	0	3289	44	0
1	H	3326	0	3294	61	0
1	I	3166	0	3145	43	0
1	J	3195	0	3169	45	0
1	K	3184	0	3159	55	0
1	L	3211	0	3182	62	0
1	M	3197	0	3174	39	0
1	N	3188	0	3159	48	0
1	O	3189	0	3161	40	0
1	P	3252	0	3225	41	0
2	A	5	0	5	0	0
2	D	5	0	5	0	0
3	A	6	0	8	1	0
3	B	12	0	16	1	0
3	O	6	0	8	0	0
4	C	5	0	0	0	0
5	A	194	0	0	8	0
5	B	220	0	0	20	0
5	C	212	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	195	0	0	11	0
5	E	217	0	0	11	0
5	F	197	0	0	9	0
5	G	207	0	0	10	0
5	H	191	0	0	11	0
5	I	195	0	0	9	0
5	J	192	0	0	12	0
5	K	181	0	0	20	0
5	L	159	0	0	5	0
5	M	166	0	0	7	0
5	N	168	0	0	5	0
5	O	193	0	0	15	0
5	P	187	0	0	7	0
All	All	55287	0	51732	646	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 6.

All (646) 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:J:84:MSE:HE1	1:J:110:GLY:C	1.70	1.16
1:K:158:ILE:CD1	1:K:318:PRO:HD3	1.79	1.11
1:H:235:LYS:CE	1:L:139:LYS:HE3	1.81	1.10
1:K:158:ILE:HD11	1:K:318:PRO:CD	1.81	1.09
1:N:84:MSE:HE3	1:N:205:LLP:H5'2	1.30	1.09
1:F:17:ASP:HB2	5:K:528:HOH:O	1.58	1.04
1:N:84:MSE:HA	1:N:84:MSE:HE2	1.37	1.03
1:L:419:GLN:O	1:L:423:SER:HB2	1.57	1.03
1:D:6:GLU:HG2	5:D:610:HOH:O	1.59	1.01
1:O:341:LEU:HD11	1:O:402:ARG:HD3	1.39	0.99
1:G:123:GLY:HA2	1:L:143:GLN:NE2	1.76	0.99
1:G:143:GLN:OE1	1:L:239:THR:HG22	1.63	0.98
1:H:235:LYS:HE2	1:L:139:LYS:HZ1	1.27	0.97
1:P:391:LEU:CD1	1:P:398:LYS:HG3	1.93	0.97
1:D:376:ILE:HD11	1:D:381:THR:HG21	1.47	0.96
1:E:376:ILE:HD11	1:E:381:THR:HG21	1.47	0.96
1:H:235:LYS:HE2	1:L:139:LYS:CE	2.00	0.92
1:H:235:LYS:HE2	1:L:139:LYS:NZ	1.84	0.92
1:I:341:LEU:HD13	1:I:368:LEU:HD13	1.49	0.91
1:H:240:PRO:HG3	5:H:566:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:376:ILE:HD11	1:H:381:THR:HG21	1.51	0.90
1:G:376:ILE:HD11	1:G:381:THR:HG21	1.52	0.90
1:B:376:ILE:HD11	1:B:381:THR:HG21	1.51	0.90
1:A:376:ILE:HD11	1:A:381:THR:HG21	1.53	0.90
1:F:376:ILE:HD11	1:F:381:THR:HG21	1.51	0.89
1:K:276:GLN:HG2	1:L:276:GLN:HG3	1.52	0.89
1:B:154:SER:OG	1:B:157:GLN:HG2	1.71	0.89
1:D:358[B]:LYS:HB2	1:D:358[B]:LYS:NZ	1.85	0.88
5:K:571[A]:HOH:O	1:L:37:LEU:HB2	1.74	0.87
1:E:381:THR:HG23	1:F:44:PHE:CE1	2.10	0.86
1:I:341:LEU:HD13	1:I:368:LEU:CD1	2.05	0.86
1:G:381:THR:HG23	1:H:44:PHE:CE1	2.11	0.85
1:M:5:LYS:HE3	1:M:71:VAL:O	1.76	0.85
1:L:5:LYS:HE3	1:L:71:VAL:O	1.76	0.85
1:H:235:LYS:CE	1:L:139:LYS:CE	2.53	0.85
1:B:381:THR:HG23	1:C:44:PHE:CE1	2.12	0.84
1:E:44:PHE:CE1	1:F:381:THR:HG23	2.13	0.84
1:H:235:LYS:HE2	1:L:139:LYS:HE3	1.56	0.84
1:M:276:GLN:HG3	1:N:276:GLN:HG2	1.57	0.84
1:N:84:MSE:HA	1:N:84:MSE:CE	2.09	0.82
1:A:44:PHE:CE1	1:D:381:THR:HG23	2.15	0.81
1:G:44:PHE:CE1	1:H:381:THR:HG23	2.16	0.81
1:K:156:PRO:HD3	5:K:523:HOH:O	1.80	0.81
1:M:45:ASN:HB2	5:M:547:HOH:O	1.79	0.81
1:A:381:THR:HG23	1:D:44:PHE:CE1	2.16	0.80
1:M:190:GLN:HG3	5:M:629:HOH:O	1.80	0.80
1:K:158:ILE:HD11	1:K:318:PRO:HD3	0.89	0.79
1:C:365:ALA:O	1:C:376:ILE:CG2	2.33	0.77
1:H:235:LYS:CD	1:L:139:LYS:HE3	2.15	0.76
1:O:248:ASN:O	1:O:251:THR:HG22	1.86	0.76
1:O:37:LEU:HD13	1:P:353:ARG:HG2	1.65	0.76
1:L:248:ASN:O	1:L:251:THR:HG22	1.87	0.75
1:B:154:SER:HG	1:B:157:GLN:HG2	1.51	0.75
1:K:353:ARG:HG2	1:L:37:LEU:HD13	1.69	0.75
1:N:248:ASN:O	1:N:251:THR:HG22	1.86	0.75
1:K:248:ASN:O	1:K:251:THR:HG22	1.87	0.75
1:M:353:ARG:HG2	1:N:37:LEU:HD13	1.67	0.75
1:K:232:ASP:HA	1:K:235:LYS:HE3	1.69	0.74
1:D:5:LYS:HE2	5:D:710:HOH:O	1.87	0.74
1:D:358[B]:LYS:HB2	1:D:358[B]:LYS:HZ2	1.52	0.73
1:H:235:LYS:NZ	1:L:139:LYS:HE3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:267:ARG:HD3	5:J:579:HOH:O	1.88	0.73
1:B:139:LYS:HE3	1:N:98:GLY:O	1.88	0.73
1:F:17:ASP:CB	5:K:528:HOH:O	2.22	0.73
1:L:336:ASN:N	5:L:556:HOH:O	2.20	0.73
1:F:105:ASN:ND2	5:F:651:HOH:O	2.22	0.72
1:P:378:PRO:HG3	5:P:548:HOH:O	1.90	0.72
1:H:232:ASP:O	1:H:235:LYS:NZ	2.21	0.72
1:M:38:ASP:OD1	1:N:353:ARG:NH1	2.22	0.72
1:I:353:ARG:HG2	1:J:37:LEU:HD13	1.72	0.71
1:K:17:ASP:HA	5:K:655:HOH:O	1.88	0.71
1:H:377:HIS:CD2	5:H:578:HOH:O	2.43	0.71
1:K:245:HIS:ND1	5:K:560:HOH:O	2.23	0.70
1:O:378:PRO:HG3	5:O:667:HOH:O	1.91	0.70
1:B:17:ASP:HB2	5:O:788:HOH:O	1.90	0.70
1:E:189:LEU:HD12	5:E:524:HOH:O	1.90	0.70
1:K:232:ASP:HA	1:K:235:LYS:CE	2.22	0.69
1:H:235:LYS:NZ	1:L:139:LYS:CE	2.56	0.69
1:J:272:SER:HB3	5:J:651:HOH:O	1.92	0.69
1:N:84:MSE:HE3	1:N:205:LLP:C5'	2.16	0.69
1:H:17:ASP:HB2	5:J:666:HOH:O	1.91	0.69
1:J:156:PRO:O	1:J:158:ILE:HD12	1.93	0.69
1:N:156:PRO:O	1:N:158:ILE:HD12	1.93	0.69
1:P:156:PRO:O	1:P:158:ILE:HD12	1.93	0.68
1:P:391:LEU:HD13	1:P:398:LYS:HG3	1.71	0.68
1:I:156:PRO:O	1:I:158:ILE:HD12	1.93	0.68
1:A:156:PRO:O	1:A:158:ILE:HD12	1.93	0.68
1:B:98:GLY:O	1:M:144:ASN:ND2	2.23	0.68
1:B:156:PRO:O	1:B:158:ILE:HD12	1.94	0.68
1:H:156:PRO:O	1:H:158:ILE:HD12	1.94	0.68
1:I:291:ARG:NH1	5:I:588:HOH:O	2.22	0.68
1:M:156:PRO:O	1:M:158:ILE:HD12	1.93	0.68
1:E:156:PRO:O	1:E:158:ILE:HD12	1.94	0.68
1:I:356:CYS:HB2	1:J:37:LEU:HD11	1.75	0.68
1:O:120:LYS:HD2	5:O:690:HOH:O	1.92	0.68
1:O:353:ARG:NH2	5:O:660:HOH:O	2.27	0.68
1:C:365:ALA:O	1:C:376:ILE:HG23	1.94	0.67
1:A:6:GLU:HG2	5:N:651:HOH:O	1.94	0.67
1:D:156:PRO:O	1:D:158:ILE:HD12	1.95	0.67
1:L:156:PRO:O	1:L:158:ILE:HD12	1.94	0.67
1:I:353:ARG:HA	1:J:37:LEU:CD1	2.24	0.67
1:J:335:LYS:HE3	5:J:652:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:685:HOH:O	1:I:17:ASP:HB2	1.93	0.67
1:G:156:PRO:O	1:G:158:ILE:HD12	1.95	0.67
1:C:156:PRO:O	1:C:158:ILE:HD12	1.95	0.67
1:F:421:ILE:C	1:F:423:SER:H	2.00	0.67
1:H:308:SER:HB2	5:H:552:HOH:O	1.94	0.67
1:M:356:CYS:HB2	1:N:37:LEU:HD11	1.77	0.67
1:F:156:PRO:O	1:F:158:ILE:HD12	1.95	0.67
1:E:417:LEU:O	1:E:421:ILE:HG23	1.95	0.66
1:N:342:LEU:HD12	1:N:342:LEU:C	2.20	0.66
1:N:103:TYR:CE2	5:N:537:HOH:O	2.48	0.66
1:F:17:ASP:CA	5:K:528:HOH:O	2.43	0.66
1:N:103:TYR:HE2	5:N:537:HOH:O	1.78	0.66
1:H:235:LYS:CE	1:L:139:LYS:NZ	2.59	0.66
1:O:253:ASP:HB2	5:O:613:HOH:O	1.95	0.66
1:B:342:LEU:HD12	1:B:342:LEU:C	2.21	0.66
5:D:766:HOH:O	1:N:17:ASP:HB2	1.94	0.66
1:A:382:THR:HG22	3:A:502:GOL:O3	1.96	0.65
1:L:342:LEU:HD12	1:L:342:LEU:C	2.20	0.65
1:P:391:LEU:HD11	1:P:398:LYS:HG3	1.78	0.65
1:F:393:LYS:NZ	5:F:623:HOH:O	2.24	0.65
1:I:164:GLU:HG2	5:I:568:HOH:O	1.95	0.65
1:P:342:LEU:HD12	1:P:342:LEU:C	2.22	0.65
1:C:331:LYS:NZ	5:C:763:HOH:O	2.29	0.65
1:B:355:ILE:CD1	1:B:421:ILE:HG22	2.27	0.65
1:D:17:ASP:HB2	5:D:783:HOH:O	1.95	0.65
1:F:342:LEU:C	1:F:342:LEU:HD12	2.22	0.65
1:K:357:ASP:HB3	5:K:638:HOH:O	1.96	0.65
1:O:37:LEU:HD11	1:P:356:CYS:HB2	1.78	0.65
1:J:342:LEU:C	1:J:342:LEU:HD12	2.22	0.64
1:H:385:GLN:HG3	5:H:635:HOH:O	1.97	0.64
1:N:229:LYS:HE3	1:N:250:ASN:O	1.97	0.64
1:K:342:LEU:C	1:K:342:LEU:HD12	2.22	0.64
1:C:376:ILE:HD12	1:C:378:PRO:HD3	1.78	0.64
1:D:342:LEU:HD12	1:D:342:LEU:C	2.23	0.64
1:H:235:LYS:HD3	1:L:139:LYS:HE3	1.78	0.64
1:I:342:LEU:HD12	1:I:342:LEU:C	2.22	0.64
5:B:648:HOH:O	1:G:418:LYS:HE2	1.97	0.64
1:G:45:ASN:ND2	5:G:682:HOH:O	2.30	0.64
1:M:353:ARG:HA	1:N:37:LEU:CD1	2.28	0.64
1:G:342:LEU:HD12	1:G:342:LEU:C	2.23	0.64
1:B:106:LYS:HB3	1:B:157:GLN:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LEU:C	1:C:342:LEU:HD12	2.24	0.63
1:P:402[A]:ARG:HD3	5:P:548:HOH:O	1.98	0.63
1:M:342:LEU:C	1:M:342:LEU:HD12	2.23	0.63
1:K:334:ASP:C	1:K:335:LYS:O	2.29	0.62
1:O:322:SER:HB2	5:O:711:HOH:O	1.98	0.62
1:O:342:LEU:C	1:O:342:LEU:HD12	2.23	0.62
1:E:342:LEU:C	1:E:342:LEU:HD12	2.24	0.62
1:H:342:LEU:C	1:H:342:LEU:HD12	2.25	0.62
1:E:6:GLU:HG2	5:E:671:HOH:O	1.98	0.62
1:O:37:LEU:CD1	1:P:353:ARG:HA	2.30	0.62
5:B:814:HOH:O	1:O:17:ASP:HB2	1.97	0.62
1:J:84:MSE:HE1	1:J:110:GLY:CA	2.28	0.62
1:A:342:LEU:C	1:A:342:LEU:HD12	2.25	0.62
1:D:240:PRO:HG3	5:D:776:HOH:O	1.99	0.62
1:P:402[B]:ARG:HG2	1:P:402[B]:ARG:HH21	1.65	0.62
1:I:341:LEU:CD1	1:I:368:LEU:HD13	2.26	0.61
1:D:358[B]:LYS:HB2	1:D:358[B]:LYS:HZ3	1.65	0.61
1:N:334:ASP:C	1:N:335:LYS:O	2.31	0.61
1:J:334:ASP:C	1:J:335:LYS:O	2.32	0.61
1:K:356:CYS:HB2	1:L:37:LEU:HD11	1.81	0.61
1:K:353:ARG:HA	1:L:37:LEU:CD1	2.31	0.61
1:F:17:ASP:HA	5:K:528:HOH:O	2.01	0.61
1:D:358[A]:LYS:HG2	1:D:420:ALA:HA	1.83	0.60
1:F:105:ASN:HD22	1:F:105:ASN:H	1.47	0.60
1:J:84:MSE:HE1	1:J:110:GLY:O	1.99	0.60
1:O:334:ASP:C	1:O:335:LYS:O	2.30	0.60
1:B:402:ARG:NH2	5:B:667:HOH:O	2.30	0.60
1:I:38:ASP:OD1	1:J:353:ARG:NH2	2.30	0.60
1:E:157:GLN:HB2	5:E:540[B]:HOH:O	2.01	0.60
1:K:157:GLN:O	1:K:158:ILE:HG23	2.01	0.60
1:K:158:ILE:HD13	1:K:317:TYR:HA	1.84	0.59
1:K:353:ARG:NH2	5:K:571[A]:HOH:O	2.34	0.59
1:A:158:ILE:HG21	1:A:318:PRO:HD3	1.84	0.59
1:P:391:LEU:CD1	1:P:398:LYS:CG	2.76	0.59
1:M:334:ASP:C	1:M:335:LYS:O	2.30	0.59
1:H:158:ILE:HG21	1:H:318:PRO:HD3	1.86	0.58
1:I:353:ARG:NH2	5:I:569:HOH:O	2.37	0.58
1:G:158:ILE:HG21	1:G:318:PRO:HD3	1.85	0.58
1:O:402:ARG:NH1	5:O:663:HOH:O	2.37	0.57
1:E:146:LYS:HE3	5:E:528:HOH:O	2.04	0.57
1:K:422:GLU:O	1:K:423:SER:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:38:ASP:OD1	1:L:353:ARG:NH2	2.32	0.57
1:M:158:ILE:HG21	1:M:318:PRO:HD3	1.86	0.57
1:M:341:LEU:HD11	1:M:402:ARG:HD2	1.86	0.57
1:O:116:SER:O	1:O:120:LYS:NZ	2.31	0.57
1:I:248:ASN:N	5:I:561:HOH:O	2.36	0.57
1:P:158:ILE:HG21	1:P:318:PRO:HD3	1.87	0.57
1:B:158:ILE:HG21	1:B:318:PRO:HD3	1.86	0.57
1:B:355:ILE:HD13	1:B:421:ILE:HG22	1.87	0.56
1:E:158:ILE:HG21	1:E:318:PRO:HD3	1.86	0.56
1:O:151:GLU:HG2	1:O:180:ASP:HB3	1.88	0.56
1:F:158:ILE:HG21	1:F:318:PRO:HD3	1.87	0.56
1:H:100:ASN:ND2	1:H:145:THR:OG1	2.34	0.56
1:I:158:ILE:HG21	1:I:318:PRO:HD3	1.86	0.56
1:K:158:ILE:CD1	1:K:317:TYR:HA	2.35	0.56
1:G:151:GLU:HG2	1:G:180:ASP:HB3	1.88	0.56
1:K:5:LYS:HE3	1:K:190:GLN:HE21	1.71	0.56
1:L:419:GLN:O	1:L:423:SER:CB	2.43	0.56
1:B:151:GLU:HG2	1:B:180:ASP:HB3	1.88	0.56
1:D:151:GLU:HG2	1:D:180:ASP:HB3	1.88	0.56
1:L:158:ILE:HG21	1:L:318:PRO:HD3	1.86	0.56
1:N:151:GLU:HG2	1:N:180:ASP:HB3	1.88	0.56
1:N:368:LEU:HD23	1:N:402:ARG:HH12	1.71	0.56
1:C:151:GLU:HG2	1:C:180:ASP:HB3	1.88	0.56
1:D:158:ILE:HG21	1:D:318:PRO:HD3	1.88	0.56
1:B:143:GLN:NE2	5:B:800[A]:HOH:O	2.39	0.56
1:I:151:GLU:HG2	1:I:180:ASP:HB3	1.88	0.56
1:P:5:LYS:HE3	1:P:186:PRO:O	2.06	0.56
1:C:158:ILE:HG21	1:C:318:PRO:HD3	1.88	0.56
1:G:240:PRO:HG3	5:G:662:HOH:O	2.06	0.56
1:J:84:MSE:CE	1:J:110:GLY:C	2.63	0.56
1:K:151:GLU:HG2	1:K:180:ASP:HB3	1.88	0.56
1:D:341:LEU:HD11	1:D:402:ARG:HD2	1.88	0.55
1:F:174:LYS:HD2	5:F:533:HOH:O	2.06	0.55
1:A:17:ASP:HB2	5:M:661:HOH:O	2.06	0.55
1:F:151:GLU:HG2	1:F:180:ASP:HB3	1.88	0.55
1:J:151:GLU:HG2	1:J:180:ASP:HB3	1.89	0.55
1:C:157:GLN:HG2	1:C:157:GLN:O	2.05	0.55
1:N:158:ILE:HG21	1:N:318:PRO:HD3	1.88	0.55
1:G:157:GLN:O	1:G:157:GLN:HG2	2.06	0.55
1:L:151:GLU:HG2	1:L:180:ASP:HB3	1.89	0.55
1:P:127:ARG:HA	5:P:632:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:O	1:A:157:GLN:HG2	2.05	0.55
1:H:157:GLN:HG2	1:H:157:GLN:O	2.05	0.55
1:J:158:ILE:HG21	1:J:318:PRO:HD3	1.89	0.55
1:D:358[B]:LYS:O	1:D:358[B]:LYS:HG3	2.06	0.55
1:M:151:GLU:HG2	1:M:180:ASP:HB3	1.89	0.55
1:P:391:LEU:HD11	1:P:398:LYS:CG	2.36	0.55
1:H:151:GLU:HG2	1:H:180:ASP:HB3	1.89	0.55
1:G:123:GLY:HA2	1:L:143:GLN:HE21	1.65	0.55
1:G:123:GLY:CA	1:L:143:GLN:NE2	2.62	0.55
1:K:351:HIS:CD2	1:K:354:ARG:HH21	2.25	0.55
1:F:157:GLN:O	1:F:157:GLN:HG2	2.06	0.55
1:H:105:ASN:HD22	1:H:393:LYS:HG3	1.72	0.55
1:D:157:GLN:O	1:D:157:GLN:HG2	2.05	0.55
1:E:381:THR:HG23	1:F:44:PHE:CD1	2.42	0.55
1:H:355:ILE:CD1	1:H:421[B]:ILE:HG22	2.36	0.55
1:I:190:GLN:HG2	5:I:654:HOH:O	2.07	0.55
1:P:4:ASN:HA	5:P:561:HOH:O	2.07	0.55
1:B:230:ASN:HA	5:B:650[A]:HOH:O	2.06	0.54
5:C:806:HOH:O	1:P:17:ASP:HB2	2.07	0.54
1:F:157:GLN:C	1:F:158:ILE:HD12	2.32	0.54
1:H:358:LYS:HE2	1:H:423:SER:OXT	2.07	0.54
1:O:158:ILE:HD11	1:O:341:LEU:HG	1.88	0.54
1:E:151:GLU:HG2	1:E:180:ASP:HB3	1.90	0.54
1:N:84:MSE:CE	1:N:205:LLP:H6	2.37	0.54
1:P:151:GLU:HG2	1:P:180:ASP:HB3	1.90	0.54
1:P:336:ASN:HB2	5:P:547:HOH:O	2.07	0.54
1:A:5:LYS:HE2	5:A:732:HOH:O	2.07	0.54
1:A:151:GLU:HG2	1:A:180:ASP:HB3	1.90	0.54
1:C:260:ARG:HD2	5:C:741:HOH:O	2.07	0.54
1:O:158:ILE:HG21	1:O:318:PRO:HD3	1.89	0.54
1:P:358:LYS:HE2	1:P:423:SER:OXT	2.08	0.54
5:D:695:HOH:O	1:M:6:GLU:HG2	2.08	0.53
1:N:358:LYS:HE2	1:N:423:SER:OXT	2.08	0.53
1:A:157:GLN:C	1:A:158:ILE:HD12	2.33	0.53
1:D:157:GLN:C	1:D:158:ILE:HD12	2.33	0.53
1:G:157:GLN:C	1:G:158:ILE:HD12	2.33	0.53
1:N:84:MSE:HE3	1:N:205:LLP:H6	1.91	0.53
1:G:157:GLN:CB	5:G:504:HOH:O	2.55	0.53
1:K:267:ARG:HD3	5:K:533:HOH:O	2.08	0.53
1:H:235:LYS:HZ3	1:L:139:LYS:HE3	1.71	0.53
1:K:157:GLN:C	1:K:158:ILE:CG2	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:331:LYS:NZ	5:P:666:HOH:O	2.28	0.53
1:O:16:PHE:HB3	1:O:20:ARG:HA	1.90	0.53
1:L:358:LYS:HE2	1:L:423:SER:OXT	2.09	0.53
1:O:358:LYS:HE2	1:O:423:SER:OXT	2.09	0.53
1:H:157:GLN:C	1:H:158:ILE:HD12	2.34	0.52
1:H:235:LYS:CE	1:L:139:LYS:HZ1	2.09	0.52
1:K:222:LYS:HG2	5:K:631:HOH:O	2.08	0.52
1:C:157:GLN:C	1:C:158:ILE:HD12	2.34	0.52
1:G:323[B]:ASN:OD1	1:G:325:TYR:N	2.34	0.52
1:J:335:LYS:N	5:J:653:HOH:O	2.21	0.52
1:H:235:LYS:HZ3	1:L:139:LYS:CE	2.23	0.52
1:M:156:PRO:O	1:M:158:ILE:CD1	2.58	0.52
1:B:105:ASN:HD22	1:B:393:LYS:HG3	1.74	0.52
1:I:5:LYS:NZ	1:I:71:VAL:O	2.43	0.52
1:G:308:SER:HB2	5:G:543:HOH:O	2.10	0.52
1:A:12:GLY:C	5:A:761:HOH:O	2.53	0.51
1:I:156:PRO:O	1:I:158:ILE:CD1	2.59	0.51
1:J:84:MSE:CE	1:J:110:GLY:HA3	2.40	0.51
1:J:154:SER:HG	1:J:157:GLN:HB2	1.75	0.51
1:K:157:GLN:O	1:K:158:ILE:CG2	2.58	0.51
5:E:709:HOH:O	1:L:17:ASP:HB2	2.11	0.51
1:L:156:PRO:O	1:L:158:ILE:CD1	2.59	0.51
1:L:341:LEU:HD11	1:L:402:ARG:CD	2.40	0.51
1:F:158:ILE:HD12	1:F:158:ILE:N	2.26	0.51
1:A:105:ASN:HD22	1:A:393:LYS:HG3	1.75	0.51
1:E:376:ILE:CD1	1:E:381:THR:HG21	2.32	0.51
1:H:232:ASP:C	1:H:235:LYS:HZ2	2.13	0.51
1:N:229:LYS:CE	1:N:250:ASN:O	2.59	0.51
1:B:16:PHE:N	5:B:687:HOH:O	2.43	0.51
1:I:131:ILE:HD12	1:I:166:ILE:HD11	1.93	0.51
1:I:368:LEU:HD12	1:I:404:SER:OG	2.11	0.51
1:J:156:PRO:O	1:J:158:ILE:CD1	2.58	0.51
1:P:341:LEU:HD11	1:P:402[B]:ARG:HD2	1.93	0.51
5:E:702:HOH:O	1:F:267:ARG:HD3	2.11	0.51
1:G:156:PRO:O	1:G:158:ILE:CD1	2.59	0.51
1:I:49:LEU:HD12	1:I:49:LEU:N	2.26	0.51
1:J:297:GLN:HB3	5:J:598:HOH:O	2.10	0.51
1:M:131:ILE:HD12	1:M:166:ILE:HD11	1.93	0.51
1:M:156:PRO:HB3	1:M:402:ARG:HD3	1.92	0.51
1:H:15:ASN:H	1:H:15:ASN:HD22	1.58	0.50
1:H:143:GLN:HG2	1:L:135:ASP:CG	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:331:LYS:NZ	5:H:643:HOH:O	2.43	0.50
1:J:84:MSE:CE	1:J:110:GLY:CA	2.89	0.50
1:N:157:GLN:C	1:N:158:ILE:HD12	2.36	0.50
1:E:157:GLN:CB	5:E:540[B]:HOH:O	2.58	0.50
1:G:158:ILE:HD12	1:G:158:ILE:N	2.26	0.50
1:L:154:SER:HG	1:L:157:GLN:HB2	1.76	0.50
1:N:156:PRO:O	1:N:158:ILE:CD1	2.58	0.50
1:C:158:ILE:HD12	1:C:158:ILE:N	2.27	0.50
1:H:156:PRO:O	1:H:158:ILE:CD1	2.59	0.50
1:I:154:SER:OG	1:I:157:GLN:HB2	2.11	0.50
1:J:157:GLN:C	1:J:158:ILE:HD12	2.36	0.50
1:O:5:LYS:NZ	1:O:71:VAL:O	2.43	0.50
1:P:156:PRO:O	1:P:158:ILE:CD1	2.58	0.50
1:P:154:SER:HG	1:P:157:GLN:HB2	1.76	0.50
1:N:157:GLN:H	1:N:157:GLN:CD	2.19	0.50
1:I:15:ASN:OD1	1:I:15:ASN:C	2.53	0.50
1:J:154:SER:OG	1:J:157:GLN:HB2	2.12	0.50
1:O:12:GLY:HA2	5:O:701:HOH:O	2.11	0.50
1:D:376:ILE:CD1	1:D:381:THR:HG21	2.32	0.50
1:E:105:ASN:HD22	1:E:393:LYS:HG3	1.76	0.50
1:H:15:ASN:ND2	5:H:622:HOH:O	2.24	0.50
1:O:331:LYS:NZ	5:O:738:HOH:O	2.44	0.50
1:P:154:SER:OG	1:P:157:GLN:HB2	2.12	0.50
1:B:5:LYS:NZ	1:B:71:VAL:O	2.43	0.50
1:B:139:LYS:HE3	1:N:98:GLY:CA	2.42	0.50
1:H:355:ILE:HD13	1:H:421[B]:ILE:HG22	1.92	0.50
1:I:5:LYS:HE3	1:I:190:GLN:CD	2.37	0.50
1:M:154:SER:OG	1:M:157:GLN:HB2	2.12	0.50
1:B:131:ILE:HD12	1:B:166:ILE:HD11	1.94	0.49
1:D:156:PRO:HB3	1:D:402:ARG:HD3	1.94	0.49
1:H:267:ARG:HD3	5:H:520:HOH:O	2.11	0.49
1:K:154:SER:OG	1:K:157:GLN:HB2	2.12	0.49
1:C:183:VAL:CG2	5:C:745:HOH:O	2.59	0.49
1:D:156:PRO:O	1:D:158:ILE:CD1	2.59	0.49
1:F:100:ASN:ND2	1:F:145:THR:OG1	2.34	0.49
1:K:294:LYS:HD3	5:K:630:HOH:O	2.11	0.49
1:L:157:GLN:C	1:L:158:ILE:HD12	2.36	0.49
1:O:154:SER:OG	1:O:157:GLN:HB2	2.12	0.49
1:D:14:TYR:HA	5:D:704:HOH:O	2.12	0.49
1:G:49:LEU:HD12	1:G:49:LEU:N	2.27	0.49
1:J:98:GLY:C	5:J:603:HOH:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:154:SER:OG	1:N:157:GLN:HB2	2.12	0.49
1:A:323[B]:ASN:OD1	1:A:325:TYR:N	2.37	0.49
1:E:5:LYS:NZ	1:E:71:VAL:O	2.44	0.49
1:D:158:ILE:HD12	1:D:158:ILE:N	2.28	0.49
1:L:154:SER:OG	1:L:157:GLN:HB2	2.12	0.49
1:L:157:GLN:H	1:L:157:GLN:CD	2.20	0.49
1:N:156:PRO:HB3	1:N:402:ARG:HD3	1.94	0.49
1:A:245:HIS:NE2	1:D:384:SER:O	2.43	0.49
1:J:157:GLN:H	1:J:157:GLN:CD	2.20	0.49
1:O:418:LYS:HD3	5:O:685:HOH:O	2.11	0.49
1:B:157:GLN:O	1:B:316:ASN:OD1	2.31	0.49
1:H:158:ILE:HD12	1:H:158:ILE:N	2.28	0.49
1:J:6:GLU:CD	5:J:547:HOH:O	2.55	0.49
1:C:156:PRO:O	1:C:158:ILE:CD1	2.60	0.49
1:C:387:SER:HB2	5:C:683:HOH:O	2.12	0.49
1:K:157:GLN:H	1:K:157:GLN:CD	2.20	0.49
1:M:152:SER:OG	5:M:626:HOH:O	2.20	0.49
1:I:341:LEU:HD13	1:I:368:LEU:HD11	1.92	0.49
1:A:158:ILE:HD12	1:A:158:ILE:N	2.28	0.49
1:D:49:LEU:N	1:D:49:LEU:HD12	2.26	0.49
1:E:157:GLN:HG3	1:E:394:ALA:O	2.13	0.49
1:F:156:PRO:O	1:F:158:ILE:CD1	2.60	0.49
1:I:157:GLN:C	1:I:158:ILE:HD12	2.37	0.49
1:I:205:LLP:OP4	1:I:205:LLP:H4'1	2.12	0.49
1:L:24:VAL:HG21	1:L:282[B]:LEU:HD21	1.93	0.49
1:O:157:GLN:H	1:O:157:GLN:CD	2.20	0.49
1:A:384:SER:O	1:D:245:HIS:NE2	2.42	0.48
1:B:49:LEU:HD12	1:B:49:LEU:N	2.28	0.48
1:K:336:ASN:HB2	5:K:675:HOH:O	2.12	0.48
1:E:49:LEU:HD12	1:E:49:LEU:N	2.28	0.48
1:G:384:SER:O	1:H:245:HIS:NE2	2.43	0.48
1:L:205:LLP:OP4	1:L:205:LLP:H4'1	2.12	0.48
1:B:381:THR:HG23	1:C:44:PHE:CD1	2.49	0.48
1:I:16:PHE:HB3	1:I:20:ARG:HA	1.95	0.48
1:P:157:GLN:C	1:P:158:ILE:HD12	2.38	0.48
1:B:235:LYS:HE2	5:B:768:HOH:O	2.12	0.48
1:E:376:ILE:HD11	1:E:381:THR:CG2	2.33	0.48
1:F:5:LYS:NZ	1:F:71:VAL:O	2.43	0.48
1:H:138:GLU:HG3	5:H:646:HOH:O	2.13	0.48
1:M:154:SER:HG	1:M:159:ALA:H	1.61	0.48
1:M:157:GLN:C	1:M:158:ILE:HD12	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PHE:CD1	1:D:381:THR:HG23	2.47	0.48
1:F:100:ASN:OD1	1:F:144:ASN:C	2.56	0.48
1:M:131:ILE:CD1	1:M:166:ILE:HD11	2.44	0.48
1:D:5:LYS:NZ	1:D:71:VAL:O	2.42	0.48
1:G:36:ASN:ND2	5:G:570:HOH:O	2.46	0.48
1:G:127:ARG:HA	5:G:578:HOH:O	2.14	0.48
1:G:381:THR:HG23	1:H:44:PHE:CD1	2.49	0.48
1:A:156:PRO:O	1:A:158:ILE:CD1	2.58	0.48
1:O:336:ASN:HB3	5:O:731:HOH:O	2.14	0.48
1:C:5:LYS:NZ	1:C:71:VAL:O	2.43	0.48
1:I:294:LYS:HD3	5:I:618:HOH:O	2.14	0.48
1:J:368:LEU:C	1:J:368:LEU:HD12	2.39	0.48
1:L:251:THR:HG21	5:L:525:HOH:O	2.14	0.48
1:J:84:MSE:HE2	1:J:110:GLY:HA3	1.95	0.48
1:J:98:GLY:CA	5:J:603:HOH:O	2.62	0.48
1:I:131:ILE:CD1	1:I:166:ILE:HD11	2.44	0.47
1:P:157:GLN:H	1:P:157:GLN:CD	2.22	0.47
1:B:156:PRO:O	1:B:158:ILE:CD1	2.59	0.47
1:I:157:GLN:H	1:I:157:GLN:CD	2.22	0.47
1:P:205:LLP:HG2	1:P:368:LEU:HG	1.95	0.47
1:I:38:ASP:CG	1:J:353:ARG:HH22	2.19	0.47
1:O:205:LLP:HG2	1:O:368:LEU:HG	1.95	0.47
1:P:42:ALA:HB1	1:P:48:GLU:HG3	1.96	0.47
1:C:42:ALA:HB1	1:C:48:GLU:HG2	1.95	0.47
5:F:554:HOH:O	1:L:6:GLU:HG2	2.13	0.47
1:M:157:GLN:CD	1:M:157:GLN:H	2.22	0.47
1:A:6:GLU:CG	5:N:651:HOH:O	2.58	0.47
1:I:154:SER:HG	1:I:159:ALA:H	1.61	0.47
1:K:157:GLN:C	1:K:158:ILE:HG22	2.40	0.47
1:N:368:LEU:C	1:N:368:LEU:HD12	2.40	0.47
1:P:423:SER:HB3	5:P:558:HOH:O	2.15	0.47
1:E:156:PRO:O	1:E:158:ILE:CD1	2.59	0.47
1:H:5:LYS:NZ	1:H:71:VAL:O	2.43	0.47
1:O:78:ILE:CD1	1:O:262:ILE:HD11	2.44	0.47
1:F:104:SER:OG	1:F:131:ILE:CG1	2.63	0.47
1:G:143:GLN:OE1	1:L:239:THR:CG2	2.49	0.47
1:G:157:GLN:HB3	5:G:504:HOH:O	2.13	0.47
1:H:205:LLP:HG2	1:H:368:LEU:HG	1.96	0.47
1:J:5:LYS:NZ	1:J:71:VAL:O	2.43	0.47
1:K:422:GLU:O	1:K:423:SER:HB3	2.14	0.47
1:L:16:PHE:HB3	1:L:20:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:LYS:NZ	1:N:71:VAL:O	2.43	0.47
1:N:84:MSE:HE2	1:N:84:MSE:CA	2.26	0.47
1:A:205:LLP:HG2	1:A:368:LEU:HG	1.96	0.47
1:F:105:ASN:HD22	1:F:105:ASN:N	2.12	0.47
1:N:156:PRO:HB3	1:N:402:ARG:CD	2.45	0.47
1:F:421:ILE:C	1:F:423:SER:N	2.72	0.47
1:K:16:PHE:HB3	1:K:20:ARG:HA	1.97	0.47
1:A:242:PRO:HG2	5:D:720:HOH:O	2.15	0.46
1:G:205:LLP:HG2	1:G:368:LEU:HG	1.96	0.46
1:A:162:ASP:OD2	5:A:746:HOH:O	2.20	0.46
1:B:205:LLP:HG2	1:B:368:LEU:HG	1.96	0.46
1:C:205:LLP:HG2	1:C:368:LEU:HG	1.96	0.46
1:J:205:LLP:HG2	1:J:368:LEU:HG	1.96	0.46
1:B:131:ILE:CD1	1:B:166:ILE:HD11	2.45	0.46
1:J:16:PHE:HB3	1:J:20:ARG:HA	1.98	0.46
1:K:368:LEU:HD12	1:K:368:LEU:C	2.41	0.46
1:N:154:SER:HG	1:N:159:ALA:H	1.63	0.46
1:E:205:LLP:HG2	1:E:368:LEU:HG	1.96	0.46
1:K:154:SER:HG	1:K:159:ALA:H	1.64	0.46
1:N:205:LLP:HG2	1:N:368:LEU:HG	1.96	0.46
1:P:368:LEU:HD12	1:P:368:LEU:C	2.41	0.46
1:A:49:LEU:N	1:A:49:LEU:HD12	2.31	0.46
1:J:164:GLU:HG2	5:J:680:HOH:O	2.15	0.46
1:K:5:LYS:NZ	1:K:71:VAL:O	2.45	0.46
1:M:205:LLP:HG2	1:M:368:LEU:HG	1.96	0.46
1:B:300:GLU:OE1	3:B:501[A]:GOL:O2	2.27	0.46
1:B:341:LEU:HD11	1:B:402:ARG:HD2	1.97	0.46
1:H:100:ASN:OD1	1:H:144:ASN:C	2.59	0.46
1:C:253:ASP:OD2	5:C:767:HOH:O	2.20	0.46
1:D:376:ILE:HD11	1:D:381:THR:CG2	2.33	0.46
1:F:205:LLP:HG2	1:F:368:LEU:HG	1.97	0.46
1:H:49:LEU:N	1:H:49:LEU:HD12	2.29	0.46
1:H:384:SER:OG	5:H:635:HOH:O	2.20	0.46
1:K:300:GLU:HG2	5:K:643:HOH:O	2.15	0.46
1:O:368:LEU:C	1:O:368:LEU:HD12	2.41	0.46
1:P:16:PHE:HB3	1:P:20:ARG:HA	1.98	0.46
1:D:16:PHE:HB3	1:D:20:ARG:HA	1.98	0.46
1:B:318:PRO:HG3	5:B:732:HOH:O	2.16	0.46
1:A:13:ALA:N	5:A:761:HOH:O	2.49	0.45
1:M:24:VAL:HG21	1:M:282[B]:LEU:HD21	1.98	0.45
5:K:556:HOH:O	1:L:276:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:5:LYS:HE2	1:M:190:GLN:HE21	1.82	0.45
1:D:6:GLU:CG	5:D:610:HOH:O	2.38	0.45
1:L:341:LEU:HD11	1:L:402:ARG:HD2	1.97	0.45
1:M:368:LEU:HD12	1:M:368:LEU:C	2.42	0.45
1:P:156:PRO:HB3	1:P:402[B]:ARG:HD3	1.98	0.45
1:G:391:LEU:HD23	1:G:392:GLN:OE1	2.16	0.45
1:H:190:GLN:HB2	1:H:193:LYS:HD3	1.99	0.45
1:K:351:HIS:HD2	1:K:354:ARG:HH21	1.63	0.45
1:G:190:GLN:HB2	1:G:193:LYS:HD3	1.99	0.45
1:K:205:LLP:HG2	1:K:368:LEU:HG	1.98	0.45
1:L:368:LEU:C	1:L:368:LEU:HD12	2.42	0.45
1:B:131:ILE:HD11	1:B:161:ALA:CB	2.47	0.45
1:C:381:THR:OG1	1:C:382:THR:N	2.47	0.45
1:A:190:GLN:HB2	1:A:193:LYS:HD3	1.99	0.45
1:A:232:ASP:HB2	5:A:763:HOH:O	2.17	0.45
1:B:409:ASN:HA	5:B:674:HOH:O	2.15	0.45
1:G:16:PHE:HB3	1:G:20:ARG:HA	1.98	0.45
1:K:18:THR:CB	5:K:528:HOH:O	2.65	0.45
1:B:378:PRO:HG3	5:B:652:HOH:O	2.17	0.45
1:E:384:SER:O	1:F:245:HIS:NE2	2.44	0.45
1:L:158:ILE:HD12	1:L:158:ILE:N	2.31	0.45
1:L:279:TRP:O	1:L:283:GLN:HG2	2.17	0.45
1:N:16:PHE:HB3	1:N:20:ARG:HA	1.99	0.45
1:D:269:LEU:HB3	5:D:752:HOH:O	2.17	0.44
1:K:152:SER:HB2	1:K:189:LEU:HD23	1.99	0.44
1:H:16:PHE:HB3	1:H:20:ARG:HA	1.99	0.44
1:B:125:GLU:HG3	1:B:126:ALA:N	2.33	0.44
1:C:308:SER:HB2	5:C:635:HOH:O	2.17	0.44
1:E:44:PHE:CD1	1:F:381:THR:HG23	2.51	0.44
1:B:380:SER:OG	5:B:719:HOH:O	2.21	0.44
1:O:154:SER:HG	1:O:159:ALA:H	1.63	0.44
1:B:47:GLN:CD	5:B:729:HOH:O	2.60	0.44
1:J:158:ILE:HD12	1:J:158:ILE:N	2.33	0.44
1:D:205:LLP:HG2	1:D:368:LEU:HG	1.99	0.44
1:E:157:GLN:C	1:E:158:ILE:HD12	2.43	0.44
1:M:16:PHE:HB3	1:M:20:ARG:HA	1.99	0.44
1:N:158:ILE:HD12	1:N:158:ILE:N	2.33	0.44
1:P:152:SER:HB2	1:P:189:LEU:HD23	2.00	0.44
1:A:381:THR:HG23	1:D:44:PHE:CD1	2.53	0.44
1:E:158:ILE:HD12	1:E:158:ILE:N	2.33	0.44
1:K:171:LYS:O	1:K:174:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:205:LLP:HG2	1:L:368:LEU:HG	1.99	0.44
5:B:674:HOH:O	1:P:6:GLU:HG2	2.18	0.44
1:I:52:ILE:HD12	5:I:666:HOH:O	2.18	0.44
1:M:45:ASN:CB	5:M:547:HOH:O	2.51	0.44
1:J:330:LYS:HD3	5:J:655:HOH:O	2.18	0.43
1:M:131:ILE:HD11	1:M:161:ALA:CB	2.48	0.43
1:O:189:LEU:HD12	5:O:689[A]:HOH:O	2.17	0.43
1:B:16:PHE:HB3	1:B:20:ARG:HA	1.99	0.43
5:B:627:HOH:O	1:G:418:LYS:HE3	2.16	0.43
1:E:213:ALA:HA	5:E:560:HOH:O	2.19	0.43
1:G:17:ASP:HB2	5:I:671:HOH:O	2.18	0.43
1:I:131:ILE:HD11	1:I:161:ALA:HB1	2.00	0.43
1:B:139:LYS:HE3	1:N:98:GLY:C	2.43	0.43
1:I:342:LEU:C	1:I:342:LEU:CD1	2.91	0.43
1:J:152:SER:HB2	1:J:189:LEU:HD23	2.01	0.43
1:M:131:ILE:HD11	1:M:161:ALA:HB1	2.00	0.43
1:A:157:GLN:CB	5:A:621:HOH:O	2.67	0.43
1:G:235:LYS:O	1:G:239:THR:HG22	2.18	0.43
1:I:131:ILE:HD11	1:I:161:ALA:CB	2.48	0.43
1:J:317:TYR:HA	1:J:318:PRO:HD3	1.93	0.43
1:O:348:ASP:HB2	5:O:632:HOH:O	2.18	0.43
1:B:16:PHE:C	5:B:687:HOH:O	2.62	0.43
1:I:330:LYS:HE3	5:I:630:HOH:O	2.17	0.43
1:M:158:ILE:HD12	1:M:158:ILE:N	2.33	0.43
1:J:279:TRP:O	1:J:283:GLN:HG2	2.18	0.43
1:M:174:LYS:HD2	5:M:612:HOH:O	2.18	0.43
1:N:152:SER:HB2	1:N:189:LEU:HD23	2.01	0.43
1:B:189:LEU:HD12	5:B:647:HOH:O	2.18	0.43
1:H:152:SER:HB2	1:H:189:LEU:HD23	2.01	0.43
1:P:391:LEU:O	1:P:396:ILE:O	2.37	0.43
5:F:694:HOH:O	1:K:17:ASP:HB2	2.18	0.43
1:G:76:PHE:HD1	5:G:698:HOH:O	2.02	0.43
1:I:353:ARG:HH22	1:J:38:ASP:CG	2.26	0.43
1:N:317:TYR:HA	1:N:318:PRO:HD3	1.93	0.43
1:F:157:GLN:CB	5:F:514:HOH:O	2.67	0.43
1:L:294:LYS:CE	5:L:544:HOH:O	2.67	0.43
1:L:323:ASN:ND2	5:L:596:HOH:O	2.41	0.43
1:O:248:ASN:O	1:O:251:THR:CG2	2.62	0.43
1:A:16:PHE:HB3	1:A:20:ARG:HA	2.00	0.42
1:B:352:ALA:HB3	5:B:737:HOH:O	2.18	0.42
1:F:57:SER:C	5:F:689:HOH:O	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:368:LEU:C	1:H:368:LEU:HD12	2.44	0.42
1:B:131:ILE:HD11	1:B:161:ALA:HB1	2.00	0.42
1:E:26:ILE:HB	1:L:26:ILE:HB	2.01	0.42
5:E:571:HOH:O	1:K:6:GLU:HB3	2.19	0.42
1:N:342:LEU:C	1:N:342:LEU:CD1	2.89	0.42
1:O:253:ASP:CB	5:O:613:HOH:O	2.63	0.42
1:D:157:GLN:HB2	5:D:658:HOH:O	2.18	0.42
1:G:368:LEU:C	1:G:368:LEU:HD12	2.44	0.42
1:P:317:TYR:HA	1:P:318:PRO:HD3	1.94	0.42
1:G:388:GLU:O	1:G:391:LEU:HB3	2.20	0.42
1:K:18:THR:HB	5:K:528:HOH:O	2.19	0.42
1:E:360:GLN:HG3	5:E:599:HOH:O	2.19	0.42
1:L:248:ASN:O	1:L:251:THR:CG2	2.62	0.42
1:M:279:TRP:O	1:M:283:GLN:HG2	2.19	0.42
1:B:26:ILE:HB	1:O:26:ILE:HB	2.02	0.42
1:D:368:LEU:HD12	1:D:368:LEU:C	2.44	0.42
1:K:113:THR:HB	5:L:566:HOH:O	2.19	0.42
1:L:152:SER:HB2	1:L:189:LEU:HD23	2.00	0.42
1:M:152:SER:HB2	1:M:189:LEU:HD23	2.01	0.42
1:N:279:TRP:O	1:N:283:GLN:HG2	2.19	0.42
1:A:279:TRP:O	1:A:283:GLN:HG2	2.20	0.42
1:G:279:TRP:O	1:G:283:GLN:HG2	2.20	0.42
1:O:402:ARG:CZ	5:O:663:HOH:O	2.67	0.42
1:B:152:SER:HB2	1:B:189:LEU:HD23	2.01	0.42
1:F:16:PHE:HB3	1:F:20:ARG:HA	2.01	0.42
1:I:353:ARG:NH2	1:J:38:ASP:OD1	2.39	0.42
1:P:342:LEU:C	1:P:342:LEU:CD1	2.90	0.42
1:B:336:ASN:HB3	5:B:700:HOH:O	2.18	0.42
1:F:152:SER:HB2	1:F:189:LEU:HD23	2.02	0.42
1:K:294:LYS:NZ	5:K:594:HOH:O	2.25	0.42
1:M:342:LEU:C	1:M:342:LEU:CD1	2.92	0.42
1:P:158:ILE:HD12	1:P:158:ILE:N	2.35	0.42
1:G:5:LYS:NZ	1:G:71:VAL:O	2.43	0.42
1:I:158:ILE:HD12	1:I:158:ILE:N	2.34	0.42
1:L:395:GLY:CA	1:L:396:ILE:HB	2.49	0.42
1:A:71:VAL:HG12	1:A:186:PRO:HB2	2.02	0.41
1:D:367:ASN:CG	1:D:368:LEU:N	2.78	0.41
1:O:402:ARG:HH11	1:O:402:ARG:HD2	1.58	0.41
1:C:376:ILE:HD12	1:C:376:ILE:C	2.45	0.41
1:G:44:PHE:CD1	1:H:381:THR:HG23	2.54	0.41
1:K:358:LYS:HE2	1:K:423:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ASN:O	1:D:15:ASN:CG	2.63	0.41
1:E:16:PHE:HB3	1:E:20:ARG:HA	2.01	0.41
1:J:17:ASP:N	5:J:610:HOH:O	2.53	0.41
1:O:342:LEU:C	1:O:342:LEU:CD1	2.92	0.41
1:B:368:LEU:C	1:B:368:LEU:HD12	2.45	0.41
1:E:279:TRP:O	1:E:283:GLN:HG2	2.20	0.41
1:F:387:SER:HB2	5:F:656:HOH:O	2.20	0.41
1:H:235:LYS:NZ	1:L:139:LYS:NZ	2.68	0.41
1:E:152:SER:HB2	1:E:189:LEU:HD23	2.02	0.41
1:F:294:LYS:HD3	5:F:603:HOH:O	2.21	0.41
1:G:381:THR:HG23	1:H:44:PHE:CZ	2.54	0.41
1:N:229:LYS:HE3	1:N:250:ASN:C	2.45	0.41
1:O:152:SER:HB2	1:O:189:LEU:HD23	2.01	0.41
1:M:294:LYS:HE3	5:M:575:HOH:O	2.20	0.41
1:B:106:LYS:HB3	1:B:157:GLN:CG	2.49	0.41
1:C:279:TRP:O	1:C:283:GLN:HG2	2.20	0.41
5:A:628:HOH:O	1:D:267:ARG:CZ	2.69	0.41
1:E:260:ARG:NH2	5:E:705:HOH:O	2.54	0.41
1:G:353:ARG:NH2	5:G:689:HOH:O	2.53	0.41
1:N:402:ARG:HD3	5:N:601:HOH:O	2.21	0.41
1:A:46[A]:LEU:HD12	1:A:46[A]:LEU:N	2.36	0.41
1:B:269:LEU:HB3	5:B:720:HOH:O	2.21	0.41
1:B:279:TRP:O	1:B:283:GLN:HG2	2.21	0.41
1:D:279:TRP:O	1:D:283:GLN:HG2	2.20	0.41
1:G:152:SER:HB2	1:G:189:LEU:HD23	2.02	0.41
1:H:157:GLN:CB	5:H:511:HOH:O	2.69	0.41
1:H:279:TRP:O	1:H:283:GLN:HG2	2.21	0.41
1:J:342:LEU:C	1:J:342:LEU:CD1	2.91	0.41
1:K:16:PHE:O	5:K:655:HOH:O	2.21	0.41
1:K:279:TRP:O	1:K:283:GLN:HG2	2.21	0.41
1:K:317:TYR:HA	1:K:318:PRO:HD3	1.95	0.41
1:K:342:LEU:C	1:K:342:LEU:CD1	2.91	0.41
1:N:155:ASN:OD1	1:N:155:ASN:C	2.63	0.41
1:B:73:GLY:C	5:B:693:HOH:O	2.63	0.41
1:B:158:ILE:HD12	1:B:158:ILE:N	2.36	0.41
1:C:16:PHE:HB3	1:C:20:ARG:HA	2.02	0.41
1:H:235:LYS:HZ3	1:L:139:LYS:CD	2.34	0.41
1:I:152:SER:HB2	1:I:189:LEU:HD23	2.02	0.41
1:C:152:SER:HB2	1:C:189:LEU:HD23	2.03	0.40
1:C:376:ILE:CD1	1:C:378:PRO:HG3	2.50	0.40
1:F:279:TRP:O	1:F:283:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ASN:CG	1:F:368:LEU:N	2.79	0.40
1:P:279:TRP:O	1:P:283:GLN:HG2	2.21	0.40
1:A:370:ASP:OD2	5:A:780:HOH:O	2.22	0.40
1:B:342:LEU:C	1:B:342:LEU:CD1	2.90	0.40
1:J:84:MSE:HE1	1:J:111:THR:N	2.27	0.40
1:A:152:SER:HB2	1:A:189:LEU:HD23	2.03	0.40
1:E:368:LEU:HD12	1:E:368:LEU:C	2.46	0.40
1:H:388:GLU:CG	5:H:625:HOH:O	2.69	0.40
1:N:84:MSE:CE	1:N:84:MSE:CA	2.91	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	423/424 (100%)	407 (96%)	16 (4%)	0	100	100
1	B	420/424 (99%)	406 (97%)	13 (3%)	1 (0%)	43	52
1	C	421/424 (99%)	406 (96%)	14 (3%)	1 (0%)	43	52
1	D	422/424 (100%)	408 (97%)	14 (3%)	0	100	100
1	E	421/424 (99%)	405 (96%)	16 (4%)	0	100	100
1	F	421/424 (99%)	404 (96%)	16 (4%)	1 (0%)	43	52
1	G	422/424 (100%)	406 (96%)	16 (4%)	0	100	100
1	H	422/424 (100%)	407 (96%)	15 (4%)	0	100	100
1	I	399/424 (94%)	386 (97%)	12 (3%)	1 (0%)	36	43
1	J	403/424 (95%)	389 (96%)	14 (4%)	0	100	100
1	K	401/424 (95%)	387 (96%)	13 (3%)	1 (0%)	43	52
1	L	405/424 (96%)	387 (96%)	17 (4%)	1 (0%)	43	52
1	M	403/424 (95%)	389 (96%)	13 (3%)	1 (0%)	43	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	401/424 (95%)	385 (96%)	16 (4%)	0	100	100
1	O	401/424 (95%)	385 (96%)	15 (4%)	1 (0%)	43	52
1	P	409/424 (96%)	393 (96%)	16 (4%)	0	100	100
All	All	6594/6784 (97%)	6350 (96%)	236 (4%)	8 (0%)	48	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	16	PHE
1	L	396	ILE
1	O	16	PHE
1	C	17	ASP
1	B	17	ASP
1	F	17	ASP
1	K	17	ASP
1	M	17	ASP

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	360/355 (101%)	357 (99%)	3 (1%)	73	84
1	B	359/355 (101%)	355 (99%)	4 (1%)	65	79
1	C	358/355 (101%)	356 (99%)	2 (1%)	78	87
1	D	359/355 (101%)	357 (99%)	2 (1%)	78	87
1	E	358/355 (101%)	356 (99%)	2 (1%)	78	87
1	F	358/355 (101%)	355 (99%)	3 (1%)	73	84
1	G	359/355 (101%)	357 (99%)	2 (1%)	78	87
1	H	359/355 (101%)	355 (99%)	4 (1%)	65	79
1	I	340/355 (96%)	337 (99%)	3 (1%)	70	82
1	J	343/355 (97%)	341 (99%)	2 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	342/355 (96%)	339 (99%)	3 (1%)	70	82
1	L	345/355 (97%)	342 (99%)	3 (1%)	70	82
1	M	343/355 (97%)	340 (99%)	3 (1%)	70	82
1	N	343/355 (97%)	339 (99%)	4 (1%)	63	77
1	O	343/355 (97%)	341 (99%)	2 (1%)	78	87
1	P	349/355 (98%)	344 (99%)	5 (1%)	59	73
All	All	5618/5680 (99%)	5571 (99%)	47 (1%)	73	84

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	A	158	ILE
1	A	342	LEU
1	B	156	PRO
1	B	157	GLN
1	B	158	ILE
1	B	342	LEU
1	C	156	PRO
1	C	158	ILE
1	D	156	PRO
1	D	158	ILE
1	E	156	PRO
1	E	158	ILE
1	F	105	ASN
1	F	156	PRO
1	F	158	ILE
1	G	156	PRO
1	G	158	ILE
1	H	15	ASN
1	H	18	THR
1	H	156	PRO
1	H	158	ILE
1	I	156	PRO
1	I	158	ILE
1	I	342	LEU
1	J	156	PRO
1	J	158	ILE
1	K	156	PRO
1	K	158	ILE

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Mol	Chain	Res	Type
1	K	342	LEU
1	L	156	PRO
1	L	158	ILE
1	L	342	LEU
1	M	156	PRO
1	M	158	ILE
1	M	342	LEU
1	N	84	MSE
1	N	156	PRO
1	N	158	ILE
1	N	342	LEU
1	O	156	PRO
1	O	342	LEU
1	P	5	LYS
1	P	15	ASN
1	P	156	PRO
1	P	158	ILE
1	P	342	LEU

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

Mol	Chain	Res	Type
1	A	143	GLN
1	A	316	ASN
1	B	4	ASN
1	B	117	HIS
1	B	276	GLN
1	B	283	GLN
1	B	392	GLN
1	C	33	ASN
1	C	117	HIS
1	C	194	HIS
1	D	190	GLN
1	D	194	HIS
1	D	276	GLN
1	E	4	ASN
1	E	117	HIS
1	E	190	GLN
1	E	307	ASN
1	F	105	ASN
1	F	117	HIS
1	F	190	GLN

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Mol	Chain	Res	Type
1	F	194	HIS
1	F	283	GLN
1	F	360	GLN
1	G	190	GLN
1	H	4	ASN
1	H	15	ASN
1	H	51	ASN
1	H	117	HIS
1	H	190	GLN
1	H	194	HIS
1	H	276	GLN
1	I	304	ASN
1	J	19	GLN
1	J	117	HIS
1	J	190	GLN
1	K	117	HIS
1	K	190	GLN
1	K	276	GLN
1	K	283	GLN
1	L	173	HIS
1	L	194	HIS
1	L	283	GLN
1	L	297	GLN
1	M	117	HIS
1	M	143	GLN
1	M	210	GLN
1	M	283	GLN
1	N	117	HIS
1	N	190	GLN
1	N	283	GLN
1	O	190	GLN
1	O	276	GLN
1	O	307	ASN
1	P	117	HIS
1	P	194	HIS
1	P	276	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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
1	LLP	P	205	1	23,24,25	1.38	1 (4%)	25,32,34	1.65	6 (24%)
1	LLP	B	205	1	23,24,25	1.26	2 (8%)	25,32,34	1.51	5 (20%)
1	LLP	J	205	1	23,24,25	1.60	1 (4%)	25,32,34	1.64	4 (16%)
1	LLP	D	205	1	23,24,25	1.47	3 (13%)	25,32,34	1.53	5 (20%)
1	LLP	M	205	1	23,24,25	1.38	2 (8%)	25,32,34	1.51	4 (16%)
1	LLP	O	205	1	23,24,25	2.05	4 (17%)	25,32,34	3.88	9 (36%)
1	LLP	G	205	1	23,24,25	1.17	2 (8%)	25,32,34	1.63	6 (24%)
1	LLP	A	205	1	23,24,25	1.49	2 (8%)	25,32,34	1.63	5 (20%)
1	LLP	C	205	1	23,24,25	1.45	3 (13%)	25,32,34	1.63	5 (20%)
1	LLP	N	205	1	23,24,25	1.61	3 (13%)	25,32,34	1.63	4 (16%)
1	LLP	E	205	1	23,24,25	1.43	2 (8%)	25,32,34	1.50	5 (20%)
1	LLP	F	205	1	23,24,25	1.37	3 (13%)	25,32,34	1.69	6 (24%)
1	LLP	K	205	1	23,24,25	1.32	2 (8%)	25,32,34	1.59	5 (20%)
1	LLP	I	205	1	23,24,25	1.62	3 (13%)	25,32,34	2.99	11 (44%)
1	LLP	H	205	1	23,24,25	1.46	3 (13%)	25,32,34	1.65	6 (24%)
1	LLP	L	205	1	23,24,25	1.81	3 (13%)	25,32,34	3.00	13 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	P	205	1	-	3/16/17/19	0/1/1/1
1	LLP	B	205	1	-	3/16/17/19	0/1/1/1
1	LLP	J	205	1	-	3/16/17/19	0/1/1/1
1	LLP	D	205	1	-	3/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	M	205	1	-	3/16/17/19	0/1/1/1
1	LLP	O	205	1	-	4/16/17/19	0/1/1/1
1	LLP	G	205	1	-	4/16/17/19	0/1/1/1
1	LLP	A	205	1	-	3/16/17/19	0/1/1/1
1	LLP	C	205	1	-	4/16/17/19	0/1/1/1
1	LLP	N	205	1	-	3/16/17/19	0/1/1/1
1	LLP	E	205	1	-	3/16/17/19	0/1/1/1
1	LLP	F	205	1	-	3/16/17/19	0/1/1/1
1	LLP	K	205	1	-	4/16/17/19	0/1/1/1
1	LLP	I	205	1	-	5/16/17/19	0/1/1/1
1	LLP	H	205	1	-	5/16/17/19	0/1/1/1
1	LLP	L	205	1	-	5/16/17/19	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	205	LLP	C3-C2	-7.59	1.33	1.41
1	J	205	LLP	C3-C2	-6.39	1.34	1.41
1	L	205	LLP	C3-C2	-6.00	1.34	1.41
1	N	205	LLP	C3-C2	-5.70	1.35	1.41
1	P	205	LLP	C3-C2	-5.03	1.35	1.41
1	I	205	LLP	C3-C2	-5.01	1.35	1.41
1	A	205	LLP	C3-C2	-4.70	1.36	1.41
1	C	205	LLP	C3-C2	-4.68	1.36	1.41
1	D	205	LLP	C3-C2	-4.67	1.36	1.41
1	M	205	LLP	C3-C2	-4.66	1.36	1.41
1	K	205	LLP	C3-C2	-4.46	1.36	1.41
1	B	205	LLP	C3-C2	-4.40	1.36	1.41
1	H	205	LLP	C4-C5	-4.33	1.35	1.42
1	E	205	LLP	C3-C2	-4.25	1.36	1.41
1	H	205	LLP	C3-C2	-4.22	1.36	1.41
1	F	205	LLP	C3-C2	-4.08	1.36	1.41
1	E	205	LLP	C4-C5	-4.00	1.36	1.42
1	A	205	LLP	C4-C5	-3.86	1.36	1.42
1	L	205	LLP	CE-NZ	-3.71	1.38	1.46
1	C	205	LLP	C4-C5	-3.65	1.36	1.42
1	F	205	LLP	C4-C5	-3.47	1.37	1.42
1	O	205	LLP	C4-C3	-3.45	1.35	1.41
1	G	205	LLP	C3-C2	-3.36	1.37	1.41
1	I	205	LLP	CE-NZ	-3.33	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	205	LLP	CD-CE	3.22	1.62	1.51
1	N	205	LLP	C4-C5	-3.10	1.37	1.42
1	L	205	LLP	CD-CE	2.91	1.61	1.51
1	D	205	LLP	C4-C5	-2.82	1.38	1.42
1	M	205	LLP	C4-C5	-2.73	1.38	1.42
1	B	205	LLP	C4-C5	-2.67	1.38	1.42
1	K	205	LLP	C4-C5	-2.64	1.38	1.42
1	O	205	LLP	C4'-NZ	-2.31	1.19	1.27
1	G	205	LLP	C4-C5	-2.31	1.38	1.42
1	O	205	LLP	C4-C4'	2.18	1.51	1.46
1	D	205	LLP	CD-CE	2.15	1.58	1.51
1	H	205	LLP	CD-CE	2.09	1.58	1.51
1	N	205	LLP	CD-CE	2.06	1.58	1.51
1	F	205	LLP	CD-CE	2.02	1.58	1.51
1	C	205	LLP	CD-CE	2.01	1.58	1.51

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	205	LLP	C5-C4-C4'	11.69	139.51	121.47
1	O	205	LLP	C3-C4-C4'	-10.20	101.98	120.40
1	I	205	LLP	CE-NZ-C4'	8.52	146.02	118.72
1	L	205	LLP	CE-NZ-C4'	8.19	144.96	118.72
1	O	205	LLP	C4-C3-C2	7.20	124.20	120.14
1	L	205	LLP	CG-CD-CE	-6.27	91.55	113.38
1	I	205	LLP	CG-CD-CE	-6.06	92.26	113.38
1	L	205	LLP	CD-CE-NZ	-4.90	97.87	110.83
1	I	205	LLP	CD-CE-NZ	-4.79	98.14	110.83
1	L	205	LLP	CD-CG-CB	4.31	129.88	113.62
1	I	205	LLP	CD-CG-CB	4.26	129.67	113.62
1	F	205	LLP	CD-CG-CB	4.16	129.30	113.62
1	B	205	LLP	CD-CG-CB	4.11	129.10	113.62
1	J	205	LLP	CD-CG-CB	4.09	129.05	113.62
1	D	205	LLP	CD-CG-CB	4.08	129.00	113.62
1	H	205	LLP	CD-CG-CB	4.06	128.93	113.62
1	C	205	LLP	CD-CG-CB	4.06	128.93	113.62
1	A	205	LLP	CD-CG-CB	4.06	128.91	113.62
1	K	205	LLP	CD-CG-CB	4.04	128.85	113.62
1	L	205	LLP	C4-C4'-NZ	4.04	142.66	124.04
1	G	205	LLP	CD-CG-CB	4.03	128.82	113.62
1	N	205	LLP	CD-CG-CB	4.03	128.80	113.62
1	E	205	LLP	CD-CG-CB	4.00	128.71	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	205	LLP	CD-CG-CB	4.00	128.70	113.62
1	I	205	LLP	C4-C4'-NZ	3.98	142.40	124.04
1	P	205	LLP	CD-CG-CB	3.97	128.59	113.62
1	O	205	LLP	CD-CG-CB	3.87	128.21	113.62
1	G	205	LLP	OP3-P-OP4	-3.66	97.12	106.67
1	C	205	LLP	C4-C3-C2	3.61	122.17	120.14
1	O	205	LLP	OP3-P-OP4	-3.60	97.28	106.67
1	A	205	LLP	C4-C3-C2	3.58	122.16	120.14
1	H	205	LLP	OP3-P-OP4	-3.57	97.37	106.67
1	F	205	LLP	C4-C3-C2	3.49	122.11	120.14
1	O	205	LLP	C2'-C2-N1	3.40	124.05	117.64
1	L	205	LLP	C4-C3-C2	3.22	121.96	120.14
1	D	205	LLP	C4-C3-C2	3.21	121.95	120.14
1	O	205	LLP	C2'-C2-C3	-3.15	117.11	120.80
1	F	205	LLP	OP2-P-OP4	-2.98	98.91	106.67
1	D	205	LLP	OP2-P-OP4	-2.97	98.92	106.67
1	I	205	LLP	OP2-P-OP4	-2.97	98.92	106.67
1	E	205	LLP	OP2-P-OP4	-2.95	98.99	106.67
1	A	205	LLP	OP2-P-OP4	-2.94	99.00	106.67
1	B	205	LLP	OP2-P-OP4	-2.93	99.03	106.67
1	J	205	LLP	CE-NZ-C4'	2.92	128.09	118.72
1	N	205	LLP	OP2-P-OP4	-2.91	99.07	106.67
1	L	205	LLP	OP2-P-OP4	-2.90	99.10	106.67
1	M	205	LLP	OP2-P-OP4	-2.88	99.15	106.67
1	P	205	LLP	OP2-P-OP4	-2.88	99.17	106.67
1	J	205	LLP	OP2-P-OP4	-2.81	99.35	106.67
1	P	205	LLP	CE-NZ-C4'	2.74	127.48	118.72
1	N	205	LLP	CE-NZ-C4'	2.71	127.40	118.72
1	H	205	LLP	C4-C3-C2	2.71	121.67	120.14
1	K	205	LLP	C3-C4-C5	2.68	120.43	118.28
1	O	205	LLP	C5'-C5-C6	-2.67	115.01	119.36
1	I	205	LLP	C5-C4-C4'	-2.59	117.47	121.47
1	L	205	LLP	C5-C4-C4'	-2.51	117.61	121.47
1	F	205	LLP	CE-NZ-C4'	2.50	126.74	118.72
1	K	205	LLP	OP2-P-OP1	2.50	120.58	110.83
1	I	205	LLP	C5-C6-N1	-2.46	119.83	123.83
1	A	205	LLP	CE-NZ-C4'	2.46	126.59	118.72
1	C	205	LLP	OP2-P-OP1	2.41	120.21	110.83
1	G	205	LLP	CE-NZ-C4'	2.38	126.34	118.72
1	B	205	LLP	CE-NZ-C4'	2.38	126.34	118.72
1	G	205	LLP	C4-C3-C2	2.38	121.48	120.14
1	M	205	LLP	CE-NZ-C4'	2.35	126.25	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	205	LLP	OP3-P-OP2	2.34	116.57	107.80
1	D	205	LLP	OP3-P-OP2	2.32	116.50	107.80
1	H	205	LLP	CE-NZ-C4'	2.29	126.06	118.72
1	E	205	LLP	OP3-P-OP2	2.29	116.40	107.80
1	N	205	LLP	OP3-P-OP2	2.29	116.38	107.80
1	L	205	LLP	C3-C4-C4'	2.28	124.52	120.40
1	J	205	LLP	OP3-P-OP2	2.28	116.35	107.80
1	H	205	LLP	OP3-P-OP1	2.26	119.65	110.83
1	B	205	LLP	OP3-P-OP2	2.26	116.28	107.80
1	F	205	LLP	C2'-C2-N1	2.26	121.90	117.64
1	M	205	LLP	OP3-P-OP2	2.25	116.24	107.80
1	L	205	LLP	C5-C6-N1	-2.24	120.19	123.83
1	I	205	LLP	C6-N1-C2	2.22	123.22	119.20
1	I	205	LLP	OP3-P-OP2	2.21	116.10	107.80
1	L	205	LLP	OP3-P-OP2	2.21	116.09	107.80
1	P	205	LLP	OP3-P-OP2	2.21	116.09	107.80
1	O	205	LLP	OP3-P-OP1	2.20	119.39	110.83
1	G	205	LLP	OP3-P-OP1	2.17	119.30	110.83
1	A	205	LLP	OP3-P-OP2	2.17	115.93	107.80
1	P	205	LLP	C2'-C2-N1	2.16	121.71	117.64
1	E	205	LLP	CE-NZ-C4'	2.16	125.63	118.72
1	L	205	LLP	C6-N1-C2	2.15	123.09	119.20
1	P	205	LLP	C6-N1-C2	2.10	123.01	119.20
1	H	205	LLP	C2'-C2-N1	2.10	121.60	117.64
1	I	205	LLP	C4-C3-C2	2.10	121.33	120.14
1	C	205	LLP	OP3-P-OP1	-2.07	102.77	110.83
1	C	205	LLP	C2'-C2-N1	2.06	121.53	117.64
1	L	205	LLP	C2'-C2-N1	2.06	121.52	117.64
1	K	205	LLP	CE-NZ-C4'	2.05	125.27	118.72
1	D	205	LLP	CE-NZ-C4'	2.02	125.18	118.72
1	K	205	LLP	OP3-P-OP1	-2.01	102.99	110.83
1	G	205	LLP	C2'-C2-N1	2.01	121.44	117.64
1	E	205	LLP	C2'-C2-N1	2.01	121.44	117.64
1	B	205	LLP	C2'-C2-N1	2.01	121.43	117.64

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	205	LLP	O-C-CA-CB
1	B	205	LLP	O-C-CA-CB
1	C	205	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	D	205	LLP	O-C-CA-CB
1	E	205	LLP	O-C-CA-CB
1	F	205	LLP	O-C-CA-CB
1	G	205	LLP	O-C-CA-CB
1	H	205	LLP	O-C-CA-CB
1	I	205	LLP	C4-C4'-NZ-CE
1	I	205	LLP	O-C-CA-CB
1	J	205	LLP	O-C-CA-CB
1	K	205	LLP	O-C-CA-CB
1	L	205	LLP	C4-C4'-NZ-CE
1	L	205	LLP	O-C-CA-CB
1	M	205	LLP	O-C-CA-CB
1	N	205	LLP	O-C-CA-CB
1	O	205	LLP	O-C-CA-CB
1	P	205	LLP	O-C-CA-CB
1	A	205	LLP	CA-CB-CG-CD
1	C	205	LLP	CA-CB-CG-CD
1	D	205	LLP	CA-CB-CG-CD
1	E	205	LLP	CA-CB-CG-CD
1	F	205	LLP	CA-CB-CG-CD
1	H	205	LLP	CA-CB-CG-CD
1	K	205	LLP	CA-CB-CG-CD
1	L	205	LLP	CA-CB-CG-CD
1	M	205	LLP	CA-CB-CG-CD
1	O	205	LLP	CA-CB-CG-CD
1	P	205	LLP	CA-CB-CG-CD
1	B	205	LLP	CA-CB-CG-CD
1	G	205	LLP	CA-CB-CG-CD
1	I	205	LLP	CA-CB-CG-CD
1	J	205	LLP	CA-CB-CG-CD
1	N	205	LLP	CA-CB-CG-CD
1	I	205	LLP	CG-CD-CE-NZ
1	L	205	LLP	CG-CD-CE-NZ
1	O	205	LLP	CG-CD-CE-NZ
1	A	205	LLP	C-CA-CB-CG
1	B	205	LLP	C-CA-CB-CG
1	C	205	LLP	C-CA-CB-CG
1	D	205	LLP	C-CA-CB-CG
1	E	205	LLP	C-CA-CB-CG
1	F	205	LLP	C-CA-CB-CG
1	G	205	LLP	C-CA-CB-CG
1	H	205	LLP	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	I	205	LLP	C-CA-CB-CG
1	J	205	LLP	C-CA-CB-CG
1	K	205	LLP	C-CA-CB-CG
1	L	205	LLP	C-CA-CB-CG
1	M	205	LLP	C-CA-CB-CG
1	N	205	LLP	C-CA-CB-CG
1	O	205	LLP	C-CA-CB-CG
1	P	205	LLP	C-CA-CB-CG
1	C	205	LLP	C5'-OP4-P-OP1
1	G	205	LLP	C5'-OP4-P-OP1
1	H	205	LLP	C5'-OP4-P-OP1
1	K	205	LLP	C5'-OP4-P-OP1
1	H	205	LLP	C5'-OP4-P-OP3

There are no ring outliers.

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	205	LLP	1	0
1	B	205	LLP	1	0
1	J	205	LLP	1	0
1	D	205	LLP	1	0
1	M	205	LLP	1	0
1	O	205	LLP	1	0
1	G	205	LLP	1	0
1	A	205	LLP	1	0
1	C	205	LLP	1	0
1	N	205	LLP	5	0
1	E	205	LLP	1	0
1	F	205	LLP	1	0
1	K	205	LLP	1	0
1	I	205	LLP	1	0
1	H	205	LLP	1	0
1	L	205	LLP	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 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	$\# Z > 2$
2	IMD	A	501	-	5,5,5	0.75	0	5,5,5	0.52	0
3	GOL	O	501	-	5,5,5	0.46	0	5,5,5	0.35	0
3	GOL	A	502	-	5,5,5	0.60	0	5,5,5	0.72	0
2	IMD	D	501	-	5,5,5	0.74	0	5,5,5	0.44	0
4	PO4	C	501	-	4,4,4	0.94	0	6,6,6	0.68	0
3	GOL	B	501[B]	-	5,5,5	0.50	0	5,5,5	0.28	0
3	GOL	B	501[A]	-	5,5,5	0.38	0	5,5,5	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	A	501	-	-	-	0/1/1/1
3	GOL	O	501	-	-	3/4/4/4	-
3	GOL	A	502	-	-	1/4/4/4	-
2	IMD	D	501	-	-	-	0/1/1/1
3	GOL	B	501[B]	-	-	2/4/4/4	-
3	GOL	B	501[A]	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501[B]	GOL	O1-C1-C2-O2
3	O	501	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	O	501	GOL	O2-C2-C3-O3
3	B	501[A]	GOL	O1-C1-C2-C3
3	B	501[A]	GOL	C1-C2-C3-O3
3	B	501[B]	GOL	O1-C1-C2-C3
3	O	501	GOL	O1-C1-C2-C3
3	B	501[A]	GOL	O1-C1-C2-O2
3	B	501[A]	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	1	0
3	B	501[A]	GOL	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	419/424 (98%)	0.12	14 (3%)	49	56	6, 18, 49, 77	5 (1%)
1	B	419/424 (98%)	0.22	13 (3%)	51	58	7, 20, 50, 79	4 (0%)
1	C	419/424 (98%)	0.17	10 (2%)	59	66	6, 18, 45, 57	3 (0%)
1	D	420/424 (99%)	0.09	8 (1%)	66	71	6, 18, 46, 85	3 (0%)
1	E	419/424 (98%)	0.21	15 (3%)	46	52	6, 19, 50, 86	3 (0%)
1	F	420/424 (99%)	0.12	9 (2%)	63	68	7, 19, 45, 76	2 (0%)
1	G	420/424 (99%)	0.24	10 (2%)	59	66	7, 22, 52, 76	3 (0%)
1	H	420/424 (99%)	0.23	12 (2%)	53	60	6, 20, 50, 76	3 (0%)
1	I	401/424 (94%)	0.14	17 (4%)	40	46	8, 20, 45, 69	1 (0%)
1	J	405/424 (95%)	0.19	14 (3%)	47	53	8, 22, 48, 71	1 (0%)
1	K	404/424 (95%)	0.28	26 (6%)	25	28	9, 22, 51, 84	0
1	L	405/424 (95%)	0.29	17 (4%)	40	46	5, 24, 54, 83	3 (0%)
1	M	405/424 (95%)	0.18	15 (3%)	45	51	4, 21, 47, 80	1 (0%)
1	N	403/424 (95%)	0.21	15 (3%)	45	51	8, 22, 48, 69	1 (0%)
1	O	403/424 (95%)	0.16	15 (3%)	45	51	8, 20, 47, 86	1 (0%)
1	P	410/424 (96%)	0.19	23 (5%)	30	35	8, 20, 52, 98	2 (0%)
All	All	6592/6784 (97%)	0.19	233 (3%)	47	53	4, 20, 49, 98	36 (0%)

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	394	ALA	5.8
1	O	41	ALA	4.9
1	M	423	SER	4.8
1	P	17	ASP	4.5
1	A	379	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	K	16	PHE	4.1
1	B	423	SER	4.1
1	N	15	ASN	3.9
1	A	394	ALA	3.8
1	M	394	ALA	3.8
1	M	336	ASN	3.8
1	F	2	ASN	3.8
1	O	16	PHE	3.8
1	K	377	HIS	3.8
1	J	394	ALA	3.7
1	O	49	LEU	3.7
1	L	336	ASN	3.7
1	M	378	PRO	3.7
1	J	16	PHE	3.7
1	L	17	ASP	3.6
1	N	377	HIS	3.6
1	J	49	LEU	3.6
1	N	396	ILE	3.5
1	G	15	ASN	3.5
1	L	49	LEU	3.5
1	I	349	TYR	3.4
1	E	379	ALA	3.4
1	K	378	PRO	3.4
1	P	423	SER	3.4
1	D	17	ASP	3.4
1	P	336	ASN	3.4
1	M	243	SER	3.4
1	B	386	LEU	3.3
1	B	394	ALA	3.2
1	J	244	TYR	3.2
1	E	386	LEU	3.2
1	C	17	ASP	3.2
1	O	17	ASP	3.2
1	A	17	ASP	3.1
1	P	42	ALA	3.1
1	I	2	ASN	3.1
1	C	16	PHE	3.1
1	E	16	PHE	3.1
1	O	15	ASN	3.1
1	D	391	LEU	3.1
1	G	387	SER	3.0
1	K	423	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	396	ILE	3.0
1	P	156	PRO	3.0
1	G	49	LEU	3.0
1	P	49	LEU	3.0
1	I	336	ASN	3.0
1	O	48	GLU	3.0
1	F	423	SER	3.0
1	I	16	PHE	2.9
1	H	17	ASP	2.9
1	K	37	LEU	2.9
1	K	49	LEU	2.9
1	M	396	ILE	2.9
1	P	396	ILE	2.9
1	B	393	LYS	2.9
1	H	394	ALA	2.9
1	L	394	ALA	2.9
1	E	388	GLU	2.9
1	K	156	PRO	2.8
1	N	157	GLN	2.8
1	O	377	HIS	2.8
1	I	46	LEU	2.8
1	C	398	LYS	2.8
1	F	17	ASP	2.8
1	J	377	HIS	2.8
1	J	157	GLN	2.8
1	E	244	TYR	2.8
1	A	46[A]	LEU	2.8
1	B	391	LEU	2.8
1	D	49	LEU	2.8
1	N	2	ASN	2.7
1	O	396	ILE	2.7
1	L	143	GLN	2.7
1	L	156	PRO	2.7
1	N	49	LEU	2.7
1	L	16	PHE	2.7
1	N	16	PHE	2.7
1	B	381	THR	2.7
1	O	322	SER	2.7
1	P	377	HIS	2.7
1	G	143	GLN	2.7
1	L	335	LYS	2.7
1	M	49	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	16	PHE	2.7
1	C	253	ASP	2.7
1	P	391	LEU	2.7
1	K	336	ASN	2.6
1	K	131	ILE	2.6
1	E	391	LEU	2.6
1	M	37	LEU	2.6
1	O	46	LEU	2.6
1	M	16	PHE	2.6
1	P	244	TYR	2.6
1	P	354	ARG	2.6
1	M	156	PRO	2.6
1	H	49	LEU	2.6
1	I	49	LEU	2.6
1	P	390	GLU	2.6
1	L	396	ILE	2.6
1	N	322	SER	2.6
1	O	143	GLN	2.6
1	H	386	LEU	2.6
1	K	17	ASP	2.6
1	F	16	PHE	2.6
1	I	156	PRO	2.6
1	I	396	ILE	2.6
1	K	139	LYS	2.6
1	H	47	GLN	2.5
1	L	41	ALA	2.5
1	G	17	ASP	2.5
1	M	2	ASN	2.5
1	K	322	SER	2.5
1	B	388	GLU	2.5
1	B	379	ALA	2.5
1	E	232	ASP	2.5
1	H	379	ALA	2.5
1	P	243	SER	2.5
1	G	386	LEU	2.5
1	D	379	ALA	2.5
1	K	314	GLY	2.5
1	M	377	HIS	2.5
1	M	244	TYR	2.5
1	D	46	LEU	2.5
1	A	393	LYS	2.5
1	A	16	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	335	LYS	2.4
1	I	17	ASP	2.4
1	N	232	ASP	2.4
1	P	2	ASN	2.4
1	E	139	LYS	2.4
1	K	15	ASN	2.4
1	K	42	ALA	2.4
1	P	393	LYS	2.4
1	J	37	LEU	2.4
1	L	46	LEU	2.4
1	A	390	GLU	2.4
1	E	17	ASP	2.4
1	P	394	ALA	2.4
1	M	335	LYS	2.4
1	H	97	SER	2.4
1	K	157	GLN	2.4
1	P	392	GLN	2.4
1	I	41	ALA	2.3
1	G	239	THR	2.3
1	J	396	ILE	2.3
1	N	314	GLY	2.3
1	A	253	ASP	2.3
1	J	336	ASN	2.3
1	P	378	PRO	2.3
1	E	246	GLY	2.3
1	I	314	GLY	2.3
1	O	158	ILE	2.3
1	O	37	LEU	2.3
1	L	45	ASN	2.3
1	K	324	ALA	2.3
1	J	423	SER	2.3
1	I	398	LYS	2.3
1	C	49	LEU	2.2
1	D	15	ASN	2.2
1	K	2	ASN	2.2
1	L	15	ASN	2.2
1	M	334	ASP	2.2
1	N	17	ASP	2.2
1	K	395	GLY	2.2
1	I	244	TYR	2.2
1	H	157	GLN	2.2
1	J	48	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	384	SER	2.2
1	P	46	LEU	2.2
1	K	253	ASP	2.2
1	N	323	ASN	2.2
1	J	243	SER	2.2
1	K	349	TYR	2.2
1	D	386	LEU	2.2
1	B	15	ASN	2.2
1	L	2	ASN	2.2
1	A	47	GLN	2.2
1	H	245	HIS	2.2
1	P	389	GLU	2.2
1	I	239	THR	2.2
1	K	244	TYR	2.2
1	A	49	LEU	2.2
1	K	134	LEU	2.2
1	C	171	LYS	2.2
1	F	393	LYS	2.2
1	A	380	SER	2.2
1	N	349	TYR	2.1
1	B	17	ASP	2.1
1	I	15	ASN	2.1
1	K	313	LYS	2.1
1	C	244	TYR	2.1
1	G	244	TYR	2.1
1	E	49	LEU	2.1
1	N	335	LYS	2.1
1	E	392	GLN	2.1
1	I	157	GLN	2.1
1	F	41	ALA	2.1
1	F	379	ALA	2.1
1	B	148	ILE	2.1
1	I	37	LEU	2.1
1	K	46	LEU	2.1
1	B	230	ASN	2.1
1	L	378	PRO	2.1
1	B	16	PHE	2.1
1	E	381	THR	2.1
1	H	380	SER	2.1
1	C	313	LYS	2.1
1	A	386	LEU	2.1
1	C	143	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	47	GLN	2.1
1	F	46	LEU	2.1
1	F	15	ASN	2.1
1	J	17	ASP	2.1
1	L	253[A]	ASP	2.1
1	J	156	PRO	2.1
1	C	50	GLY	2.1
1	A	381	THR	2.0
1	G	384	SER	2.0
1	P	157	GLN	2.0
1	A	391	LEU	2.0
1	N	336	ASN	2.0
1	L	244	TYR	2.0
1	G	16	PHE	2.0
1	H	16	PHE	2.0
1	H	389	GLU	2.0
1	O	45	ASN	2.0
1	O	313	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	N	205	24/25	0.91	0.12	15,23,30,32	0
1	LLP	K	205	24/25	0.92	0.10	14,21,25,26	0
1	LLP	F	205	24/25	0.93	0.09	13,16,19,21	0
1	LLP	A	205	24/25	0.93	0.09	12,15,18,24	0
1	LLP	L	205	24/25	0.93	0.09	14,23,26,29	0
1	LLP	C	205	24/25	0.93	0.09	11,14,17,23	0
1	LLP	O	205	24/25	0.93	0.10	13,23,29,37	0
1	LLP	J	205	24/25	0.94	0.09	16,19,22,24	0
1	LLP	D	205	24/25	0.94	0.09	13,16,18,20	0
1	LLP	B	205	24/25	0.94	0.09	12,16,17,20	0
1	LLP	H	205	24/25	0.94	0.08	13,17,20,23	0
1	LLP	I	205	24/25	0.94	0.10	13,18,24,27	0
1	LLP	G	205	24/25	0.95	0.09	13,18,21,24	0
1	LLP	E	205	24/25	0.95	0.07	12,15,18,19	0
1	LLP	P	205	24/25	0.95	0.09	12,19,24,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	M	205	24/25	0.96	0.08	12,14,18,18	0

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($\text{\AA}^2$)	Q<0.9
2	IMD	D	501	5/5	0.65	0.17	38,38,43,45	0
2	IMD	A	501	5/5	0.84	0.13	26,28,30,31	0
3	GOL	B	501[A]	6/6	0.84	0.13	11,11,12,13	6
3	GOL	B	501[B]	6/6	0.84	0.13	19,20,21,21	6
3	GOL	A	502	6/6	0.89	0.11	26,27,31,31	0
3	GOL	O	501	6/6	0.92	0.12	26,27,28,33	0
4	PO4	C	501	5/5	0.92	0.08	45,47,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.