



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:47 PM UTC

PDB ID : 7O49 / pdb_00007o49
Title : Crystal structure of Penicillin-Binding Protein 1 (PBP1) from *Staphylococcus aureus*
Authors : Martinez Caballero, S.; Hermoso, J.A.
Deposited on : 2021-04-05
Resolution : 3.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

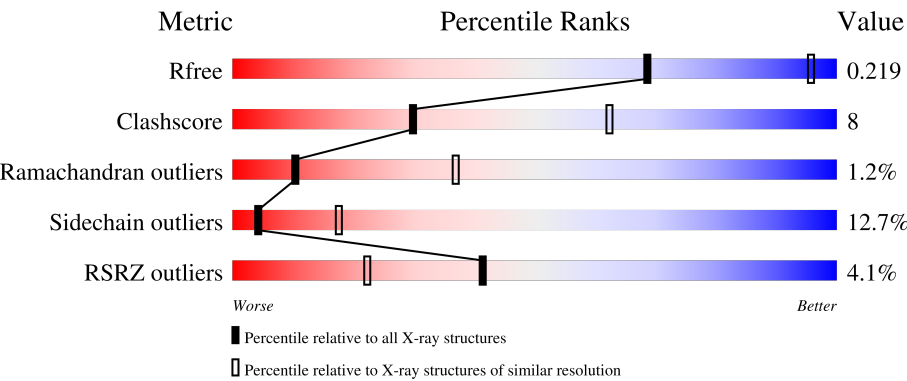
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	650	3% 60% 18% • 20%
1	B	650	3% 59% 19% • 19%
1	C	650	2% 61% 16% • 20%
1	D	650	5% 58% 16% • 23%
1	E	650	2% 58% 18% • 20%

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Mol	Chain	Length	Quality of chain
1	F	650	
1	G	650	
1	H	650	
1	I	650	
1	J	650	
1	K	650	
1	L	650	

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
4	CL	C	802	-	-	X	-
4	CL	E	802	-	-	X	-
4	CL	K	801	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48707 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 Penicillin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4105	2609	706	774	16			
1	B	527	Total	C	N	O	S	0	0	0
			4156	2639	716	785	16			
1	C	520	Total	C	N	O	S	0	0	0
			4098	2604	705	773	16			
1	D	502	Total	C	N	O	S	0	0	0
			3958	2514	677	751	16			
1	E	523	Total	C	N	O	S	0	0	0
			4120	2617	709	778	16			
1	F	528	Total	C	N	O	S	0	0	0
			4165	2645	718	786	16			
1	G	520	Total	C	N	O	S	0	0	0
			4098	2604	705	773	16			
1	H	471	Total	C	N	O	S	0	0	0
			3703	2355	631	702	15			
1	I	518	Total	C	N	O	S	0	0	0
			4083	2595	702	770	16			
1	J	518	Total	C	N	O	S	0	0	0
			4080	2592	701	771	16			
1	K	511	Total	C	N	O	S	0	0	0
			4029	2562	690	761	16			
1	L	494	Total	C	N	O	S	0	0	0
			3894	2479	662	737	16			

There are 12 discrepancies between the modelled and reference sequences:

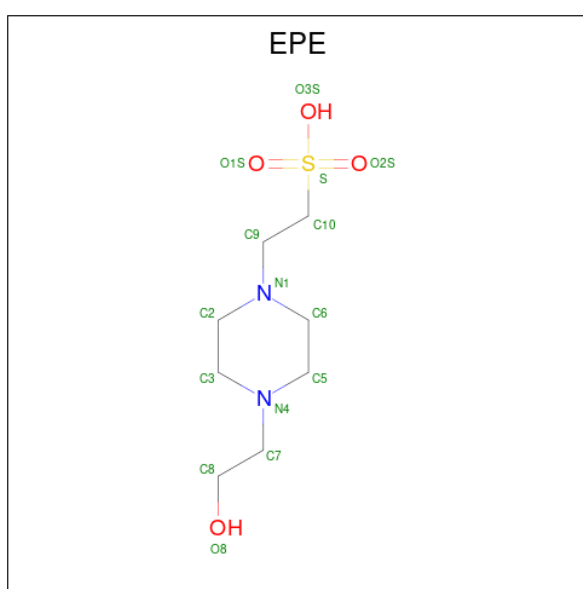
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	MET	-	initiating methionine	UNP A0A0H2WVW5
B	64	MET	-	initiating methionine	UNP A0A0H2WVW5
C	64	MET	-	initiating methionine	UNP A0A0H2WVW5
D	64	MET	-	initiating methionine	UNP A0A0H2WVW5
E	64	MET	-	initiating methionine	UNP A0A0H2WVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	64	MET	-	initiating methionine	UNP A0A0H2WVW5
G	64	MET	-	initiating methionine	UNP A0A0H2WVW5
H	64	MET	-	initiating methionine	UNP A0A0H2WVW5
I	64	MET	-	initiating methionine	UNP A0A0H2WVW5
J	64	MET	-	initiating methionine	UNP A0A0H2WVW5
K	64	MET	-	initiating methionine	UNP A0A0H2WVW5
L	64	MET	-	initiating methionine	UNP A0A0H2WVW5

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	I	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cd	0	0
			1	1		
3	B	1	Total	Cd	0	0
			1	1		
3	C	1	Total	Cd	0	0
			1	1		
3	D	1	Total	Cd	0	0
			1	1		
3	E	1	Total	Cd	0	0
			1	1		
3	F	1	Total	Cd	0	0
			1	1		
3	G	1	Total	Cd	0	0
			1	1		
3	H	1	Total	Cd	0	0
			1	1		
3	I	1	Total	Cd	0	0
			1	1		
3	J	1	Total	Cd	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

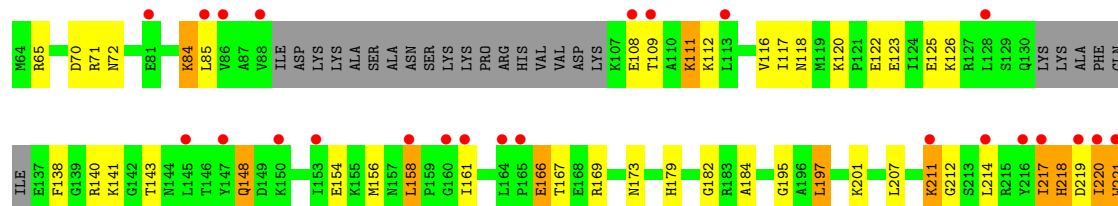
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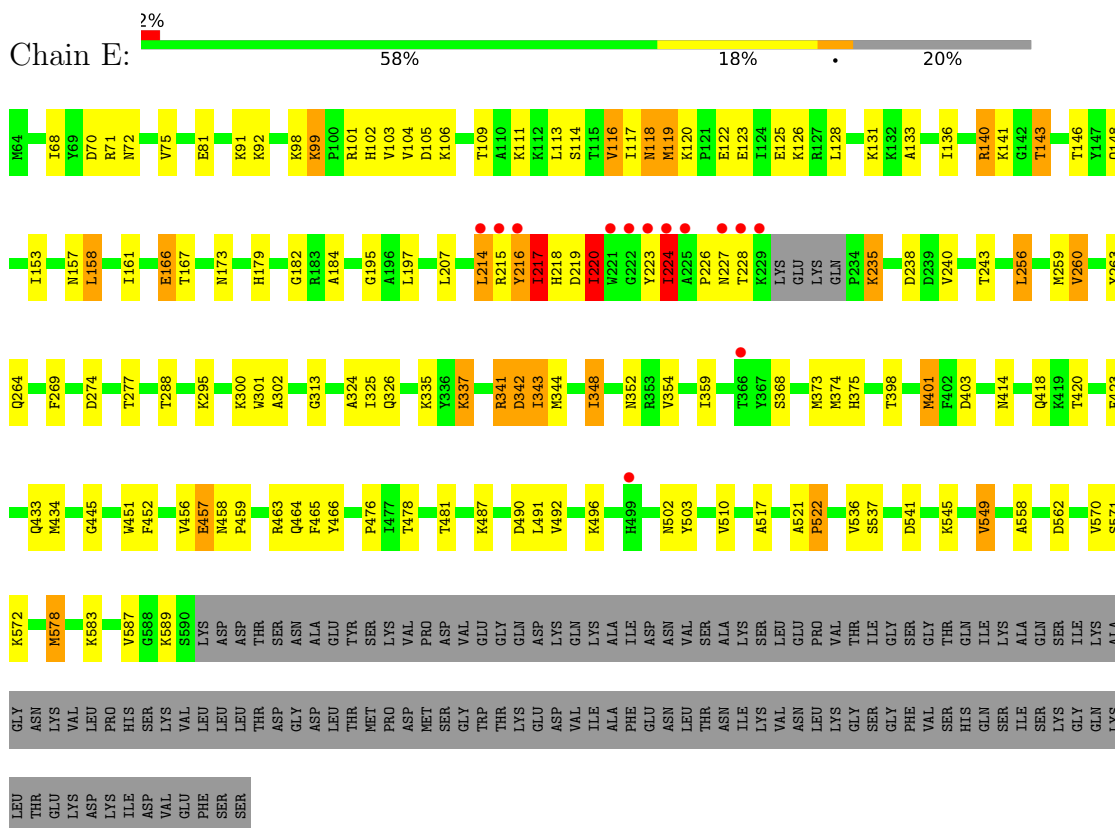
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Cl 1	0	0
4	J	1	Total 1	Cl 1	0	0
4	K	1	Total 1	Cl 1	0	0
4	L	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

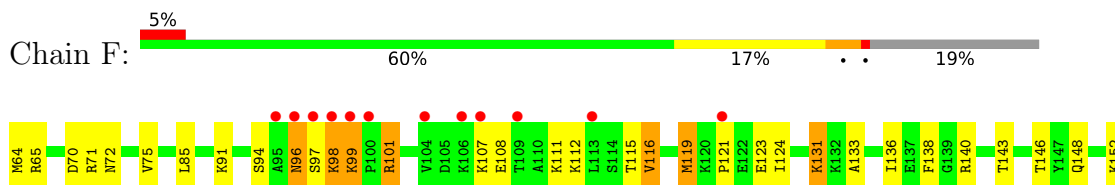
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	3	Total 3	O 3	0	0
5	C	6	Total 6	O 6	0	0
5	D	3	Total 3	O 3	0	0
5	E	7	Total 7	O 7	0	0
5	F	8	Total 8	O 8	0	0
5	G	5	Total 5	O 5	0	0
5	H	3	Total 3	O 3	0	0
5	I	4	Total 4	O 4	0	0
5	J	4	Total 4	O 4	0	0
5	K	3	Total 3	O 3	0	0
5	L	1	Total 1	O 1	0	0

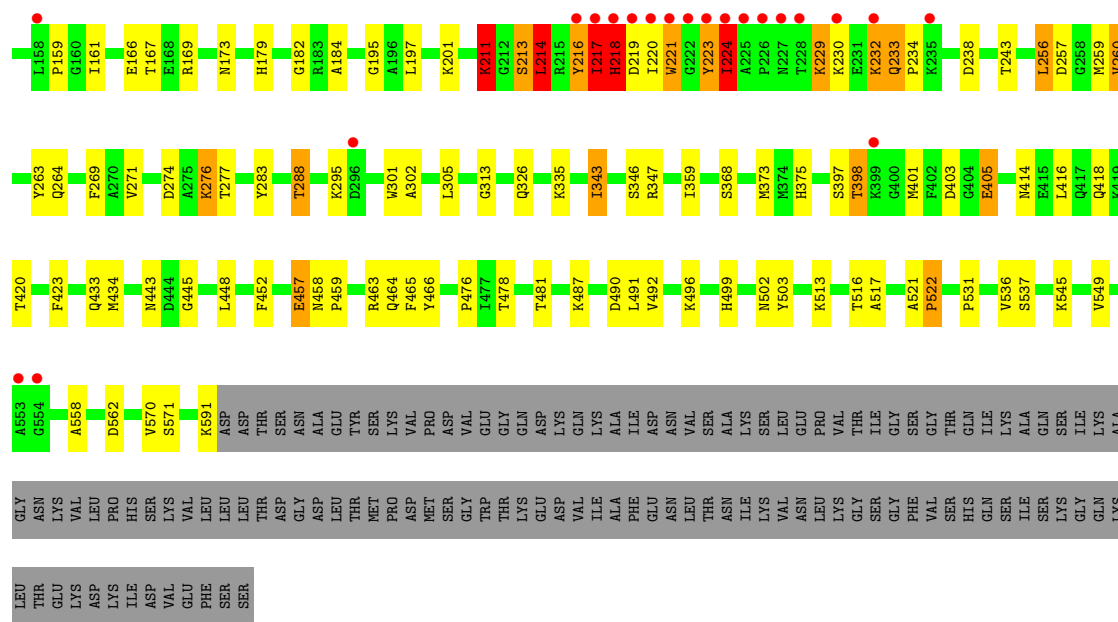


- Molecule 1: Penicillin-binding protein 1

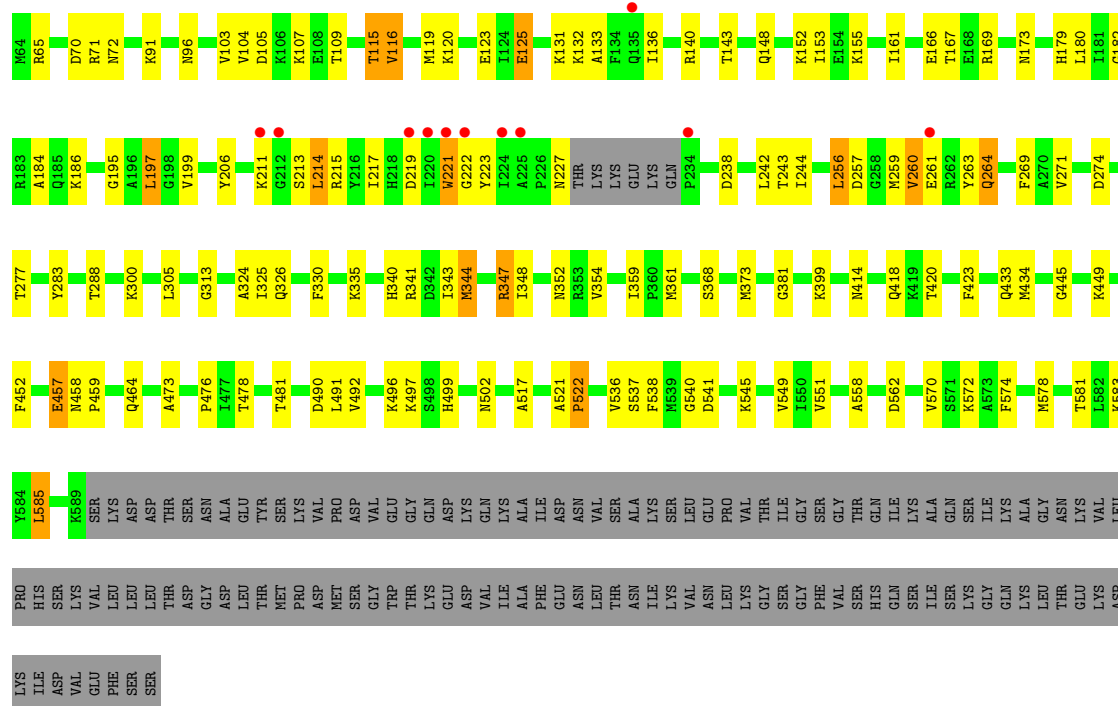


- Molecule 1: Penicillin-binding protein 1

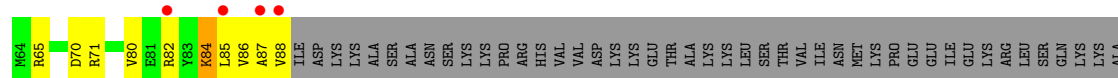


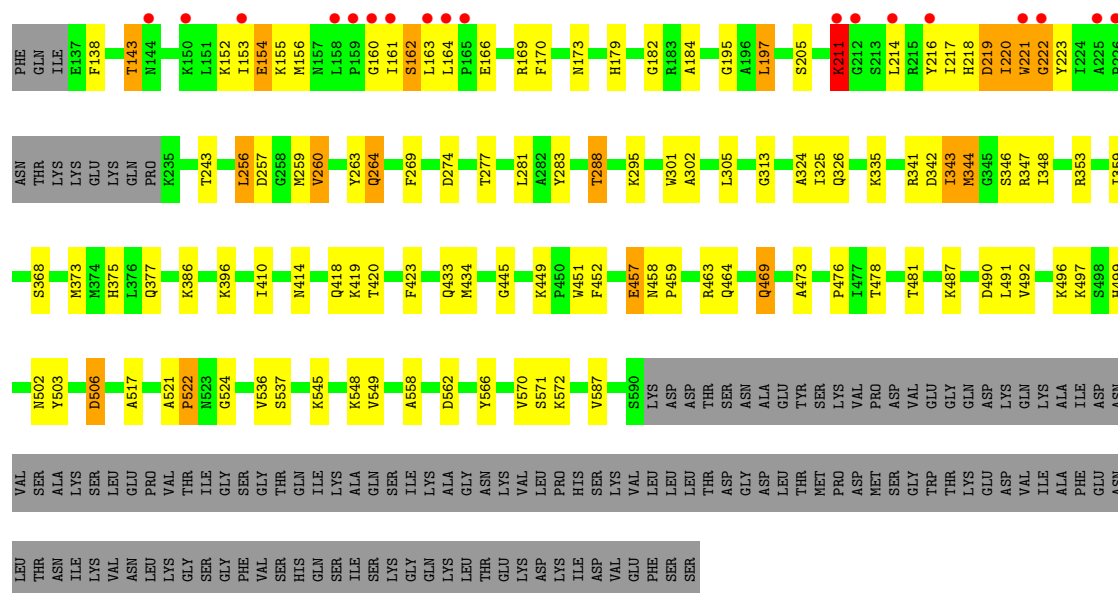


- Molecule 1: Penicillin-binding protein 1

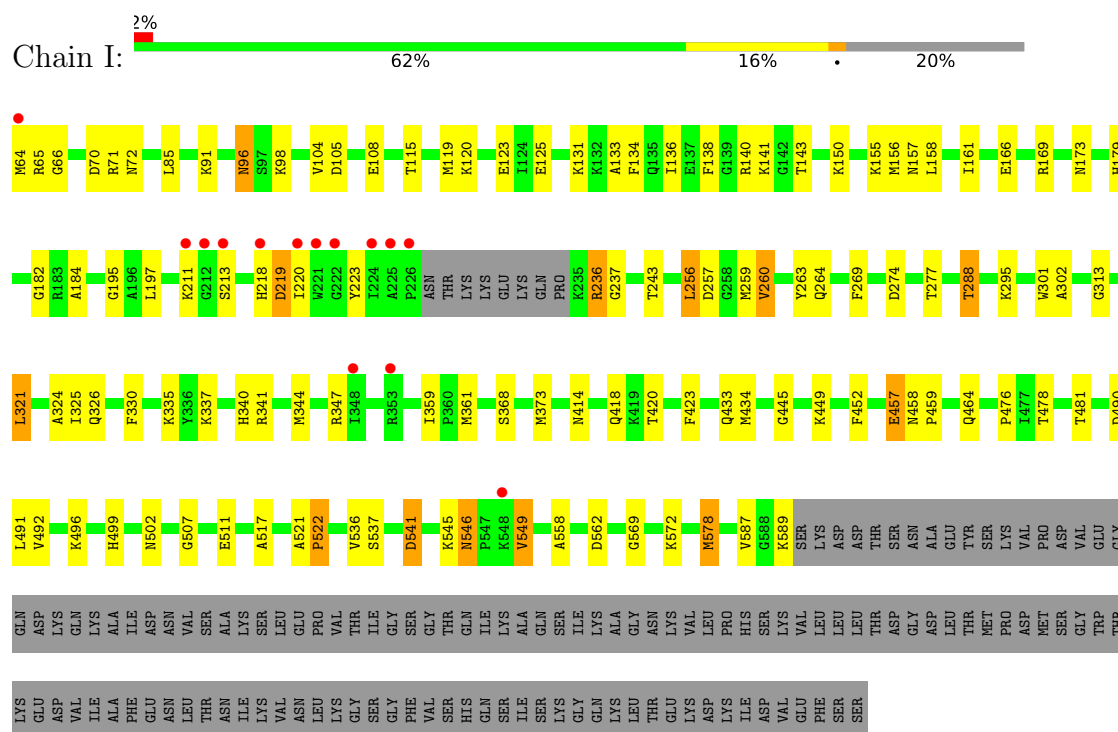


- Molecule 1: Penicillin-binding protein 1

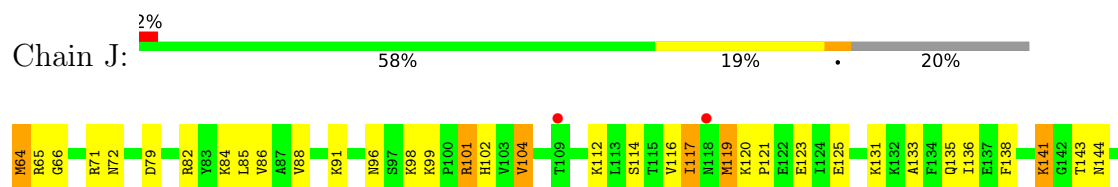


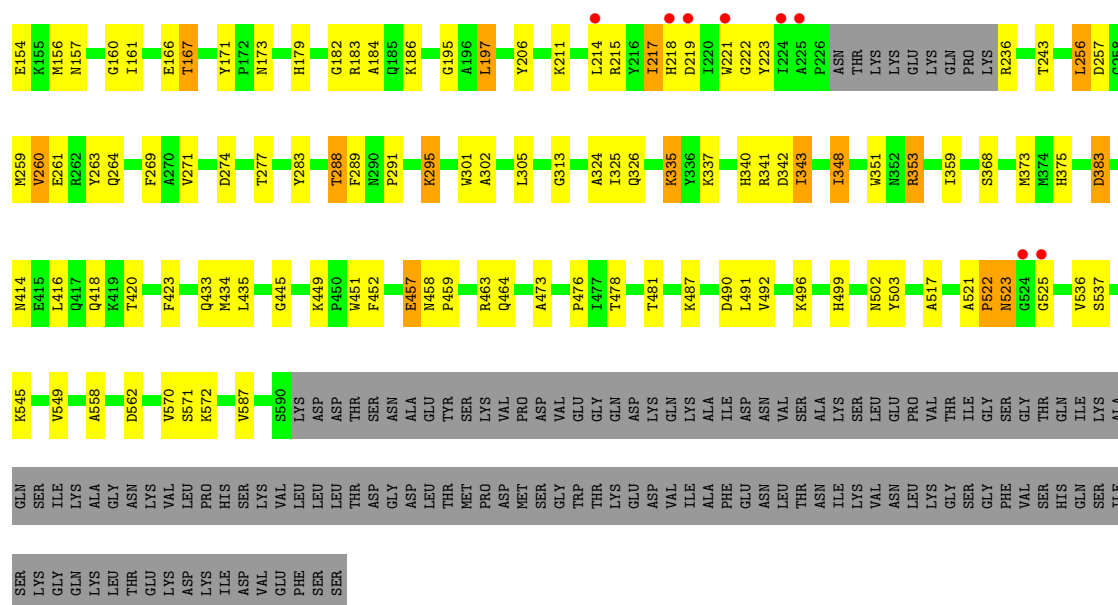


- Molecule 1: Penicillin-binding protein 1

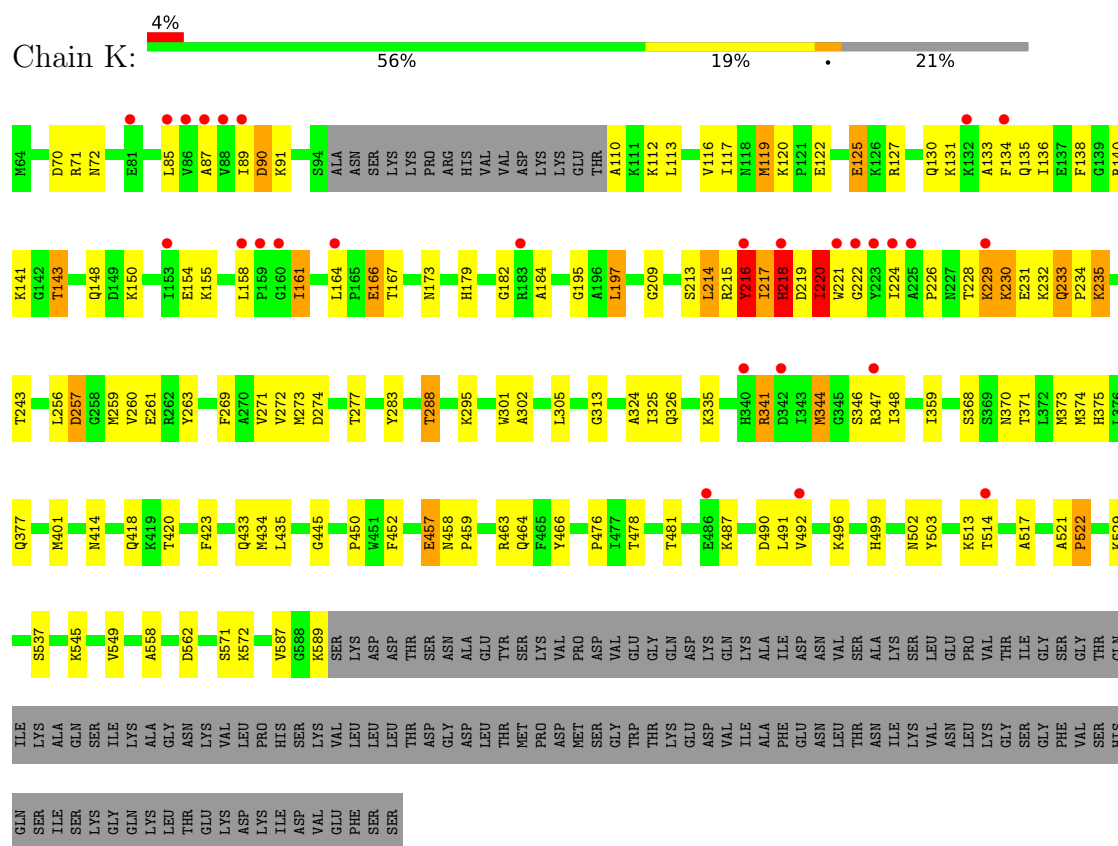


- Molecule 1: Penicillin-binding protein 1



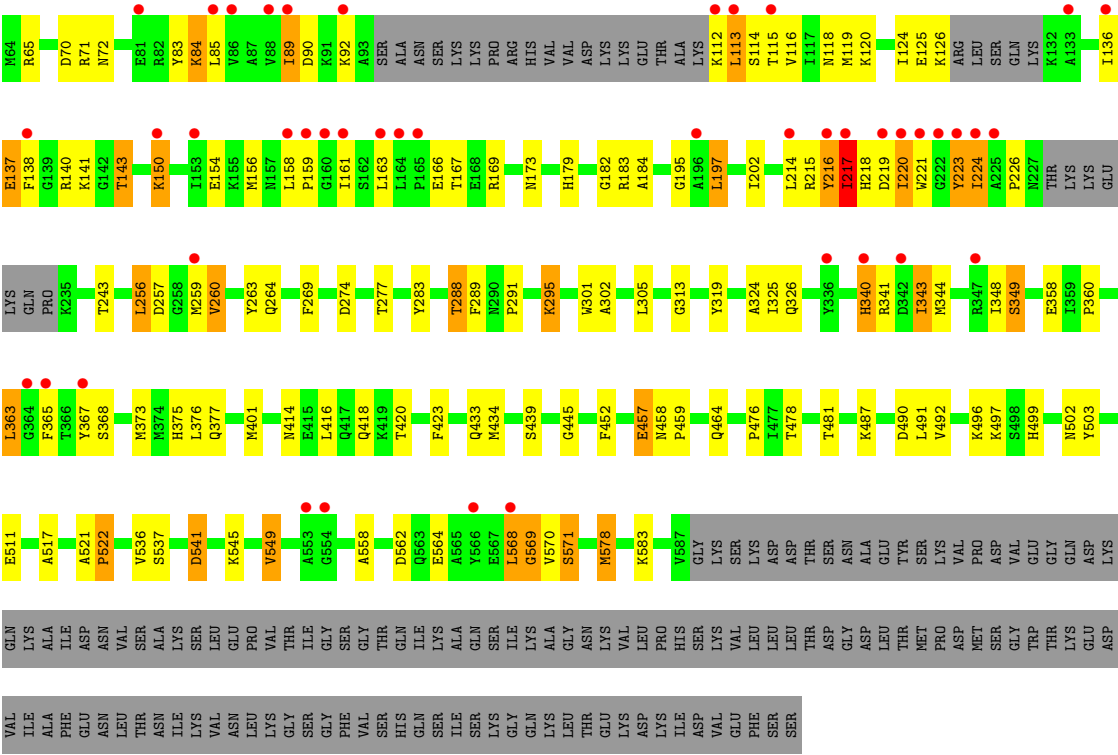


• Molecule 1: Penicillin-binding protein 1



• Molecule 1: Penicillin-binding protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	311.86Å 197.15Å 221.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.03 49.00 – 3.03	Depositor EDS
% Data completeness (in resolution range)	55.2 (49.00-3.03) 55.2 (49.00-3.03)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.246 (Not available) , 0.219	Depositor DCC
R_{free} test set	7237 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	81.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 97.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	48707	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: CL, EPE, CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	1/4195 (0.0%)	1.44	11/5641 (0.2%)
1	B	1.04	4/4247 (0.1%)	1.45	8/5712 (0.1%)
1	C	1.02	1/4188 (0.0%)	1.45	4/5633 (0.1%)
1	D	1.02	1/4044 (0.0%)	1.44	5/5440 (0.1%)
1	E	1.03	2/4210 (0.0%)	1.43	2/5662 (0.0%)
1	F	1.04	2/4256 (0.0%)	1.45	9/5723 (0.2%)
1	G	1.01	1/4188 (0.0%)	1.42	2/5633 (0.0%)
1	H	1.04	2/3787 (0.1%)	1.43	9/5099 (0.2%)
1	I	1.02	3/4172 (0.1%)	1.43	4/5611 (0.1%)
1	J	1.03	1/4169 (0.0%)	1.44	11/5608 (0.2%)
1	K	1.06	3/4117 (0.1%)	1.43	7/5537 (0.1%)
1	L	1.08	4/3979 (0.1%)	1.45	8/5354 (0.1%)
All	All	1.03	25/49552 (0.1%)	1.44	80/66653 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	218	HIS	CE1-NE2	11.29	1.43	1.32
1	L	340	HIS	CE1-NE2	8.34	1.40	1.32
1	I	340	HIS	CE1-NE2	8.33	1.40	1.32
1	K	89	ILE	C-O	7.49	1.31	1.23
1	B	218	HIS	CE1-NE2	6.85	1.39	1.32
1	K	87	ALA	C-O	6.49	1.31	1.24
1	L	363	LEU	C-O	6.48	1.32	1.23
1	F	224	ILE	C-O	6.32	1.31	1.24
1	E	224	ILE	C-O	6.16	1.31	1.24
1	H	342	ASP	CG-OD2	5.98	1.36	1.25
1	B	218	HIS	CG-ND1	5.57	1.44	1.38
1	I	264	GLN	N-CA	5.41	1.50	1.46
1	I	340	HIS	CG-ND1	5.37	1.44	1.38
1	F	264	GLN	N-CA	5.32	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	GLN	N-CA	5.25	1.50	1.46
1	L	264	GLN	N-CA	5.22	1.50	1.46
1	L	360	PRO	C-O	-5.10	1.17	1.23
1	J	219	ASP	CG-OD1	5.10	1.35	1.25
1	G	264	GLN	N-CA	5.08	1.50	1.46
1	E	264	GLN	N-CA	5.08	1.50	1.46
1	H	264	GLN	N-CA	5.05	1.50	1.46
1	D	264	GLN	N-CA	5.02	1.50	1.46
1	A	264	GLN	N-CA	5.02	1.50	1.46
1	B	236	ARG	C-O	5.01	1.30	1.23
1	C	264	GLN	N-CA	5.00	1.50	1.46

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	342	ASP	CA-CB-CG	9.05	121.65	112.60
1	B	342	ASP	CA-CB-CG	8.57	121.17	112.60
1	L	568	LEU	CA-C-O	-8.15	112.91	122.13
1	F	405	GLU	CB-CG-CD	7.92	126.06	112.60
1	A	131	LYS	CB-CA-C	-7.84	105.36	116.34
1	J	523	ASN	N-CA-C	-7.55	103.14	112.88
1	J	342	ASP	CA-CB-CG	7.46	120.06	112.60
1	H	587	VAL	CA-C-O	-7.12	113.31	120.85
1	B	218	HIS	CA-C-O	-6.92	110.61	120.51
1	L	365	PHE	N-CA-C	-6.88	103.22	111.69
1	H	162	SER	CA-C-O	-6.74	111.11	120.21
1	D	342	ASP	CA-CB-CG	6.40	119.00	112.60
1	J	587	VAL	CA-C-O	-6.37	114.09	120.85
1	A	117	ILE	CA-C-O	-6.36	112.83	120.78
1	H	219	ASP	CA-CB-CG	6.29	118.89	112.60
1	F	513	LYS	CG-CD-CE	5.95	124.98	111.30
1	A	219	ASP	CA-CB-CG	5.91	118.51	112.60
1	H	220	ILE	CA-C-O	-5.90	113.41	120.78
1	A	115	THR	N-CA-C	-5.83	106.02	114.12
1	I	546	ASN	CA-CB-CG	5.80	118.40	112.60
1	F	214	LEU	CA-C-O	-5.65	112.43	120.51
1	J	157	ASN	CA-CB-CG	5.59	118.19	112.60
1	D	524	GLY	CA-C-O	-5.52	115.37	121.94
1	F	218	HIS	CA-CB-CG	5.51	119.31	113.80
1	J	215	ARG	CA-C-O	-5.43	114.50	120.69
1	A	342	ASP	CA-CB-CG	5.40	118.00	112.60
1	L	568	LEU	CB-CA-C	-5.40	103.85	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	ASP	CA-C-N	5.40	126.09	119.99
1	D	257	ASP	C-N-CA	5.40	126.09	119.99
1	I	257	ASP	CA-C-N	5.36	126.05	119.99
1	I	257	ASP	C-N-CA	5.36	126.05	119.99
1	A	215	ARG	CB-CG-CD	5.35	123.59	111.30
1	B	257	ASP	CA-C-N	5.33	126.02	119.99
1	B	257	ASP	C-N-CA	5.33	126.02	119.99
1	C	257	ASP	CA-C-N	5.33	126.02	119.99
1	C	257	ASP	C-N-CA	5.33	126.02	119.99
1	K	216	TYR	CA-C-O	-5.33	115.34	121.47
1	J	257	ASP	CA-C-N	5.30	125.98	119.99
1	J	257	ASP	C-N-CA	5.30	125.98	119.99
1	K	89	ILE	N-CA-C	-5.30	107.61	111.90
1	F	96	ASN	CB-CA-C	5.29	117.95	109.07
1	H	257	ASP	CA-C-N	5.27	125.95	119.99
1	H	257	ASP	C-N-CA	5.27	125.95	119.99
1	B	218	HIS	CA-C-N	5.27	130.60	121.64
1	B	218	HIS	C-N-CA	5.27	130.60	121.64
1	A	257	ASP	CA-C-N	5.26	125.94	119.99
1	A	257	ASP	C-N-CA	5.26	125.94	119.99
1	G	257	ASP	CA-C-N	5.26	125.93	119.99
1	G	257	ASP	C-N-CA	5.26	125.93	119.99
1	B	288	THR	CB-CA-C	5.24	121.81	113.37
1	K	219	ASP	N-CA-CB	-5.24	102.70	111.20
1	A	171	TYR	CB-CA-C	5.20	115.64	110.33
1	F	211	LYS	CA-C-O	-5.20	113.52	119.60
1	E	235	LYS	CB-CA-C	5.17	118.31	109.72
1	A	219	ASP	N-CA-C	-5.17	107.99	114.56
1	H	524	GLY	CA-C-O	-5.17	115.25	121.67
1	F	288	THR	CB-CA-C	5.16	121.68	113.37
1	L	288	THR	CB-CA-C	5.15	121.66	113.37
1	B	409	GLN	N-CA-CB	-5.11	101.89	111.13
1	K	257	ASP	CA-C-N	5.10	125.76	119.99
1	K	257	ASP	C-N-CA	5.10	125.76	119.99
1	J	171	TYR	CB-CA-C	5.09	115.53	110.33
1	C	288	THR	CB-CA-C	5.09	121.57	113.37
1	I	288	THR	CB-CA-C	5.09	121.57	113.37
1	J	288	THR	CB-CA-C	5.09	121.57	113.37
1	J	104	VAL	N-CA-CB	5.08	116.74	110.64
1	F	257	ASP	CA-C-N	5.08	125.73	119.99
1	F	257	ASP	C-N-CA	5.08	125.73	119.99
1	L	363	LEU	N-CA-C	-5.07	103.71	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	SER	CA-C-O	-5.06	115.97	121.89
1	K	89	ILE	CB-CA-C	5.05	116.15	111.30
1	L	257	ASP	CA-C-N	5.04	125.69	119.99
1	L	257	ASP	C-N-CA	5.04	125.69	119.99
1	D	221	TRP	CB-CA-C	5.04	117.81	110.26
1	L	568	LEU	N-CA-C	-5.03	99.14	108.24
1	A	288	THR	CB-CA-C	5.03	121.46	113.37
1	K	288	THR	CB-CA-C	5.02	121.45	113.37
1	H	342	ASP	CA-CB-CG	5.01	117.61	112.60
1	J	383	ASP	CA-CB-CG	5.01	117.61	112.60
1	H	288	THR	CB-CA-C	5.01	121.43	113.37

There are no chirality outliers.

There are no planarity outliers.

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	4105	0	4096	73	0
1	B	4156	0	4149	80	0
1	C	4098	0	4084	65	0
1	D	3958	0	3928	67	0
1	E	4120	0	4109	85	0
1	F	4165	0	4162	79	0
1	G	4098	0	4084	75	0
1	H	3703	0	3646	67	0
1	I	4083	0	4070	61	0
1	J	4080	0	4062	67	0
1	K	4029	0	4013	80	0
1	L	3894	0	3855	65	0
2	A	15	0	18	0	0
2	B	15	0	18	0	0
2	C	15	0	17	0	0
2	D	15	0	17	0	0
2	E	15	0	17	0	0
2	F	15	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	15	0	17	0	0
2	H	15	0	18	1	0
2	I	15	0	18	1	0
2	J	15	0	18	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	C	1	0	0	2	0
4	D	1	0	0	1	0
4	E	1	0	0	2	0
4	F	1	0	0	1	0
4	H	1	0	0	1	0
4	J	1	0	0	1	0
4	K	1	0	0	2	0
4	L	1	0	0	1	0
5	A	3	0	0	1	0
5	B	3	0	0	0	0
5	C	6	0	0	0	0
5	D	3	0	0	1	0
5	E	7	0	0	0	0
5	F	8	0	0	1	0
5	G	5	0	0	0	0
5	H	3	0	0	0	0
5	I	4	0	0	1	0
5	J	4	0	0	1	0
5	K	3	0	0	1	0
5	L	1	0	0	0	0
All	All	48707	0	48433	824	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 8.

All (824) 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:E:343:ILE:HG21	1:E:348:ILE:HD11	1.16	1.15
1:J:117:ILE:HD11	1:J:141:LYS:O	1.51	1.11
1:H:85:LEU:HD12	1:H:163:LEU:HD21	1.40	1.02
1:F:223:TYR:O	1:F:224:ILE:HG12	1.58	1.01
1:A:437:ALA:HA	1:A:447:MET:HE2	1.42	1.01
1:K:110:ALA:HB3	1:K:125:GLU:OE2	1.65	0.95
1:E:343:ILE:CG2	1:E:348:ILE:HD11	1.96	0.95
1:K:375:HIS:ND1	4:K:801:CL:CL	2.36	0.94
1:D:225:ALA:HB2	1:H:219:ASP:OD1	1.67	0.93
1:L:158:LEU:HG	1:L:159:PRO:HD2	1.50	0.93
1:E:215:ARG:NH1	1:E:224:ILE:HG23	1.86	0.91
1:A:392:PHE:HA	1:A:447:MET:HE1	1.53	0.88
1:A:392:PHE:CA	1:A:447:MET:HE1	2.02	0.88
1:B:463:ARG:HG2	1:H:473:ALA:O	1.72	0.87
1:F:221:TRP:HB3	1:J:222:GLY:HA2	1.55	0.87
1:D:223:TYR:O	1:D:224:ILE:HG13	1.74	0.86
1:I:66:GLY:HA2	1:I:236:ARG:NH2	1.91	0.86
1:C:375:HIS:ND1	4:C:802:CL:CL	2.45	0.84
1:H:375:HIS:ND1	4:H:802:CL:CL	2.49	0.82
1:E:343:ILE:HG21	1:E:348:ILE:CD1	2.06	0.81
1:B:343:ILE:HD11	1:B:416:LEU:HA	1.62	0.81
1:K:217:ILE:HB	1:K:466:TYR:HB2	1.60	0.80
1:A:539:MET:CE	1:A:550:ILE:CG2	2.60	0.80
1:A:392:PHE:CD1	1:A:447:MET:CE	2.65	0.79
1:F:112:LYS:O	1:F:115:THR:HG22	1.82	0.79
1:G:551:VAL:CG1	1:G:574:PHE:CE1	2.65	0.79
1:E:348:ILE:HD12	1:E:374:MET:SD	2.23	0.79
1:D:375:HIS:ND1	4:D:802:CL:CL	2.52	0.79
1:E:375:HIS:ND1	4:E:802:CL:CL	2.52	0.79
1:F:443:ASN:OD1	1:F:448:LEU:HD11	1.83	0.79
1:A:392:PHE:HA	1:A:447:MET:CE	2.13	0.79
1:F:119:MET:HE3	1:F:124:ILE:HG12	1.65	0.78
1:K:272:VAL:CG1	1:K:549:VAL:HG21	2.14	0.78
1:B:220:ILE:HD12	1:B:220:ILE:O	1.84	0.77
1:E:223:TYR:HE1	1:E:403:ASP:HB2	1.49	0.76
1:J:260:VAL:O	1:J:264:GLN:HG3	1.85	0.76
1:K:110:ALA:CB	1:K:125:GLU:OE2	2.34	0.76
1:B:271:VAL:HG11	1:B:305:LEU:HD13	1.67	0.75
1:B:217:ILE:HG23	1:B:224:ILE:HG21	1.68	0.74
1:D:217:ILE:HB	1:D:466:TYR:HB2	1.68	0.74
1:A:392:PHE:HD1	1:A:447:MET:CE	2.01	0.74
1:L:220:ILE:HG12	1:L:224:ILE:HG13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:LEU:HD22	1:K:117:ILE:HD11	1.69	0.73
1:G:551:VAL:CG1	1:G:574:PHE:HE1	2.03	0.72
1:L:217:ILE:HD11	1:L:401:MET:HE1	1.70	0.72
1:C:84:LYS:HD2	1:C:164:LEU:HD11	1.72	0.71
1:F:223:TYR:C	1:F:224:ILE:HG12	2.14	0.71
1:I:321:LEU:CD2	1:I:325:ILE:HG13	2.22	0.70
1:L:217:ILE:HA	1:L:224:ILE:HG21	1.73	0.70
1:E:226:PRO:C	1:E:228:THR:H	1.98	0.70
1:I:321:LEU:HD22	1:I:325:ILE:HG13	1.73	0.70
1:A:539:MET:CE	1:A:550:ILE:HG23	2.22	0.69
1:F:443:ASN:OD1	1:F:448:LEU:CD1	2.39	0.69
1:J:88:VAL:HG11	1:J:101:ARG:O	1.93	0.69
1:G:551:VAL:HG11	1:G:574:PHE:CE1	2.27	0.69
1:J:82:ARG:NH2	1:J:144:ASN:ND2	2.41	0.69
1:A:392:PHE:CD1	1:A:447:MET:HE3	2.28	0.68
1:F:218:HIS:HB3	1:J:223:TYR:CE2	2.28	0.68
1:G:116:VAL:HG11	1:G:153:ILE:HG12	1.76	0.68
1:B:88:VAL:HG11	1:B:101:ARG:O	1.94	0.67
1:F:463:ARG:HD2	1:J:473:ALA:O	1.94	0.67
1:E:343:ILE:CG2	1:E:348:ILE:CD1	2.69	0.66
1:G:551:VAL:HG12	1:G:578:MET:HE2	1.76	0.66
1:K:113:LEU:HD21	1:K:161:ILE:CD1	2.25	0.66
1:B:217:ILE:HB	1:B:466:TYR:HB2	1.77	0.66
1:A:271:VAL:HG22	1:A:283:TYR:HD1	1.60	0.66
1:E:223:TYR:CE1	1:E:403:ASP:HB2	2.31	0.66
1:G:551:VAL:CG1	1:G:578:MET:HE2	2.25	0.66
1:E:220:ILE:HG23	1:E:401:MET:HG3	1.78	0.65
1:G:271:VAL:HG22	1:G:283:TYR:HD1	1.61	0.65
1:F:443:ASN:CG	1:F:448:LEU:HD11	2.20	0.65
1:L:84:LYS:HE2	1:L:137:GLU:HB3	1.78	0.65
1:F:271:VAL:HG22	1:F:283:TYR:HD1	1.62	0.64
1:K:273:MET:CE	1:K:435:LEU:HB3	2.27	0.64
1:A:218:HIS:NE2	1:B:223:TYR:CE1	2.66	0.64
1:C:272:VAL:HG13	1:C:549:VAL:CG1	2.27	0.64
1:J:88:VAL:CG1	1:J:101:ARG:O	2.46	0.64
1:F:375:HIS:ND1	4:F:802:CL:CL	2.66	0.64
1:I:66:GLY:HA2	1:I:236:ARG:HH21	1.61	0.64
1:J:86:VAL:HG21	1:J:135:GLN:OE1	1.98	0.64
1:C:272:VAL:HG13	1:C:549:VAL:HG11	1.79	0.64
1:A:539:MET:HE3	1:A:550:ILE:HG23	1.80	0.63
1:A:539:MET:CE	1:A:550:ILE:HG21	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:VAL:HG23	1:E:578:MET:CE	2.29	0.62
1:A:539:MET:HE1	1:A:550:ILE:CG2	2.28	0.62
1:B:88:VAL:CG1	1:B:101:ARG:O	2.47	0.62
1:L:220:ILE:HG12	1:L:224:ILE:CG1	2.28	0.62
1:E:217:ILE:HB	1:E:466:TYR:HB2	1.82	0.62
1:K:273:MET:HE3	1:K:435:LEU:HB3	1.81	0.62
1:I:549:VAL:HG23	1:I:578:MET:CE	2.29	0.62
1:I:549:VAL:HG23	1:I:578:MET:HE1	1.82	0.62
1:A:443:ASN:CG	1:A:448:LEU:HD11	2.24	0.62
1:K:90:ASP:HB2	1:K:134:PHE:HA	1.82	0.62
1:E:549:VAL:HG23	1:E:578:MET:HE1	1.82	0.62
1:K:214:LEU:H	1:K:226:PRO:HB2	1.65	0.62
1:B:271:VAL:HG13	1:B:283:TYR:HD1	1.65	0.61
1:L:375:HIS:ND1	4:L:801:CL:CL	2.68	0.61
1:D:313:GLY:HA3	1:D:517:ALA:HB2	1.83	0.61
1:K:217:ILE:HG23	1:K:224:ILE:HG12	1.82	0.60
1:L:83:TYR:HB3	1:L:163:LEU:HG	1.83	0.60
1:A:392:PHE:C	1:A:447:MET:HE1	2.26	0.60
1:I:313:GLY:HA3	1:I:517:ALA:HB2	1.84	0.60
1:G:242:LEU:HB3	1:G:244:ILE:HD12	1.82	0.60
1:A:313:GLY:HA3	1:A:517:ALA:HB2	1.83	0.60
1:G:271:VAL:HG21	1:G:305:LEU:HD13	1.84	0.60
1:K:273:MET:HE2	1:K:450:PRO:HB3	1.84	0.60
1:K:313:GLY:HA3	1:K:517:ALA:HB2	1.83	0.60
1:E:313:GLY:HA3	1:E:517:ALA:HB2	1.83	0.60
1:F:217:ILE:HB	1:F:466:TYR:HB2	1.83	0.60
1:G:222:GLY:HA2	1:K:221:TRP:HB2	1.84	0.60
1:I:321:LEU:CD2	1:I:321:LEU:C	2.74	0.60
1:C:313:GLY:HA3	1:C:517:ALA:HB2	1.83	0.60
1:F:313:GLY:HA3	1:F:517:ALA:HB2	1.83	0.60
1:J:313:GLY:HA3	1:J:517:ALA:HB2	1.83	0.60
1:L:158:LEU:HG	1:L:159:PRO:CD	2.28	0.60
1:G:313:GLY:HA3	1:G:517:ALA:HB2	1.83	0.59
1:C:214:LEU:HD21	1:G:214:LEU:HD11	1.83	0.59
1:E:240:VAL:HG12	1:E:456:VAL:HG22	1.84	0.59
1:F:343:ILE:HD11	1:F:416:LEU:HA	1.84	0.59
1:G:206:TYR:OH	1:G:223:TYR:O	2.21	0.59
1:J:243:THR:OG1	1:J:452:PHE:HA	2.02	0.59
1:A:243:THR:OG1	1:A:452:PHE:HA	2.02	0.59
1:B:209:GLY:O	1:B:210:SER:CB	2.50	0.59
1:H:313:GLY:HA3	1:H:517:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:LEU:HD12	1:J:138:PHE:CD2	2.37	0.59
1:D:243:THR:OG1	1:D:452:PHE:HA	2.03	0.59
1:C:103:VAL:O	1:C:103:VAL:HG13	2.02	0.59
1:E:116:VAL:HG21	1:E:153:ILE:HD11	1.84	0.59
1:G:243:THR:OG1	1:G:452:PHE:HA	2.03	0.59
1:L:313:GLY:HA3	1:L:517:ALA:HB2	1.84	0.59
1:B:313:GLY:HA3	1:B:517:ALA:HB2	1.84	0.59
1:F:223:TYR:CE2	1:F:403:ASP:HB2	2.37	0.59
1:I:511:GLU:HG3	1:I:541:ASP:OD1	2.03	0.59
1:K:113:LEU:HD21	1:K:161:ILE:HD12	1.85	0.58
1:K:243:THR:OG1	1:K:452:PHE:HA	2.02	0.58
1:C:140:ARG:HH12	1:C:144:ASN:HD22	1.51	0.58
1:F:243:THR:OG1	1:F:452:PHE:HA	2.02	0.58
1:L:243:THR:OG1	1:L:452:PHE:HA	2.03	0.58
1:L:511:GLU:HG3	1:L:541:ASP:OD1	2.03	0.58
1:A:103:VAL:O	1:A:103:VAL:HG13	2.02	0.58
1:D:220:ILE:HA	1:D:223:TYR:O	2.04	0.58
1:A:539:MET:HE1	1:A:550:ILE:HG21	1.86	0.58
1:K:272:VAL:HG12	1:K:549:VAL:HG21	1.85	0.58
1:B:199:VAL:HA	1:B:202:ILE:HD11	1.86	0.58
1:A:271:VAL:HG21	1:A:305:LEU:HD13	1.84	0.58
1:E:215:ARG:NH2	1:E:217:ILE:O	2.36	0.58
1:I:115:THR:OG1	1:I:156:MET:HE1	2.04	0.58
1:I:449:LYS:HD3	1:L:216:TYR:HE2	1.68	0.58
1:A:448:LEU:HD12	1:A:448:LEU:N	2.19	0.58
1:B:216:TYR:HE2	1:H:449:LYS:HD3	1.68	0.58
1:B:243:THR:OG1	1:B:452:PHE:HA	2.03	0.58
1:D:84:LYS:HG2	1:D:166:GLU:HG2	1.86	0.58
1:I:243:THR:OG1	1:I:452:PHE:HA	2.03	0.58
1:H:243:THR:OG1	1:H:452:PHE:HA	2.03	0.58
1:G:132:LYS:HE3	1:G:132:LYS:HA	1.85	0.57
1:C:243:THR:OG1	1:C:452:PHE:HA	2.03	0.57
1:C:511:GLU:HG3	1:C:541:ASP:OD1	2.03	0.57
1:C:528:VAL:HG13	1:C:533:PRO:HB2	1.85	0.57
1:H:205:SER:HA	1:H:211:LYS:HE2	1.87	0.57
1:H:458:ASN:OD1	1:H:459:PRO:HD2	2.05	0.57
1:A:443:ASN:ND2	1:A:448:LEU:HD11	2.19	0.57
1:C:458:ASN:OD1	1:C:459:PRO:HD2	2.04	0.57
1:K:513:LYS:HZ2	1:K:514:THR:HG22	1.70	0.57
1:L:319:TYR:HE2	1:L:434:MET:HE2	1.70	0.57
1:C:274:ASP:HB3	1:C:277:THR:OG1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:THR:OG1	1:E:452:PHE:HA	2.03	0.57
1:G:458:ASN:OD1	1:G:459:PRO:HD2	2.04	0.57
1:A:274:ASP:HB3	1:A:277:THR:OG1	2.05	0.57
1:E:106:LYS:HE3	1:E:128:LEU:O	2.04	0.57
1:F:111:LYS:HD3	1:F:121:PRO:HB3	1.85	0.57
1:F:159:PRO:HA	5:F:906:HOH:O	2.05	0.57
1:G:551:VAL:CG1	1:G:574:PHE:CD1	2.88	0.57
1:J:458:ASN:OD1	1:J:459:PRO:HD2	2.04	0.57
1:A:458:ASN:OD1	1:A:459:PRO:HD2	2.04	0.56
1:E:217:ILE:HA	1:E:224:ILE:HG21	1.87	0.56
1:E:274:ASP:HB3	1:E:277:THR:OG1	2.05	0.56
1:J:274:ASP:HB3	1:J:277:THR:OG1	2.05	0.56
1:L:274:ASP:HB3	1:L:277:THR:OG1	2.05	0.56
1:B:458:ASN:OD1	1:B:459:PRO:HD2	2.05	0.56
1:D:458:ASN:OD1	1:D:459:PRO:HD2	2.05	0.56
1:E:337:LYS:O	1:E:341:ARG:NH2	2.39	0.56
1:G:352:ASN:HB2	1:I:105:ASP:HB2	1.86	0.56
1:I:274:ASP:HB3	1:I:277:THR:OG1	2.05	0.56
1:J:85:LEU:HD12	1:J:138:PHE:CE2	2.40	0.56
1:A:507:GLY:HA3	1:A:589:LYS:HG3	1.88	0.56
1:K:326:GLN:OE1	1:K:478:THR:HG23	2.06	0.56
1:J:206:TYR:OH	1:J:223:TYR:O	2.22	0.56
1:F:274:ASP:HB3	1:F:277:THR:OG1	2.06	0.56
1:F:458:ASN:OD1	1:F:459:PRO:HD2	2.05	0.56
1:I:478:THR:HG1	1:I:481:THR:H	1.54	0.56
1:L:458:ASN:OD1	1:L:459:PRO:HD2	2.05	0.56
1:B:274:ASP:HB3	1:B:277:THR:OG1	2.05	0.56
1:B:326:GLN:OE1	1:B:478:THR:HG23	2.06	0.56
1:F:271:VAL:HG21	1:F:305:LEU:HD13	1.87	0.56
1:H:326:GLN:OE1	1:H:478:THR:HG23	2.06	0.56
1:B:202:ILE:HG13	1:B:203:PHE:CD2	2.41	0.56
1:G:107:LYS:HG2	1:G:125:GLU:OE2	2.06	0.56
1:G:274:ASP:HB3	1:G:277:THR:OG1	2.05	0.56
1:J:326:GLN:OE1	1:J:478:THR:HG23	2.06	0.56
1:E:458:ASN:OD1	1:E:459:PRO:HD2	2.06	0.56
1:E:478:THR:HG1	1:E:481:THR:H	1.54	0.56
1:G:326:GLN:OE1	1:G:478:THR:HG23	2.06	0.56
1:I:458:ASN:OD1	1:I:459:PRO:HD2	2.05	0.56
1:K:233:GLN:HB3	1:K:234:PRO:HD2	1.88	0.56
1:L:326:GLN:OE1	1:L:478:THR:HG23	2.07	0.56
1:D:326:GLN:OE1	1:D:478:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:274:ASP:HB3	1:H:277:THR:OG1	2.05	0.55
1:C:326:GLN:OE1	1:C:478:THR:HG23	2.06	0.55
1:H:182:GLY:HA3	1:H:197:LEU:O	2.06	0.55
1:I:347:ARG:NH2	5:I:901:HOH:O	2.37	0.55
1:K:274:ASP:HB3	1:K:277:THR:OG1	2.06	0.55
1:A:326:GLN:OE1	1:A:478:THR:HG23	2.06	0.55
1:C:182:GLY:HA3	1:C:197:LEU:O	2.07	0.55
1:E:182:GLY:HA3	1:E:197:LEU:O	2.07	0.55
1:K:113:LEU:HD21	1:K:161:ILE:HD11	1.88	0.55
1:B:199:VAL:HA	1:B:202:ILE:CG1	2.36	0.55
1:F:326:GLN:OE1	1:F:478:THR:HG23	2.06	0.55
1:D:274:ASP:HB3	1:D:277:THR:OG1	2.05	0.55
1:F:448:LEU:N	1:F:448:LEU:HD12	2.22	0.55
1:K:458:ASN:OD1	1:K:459:PRO:HD2	2.06	0.55
1:B:105:ASP:HB2	1:E:352:ASN:HB2	1.89	0.55
1:E:68:ILE:HG12	1:E:240:VAL:CG2	2.37	0.55
1:G:478:THR:HG1	1:G:481:THR:H	1.54	0.55
1:G:551:VAL:HG11	1:G:574:PHE:CD1	2.42	0.55
1:L:182:GLY:HA3	1:L:197:LEU:O	2.07	0.55
1:F:182:GLY:HA3	1:F:197:LEU:O	2.07	0.54
1:F:216:TYR:HE2	1:J:449:LYS:HD3	1.72	0.54
1:K:272:VAL:CG1	1:K:549:VAL:CG2	2.85	0.54
1:A:206:TYR:OH	1:A:223:TYR:O	2.24	0.54
1:J:182:GLY:HA3	1:J:197:LEU:O	2.07	0.54
1:B:414:ASN:C	1:B:414:ASN:OD1	2.51	0.54
1:D:182:GLY:HA3	1:D:197:LEU:O	2.06	0.54
1:J:414:ASN:OD1	1:J:414:ASN:C	2.51	0.54
1:E:343:ILE:CG2	1:E:348:ILE:CG1	2.85	0.54
1:H:414:ASN:OD1	1:H:414:ASN:C	2.50	0.54
1:C:206:TYR:OH	1:C:223:TYR:O	2.24	0.54
1:E:326:GLN:OE1	1:E:478:THR:HG23	2.06	0.54
1:G:182:GLY:HA3	1:G:197:LEU:O	2.07	0.54
1:H:87:ALA:HA	1:H:160:GLY:O	2.07	0.54
1:I:326:GLN:OE1	1:I:478:THR:HG23	2.07	0.54
1:I:414:ASN:C	1:I:414:ASN:OD1	2.51	0.54
1:F:99:LYS:HG3	1:F:101:ARG:HD3	1.90	0.54
1:J:117:ILE:HG23	1:J:119:MET:H	1.71	0.54
1:J:457:GLU:HB3	1:J:464:GLN:HA	1.90	0.54
1:L:414:ASN:C	1:L:414:ASN:OD1	2.50	0.54
1:A:182:GLY:HA3	1:A:197:LEU:O	2.08	0.54
1:A:392:PHE:O	1:A:447:MET:HE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLY:HA3	1:B:197:LEU:O	2.07	0.54
1:C:214:LEU:HD13	1:K:221:TRP:CH2	2.43	0.54
1:E:259:MET:HE1	1:E:572:LYS:CB	2.38	0.54
1:F:116:VAL:HG22	1:F:152:LYS:CE	2.37	0.54
1:G:551:VAL:HG13	1:G:574:PHE:CE1	2.43	0.54
1:I:182:GLY:HA3	1:I:197:LEU:O	2.07	0.54
1:K:182:GLY:HA3	1:K:197:LEU:O	2.07	0.54
1:L:377:GLN:HE22	1:L:418:GLN:HB3	1.73	0.54
1:A:414:ASN:OD1	1:A:414:ASN:C	2.51	0.54
1:E:414:ASN:OD1	1:E:414:ASN:C	2.51	0.54
1:K:272:VAL:HG12	1:K:549:VAL:CG2	2.38	0.54
1:K:414:ASN:OD1	1:K:414:ASN:C	2.50	0.54
1:C:414:ASN:OD1	1:C:414:ASN:C	2.50	0.53
1:K:229:LYS:O	1:K:230:LYS:C	2.50	0.53
1:A:478:THR:HG1	1:A:481:THR:H	1.57	0.53
1:B:199:VAL:O	1:B:202:ILE:HG12	2.09	0.53
1:G:473:ALA:O	1:K:463:ARG:HD2	2.09	0.53
1:F:414:ASN:OD1	1:F:414:ASN:C	2.51	0.53
1:F:516:THR:HB	2:F:801:EPE:H71	1.91	0.53
1:G:414:ASN:C	1:G:414:ASN:OD1	2.51	0.53
1:D:414:ASN:C	1:D:414:ASN:OD1	2.50	0.53
1:H:85:LEU:HA	1:H:163:LEU:HD23	1.91	0.53
1:L:217:ILE:HA	1:L:224:ILE:CG2	2.39	0.53
1:C:216:TYR:CD2	1:K:222:GLY:HA2	2.43	0.53
1:G:259:MET:HE1	1:G:572:LYS:CB	2.39	0.53
1:H:85:LEU:HD12	1:H:163:LEU:CD2	2.27	0.53
1:L:478:THR:HG1	1:L:481:THR:H	1.57	0.52
1:A:259:MET:HE1	1:A:572:LYS:CB	2.39	0.52
1:A:443:ASN:ND2	1:A:448:LEU:CD1	2.72	0.52
1:B:199:VAL:HA	1:B:202:ILE:HG12	1.91	0.52
1:F:238:ASP:OD2	1:F:465:PHE:CE2	2.63	0.52
1:F:457:GLU:HB3	1:F:464:GLN:HA	1.91	0.52
1:I:321:LEU:CD2	1:I:325:ILE:CG1	2.87	0.52
1:K:259:MET:HE1	1:K:572:LYS:CB	2.40	0.52
1:C:161:ILE:HD12	1:C:161:ILE:O	2.10	0.52
1:C:457:GLU:HB3	1:C:464:GLN:HA	1.92	0.52
1:D:259:MET:HE1	1:D:572:LYS:CB	2.40	0.52
1:B:259:MET:HE1	1:B:572:LYS:CB	2.39	0.52
1:H:259:MET:HE1	1:H:572:LYS:CB	2.40	0.52
1:E:226:PRO:C	1:E:228:THR:N	2.66	0.52
1:B:457:GLU:HB3	1:B:464:GLN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:478:THR:HG1	1:H:481:THR:H	1.57	0.52
1:L:457:GLU:HB3	1:L:464:GLN:HA	1.91	0.52
1:I:259:MET:HE1	1:I:572:LYS:CB	2.40	0.52
1:K:457:GLU:HB3	1:K:464:GLN:HA	1.92	0.52
1:C:259:MET:HE1	1:C:572:LYS:CB	2.40	0.52
1:H:457:GLU:HB3	1:H:464:GLN:HA	1.91	0.52
1:K:221:TRP:HA	1:K:221:TRP:CE3	2.44	0.52
1:B:214:LEU:H	1:B:226:PRO:HB2	1.75	0.51
1:G:551:VAL:HG12	1:G:578:MET:CE	2.39	0.51
1:G:551:VAL:HG13	1:G:551:VAL:O	2.10	0.51
1:L:217:ILE:CA	1:L:224:ILE:HG21	2.40	0.51
1:F:96:ASN:C	1:F:98:LYS:H	2.17	0.51
1:C:375:HIS:CE1	4:C:802:CL:CL	3.00	0.51
1:E:226:PRO:O	1:E:228:THR:N	2.40	0.51
1:E:215:ARG:HH11	1:E:224:ILE:HG23	1.70	0.51
1:H:205:SER:O	1:H:211:LYS:HG2	2.10	0.51
1:A:207:LEU:CD1	1:A:240:VAL:HG23	2.40	0.51
1:F:221:TRP:CB	1:J:222:GLY:HA2	2.35	0.51
1:B:216:TYR:HE2	1:H:449:LYS:CD	2.24	0.51
1:C:272:VAL:CG1	1:C:549:VAL:HG11	2.40	0.51
1:E:103:VAL:HG23	1:E:103:VAL:O	2.10	0.51
1:G:457:GLU:HB3	1:G:464:GLN:HA	1.92	0.51
1:D:478:THR:HG1	1:D:481:THR:H	1.58	0.51
1:E:457:GLU:HB3	1:E:464:GLN:HA	1.92	0.51
1:G:449:LYS:HD3	1:K:216:TYR:HE2	1.76	0.51
1:K:478:THR:HG1	1:K:481:THR:H	1.57	0.51
1:L:568:LEU:O	1:L:569:GLY:O	2.28	0.51
1:C:343:ILE:HG12	1:C:419:LYS:HG3	1.93	0.51
1:H:84:LYS:HD2	1:H:143:THR:HG23	1.92	0.51
1:J:259:MET:HE1	1:J:572:LYS:CB	2.40	0.51
1:B:216:TYR:CE2	1:H:449:LYS:HD3	2.46	0.50
1:E:375:HIS:CE1	4:E:802:CL:CL	3.01	0.50
1:D:223:TYR:CD1	1:D:223:TYR:N	2.79	0.50
1:H:343:ILE:HG12	1:H:419:LYS:HG3	1.94	0.50
1:B:271:VAL:HG13	1:B:283:TYR:CD1	2.46	0.50
1:A:392:PHE:HD1	1:A:447:MET:HE2	1.76	0.50
1:E:104:VAL:HG23	1:E:105:ASP:N	2.26	0.50
1:G:221:TRP:HH2	1:G:399:LYS:HD2	1.76	0.50
1:A:448:LEU:HD12	1:A:448:LEU:H	1.77	0.50
1:J:375:HIS:ND1	4:J:802:CL:CL	2.69	0.50
1:I:321:LEU:HD22	1:I:325:ILE:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ASP:OD2	1:E:465:PHE:CE2	2.64	0.50
1:A:209:GLY:O	1:A:235:LYS:HB2	2.12	0.49
1:F:233:GLN:CB	1:F:234:PRO:CD	2.90	0.49
1:I:457:GLU:HB3	1:I:464:GLN:HA	1.93	0.49
1:K:112:LYS:CE	1:K:158:LEU:HD21	2.41	0.49
1:B:199:VAL:HA	1:B:202:ILE:CD1	2.42	0.49
1:B:209:GLY:O	1:B:210:SER:OG	2.27	0.49
1:F:420:THR:HA	1:F:423:PHE:CZ	2.47	0.49
1:G:538:PHE:HE1	1:G:540:GLY:HA3	1.77	0.49
1:D:420:THR:HA	1:D:423:PHE:CZ	2.48	0.49
1:E:420:THR:HA	1:E:423:PHE:CZ	2.48	0.49
1:J:420:THR:HA	1:J:423:PHE:CZ	2.48	0.49
1:C:478:THR:HG1	1:C:481:THR:H	1.58	0.49
1:D:212:GLY:HA3	1:D:229:LYS:HB3	1.93	0.49
1:G:223:TYR:CE2	1:K:218:HIS:HB3	2.48	0.49
1:A:223:TYR:CE2	1:D:218:HIS:HB3	2.48	0.49
1:F:269:PHE:C	1:F:269:PHE:CD1	2.91	0.49
1:G:420:THR:HA	1:G:423:PHE:CZ	2.48	0.49
1:B:463:ARG:CG	1:H:473:ALA:O	2.53	0.49
1:D:377:GLN:HE22	1:D:418:GLN:HB3	1.78	0.49
1:I:104:VAL:HG23	1:I:105:ASP:N	2.28	0.49
1:K:420:THR:HA	1:K:423:PHE:CZ	2.48	0.49
1:L:269:PHE:CD1	1:L:269:PHE:C	2.91	0.49
1:A:420:THR:HA	1:A:423:PHE:CZ	2.47	0.49
1:A:457:GLU:HB3	1:A:464:GLN:HA	1.93	0.49
1:B:269:PHE:CD1	1:B:269:PHE:C	2.91	0.49
1:C:420:THR:HA	1:C:423:PHE:CZ	2.48	0.49
1:D:201:LYS:HG2	1:D:223:TYR:HE2	1.78	0.49
1:D:269:PHE:CD1	1:D:269:PHE:C	2.91	0.49
1:E:109:THR:HG22	1:E:158:LEU:HG	1.95	0.49
1:F:448:LEU:HD12	1:F:448:LEU:H	1.77	0.49
1:A:89:ILE:HA	1:A:103:VAL:HG12	1.95	0.49
1:A:127:ARG:NH1	5:A:901:HOH:O	2.45	0.49
1:B:420:THR:HA	1:B:423:PHE:CZ	2.48	0.49
1:D:457:GLU:HB3	1:D:464:GLN:HA	1.93	0.49
1:F:301:TRP:CE3	1:F:302:ALA:N	2.81	0.49
1:F:478:THR:HG1	1:F:481:THR:H	1.58	0.49
1:H:420:THR:HA	1:H:423:PHE:CZ	2.48	0.49
1:J:217:ILE:HG13	1:J:223:TYR:HB2	1.95	0.49
1:A:207:LEU:HD13	1:A:240:VAL:HG23	1.95	0.49
1:B:478:THR:HG1	1:B:481:THR:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:TYR:N	1:D:223:TYR:HD1	2.11	0.49
1:H:377:GLN:HE22	1:H:418:GLN:HB3	1.78	0.49
1:I:420:THR:HA	1:I:423:PHE:CZ	2.48	0.49
1:C:377:GLN:HE22	1:C:418:GLN:HB3	1.78	0.48
1:G:115:THR:HG23	1:G:152:LYS:HE2	1.95	0.48
1:H:86:VAL:HG23	1:H:162:SER:HB3	1.95	0.48
1:I:301:TRP:CE3	1:I:302:ALA:N	2.81	0.48
1:J:269:PHE:CD1	1:J:269:PHE:C	2.91	0.48
1:J:478:THR:HG1	1:J:481:THR:H	1.59	0.48
1:A:301:TRP:CE3	1:A:302:ALA:N	2.81	0.48
1:B:301:TRP:CE3	1:B:302:ALA:N	2.81	0.48
1:D:223:TYR:C	1:D:224:ILE:HG13	2.37	0.48
1:H:220:ILE:CG2	1:H:220:ILE:O	2.61	0.48
1:I:269:PHE:CD1	1:I:269:PHE:C	2.91	0.48
1:K:341:ARG:HH21	1:K:371:THR:HB	1.77	0.48
1:L:301:TRP:CE3	1:L:302:ALA:N	2.81	0.48
1:E:117:ILE:HG23	1:E:119:MET:H	1.79	0.48
1:D:217:ILE:HA	1:D:224:ILE:HG21	1.95	0.48
1:G:269:PHE:CD1	1:G:269:PHE:C	2.91	0.48
1:J:167:THR:O	1:J:186:LYS:HE3	2.13	0.48
1:E:301:TRP:CE3	1:E:302:ALA:N	2.81	0.48
1:K:301:TRP:CE3	1:K:302:ALA:N	2.81	0.48
1:L:420:THR:HA	1:L:423:PHE:CZ	2.48	0.48
1:A:271:VAL:HG22	1:A:283:TYR:CD1	2.44	0.48
1:K:209:GLY:O	1:K:235:LYS:HB2	2.14	0.48
1:C:301:TRP:CE3	1:C:302:ALA:N	2.81	0.48
1:E:146:THR:OG1	1:E:148:GLN:HG2	2.14	0.48
1:F:259:MET:HE1	1:F:570:VAL:HA	1.95	0.48
1:C:269:PHE:CD1	1:C:269:PHE:C	2.91	0.48
1:D:301:TRP:CE3	1:D:302:ALA:N	2.81	0.48
1:H:269:PHE:CD1	1:H:269:PHE:C	2.91	0.48
1:A:269:PHE:C	1:A:269:PHE:CD1	2.91	0.48
1:E:269:PHE:CD1	1:E:269:PHE:C	2.91	0.48
1:F:301:TRP:CE3	1:F:302:ALA:HA	2.49	0.48
1:H:301:TRP:CE3	1:H:302:ALA:N	2.82	0.48
1:I:220:ILE:O	1:I:220:ILE:CG2	2.61	0.48
1:B:231:GLU:O	1:B:231:GLU:HG2	2.13	0.47
1:L:259:MET:HE1	1:L:570:VAL:HA	1.96	0.47
1:E:301:TRP:CE3	1:E:302:ALA:HA	2.50	0.47
1:F:96:ASN:O	1:F:98:LYS:N	2.42	0.47
1:G:104:VAL:HG23	1:G:105:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:269:PHE:CD1	1:K:269:PHE:C	2.91	0.47
1:E:215:ARG:HH12	1:E:224:ILE:HG23	1.71	0.47
1:D:156:MET:O	1:D:158:LEU:HD13	2.14	0.47
1:G:215:ARG:NH2	1:G:238:ASP:OD2	2.48	0.47
1:K:377:GLN:HE22	1:K:418:GLN:HB3	1.78	0.47
1:D:108:GLU:HA	1:D:111:LYS:HE3	1.96	0.47
1:F:116:VAL:HG22	1:F:152:LYS:HE3	1.95	0.47
1:J:301:TRP:CE3	1:J:302:ALA:N	2.81	0.47
1:L:202:ILE:HA	1:L:223:TYR:HD2	1.79	0.47
1:A:437:ALA:CA	1:A:447:MET:HE2	2.30	0.47
1:C:272:VAL:CG1	1:C:549:VAL:CG1	2.93	0.47
1:D:108:GLU:HG3	1:D:112:LYS:NZ	2.29	0.47
1:E:214:LEU:H	1:E:226:PRO:HB2	1.80	0.47
1:F:271:VAL:HG22	1:F:283:TYR:CD1	2.45	0.47
1:F:274:ASP:OD1	1:F:276:LYS:HD3	2.15	0.47
1:F:531:PRO:HG3	1:I:134:PHE:CD2	2.49	0.47
1:K:401:MET:HB2	5:K:903:HOH:O	2.15	0.47
1:L:89:ILE:HG12	1:L:90:ASP:N	2.30	0.47
1:L:301:TRP:CE3	1:L:302:ALA:HA	2.50	0.47
1:B:434:MET:HE3	1:B:434:MET:HB3	1.78	0.47
1:I:507:GLY:HA3	1:I:589:LYS:HG3	1.96	0.47
1:L:549:VAL:HG23	1:L:578:MET:CE	2.45	0.47
1:B:301:TRP:CE3	1:B:302:ALA:HA	2.50	0.47
1:D:377:GLN:NE2	1:D:418:GLN:HB3	2.30	0.47
1:G:551:VAL:HG13	1:G:574:PHE:CD1	2.49	0.47
1:A:301:TRP:CE3	1:A:302:ALA:HA	2.50	0.47
1:B:220:ILE:HA	1:B:224:ILE:HG23	1.96	0.47
1:D:301:TRP:CE3	1:D:302:ALA:HA	2.49	0.47
1:E:341:ARG:O	1:E:348:ILE:HG13	2.15	0.47
1:F:218:HIS:HB3	1:J:223:TYR:CZ	2.50	0.47
1:F:233:GLN:HB3	1:F:234:PRO:CD	2.45	0.47
1:H:152:LYS:HB2	1:H:152:LYS:HE2	1.65	0.47
1:J:301:TRP:CE3	1:J:302:ALA:HA	2.50	0.47
1:J:451:TRP:HA	5:J:903:HOH:O	2.15	0.47
1:K:301:TRP:CE3	1:K:302:ALA:HA	2.50	0.47
1:C:214:LEU:HD13	1:K:221:TRP:HH2	1.80	0.46
1:C:377:GLN:NE2	1:C:418:GLN:HB3	2.30	0.46
1:F:146:THR:OG1	1:F:148:GLN:HG2	2.14	0.46
1:K:272:VAL:HG13	1:K:549:VAL:HG21	1.94	0.46
1:D:207:LEU:HD21	1:D:240:VAL:HG12	1.97	0.46
1:G:330:PHE:CE1	1:G:361:MET:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:301:TRP:CE3	1:H:302:ALA:HA	2.50	0.46
1:D:451:TRP:HA	5:D:903:HOH:O	2.16	0.46
1:L:217:ILE:CB	1:L:224:ILE:HG21	2.44	0.46
1:D:108:GLU:HG3	1:D:112:LYS:HZ1	1.81	0.46
1:H:377:GLN:NE2	1:H:418:GLN:HB3	2.30	0.46
1:C:184:ALA:HA	1:C:195:GLY:HA2	1.98	0.46
1:E:116:VAL:HG21	1:E:153:ILE:CD1	2.45	0.46
1:J:117:ILE:HD12	1:J:117:ILE:HA	1.72	0.46
1:J:184:ALA:HA	1:J:195:GLY:HA2	1.97	0.46
1:B:80:VAL:HG21	1:B:82:ARG:HH21	1.81	0.46
1:B:271:VAL:HG12	1:B:283:TYR:HB2	1.98	0.46
1:C:344:MET:HE3	1:C:344:MET:HB3	1.79	0.46
1:D:220:ILE:C	1:D:223:TYR:O	2.58	0.46
1:E:104:VAL:HG23	1:E:105:ASP:H	1.80	0.46
1:F:211:LYS:O	1:F:229:LYS:HB3	2.16	0.46
1:L:113:LEU:HB2	1:L:124:ILE:HG21	1.96	0.46
1:B:184:ALA:HA	1:B:195:GLY:HA2	1.98	0.46
1:B:256:LEU:O	1:B:260:VAL:HG23	2.16	0.46
1:C:216:TYR:CE2	1:K:222:GLY:HA2	2.50	0.46
1:E:434:MET:HE3	1:E:434:MET:HB3	1.79	0.46
1:B:143:THR:HG22	1:B:166:GLU:OE2	2.15	0.46
1:C:199:VAL:HG21	1:C:242:LEU:HD21	1.98	0.46
1:D:184:ALA:HA	1:D:195:GLY:HA2	1.97	0.46
1:D:207:LEU:HD21	1:D:240:VAL:CG1	2.45	0.46
1:D:221:TRP:HZ3	1:H:216:TYR:HB3	1.81	0.46
1:G:184:ALA:HA	1:G:195:GLY:HA2	1.98	0.46
1:G:271:VAL:HG22	1:G:283:TYR:CD1	2.44	0.46
1:A:392:PHE:CB	1:A:447:MET:HE1	2.46	0.46
1:H:71:ARG:NH1	1:H:243:THR:O	2.48	0.46
1:K:377:GLN:NE2	1:K:418:GLN:HB3	2.31	0.45
1:A:301:TRP:CE3	1:A:302:ALA:CA	3.00	0.45
1:E:445:GLY:O	1:E:476:PRO:HD2	2.17	0.45
1:F:131:LYS:C	1:F:133:ALA:H	2.23	0.45
1:F:217:ILE:HG23	1:F:224:ILE:HD12	1.98	0.45
1:I:301:TRP:CE3	1:I:302:ALA:HA	2.51	0.45
1:L:150:LYS:HB2	1:L:163:LEU:HD21	1.99	0.45
1:B:216:TYR:CE1	1:B:463:ARG:NH1	2.85	0.45
1:B:330:PHE:CE1	1:B:361:MET:HB3	2.51	0.45
1:H:434:MET:HE3	1:H:434:MET:HB3	1.78	0.45
1:I:218:HIS:O	1:I:219:ASP:HB3	2.16	0.45
1:K:184:ALA:HA	1:K:195:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:271:VAL:HG11	1:K:435:LEU:HD11	1.97	0.45
1:L:217:ILE:HB	1:L:224:ILE:HG21	1.98	0.45
1:F:184:ALA:HA	1:F:195:GLY:HA2	1.98	0.45
1:I:236:ARG:HE	1:I:237:GLY:H	1.65	0.45
1:I:256:LEU:O	1:I:260:VAL:HG23	2.16	0.45
1:J:71:ARG:NH1	1:J:243:THR:O	2.49	0.45
1:L:301:TRP:CE3	1:L:302:ALA:CA	3.00	0.45
1:F:301:TRP:CE3	1:F:302:ALA:CA	2.99	0.45
1:H:184:ALA:HA	1:H:195:GLY:HA2	1.98	0.45
1:I:445:GLY:O	1:I:476:PRO:HD2	2.17	0.45
1:L:503:TYR:CE1	1:L:571:SER:HA	2.51	0.45
1:A:218:HIS:CD2	1:B:223:TYR:CE1	3.05	0.45
1:B:218:HIS:HB2	1:H:223:TYR:OH	2.16	0.45
1:C:301:TRP:CE3	1:C:302:ALA:HA	2.51	0.45
1:J:66:GLY:HA2	1:J:236:ARG:HH12	1.81	0.45
1:J:343:ILE:CG2	1:J:348:ILE:HG13	2.46	0.45
1:G:199:VAL:HG21	1:G:242:LEU:HD21	1.99	0.45
1:G:434:MET:HE3	1:G:434:MET:HB3	1.77	0.45
1:H:445:GLY:O	1:H:476:PRO:HD2	2.17	0.45
1:I:104:VAL:HG23	1:I:105:ASP:H	1.82	0.45
1:I:321:LEU:HD22	1:I:321:LEU:C	2.42	0.45
1:K:414:ASN:O	1:K:418:GLN:HG3	2.17	0.45
1:A:70:ASP:OD1	1:A:70:ASP:C	2.60	0.45
1:B:80:VAL:HG21	1:B:82:ARG:NH2	2.32	0.45
1:E:70:ASP:OD1	1:E:70:ASP:C	2.60	0.45
1:E:143:THR:HG22	1:E:166:GLU:OE2	2.17	0.45
1:E:301:TRP:CE3	1:E:302:ALA:CA	3.00	0.45
1:F:221:TRP:HB3	1:J:222:GLY:CA	2.38	0.45
1:F:521:ALA:O	1:F:522:PRO:C	2.60	0.45
1:J:301:TRP:CE3	1:J:302:ALA:CA	3.00	0.45
1:L:256:LEU:O	1:L:260:VAL:HG23	2.17	0.45
1:L:414:ASN:O	1:L:418:GLN:HG3	2.17	0.45
1:A:184:ALA:HA	1:A:195:GLY:HA2	1.98	0.45
1:A:256:LEU:O	1:A:260:VAL:HG23	2.17	0.45
1:B:70:ASP:C	1:B:70:ASP:OD1	2.60	0.45
1:B:301:TRP:CE3	1:B:302:ALA:CA	3.00	0.45
1:D:220:ILE:CA	1:D:223:TYR:O	2.65	0.45
1:G:70:ASP:C	1:G:70:ASP:OD1	2.60	0.45
1:H:414:ASN:O	1:H:418:GLN:HG3	2.17	0.45
1:L:564:GLU:HG3	1:L:568:LEU:HD12	1.97	0.45
1:A:521:ALA:O	1:A:522:PRO:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:HB2	1:C:161:ILE:HG12	1.97	0.45
1:E:184:ALA:HA	1:E:195:GLY:HA2	1.98	0.45
1:K:301:TRP:CE3	1:K:302:ALA:CA	3.00	0.45
1:L:184:ALA:HA	1:L:195:GLY:HA2	1.99	0.45
1:D:301:TRP:CE3	1:D:302:ALA:CA	3.00	0.44
1:E:414:ASN:O	1:E:418:GLN:HG3	2.17	0.44
1:F:256:LEU:O	1:F:260:VAL:HG23	2.17	0.44
1:G:551:VAL:HG11	1:G:578:MET:HE2	1.98	0.44
1:H:256:LEU:O	1:H:260:VAL:HG23	2.17	0.44
1:H:506:ASP:OD1	1:H:506:ASP:N	2.50	0.44
1:I:521:ALA:O	1:I:522:PRO:C	2.60	0.44
1:J:256:LEU:O	1:J:260:VAL:HG23	2.17	0.44
1:H:521:ALA:O	1:H:522:PRO:C	2.61	0.44
1:I:184:ALA:HA	1:I:195:GLY:HA2	1.97	0.44
1:I:414:ASN:O	1:I:418:GLN:HG3	2.18	0.44
1:J:351:TRP:O	1:J:353:ARG:NH1	2.51	0.44
1:K:445:GLY:O	1:K:476:PRO:HD2	2.17	0.44
1:B:445:GLY:O	1:B:476:PRO:HD2	2.17	0.44
1:E:521:ALA:O	1:E:522:PRO:C	2.60	0.44
1:F:71:ARG:NH1	1:F:243:THR:O	2.49	0.44
1:H:70:ASP:OD1	1:H:70:ASP:C	2.60	0.44
1:H:301:TRP:CE3	1:H:302:ALA:CA	3.00	0.44
1:L:445:GLY:O	1:L:476:PRO:HD2	2.17	0.44
1:K:213:SER:HA	1:K:226:PRO:HB2	2.00	0.44
1:B:271:VAL:CG1	1:B:283:TYR:HD1	2.29	0.44
1:C:301:TRP:CE3	1:C:302:ALA:CA	3.00	0.44
1:C:521:ALA:O	1:C:522:PRO:C	2.61	0.44
1:D:256:LEU:O	1:D:260:VAL:HG23	2.17	0.44
1:I:70:ASP:C	1:I:70:ASP:OD1	2.60	0.44
1:K:70:ASP:OD1	1:K:70:ASP:C	2.60	0.44
1:L:156:MET:HE2	1:L:156:MET:HB3	1.79	0.44
1:D:521:ALA:O	1:D:522:PRO:C	2.61	0.44
1:F:70:ASP:OD1	1:F:70:ASP:C	2.60	0.44
1:G:105:ASP:O	1:G:109:THR:HG23	2.18	0.44
1:G:256:LEU:O	1:G:260:VAL:HG23	2.17	0.44
1:I:330:PHE:CE1	1:I:361:MET:HB3	2.52	0.44
1:K:119:MET:SD	1:K:127:ARG:NH1	2.91	0.44
1:K:273:MET:HE1	1:K:435:LEU:HB3	1.96	0.44
1:L:70:ASP:OD1	1:L:70:ASP:C	2.60	0.44
1:L:340:HIS:HA	1:L:349:SER:HA	1.99	0.44
1:B:105:ASP:OD2	1:E:352:ASN:ND2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASP:OD1	1:C:70:ASP:C	2.60	0.44
1:C:445:GLY:O	1:C:476:PRO:HD2	2.17	0.44
1:D:220:ILE:HG22	1:D:224:ILE:HD11	1.98	0.44
1:F:414:ASN:O	1:F:418:GLN:HG3	2.17	0.44
1:K:521:ALA:O	1:K:522:PRO:C	2.60	0.44
1:E:113:LEU:O	1:E:116:VAL:HG22	2.18	0.44
1:G:414:ASN:O	1:G:418:GLN:HG3	2.17	0.44
1:C:414:ASN:O	1:C:418:GLN:HG3	2.17	0.44
1:F:213:SER:O	1:F:214:LEU:HB3	2.17	0.44
1:G:180:LEU:HD23	1:G:244:ILE:HD11	2.00	0.44
1:G:354:VAL:HG21	1:I:108:GLU:HB2	2.00	0.44
1:G:521:ALA:O	1:G:522:PRO:C	2.61	0.44
1:D:109:THR:HG23	1:D:158:LEU:HD23	1.99	0.43
1:D:220:ILE:HA	1:D:224:ILE:HG13	2.00	0.43
1:D:335:LYS:HA	1:D:359:ILE:O	2.19	0.43
1:G:263:TYR:HB3	1:G:558:ALA:HB1	2.00	0.43
1:G:445:GLY:O	1:G:476:PRO:HD2	2.17	0.43
1:I:511:GLU:CG	1:I:541:ASP:OD1	2.65	0.43
1:J:183:ARG:HD2	1:J:291:PRO:O	2.18	0.43
1:J:414:ASN:O	1:J:418:GLN:HG3	2.18	0.43
1:K:335:LYS:HA	1:K:359:ILE:O	2.18	0.43
1:L:521:ALA:O	1:L:522:PRO:C	2.60	0.43
1:A:414:ASN:O	1:A:418:GLN:HG3	2.17	0.43
1:B:414:ASN:O	1:B:418:GLN:HG3	2.18	0.43
1:B:183:ARG:HD2	1:B:291:PRO:O	2.18	0.43
1:C:71:ARG:NH1	1:C:243:THR:O	2.49	0.43
1:C:256:LEU:O	1:C:260:VAL:HG23	2.17	0.43
1:D:445:GLY:O	1:D:476:PRO:HD2	2.18	0.43
1:E:99:LYS:HA	1:E:99:LYS:HD3	1.79	0.43
1:G:381:GLY:HA3	1:H:347:ARG:HH22	1.83	0.43
1:J:491:LEU:O	1:J:492:VAL:C	2.61	0.43
1:J:521:ALA:O	1:J:522:PRO:C	2.61	0.43
1:A:335:LYS:HA	1:A:359:ILE:O	2.18	0.43
1:B:467:LYS:HD3	1:H:469:GLN:NE2	2.33	0.43
1:C:89:ILE:HA	1:C:103:VAL:HG12	2.00	0.43
1:F:445:GLY:O	1:F:476:PRO:HD2	2.17	0.43
1:G:491:LEU:O	1:G:492:VAL:C	2.61	0.43
1:H:80:VAL:HG22	1:H:170:PHE:HB2	2.00	0.43
2:I:801:EPE:H62	2:I:801:EPE:H102	1.89	0.43
1:A:189:ASP:O	1:B:522:PRO:HG3	2.18	0.43
1:B:491:LEU:O	1:B:492:VAL:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:301:TRP:CE3	1:I:302:ALA:CA	3.00	0.43
1:L:183:ARG:HD2	1:L:291:PRO:O	2.19	0.43
1:B:335:LYS:HA	1:B:359:ILE:O	2.18	0.43
1:C:335:LYS:HA	1:C:359:ILE:O	2.19	0.43
1:D:70:ASP:C	1:D:70:ASP:OD1	2.60	0.43
1:E:491:LEU:O	1:E:492:VAL:C	2.61	0.43
1:F:335:LYS:HA	1:F:359:ILE:O	2.19	0.43
1:H:491:LEU:O	1:H:492:VAL:C	2.61	0.43
1:K:263:TYR:HB3	1:K:558:ALA:HB1	2.01	0.43
1:C:491:LEU:O	1:C:492:VAL:C	2.61	0.43
1:D:414:ASN:O	1:D:418:GLN:HG3	2.18	0.43
1:E:131:LYS:C	1:E:133:ALA:H	2.26	0.43
1:E:335:LYS:HA	1:E:359:ILE:O	2.18	0.43
1:F:116:VAL:HG22	1:F:152:LYS:HE2	2.00	0.43
1:I:263:TYR:HB3	1:I:558:ALA:HB1	2.01	0.43
1:I:491:LEU:O	1:I:492:VAL:C	2.61	0.43
1:J:112:LYS:HD3	1:J:156:MET:HE2	2.01	0.43
1:L:491:LEU:O	1:L:492:VAL:C	2.62	0.43
1:A:363:LEU:HD12	1:A:363:LEU:HA	1.79	0.43
1:D:223:TYR:CD1	1:H:218:HIS:CE1	3.06	0.43
1:E:256:LEU:O	1:E:260:VAL:HG23	2.18	0.43
1:K:220:ILE:N	1:K:401:MET:HE1	2.34	0.43
1:A:71:ARG:NH1	1:A:243:THR:O	2.49	0.43
1:E:263:TYR:HB3	1:E:558:ALA:HB1	2.01	0.43
1:G:71:ARG:NH1	1:G:243:THR:O	2.49	0.43
1:G:340:HIS:HB2	1:G:347:ARG:HD2	2.00	0.43
1:H:386:LYS:HG3	1:H:410:ILE:HD12	2.01	0.43
1:D:434:MET:HE3	1:D:434:MET:HB3	1.77	0.43
1:H:221:TRP:HB2	1:H:222:GLY:H	1.72	0.43
1:K:491:LEU:O	1:K:492:VAL:C	2.61	0.43
1:C:263:TYR:HB3	1:C:558:ALA:HB1	2.01	0.42
1:C:497:LYS:HE2	1:C:497:LYS:HB3	1.90	0.42
1:C:511:GLU:CG	1:C:541:ASP:OD1	2.66	0.42
1:G:259:MET:HE1	1:G:572:LYS:HB3	2.01	0.42
1:G:335:LYS:HA	1:G:359:ILE:O	2.19	0.42
1:A:503:TYR:CE1	1:A:571:SER:HA	2.54	0.42
1:C:161:ILE:HD12	1:C:161:ILE:C	2.44	0.42
1:E:71:ARG:NH1	1:E:243:THR:O	2.49	0.42
1:H:281:LEU:N	1:H:281:LEU:HD12	2.33	0.42
1:J:445:GLY:O	1:J:476:PRO:HD2	2.19	0.42
1:J:503:TYR:CE1	1:J:571:SER:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:215:ARG:NH2	1:K:217:ILE:O	2.46	0.42
1:B:199:VAL:CA	1:B:202:ILE:HG12	2.49	0.42
1:B:503:TYR:CE1	1:B:571:SER:HA	2.55	0.42
1:B:521:ALA:O	1:B:522:PRO:C	2.62	0.42
1:E:503:TYR:CE1	1:E:571:SER:HA	2.55	0.42
1:F:263:TYR:HB3	1:F:558:ALA:HB1	2.01	0.42
1:F:434:MET:HE3	1:F:434:MET:HB3	1.78	0.42
1:I:335:LYS:HA	1:I:359:ILE:O	2.19	0.42
1:D:156:MET:HB3	1:D:158:LEU:HD22	2.02	0.42
1:D:263:TYR:HB3	1:D:558:ALA:HB1	2.02	0.42
1:E:215:ARG:HG2	1:E:226:PRO:HA	2.01	0.42
1:I:434:MET:HE3	1:I:434:MET:HB3	1.79	0.42
1:A:445:GLY:O	1:A:476:PRO:HD2	2.18	0.42
1:D:491:LEU:O	1:D:492:VAL:C	2.61	0.42
1:F:96:ASN:O	1:F:98:LYS:HG2	2.20	0.42
1:F:491:LEU:O	1:F:492:VAL:C	2.61	0.42
1:F:503:TYR:CE1	1:F:571:SER:HA	2.55	0.42
1:K:503:TYR:CE1	1:K:571:SER:HA	2.54	0.42
1:A:491:LEU:O	1:A:492:VAL:C	2.61	0.42
1:E:259:MET:HE1	1:E:572:LYS:HB3	2.01	0.42
1:F:223:TYR:CD1	1:F:223:TYR:N	2.86	0.42
1:G:104:VAL:HG23	1:G:105:ASP:H	1.84	0.42
1:H:335:LYS:HA	1:H:359:ILE:O	2.18	0.42
1:H:344:MET:HE3	1:H:344:MET:HB3	1.82	0.42
1:L:71:ARG:NH1	1:L:243:THR:O	2.49	0.42
1:L:223:TYR:N	1:L:223:TYR:CD1	2.87	0.42
1:C:155:LYS:HD3	1:C:155:LYS:HA	1.77	0.42
1:G:131:LYS:C	1:G:133:ALA:H	2.27	0.42
1:G:344:MET:HE3	1:G:344:MET:HB3	1.81	0.42
1:J:112:LYS:HD3	1:J:156:MET:CE	2.49	0.42
1:L:511:GLU:CG	1:L:541:ASP:OD1	2.66	0.42
1:B:223:TYR:N	1:B:223:TYR:CD1	2.88	0.42
1:D:211:LYS:HA	1:D:211:LYS:HD3	1.71	0.42
1:E:207:LEU:HD21	1:E:240:VAL:HG22	2.02	0.42
1:E:549:VAL:HG23	1:E:578:MET:HE2	2.01	0.42
1:B:71:ARG:NH1	1:B:243:THR:O	2.49	0.42
1:B:271:VAL:CG1	1:B:283:TYR:CD1	3.03	0.42
1:C:131:LYS:C	1:C:133:ALA:H	2.26	0.42
1:D:503:TYR:CE1	1:D:571:SER:HA	2.54	0.42
1:E:216:TYR:HE1	1:E:463:ARG:CZ	2.33	0.42
1:F:536:VAL:HG23	1:F:570:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:C	1:B:133:ALA:H	2.28	0.42
1:I:321:LEU:C	1:I:321:LEU:HD23	2.45	0.42
1:J:120:LYS:HG3	1:J:121:PRO:HD2	2.01	0.42
1:D:260:VAL:O	1:D:264:GLN:HG3	2.20	0.41
1:E:343:ILE:CG2	1:E:348:ILE:HG12	2.50	0.41
1:G:103:VAL:HG13	1:G:109:THR:HG21	2.01	0.41
1:J:263:TYR:HB3	1:J:558:ALA:HB1	2.01	0.41
1:D:341:ARG:HB3	1:D:343:ILE:HD12	2.02	0.41
1:I:259:MET:HE1	1:I:572:LYS:HB2	2.03	0.41
1:B:85:LEU:HD23	1:B:138:PHE:CD2	2.56	0.41
1:E:119:MET:SD	1:E:123:GLU:HG2	2.61	0.41
1:E:343:ILE:HG22	1:E:348:ILE:CG1	2.50	0.41
1:G:65:ARG:HD3	1:G:169:ARG:NH1	2.35	0.41
1:H:65:ARG:HD3	1:H:169:ARG:NH1	2.35	0.41
1:J:340:HIS:O	1:J:341:ARG:HG2	2.20	0.41
1:J:434:MET:HE3	1:J:434:MET:HB3	1.77	0.41
1:K:71:ARG:NH1	1:K:243:THR:O	2.49	0.41
1:A:399:LYS:HA	1:A:399:LYS:HD3	1.96	0.41
1:D:271:VAL:HG11	1:D:435:LEU:HD11	2.03	0.41
1:E:140:ARG:HE	1:E:140:ARG:HB3	1.80	0.41
1:J:88:VAL:HG12	1:J:160:GLY:O	2.20	0.41
1:L:84:LYS:HD2	1:L:143:THR:HG23	2.03	0.41
1:L:263:TYR:HB3	1:L:558:ALA:HB1	2.01	0.41
1:C:313:GLY:CA	1:C:517:ALA:HB2	2.50	0.41
1:E:536:VAL:HG23	1:E:570:VAL:HG13	2.03	0.41
1:F:232:LYS:HD3	1:F:232:LYS:HA	1.93	0.41
1:K:283:TYR:CE1	1:K:305:LEU:HB2	2.56	0.41
1:L:150:LYS:HA	1:L:163:LEU:HD21	2.02	0.41
1:A:219:ASP:OD1	1:B:225:ALA:HB2	2.20	0.41
1:B:263:TYR:HB3	1:B:558:ALA:HB1	2.01	0.41
1:C:85:LEU:HD23	1:C:138:PHE:CD2	2.56	0.41
1:C:281:LEU:N	1:C:281:LEU:HD12	2.36	0.41
1:D:344:MET:HE3	1:D:344:MET:HB3	1.93	0.41
1:F:223:TYR:CD1	1:I:218:HIS:CE1	3.08	0.41
1:G:260:VAL:O	1:G:264:GLN:HG3	2.21	0.41
1:G:581:THR:O	1:G:585:LEU:HD22	2.20	0.41
1:H:503:TYR:CE1	1:H:571:SER:HA	2.55	0.41
1:J:131:LYS:C	1:J:133:ALA:H	2.28	0.41
1:L:113:LEU:C	1:L:115:THR:H	2.29	0.41
1:B:88:VAL:CG1	1:B:160:GLY:HA2	2.50	0.41
1:B:536:VAL:HG21	1:B:569:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HA	1:C:140:ARG:HD2	1.67	0.41
1:C:324:ALA:O	1:C:325:ILE:C	2.64	0.41
1:D:71:ARG:NH1	1:D:243:THR:O	2.49	0.41
1:I:96:ASN:HD22	1:I:96:ASN:HA	1.67	0.41
1:K:257:ASP:O	1:K:260:VAL:HG12	2.20	0.41
1:K:344:MET:HE3	1:K:344:MET:HB3	1.67	0.41
1:L:85:LEU:HD23	1:L:138:PHE:CD2	2.55	0.41
1:C:81:GLU:H	1:C:81:GLU:HG2	1.68	0.41
1:D:85:LEU:HD23	1:D:138:PHE:CD2	2.56	0.41
1:J:88:VAL:CG1	1:J:160:GLY:HA2	2.51	0.41
1:J:335:LYS:HA	1:J:359:ILE:O	2.20	0.41
1:K:143:THR:HG22	1:K:166:GLU:OE2	2.20	0.41
1:K:434:MET:HE3	1:K:434:MET:HB3	1.77	0.41
1:L:221:TRP:CD1	1:L:221:TRP:H	2.37	0.41
1:A:263:TYR:HB3	1:A:558:ALA:HB1	2.02	0.41
1:A:281:LEU:N	1:A:281:LEU:HD12	2.36	0.41
1:B:108:GLU:HB2	1:E:354:VAL:HG21	2.03	0.41
1:B:289:PHE:HB2	1:B:295:LYS:O	2.21	0.41
1:B:324:ALA:O	1:B:325:ILE:C	2.64	0.41
1:E:324:ALA:O	1:E:325:ILE:C	2.64	0.41
1:F:213:SER:O	1:F:214:LEU:CB	2.68	0.41
1:G:116:VAL:HG11	1:G:153:ILE:CG1	2.50	0.41
1:H:260:VAL:O	1:H:264:GLN:HG3	2.21	0.41
1:H:263:TYR:HB3	1:H:558:ALA:HB1	2.02	0.41
1:H:324:ALA:O	1:H:325:ILE:C	2.64	0.41
1:H:536:VAL:HG23	1:H:570:VAL:HG13	2.03	0.41
1:I:85:LEU:HD23	1:I:138:PHE:CD2	2.55	0.41
1:L:343:ILE:HD11	1:L:416:LEU:HA	2.03	0.41
1:A:260:VAL:O	1:A:264:GLN:HG3	2.20	0.41
1:C:260:VAL:O	1:C:264:GLN:HG3	2.21	0.41
1:F:398:THR:HG22	1:F:405:GLU:OE2	2.22	0.41
1:G:324:ALA:O	1:G:325:ILE:C	2.64	0.41
1:G:352:ASN:ND2	1:I:105:ASP:OD2	2.50	0.41
1:I:536:VAL:HG21	1:I:569:GLY:HA2	2.03	0.41
1:J:271:VAL:HG11	1:J:435:LEU:HD11	2.02	0.41
1:K:131:LYS:C	1:K:133:ALA:H	2.29	0.41
1:L:65:ARG:HD3	1:L:169:ARG:NH1	2.36	0.41
1:D:65:ARG:HD3	1:D:169:ARG:NH1	2.36	0.40
1:D:283:TYR:CE1	1:D:305:LEU:HB2	2.56	0.40
1:F:85:LEU:HD23	1:F:138:PHE:CD2	2.56	0.40
1:G:132:LYS:HA	1:G:132:LYS:CE	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:LEU:HD23	1:H:138:PHE:CD2	2.56	0.40
1:J:536:VAL:HG23	1:J:570:VAL:HG13	2.03	0.40
1:K:113:LEU:CD2	1:K:161:ILE:HD11	2.50	0.40
1:L:289:PHE:HB2	1:L:295:LYS:O	2.20	0.40
1:A:136:ILE:HD12	1:A:138:PHE:CZ	2.56	0.40
1:H:283:TYR:CE1	1:H:305:LEU:HB2	2.57	0.40
1:H:451:TRP:CD1	1:H:451:TRP:N	2.90	0.40
1:I:549:VAL:HG23	1:I:578:MET:HE2	2.01	0.40
1:J:64:MET:HE3	1:J:79:ASP:HB2	2.04	0.40
1:J:343:ILE:HD11	1:J:416:LEU:HA	2.04	0.40
1:J:451:TRP:CD1	1:J:451:TRP:N	2.90	0.40
1:L:324:ALA:O	1:L:325:ILE:C	2.64	0.40
1:L:536:VAL:HG23	1:L:570:VAL:HG13	2.04	0.40
1:A:324:ALA:O	1:A:325:ILE:C	2.64	0.40
1:A:434:MET:HE3	1:A:434:MET:HB3	1.76	0.40
1:E:114:SER:HA	1:E:117:ILE:HG22	2.03	0.40
1:E:451:TRP:CD1	1:E:451:TRP:N	2.90	0.40
1:H:313:GLY:CA	1:H:517:ALA:HB2	2.50	0.40
1:H:566:TYR:CZ	2:H:801:EPE:H61	2.56	0.40
1:I:65:ARG:HD3	1:I:169:ARG:NH1	2.37	0.40
1:I:131:LYS:C	1:I:133:ALA:H	2.28	0.40
1:J:283:TYR:CE1	1:J:305:LEU:HB2	2.57	0.40
1:K:85:LEU:HD23	1:K:138:PHE:CD2	2.56	0.40
1:K:375:HIS:CE1	4:K:801:CL:CL	3.09	0.40
1:C:283:TYR:CE1	1:C:305:LEU:HB2	2.56	0.40
1:C:536:VAL:HG23	1:C:570:VAL:HG13	2.03	0.40
1:D:148:GLN:HE21	1:D:148:GLN:HB2	1.77	0.40
1:D:324:ALA:O	1:D:325:ILE:C	2.64	0.40
1:E:118:ASN:HD22	1:E:118:ASN:HA	1.63	0.40
1:F:65:ARG:HD3	1:F:169:ARG:NH1	2.37	0.40
1:L:283:TYR:CE1	1:L:305:LEU:HB2	2.56	0.40
1:A:536:VAL:HG23	1:A:570:VAL:HG13	2.04	0.40
1:B:88:VAL:HG13	1:B:101:ARG:O	2.21	0.40
1:B:313:GLY:CA	1:B:517:ALA:HB2	2.50	0.40
1:C:218:HIS:O	1:C:219:ASP:HB2	2.21	0.40
1:F:283:TYR:CE1	1:F:305:LEU:HB2	2.56	0.40
1:G:214:LEU:HA	1:G:214:LEU:HD12	1.89	0.40
1:G:536:VAL:HG23	1:G:570:VAL:HG13	2.03	0.40
1:I:324:ALA:O	1:I:325:ILE:C	2.64	0.40
1:J:289:PHE:HB2	1:J:295:LYS:O	2.22	0.40
1:J:324:ALA:O	1:J:325:ILE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:257:ASP:HA	1:K:260:VAL:HG12	2.04	0.40
1:K:324:ALA:O	1:K:325:ILE:C	2.64	0.40
1:K:370:ASN:O	1:K:374:MET:HG3	2.22	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	517/650 (80%)	454 (88%)	59 (11%)	4 (1%)	16	46
1	B	525/650 (81%)	455 (87%)	63 (12%)	7 (1%)	9	35
1	C	516/650 (79%)	452 (88%)	59 (11%)	5 (1%)	12	41
1	D	496/650 (76%)	429 (86%)	59 (12%)	8 (2%)	7	30
1	E	519/650 (80%)	456 (88%)	56 (11%)	7 (1%)	9	35
1	F	526/650 (81%)	456 (87%)	61 (12%)	9 (2%)	7	29
1	G	516/650 (79%)	453 (88%)	59 (11%)	4 (1%)	16	46
1	H	465/650 (72%)	403 (87%)	57 (12%)	5 (1%)	11	39
1	I	514/650 (79%)	449 (87%)	59 (12%)	6 (1%)	10	37
1	J	514/650 (79%)	449 (87%)	61 (12%)	4 (1%)	16	46
1	K	507/650 (78%)	438 (86%)	63 (12%)	6 (1%)	10	37
1	L	486/650 (75%)	424 (87%)	53 (11%)	9 (2%)	6	27
All	All	6101/7800 (78%)	5318 (87%)	709 (12%)	74 (1%)	10	37

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	SER

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Mol	Chain	Res	Type
1	D	232	LYS
1	F	97	SER
1	F	214	LEU
1	F	233	GLN
1	G	213	SER
1	H	154	GLU
1	H	211	LYS
1	H	222	GLY
1	I	213	SER
1	L	569	GLY
1	A	213	SER
1	B	210	SER
1	B	217	ILE
1	B	368	SER
1	C	368	SER
1	D	226	PRO
1	D	228	THR
1	D	368	SER
1	E	217	ILE
1	E	368	SER
1	F	217	ILE
1	F	368	SER
1	G	368	SER
1	H	368	SER
1	I	368	SER
1	J	218	HIS
1	J	368	SER
1	J	525	GLY
1	K	230	LYS
1	K	233	GLN
1	K	368	SER
1	A	211	LYS
1	B	224	ILE
1	B	523	ASN
1	C	211	LYS
1	C	219	ASP
1	G	219	ASP
1	I	211	LYS
1	I	219	ASP
1	L	217	ILE
1	L	218	HIS
1	A	117	ILE

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Mol	Chain	Res	Type
1	B	226	PRO
1	D	218	HIS
1	D	220	ILE
1	E	218	HIS
1	E	220	ILE
1	E	227	ASN
1	F	218	HIS
1	F	221	TRP
1	H	522	PRO
1	K	218	HIS
1	L	89	ILE
1	L	92	LYS
1	L	114	SER
1	L	226	PRO
1	F	213	SER
1	I	223	TYR
1	L	367	TYR
1	A	522	PRO
1	C	522	PRO
1	D	522	PRO
1	G	522	PRO
1	I	522	PRO
1	D	224	ILE
1	E	522	PRO
1	F	522	PRO
1	K	220	ILE
1	K	522	PRO
1	L	522	PRO
1	E	224	ILE
1	J	522	PRO
1	B	233	GLN

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/552 (79%)	381 (87%)	57 (13%)	4	17
1	B	444/552 (80%)	383 (86%)	61 (14%)	3	15
1	C	437/552 (79%)	388 (89%)	49 (11%)	6	22
1	D	422/552 (76%)	371 (88%)	51 (12%)	5	19
1	E	440/552 (80%)	375 (85%)	65 (15%)	3	13
1	F	445/552 (81%)	388 (87%)	57 (13%)	4	17
1	G	437/552 (79%)	386 (88%)	51 (12%)	5	20
1	H	392/552 (71%)	346 (88%)	46 (12%)	5	20
1	I	435/552 (79%)	389 (89%)	46 (11%)	6	24
1	J	435/552 (79%)	379 (87%)	56 (13%)	4	17
1	K	429/552 (78%)	372 (87%)	57 (13%)	4	16
1	L	414/552 (75%)	352 (85%)	62 (15%)	3	12
All	All	5168/6624 (78%)	4510 (87%)	658 (13%)	4	17

All (658) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	MET
1	A	72	ASN
1	A	75	VAL
1	A	82	ARG
1	A	91	LYS
1	A	96	ASN
1	A	98	LYS
1	A	99	LYS
1	A	101	ARG
1	A	102	HIS
1	A	107	LYS
1	A	120	LYS
1	A	125	GLU
1	A	126	LYS
1	A	136	ILE
1	A	140	ARG
1	A	143	THR
1	A	158	LEU
1	A	161	ILE

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Mol	Chain	Res	Type
1	A	166	GLU
1	A	167	THR
1	A	168	GLU
1	A	173	ASN
1	A	179	HIS
1	A	207	LEU
1	A	211	LYS
1	A	215	ARG
1	A	217	ILE
1	A	219	ASP
1	A	220	ILE
1	A	235	LYS
1	A	236	ARG
1	A	256	LEU
1	A	260	VAL
1	A	288	THR
1	A	295	LYS
1	A	343	ILE
1	A	344	MET
1	A	362	SER
1	A	368	SER
1	A	373	MET
1	A	397	SER
1	A	433	GLN
1	A	457	GLU
1	A	463	ARG
1	A	478	THR
1	A	487	LYS
1	A	490	ASP
1	A	496	LYS
1	A	499	HIS
1	A	502	ASN
1	A	537	SER
1	A	545	LYS
1	A	549	VAL
1	A	562	ASP
1	A	587	VAL
1	A	591	LYS
1	B	64	MET
1	B	72	ASN
1	B	74	LYS
1	B	91	LYS

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Mol	Chain	Res	Type
1	B	92	LYS
1	B	99	LYS
1	B	101	ARG
1	B	116	VAL
1	B	119	MET
1	B	122	GLU
1	B	123	GLU
1	B	125	GLU
1	B	126	LYS
1	B	130	GLN
1	B	136	ILE
1	B	140	ARG
1	B	141	LYS
1	B	143	THR
1	B	155	LYS
1	B	158	LEU
1	B	161	ILE
1	B	166	GLU
1	B	167	THR
1	B	173	ASN
1	B	179	HIS
1	B	197	LEU
1	B	216	TYR
1	B	217	ILE
1	B	224	ILE
1	B	229	LYS
1	B	230	LYS
1	B	231	GLU
1	B	232	LYS
1	B	256	LEU
1	B	260	VAL
1	B	271	VAL
1	B	288	THR
1	B	295	LYS
1	B	300	LYS
1	B	337	LYS
1	B	341	ARG
1	B	342	ASP
1	B	343	ILE
1	B	353	ARG
1	B	373	MET
1	B	398	THR

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Mol	Chain	Res	Type
1	B	433	GLN
1	B	457	GLU
1	B	463	ARG
1	B	487	LYS
1	B	490	ASP
1	B	496	LYS
1	B	499	HIS
1	B	502	ASN
1	B	537	SER
1	B	545	LYS
1	B	548	LYS
1	B	549	VAL
1	B	562	ASP
1	B	583	LYS
1	B	587	VAL
1	C	72	ASN
1	C	81	GLU
1	C	86	VAL
1	C	96	ASN
1	C	102	HIS
1	C	107	LYS
1	C	108	GLU
1	C	113	LEU
1	C	119	MET
1	C	120	LYS
1	C	123	GLU
1	C	125	GLU
1	C	126	LYS
1	C	131	LYS
1	C	140	ARG
1	C	143	THR
1	C	155	LYS
1	C	164	LEU
1	C	166	GLU
1	C	173	ASN
1	C	179	HIS
1	C	197	LEU
1	C	217	ILE
1	C	256	LEU
1	C	260	VAL
1	C	261	GLU
1	C	288	THR

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Mol	Chain	Res	Type
1	C	337	LYS
1	C	341	ARG
1	C	343	ILE
1	C	344	MET
1	C	348	ILE
1	C	373	MET
1	C	409	GLN
1	C	433	GLN
1	C	457	GLU
1	C	487	LYS
1	C	490	ASP
1	C	496	LYS
1	C	497	LYS
1	C	499	HIS
1	C	502	ASN
1	C	510	VAL
1	C	529	LYS
1	C	537	SER
1	C	541	ASP
1	C	545	LYS
1	C	548	LYS
1	C	562	ASP
1	D	72	ASN
1	D	84	LYS
1	D	111	LYS
1	D	116	VAL
1	D	117	ILE
1	D	118	ASN
1	D	120	LYS
1	D	122	GLU
1	D	123	GLU
1	D	125	GLU
1	D	126	LYS
1	D	140	ARG
1	D	141	LYS
1	D	143	THR
1	D	148	GLN
1	D	154	GLU
1	D	158	LEU
1	D	161	ILE
1	D	166	GLU
1	D	167	THR

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Mol	Chain	Res	Type
1	D	173	ASN
1	D	179	HIS
1	D	197	LEU
1	D	211	LYS
1	D	214	LEU
1	D	217	ILE
1	D	219	ASP
1	D	223	TYR
1	D	231	GLU
1	D	232	LYS
1	D	233	GLN
1	D	235	LYS
1	D	240	VAL
1	D	256	LEU
1	D	260	VAL
1	D	288	THR
1	D	337	LYS
1	D	341	ARG
1	D	343	ILE
1	D	344	MET
1	D	358	GLU
1	D	373	MET
1	D	433	GLN
1	D	457	GLU
1	D	490	ASP
1	D	496	LYS
1	D	502	ASN
1	D	537	SER
1	D	545	LYS
1	D	549	VAL
1	D	562	ASP
1	E	72	ASN
1	E	75	VAL
1	E	81	GLU
1	E	91	LYS
1	E	92	LYS
1	E	98	LYS
1	E	99	LYS
1	E	101	ARG
1	E	102	HIS
1	E	111	LYS
1	E	116	VAL

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Mol	Chain	Res	Type
1	E	118	ASN
1	E	119	MET
1	E	120	LYS
1	E	122	GLU
1	E	125	GLU
1	E	126	LYS
1	E	136	ILE
1	E	140	ARG
1	E	141	LYS
1	E	143	THR
1	E	157	ASN
1	E	158	LEU
1	E	161	ILE
1	E	166	GLU
1	E	167	THR
1	E	173	ASN
1	E	179	HIS
1	E	214	LEU
1	E	216	TYR
1	E	217	ILE
1	E	219	ASP
1	E	220	ILE
1	E	224	ILE
1	E	235	LYS
1	E	256	LEU
1	E	260	VAL
1	E	288	THR
1	E	295	LYS
1	E	300	LYS
1	E	337	LYS
1	E	341	ARG
1	E	342	ASP
1	E	343	ILE
1	E	344	MET
1	E	348	ILE
1	E	373	MET
1	E	398	THR
1	E	401	MET
1	E	433	GLN
1	E	457	GLU
1	E	487	LYS
1	E	490	ASP

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Mol	Chain	Res	Type
1	E	496	LYS
1	E	502	ASN
1	E	510	VAL
1	E	537	SER
1	E	541	ASP
1	E	545	LYS
1	E	549	VAL
1	E	562	ASP
1	E	578	MET
1	E	583	LYS
1	E	587	VAL
1	E	589	LYS
1	F	64	MET
1	F	72	ASN
1	F	75	VAL
1	F	91	LYS
1	F	94	SER
1	F	98	LYS
1	F	99	LYS
1	F	101	ARG
1	F	107	LYS
1	F	108	GLU
1	F	116	VAL
1	F	119	MET
1	F	123	GLU
1	F	131	LYS
1	F	136	ILE
1	F	140	ARG
1	F	143	THR
1	F	161	ILE
1	F	166	GLU
1	F	167	THR
1	F	173	ASN
1	F	179	HIS
1	F	201	LYS
1	F	211	LYS
1	F	216	TYR
1	F	217	ILE
1	F	219	ASP
1	F	220	ILE
1	F	223	TYR
1	F	224	ILE

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Mol	Chain	Res	Type
1	F	229	LYS
1	F	230	LYS
1	F	232	LYS
1	F	256	LEU
1	F	260	VAL
1	F	276	LYS
1	F	288	THR
1	F	295	LYS
1	F	343	ILE
1	F	346	SER
1	F	347	ARG
1	F	373	MET
1	F	397	SER
1	F	398	THR
1	F	401	MET
1	F	433	GLN
1	F	457	GLU
1	F	487	LYS
1	F	490	ASP
1	F	496	LYS
1	F	499	HIS
1	F	502	ASN
1	F	537	SER
1	F	545	LYS
1	F	549	VAL
1	F	562	ASP
1	F	591	LYS
1	G	72	ASN
1	G	91	LYS
1	G	96	ASN
1	G	115	THR
1	G	116	VAL
1	G	119	MET
1	G	120	LYS
1	G	123	GLU
1	G	125	GLU
1	G	136	ILE
1	G	140	ARG
1	G	143	THR
1	G	148	GLN
1	G	155	LYS
1	G	161	ILE

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Mol	Chain	Res	Type
1	G	166	GLU
1	G	167	THR
1	G	173	ASN
1	G	179	HIS
1	G	186	LYS
1	G	197	LEU
1	G	211	LYS
1	G	214	LEU
1	G	217	ILE
1	G	221	TRP
1	G	227	ASN
1	G	256	LEU
1	G	260	VAL
1	G	261	GLU
1	G	288	THR
1	G	300	LYS
1	G	341	ARG
1	G	343	ILE
1	G	344	MET
1	G	347	ARG
1	G	348	ILE
1	G	373	MET
1	G	433	GLN
1	G	457	GLU
1	G	490	ASP
1	G	496	LYS
1	G	497	LYS
1	G	499	HIS
1	G	502	ASN
1	G	537	SER
1	G	541	ASP
1	G	545	LYS
1	G	549	VAL
1	G	562	ASP
1	G	583	LYS
1	G	585	LEU
1	H	82	ARG
1	H	84	LYS
1	H	88	VAL
1	H	143	THR
1	H	153	ILE
1	H	154	GLU

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Mol	Chain	Res	Type
1	H	155	LYS
1	H	156	MET
1	H	161	ILE
1	H	164	LEU
1	H	166	GLU
1	H	173	ASN
1	H	179	HIS
1	H	197	LEU
1	H	211	LYS
1	H	214	LEU
1	H	217	ILE
1	H	221	TRP
1	H	256	LEU
1	H	260	VAL
1	H	288	THR
1	H	295	LYS
1	H	341	ARG
1	H	343	ILE
1	H	344	MET
1	H	346	SER
1	H	348	ILE
1	H	353	ARG
1	H	373	MET
1	H	396	LYS
1	H	433	GLN
1	H	457	GLU
1	H	463	ARG
1	H	469	GLN
1	H	487	LYS
1	H	490	ASP
1	H	496	LYS
1	H	497	LYS
1	H	499	HIS
1	H	502	ASN
1	H	506	ASP
1	H	537	SER
1	H	545	LYS
1	H	548	LYS
1	H	549	VAL
1	H	562	ASP
1	I	64	MET
1	I	71	ARG

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Mol	Chain	Res	Type
1	I	72	ASN
1	I	91	LYS
1	I	96	ASN
1	I	98	LYS
1	I	119	MET
1	I	120	LYS
1	I	123	GLU
1	I	125	GLU
1	I	136	ILE
1	I	140	ARG
1	I	141	LYS
1	I	143	THR
1	I	150	LYS
1	I	155	LYS
1	I	157	ASN
1	I	158	LEU
1	I	161	ILE
1	I	166	GLU
1	I	173	ASN
1	I	179	HIS
1	I	236	ARG
1	I	256	LEU
1	I	260	VAL
1	I	288	THR
1	I	295	LYS
1	I	321	LEU
1	I	337	LYS
1	I	341	ARG
1	I	344	MET
1	I	373	MET
1	I	433	GLN
1	I	457	GLU
1	I	490	ASP
1	I	496	LYS
1	I	499	HIS
1	I	502	ASN
1	I	537	SER
1	I	541	ASP
1	I	545	LYS
1	I	546	ASN
1	I	549	VAL
1	I	562	ASP

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Mol	Chain	Res	Type
1	I	578	MET
1	I	587	VAL
1	J	64	MET
1	J	65	ARG
1	J	72	ASN
1	J	84	LYS
1	J	91	LYS
1	J	96	ASN
1	J	98	LYS
1	J	99	LYS
1	J	101	ARG
1	J	102	HIS
1	J	104	VAL
1	J	114	SER
1	J	116	VAL
1	J	117	ILE
1	J	119	MET
1	J	123	GLU
1	J	125	GLU
1	J	136	ILE
1	J	141	LYS
1	J	143	THR
1	J	154	GLU
1	J	161	ILE
1	J	166	GLU
1	J	167	THR
1	J	173	ASN
1	J	179	HIS
1	J	197	LEU
1	J	211	LYS
1	J	214	LEU
1	J	217	ILE
1	J	221	TRP
1	J	256	LEU
1	J	260	VAL
1	J	261	GLU
1	J	288	THR
1	J	295	LYS
1	J	335	LYS
1	J	337	LYS
1	J	343	ILE
1	J	348	ILE

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Mol	Chain	Res	Type
1	J	353	ARG
1	J	373	MET
1	J	383	ASP
1	J	433	GLN
1	J	457	GLU
1	J	463	ARG
1	J	487	LYS
1	J	490	ASP
1	J	496	LYS
1	J	499	HIS
1	J	502	ASN
1	J	523	ASN
1	J	537	SER
1	J	545	LYS
1	J	549	VAL
1	J	562	ASP
1	K	72	ASN
1	K	90	ASP
1	K	91	LYS
1	K	116	VAL
1	K	119	MET
1	K	120	LYS
1	K	122	GLU
1	K	125	GLU
1	K	130	GLN
1	K	135	GLN
1	K	136	ILE
1	K	140	ARG
1	K	141	LYS
1	K	143	THR
1	K	148	GLN
1	K	150	LYS
1	K	154	GLU
1	K	155	LYS
1	K	161	ILE
1	K	164	LEU
1	K	166	GLU
1	K	167	THR
1	K	173	ASN
1	K	179	HIS
1	K	197	LEU
1	K	214	LEU

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Mol	Chain	Res	Type
1	K	216	TYR
1	K	217	ILE
1	K	220	ILE
1	K	228	THR
1	K	229	LYS
1	K	231	GLU
1	K	232	LYS
1	K	235	LYS
1	K	256	LEU
1	K	261	GLU
1	K	288	THR
1	K	295	LYS
1	K	341	ARG
1	K	344	MET
1	K	346	SER
1	K	347	ARG
1	K	348	ILE
1	K	373	MET
1	K	433	GLN
1	K	457	GLU
1	K	487	LYS
1	K	490	ASP
1	K	496	LYS
1	K	499	HIS
1	K	502	ASN
1	K	529	LYS
1	K	537	SER
1	K	545	LYS
1	K	562	ASP
1	K	587	VAL
1	K	589	LYS
1	L	72	ASN
1	L	84	LYS
1	L	112	LYS
1	L	113	LEU
1	L	116	VAL
1	L	118	ASN
1	L	119	MET
1	L	120	LYS
1	L	125	GLU
1	L	126	LYS
1	L	136	ILE

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Mol	Chain	Res	Type
1	L	137	GLU
1	L	140	ARG
1	L	141	LYS
1	L	143	THR
1	L	150	LYS
1	L	154	GLU
1	L	161	ILE
1	L	166	GLU
1	L	167	THR
1	L	173	ASN
1	L	179	HIS
1	L	197	LEU
1	L	214	LEU
1	L	215	ARG
1	L	216	TYR
1	L	217	ILE
1	L	219	ASP
1	L	220	ILE
1	L	223	TYR
1	L	224	ILE
1	L	256	LEU
1	L	260	VAL
1	L	288	THR
1	L	295	LYS
1	L	341	ARG
1	L	343	ILE
1	L	344	MET
1	L	348	ILE
1	L	349	SER
1	L	358	GLU
1	L	363	LEU
1	L	368	SER
1	L	373	MET
1	L	376	LEU
1	L	433	GLN
1	L	439	SER
1	L	457	GLU
1	L	487	LYS
1	L	490	ASP
1	L	496	LYS
1	L	497	LYS
1	L	499	HIS

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Mol	Chain	Res	Type
1	L	502	ASN
1	L	537	SER
1	L	541	ASP
1	L	545	LYS
1	L	549	VAL
1	L	562	ASP
1	L	571	SER
1	L	578	MET
1	L	583	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	130	GLN
1	A	375	HIS
1	A	409	GLN
1	A	433	GLN
1	A	443	ASN
1	A	499	HIS
1	A	523	ASN
1	A	532	ASN
1	A	559	GLN
1	B	218	HIS
1	B	227	ASN
1	B	433	GLN
1	B	443	ASN
1	B	499	HIS
1	B	532	ASN
1	C	96	ASN
1	C	241	HIS
1	C	377	GLN
1	C	433	GLN
1	C	436	GLN
1	C	443	ASN
1	C	499	HIS
1	C	532	ASN
1	D	148	GLN
1	D	241	HIS
1	D	377	GLN
1	D	409	GLN
1	D	433	GLN

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Mol	Chain	Res	Type
1	D	436	GLN
1	D	443	ASN
1	D	499	HIS
1	D	532	ASN
1	D	559	GLN
1	E	72	ASN
1	E	118	ASN
1	E	218	HIS
1	E	227	ASN
1	E	409	GLN
1	E	433	GLN
1	E	443	ASN
1	E	532	ASN
1	E	559	GLN
1	F	118	ASN
1	F	227	ASN
1	F	340	HIS
1	F	409	GLN
1	F	433	GLN
1	F	436	GLN
1	F	446	ASN
1	F	532	ASN
1	F	559	GLN
1	G	241	HIS
1	G	409	GLN
1	G	433	GLN
1	G	443	ASN
1	G	499	HIS
1	G	532	ASN
1	G	546	ASN
1	G	559	GLN
1	G	561	ASN
1	H	218	HIS
1	H	409	GLN
1	H	433	GLN
1	H	436	GLN
1	H	443	ASN
1	H	471	GLN
1	H	494	ASN
1	H	499	HIS
1	H	518	GLN
1	H	532	ASN

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Mol	Chain	Res	Type
1	I	72	ASN
1	I	96	ASN
1	I	409	GLN
1	I	433	GLN
1	I	436	GLN
1	I	443	ASN
1	I	464	GLN
1	I	471	GLN
1	I	499	HIS
1	I	532	ASN
1	I	546	ASN
1	J	102	HIS
1	J	409	GLN
1	J	433	GLN
1	J	436	GLN
1	J	443	ASN
1	J	469	GLN
1	J	471	GLN
1	J	499	HIS
1	J	532	ASN
1	J	561	ASN
1	K	144	ASN
1	K	218	HIS
1	K	227	ASN
1	K	241	HIS
1	K	377	GLN
1	K	409	GLN
1	K	433	GLN
1	K	436	GLN
1	K	443	ASN
1	K	499	HIS
1	K	523	ASN
1	K	532	ASN
1	K	546	ASN
1	K	580	ASN
1	L	340	HIS
1	L	377	GLN
1	L	409	GLN
1	L	433	GLN
1	L	443	ASN
1	L	488	GLN
1	L	499	HIS

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Mol	Chain	Res	Type
1	L	518	GLN
1	L	532	ASN
1	L	580	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 18 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EPE	D	801	-	15,15,15	1.14	1 (6%)	19,20,20	1.26	1 (5%)
2	EPE	B	801	-	15,15,15	0.64	1 (6%)	19,20,20	0.81	0
2	EPE	E	801	-	15,15,15	0.99	1 (6%)	19,20,20	0.89	2 (10%)
2	EPE	G	801	-	15,15,15	1.03	1 (6%)	19,20,20	1.03	2 (10%)
2	EPE	H	801	-	15,15,15	0.63	1 (6%)	19,20,20	0.65	0
2	EPE	I	801	-	15,15,15	0.79	1 (6%)	19,20,20	0.88	0
2	EPE	A	801	-	15,15,15	0.68	1 (6%)	19,20,20	0.72	0
2	EPE	C	801	-	15,15,15	1.05	1 (6%)	19,20,20	1.13	1 (5%)
2	EPE	J	801	-	15,15,15	0.70	1 (6%)	19,20,20	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPE	F	801	-	15,15,15	1.03	1 (6%)	19,20,20	0.95	2 (10%)

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	EPE	D	801	-	-	4/9/19/19	0/1/1/1
2	EPE	B	801	-	-	7/9/19/19	0/1/1/1
2	EPE	E	801	-	-	6/9/19/19	0/1/1/1
2	EPE	G	801	-	-	3/9/19/19	0/1/1/1
2	EPE	H	801	-	-	6/9/19/19	0/1/1/1
2	EPE	I	801	-	-	5/9/19/19	0/1/1/1
2	EPE	A	801	-	-	5/9/19/19	0/1/1/1
2	EPE	C	801	-	-	6/9/19/19	0/1/1/1
2	EPE	J	801	-	-	5/9/19/19	0/1/1/1
2	EPE	F	801	-	-	5/9/19/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	EPE	O1S-S	3.76	1.55	1.45
2	G	801	EPE	O1S-S	3.66	1.55	1.45
2	F	801	EPE	O2S-S	3.65	1.55	1.45
2	E	801	EPE	O2S-S	3.59	1.55	1.45
2	D	801	EPE	O1S-S	3.58	1.55	1.45
2	I	801	EPE	O3S-S	2.36	1.56	1.47
2	A	801	EPE	O3S-S	2.25	1.55	1.47
2	B	801	EPE	O3S-S	2.24	1.55	1.47
2	H	801	EPE	O3S-S	2.23	1.55	1.47
2	J	801	EPE	O3S-S	2.17	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	EPE	O3S-S-O2S	3.13	119.22	111.40
2	F	801	EPE	O3S-S-O1S	2.72	118.20	111.40
2	E	801	EPE	O3S-S-O1S	2.66	118.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	EPE	O3S-S-O2S	2.54	117.76	111.40
2	D	801	EPE	O3S-S-O2S	2.37	117.33	111.40
2	G	801	EPE	O1S-S-C10	-2.25	103.33	106.73
2	F	801	EPE	O2S-S-O1S	-2.12	106.92	113.82
2	E	801	EPE	O2S-S-C10	-2.03	103.67	106.73

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	EPE	C10-C9-N1-C2
2	A	801	EPE	C10-C9-N1-C6
2	B	801	EPE	S-C10-C9-N1
2	B	801	EPE	C9-C10-S-O1S
2	D	801	EPE	C10-C9-N1-C6
2	D	801	EPE	C8-C7-N4-C5
2	D	801	EPE	S-C10-C9-N1
2	E	801	EPE	C10-C9-N1-C2
2	E	801	EPE	C10-C9-N1-C6
2	G	801	EPE	C8-C7-N4-C5
2	H	801	EPE	S-C10-C9-N1
2	H	801	EPE	C9-C10-S-O1S
2	I	801	EPE	C10-C9-N1-C6
2	J	801	EPE	C10-C9-N1-C6
2	A	801	EPE	C8-C7-N4-C5
2	C	801	EPE	C8-C7-N4-C5
2	I	801	EPE	C8-C7-N4-C5
2	J	801	EPE	C8-C7-N4-C5
2	J	801	EPE	C8-C7-N4-C3
2	B	801	EPE	C9-C10-S-O3S
2	C	801	EPE	C9-C10-S-O3S
2	E	801	EPE	N4-C7-C8-O8
2	B	801	EPE	N4-C7-C8-O8
2	C	801	EPE	C10-C9-N1-C2
2	I	801	EPE	C10-C9-N1-C2
2	J	801	EPE	C10-C9-N1-C2
2	H	801	EPE	C9-C10-S-O3S
2	A	801	EPE	C8-C7-N4-C3
2	B	801	EPE	C8-C7-N4-C5
2	G	801	EPE	C8-C7-N4-C3
2	B	801	EPE	C9-C10-S-O2S
2	E	801	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
2	H	801	EPE	C9-C10-S-O2S
2	A	801	EPE	S-C10-C9-N1
2	G	801	EPE	S-C10-C9-N1
2	I	801	EPE	S-C10-C9-N1
2	J	801	EPE	S-C10-C9-N1
2	I	801	EPE	C8-C7-N4-C3
2	F	801	EPE	C9-C10-S-O3S
2	C	801	EPE	C10-C9-N1-C6
2	F	801	EPE	C10-C9-N1-C2
2	F	801	EPE	C10-C9-N1-C6
2	F	801	EPE	C8-C7-N4-C5
2	D	801	EPE	N4-C7-C8-O8
2	B	801	EPE	C8-C7-N4-C3
2	E	801	EPE	C8-C7-N4-C5
2	E	801	EPE	C8-C7-N4-C3
2	F	801	EPE	C8-C7-N4-C3
2	H	801	EPE	C8-C7-N4-C3
2	C	801	EPE	C9-C10-S-O1S
2	H	801	EPE	C8-C7-N4-C5
2	C	801	EPE	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	801	EPE	1	0
2	I	801	EPE	1	0
2	F	801	EPE	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	521/650 (80%)	0.10	19 (3%)	46	25	42, 79, 150, 203	0
1	B	527/650 (81%)	-0.02	18 (3%)	48	27	44, 82, 132, 200	1 (0%)
1	C	520/650 (80%)	0.06	11 (2%)	63	39	44, 86, 162, 191	0
1	D	502/650 (77%)	0.16	32 (6%)	25	13	41, 83, 199, 280	0
1	E	523/650 (80%)	0.06	13 (2%)	58	34	43, 90, 135, 185	1 (0%)
1	F	528/650 (81%)	0.21	33 (6%)	26	13	46, 93, 164, 196	1 (0%)
1	G	520/650 (80%)	0.03	11 (2%)	63	39	50, 84, 136, 198	0
1	H	471/650 (72%)	0.14	22 (4%)	36	19	46, 85, 166, 213	0
1	I	518/650 (79%)	0.02	14 (2%)	56	32	42, 88, 134, 186	0
1	J	518/650 (79%)	0.11	10 (1%)	66	42	40, 93, 174, 230	0
1	K	511/650 (78%)	0.47	28 (5%)	30	15	49, 110, 192, 273	0
1	L	494/650 (76%)	0.58	44 (8%)	15	8	64, 122, 194, 253	0
All	All	6153/7800 (78%)	0.16	255 (4%)	41	22	40, 90, 166, 280	3 (0%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	225	ALA	6.3
1	C	221	TRP	6.1
1	E	221	TRP	6.1
1	D	216	TYR	5.7
1	F	100	PRO	5.7
1	K	88	VAL	5.3
1	L	221	TRP	5.3
1	I	225	ALA	5.3
1	F	222	GLY	5.3
1	L	85	LEU	5.2
1	H	221	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	221	TRP	5.0
1	J	214	LEU	5.0
1	G	221	TRP	5.0
1	H	225	ALA	5.0
1	D	108	GLU	4.9
1	L	214	LEU	4.8
1	E	229	LYS	4.8
1	F	553	ALA	4.7
1	D	85	LEU	4.6
1	D	88	VAL	4.6
1	D	222	GLY	4.6
1	L	89	ILE	4.5
1	L	342	ASP	4.5
1	E	222	GLY	4.5
1	H	163	LEU	4.5
1	B	227	ASN	4.4
1	J	218	HIS	4.4
1	I	222	GLY	4.4
1	L	88	VAL	4.3
1	H	161	ILE	4.3
1	L	222	GLY	4.3
1	K	221	TRP	4.2
1	F	221	TRP	4.2
1	L	219	ASP	4.1
1	B	218	HIS	4.1
1	K	342	ASP	4.0
1	F	223	TYR	4.0
1	B	215	ARG	3.9
1	K	347	ARG	3.9
1	A	212	GLY	3.9
1	K	89	ILE	3.9
1	H	85	LEU	3.9
1	H	158	LEU	3.9
1	K	223	TYR	3.9
1	F	216	TYR	3.8
1	D	164	LEU	3.8
1	L	225	ALA	3.8
1	K	216	TYR	3.8
1	H	88	VAL	3.8
1	K	222	GLY	3.8
1	B	230	LYS	3.7
1	H	160	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	226	PRO	3.7
1	B	216	TYR	3.7
1	L	217	ILE	3.7
1	D	113	LEU	3.6
1	D	153	ILE	3.6
1	L	136	ILE	3.6
1	B	229	LYS	3.6
1	D	230	LYS	3.6
1	A	225	ALA	3.5
1	K	225	ALA	3.5
1	L	223	TYR	3.5
1	F	226	PRO	3.5
1	K	159	PRO	3.5
1	L	159	PRO	3.5
1	K	229	LYS	3.4
1	F	227	ASN	3.4
1	F	104	VAL	3.4
1	D	161	ILE	3.4
1	L	113	LEU	3.4
1	D	109	THR	3.4
1	K	340	HIS	3.4
1	L	81	GLU	3.3
1	J	225	ALA	3.3
1	L	220	ILE	3.3
1	H	82	ARG	3.3
1	F	98	LYS	3.3
1	L	367	TYR	3.3
1	D	228	THR	3.3
1	B	214	LEU	3.2
1	G	211	LYS	3.2
1	G	219	ASP	3.2
1	L	92	LYS	3.2
1	B	221	TRP	3.2
1	L	364	GLY	3.2
1	A	226	PRO	3.2
1	F	218	HIS	3.2
1	C	222	GLY	3.1
1	H	222	GLY	3.1
1	L	259	MET	3.1
1	C	225	ALA	3.1
1	F	220	ILE	3.1
1	C	183	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	368	SER	3.0
1	I	224	ILE	3.0
1	B	212	GLY	3.0
1	L	160	GLY	3.0
1	F	232	LYS	3.0
1	D	219	ASP	3.0
1	A	221	TRP	2.9
1	H	159	PRO	2.9
1	J	219	ASP	2.9
1	L	164	LEU	2.9
1	L	347	ARG	2.9
1	E	216	TYR	2.9
1	F	97	SER	2.9
1	H	212	GLY	2.9
1	K	160	GLY	2.9
1	K	164	LEU	2.9
1	L	112	LYS	2.9
1	D	165	PRO	2.9
1	K	153	ILE	2.9
1	D	229	LYS	2.9
1	E	224	ILE	2.9
1	D	86	VAL	2.8
1	D	211	LYS	2.8
1	A	213	SER	2.8
1	F	219	ASP	2.8
1	F	96	ASN	2.8
1	I	218	HIS	2.8
1	F	109	THR	2.8
1	L	224	ILE	2.8
1	C	216	TYR	2.7
1	E	225	ALA	2.7
1	G	261	GLU	2.7
1	F	554	GLY	2.7
1	D	147	TYR	2.7
1	D	227	ASN	2.7
1	L	158	LEU	2.7
1	L	163	LEU	2.7
1	K	81	GLU	2.7
1	A	219	ASP	2.7
1	C	299	LYS	2.7
1	A	159	PRO	2.7
1	C	234	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	218	HIS	2.7
1	B	232	LYS	2.6
1	J	524	GLY	2.6
1	K	514	THR	2.6
1	A	115	THR	2.6
1	D	150	LYS	2.6
1	H	226	PRO	2.6
1	E	228	THR	2.6
1	H	153	ILE	2.6
1	H	211	LYS	2.6
1	L	86	VAL	2.6
1	F	228	THR	2.6
1	F	99	LYS	2.6
1	L	153	ILE	2.6
1	K	134	PHE	2.5
1	L	165	PRO	2.5
1	H	164	LEU	2.5
1	K	158	LEU	2.5
1	A	109	THR	2.5
1	J	224	ILE	2.5
1	G	212	GLY	2.5
1	K	85	LEU	2.5
1	H	144	ASN	2.5
1	L	553	ALA	2.5
1	F	106	LYS	2.5
1	D	217	ILE	2.5
1	A	103	VAL	2.5
1	H	150	LYS	2.4
1	D	160	GLY	2.4
1	I	212	GLY	2.4
1	F	224	ILE	2.4
1	K	183	ARG	2.4
1	D	214	LEU	2.4
1	L	196	ALA	2.4
1	D	81	GLU	2.4
1	E	227	ASN	2.4
1	C	131	LYS	2.4
1	C	211	LYS	2.4
1	B	415	GLU	2.4
1	D	158	LEU	2.4
1	D	411	GLY	2.4
1	K	132	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	2.4
1	G	234	PRO	2.4
1	B	409	GLN	2.3
1	F	113	LEU	2.3
1	G	135	GLN	2.3
1	H	214	LEU	2.3
1	L	138	PHE	2.3
1	D	225	ALA	2.3
1	F	107	LYS	2.3
1	F	121	PRO	2.3
1	F	217	ILE	2.3
1	L	161	ILE	2.3
1	B	228	THR	2.3
1	A	499	HIS	2.3
1	D	145	LEU	2.3
1	E	499	HIS	2.3
1	L	216	TYR	2.3
1	F	296	ASP	2.3
1	A	211	LYS	2.3
1	H	87	ALA	2.3
1	J	525	GLY	2.3
1	L	133	ALA	2.3
1	A	210	SER	2.3
1	E	223	TYR	2.3
1	J	118	ASN	2.2
1	E	214	LEU	2.2
1	I	64	MET	2.2
1	I	221	TRP	2.2
1	J	109	THR	2.2
1	I	353	ARG	2.2
1	G	222	GLY	2.2
1	A	152	LYS	2.2
1	I	548	LYS	2.2
1	A	218	HIS	2.2
1	A	234	PRO	2.2
1	C	212	GLY	2.2
1	F	230	LYS	2.2
1	L	365	PHE	2.2
1	K	86	VAL	2.2
1	I	213	SER	2.2
1	K	224	ILE	2.2
1	B	222	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	492	VAL	2.1
1	L	566	TYR	2.1
1	B	224	ILE	2.1
1	D	128	LEU	2.1
1	G	225	ALA	2.1
1	B	353	ARG	2.1
1	K	486	GLU	2.1
1	K	218	HIS	2.1
1	E	366	THR	2.1
1	L	115	THR	2.1
1	B	217	ILE	2.1
1	D	232	LYS	2.1
1	F	399	LYS	2.1
1	A	133	ALA	2.1
1	F	95	ALA	2.1
1	H	165	PRO	2.1
1	F	235	LYS	2.1
1	L	336	TYR	2.1
1	L	568	LEU	2.1
1	F	158	LEU	2.1
1	G	224	ILE	2.1
1	L	340	HIS	2.1
1	B	140	ARG	2.1
1	I	211	LYS	2.1
1	G	220	ILE	2.1
1	J	221	TRP	2.1
1	H	216	TYR	2.1
1	K	87	ALA	2.1
1	L	150	LYS	2.0
1	I	348	ILE	2.0
1	L	554	GLY	2.0
1	D	220	ILE	2.0
1	I	220	ILE	2.0
1	E	215	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EPE	F	801	15/15	0.76	0.24	144,157,176,177	0
2	EPE	J	801	15/15	0.79	0.20	83,113,191,192	0
2	EPE	E	801	15/15	0.82	0.21	85,140,193,198	0
3	CD	H	803	1/1	0.82	0.16	37,37,37,37	0
2	EPE	C	801	15/15	0.84	0.19	86,113,196,197	0
2	EPE	G	801	15/15	0.84	0.19	86,121,204,211	0
2	EPE	D	801	15/15	0.85	0.18	79,123,194,197	0
2	EPE	H	801	15/15	0.85	0.21	96,123,197,213	0
2	EPE	A	801	15/15	0.86	0.20	100,111,190,196	0
3	CD	G	802	1/1	0.86	0.10	108,108,108,108	0
2	EPE	I	801	15/15	0.86	0.18	73,111,167,179	0
2	EPE	B	801	15/15	0.88	0.17	89,134,175,176	0
4	CL	H	802	1/1	0.91	0.07	76,76,76,76	0
4	CL	K	801	1/1	0.92	0.06	93,93,93,93	0
4	CL	L	801	1/1	0.93	0.05	87,87,87,87	0
4	CL	F	802	1/1	0.94	0.05	88,88,88,88	0
4	CL	J	802	1/1	0.94	0.07	70,70,70,70	0
4	CL	C	802	1/1	0.95	0.09	72,72,72,72	0
4	CL	D	802	1/1	0.96	0.07	82,82,82,82	0
3	CD	I	802	1/1	0.96	0.05	101,101,101,101	0
3	CD	A	802	1/1	0.97	0.05	98,98,98,98	0
3	CD	B	802	1/1	0.97	0.05	131,131,131,131	0
4	CL	E	802	1/1	0.97	0.05	102,102,102,102	0
3	CD	C	803	1/1	0.97	0.07	94,94,94,94	0
3	CD	D	803	1/1	0.99	0.05	97,97,97,97	0
3	CD	E	803	1/1	0.99	0.02	110,110,110,110	0
3	CD	F	803	1/1	0.99	0.02	131,131,131,131	0
3	CD	J	803	1/1	0.99	0.05	102,102,102,102	0

6.5 Other polymers ⓘ

There are no such residues in this entry.