



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 10:38 PM EDT

PDB ID : 4X2T  
Title : X-ray crystal structure of the orally available aminopeptidase inhibitor, Tosedostat, bound to the M17 Leucyl Aminopeptidase from *P. falciparum*  
Authors : Drinkwater, N.; McGowan, S.  
Deposited on : unknown  
Resolution : 2.73 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

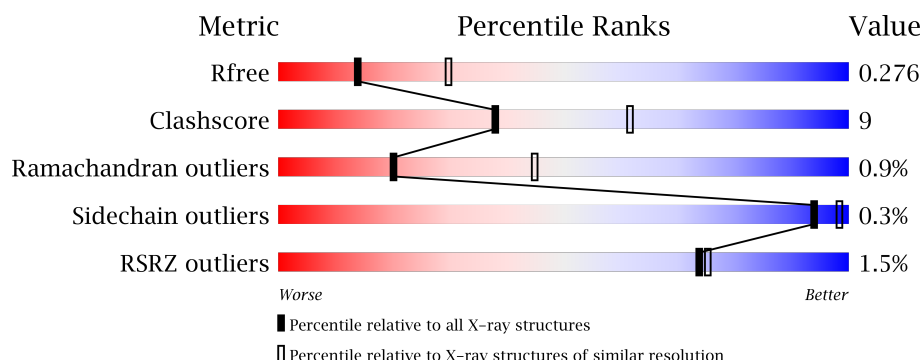
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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))
$R_{free}$	100719	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (2.74-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	519	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 87%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>100%</span> <span>87%</span> <span>12%</span> <span>.</span> </div> </div>
1	B	519	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 14%, green 81%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>100%</span> <span>81%</span> <span>14%</span> <span>...</span> </div> </div>
1	C	519	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 14%, green 83%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>100%</span> <span>83%</span> <span>14%</span> <span>.</span> </div> </div>
1	D	519	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 83%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>100%</span> <span>83%</span> <span>15%</span> <span>.</span> </div> </div>
1	E	519	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 14%, green 83%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>100%</span> <span>83%</span> <span>14%</span> <span>..</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	
1	G	519	
1	H	519	
1	I	519	
1	J	519	
1	K	519	
1	L	519	

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
3	TOD	A	703	-	-	-	X
3	TOD	I	703	-	-	-	X
4	CO3	A	704	-	-	X	X
4	CO3	E	704	-	-	-	X
4	CO3	G	704	-	-	X	X
4	CO3	I	704	-	-	-	X
4	CO3	J	704	-	-	X	X
4	CO3	K	704	-	-	X	-
5	SO4	D	704	-	-	-	X
5	SO4	E	706	-	-	-	X
6	1PE	A	708	-	-	-	X
6	1PE	B	1006	-	-	-	X
6	1PE	C	706	-	-	X	-
6	1PE	D	705	-	-	-	X
6	1PE	G	707	-	-	-	X
6	1PE	H	705	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 48055 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	1	0
			3928	2527	628	754	19			
1	B	510	Total	C	N	O	S	0	0	0
			3837	2475	619	724	19			
1	C	517	Total	C	N	O	S	0	0	0
			3942	2537	636	750	19			
1	D	511	Total	C	N	O	S	0	0	0
			3899	2511	628	741	19			
1	E	509	Total	C	N	O	S	0	0	0
			3884	2500	622	743	19			
1	F	509	Total	C	N	O	S	0	0	0
			3762	2421	606	716	19			
1	G	519	Total	C	N	O	S	0	0	0
			3979	2554	637	768	20			
1	H	510	Total	C	N	O	S	0	0	0
			3855	2480	621	735	19			
1	I	515	Total	C	N	O	S	0	0	0
			3912	2520	631	742	19			
1	J	511	Total	C	N	O	S	0	0	0
			3875	2499	624	733	19			
1	K	509	Total	C	N	O	S	0	0	0
			3878	2496	621	742	19			
1	L	508	Total	C	N	O	S	0	0	0
			3806	2447	612	728	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

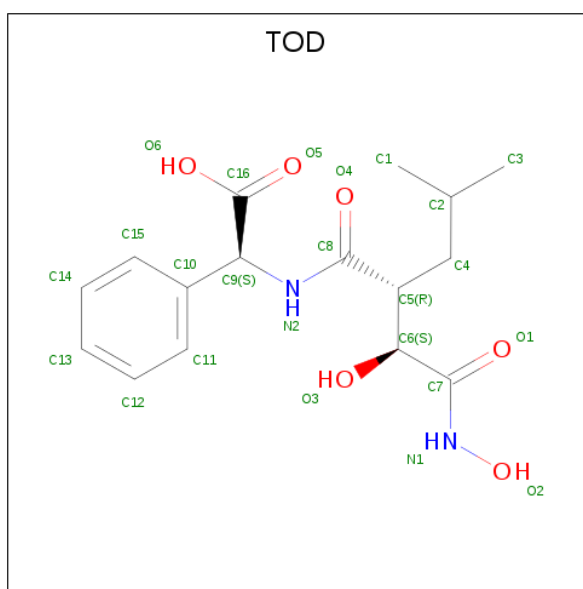
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	I	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	L	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is (2S)-({(2R)-2-[(1S)-1-hydroxy-2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}amino)(phenyl)ethanoic acid (three-letter code: TOD) (formula: C<sub>16</sub>H<sub>22</sub>N<sub>2</sub>O<sub>6</sub>).



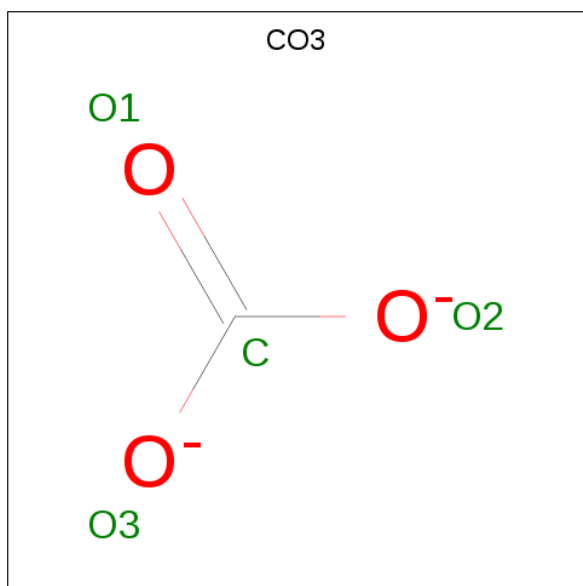
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	16	2	6		
3	B	1	Total	C	N	O	0	0
			24	16	2	6		
3	C	1	Total	C	N	O	0	0
			17	11	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			15	9	2	4		
3	F	1	Total	C	N	O	0	0
			24	16	2	6		
3	G	1	Total	C	N	O	0	0
			22	16	2	4		
3	H	1	Total	C	N	O	0	0
			14	8	2	4		
3	I	1	Total	C	N	O	0	0
			24	16	2	6		
3	J	1	Total	C	N	O	0	0
			22	16	2	4		
3	K	1	Total	C	N	O	0	0
			22	16	2	4		
3	L	1	Total	C	N	O	0	0
			24	16	2	6		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



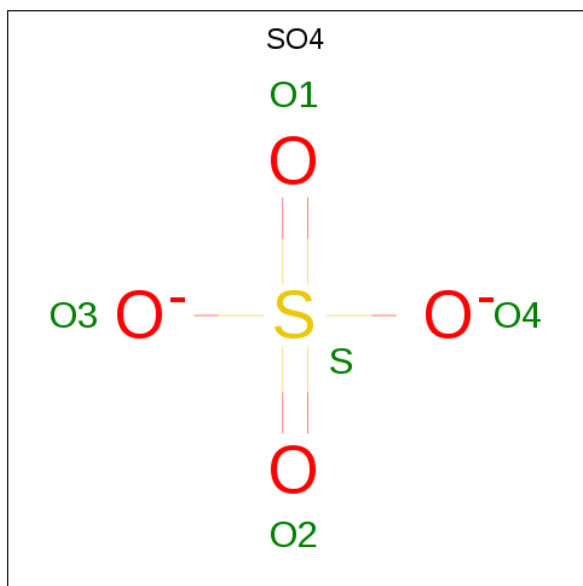
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		
4	C	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0
4	K	1	Total C O 4 1 3	0	0
4	L	1	Total C O 4 1 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

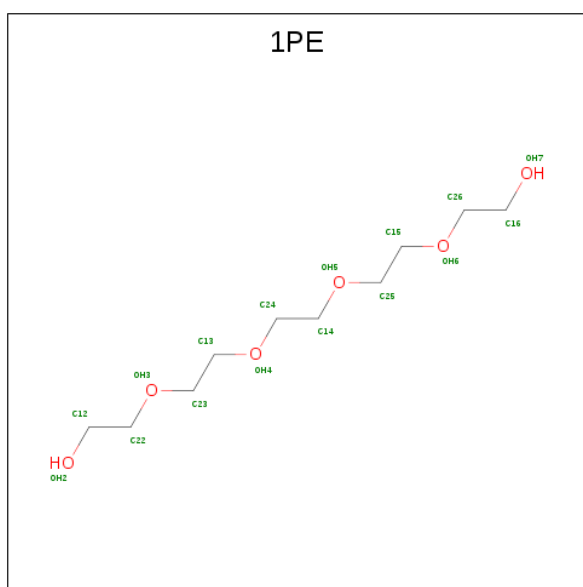
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 6 3	0	0
6	B	1	Total C O 7 5 2	0	0
6	C	1	Total C O 13 9 4	0	0
6	C	1	Total C O 9 6 3	0	0
6	D	1	Total C O 10 7 3	0	0
6	D	1	Total C O 10 7 3	0	0
6	E	1	Total C O 12 8 4	0	0
6	G	1	Total C O 9 6 3	0	0
6	G	1	Total C O 9 6 3	0	0
6	H	1	Total C O 10 7 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	102	Total O 102 102	0	0
7	B	74	Total O 74 74	0	0
7	C	70	Total O 70 70	0	0
7	D	80	Total O 80 80	0	0
7	E	113	Total O 113 113	0	0
7	F	88	Total O 88 88	0	0
7	G	93	Total O 93 93	0	0
7	H	74	Total O 74 74	0	0
7	I	91	Total O 91 91	0	0
7	J	86	Total O 86 86	0	0

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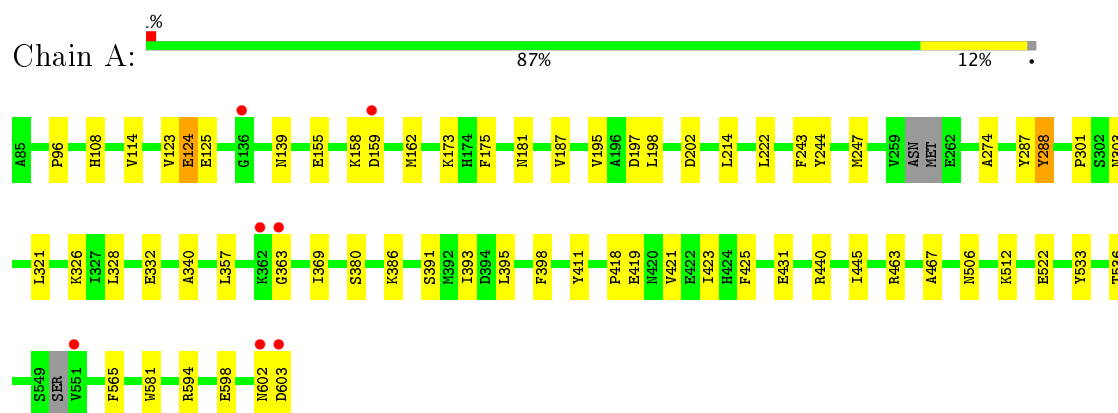
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	91	Total 91	O 91	0	0
7	L	69	Total 69	O 69	0	0

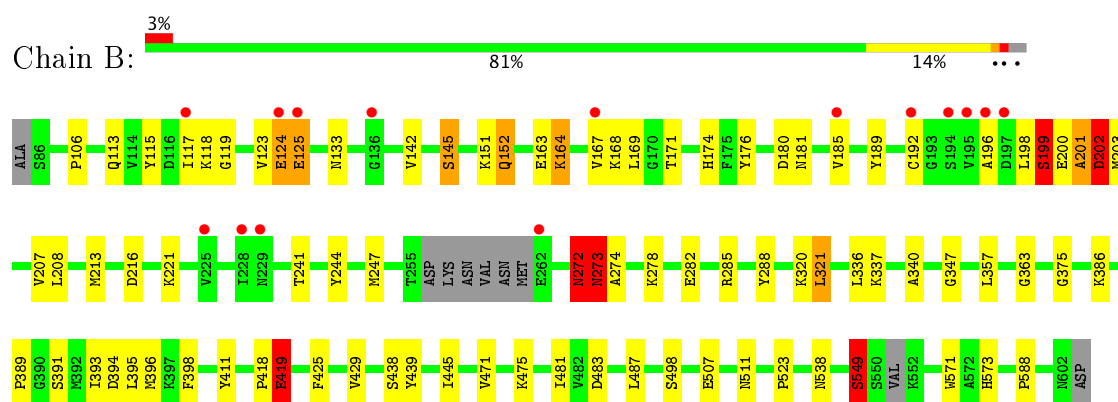
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

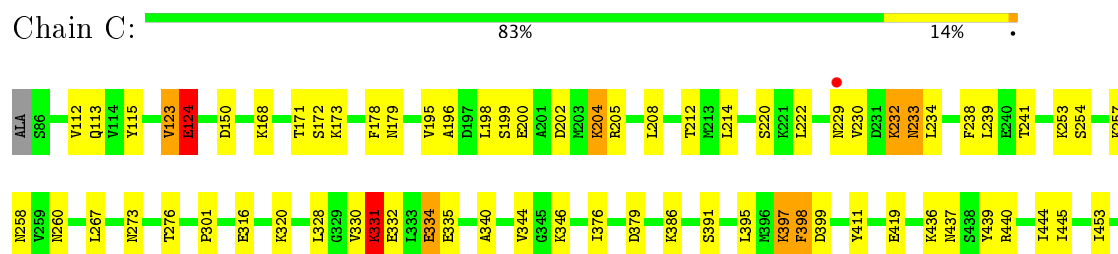
- Molecule 1: M17 leucyl aminopeptidase



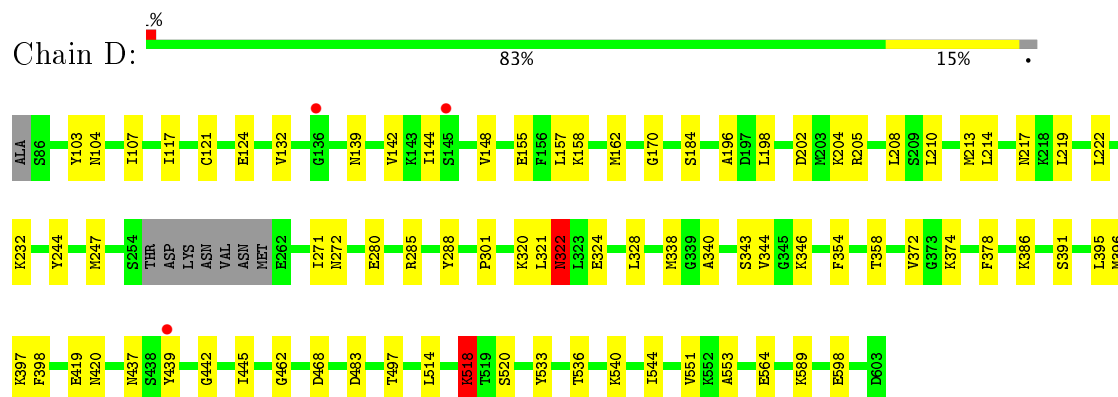
- Molecule 1: M17 leucyl aminopeptidase



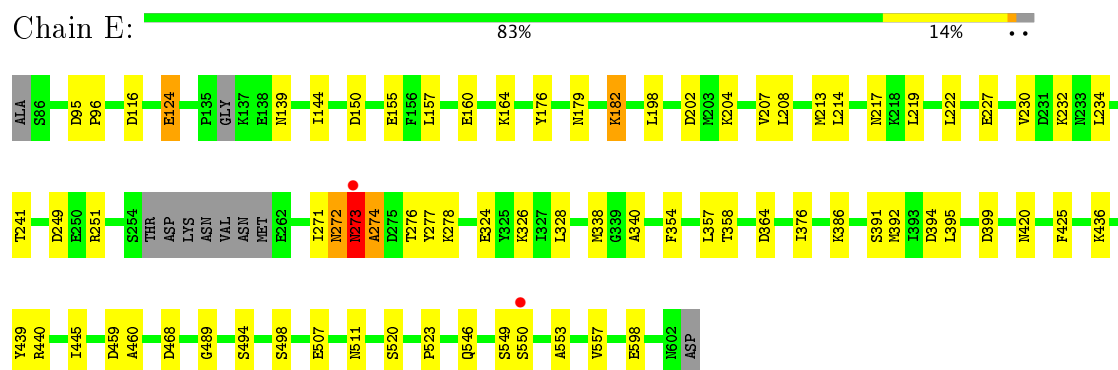
- Molecule 1: M17 leucyl aminopeptidase



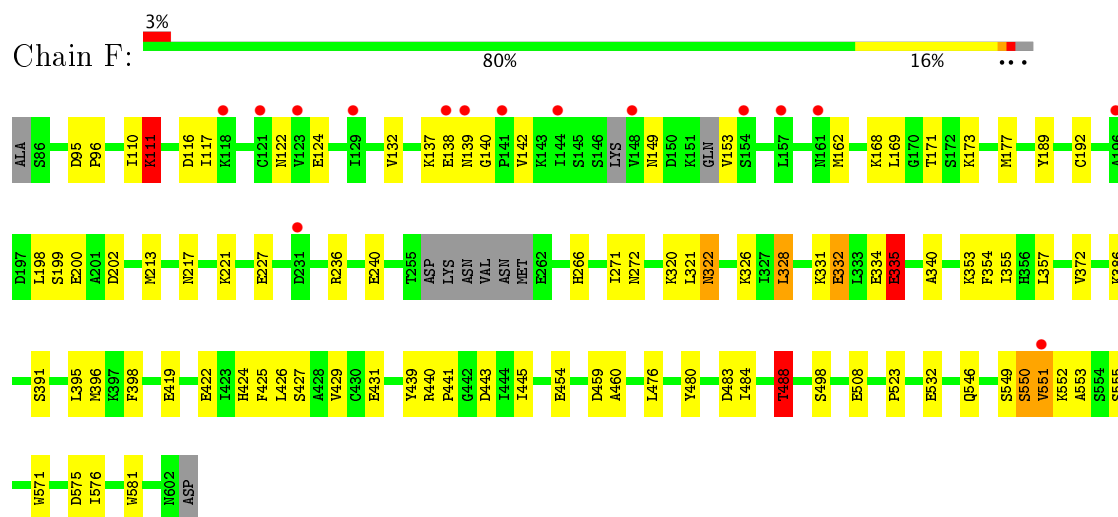
- 
- Molecule 1: M17 leucyl aminopeptidase



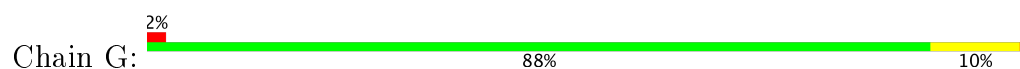
- Molecule 1: M17 leucyl aminopeptidase

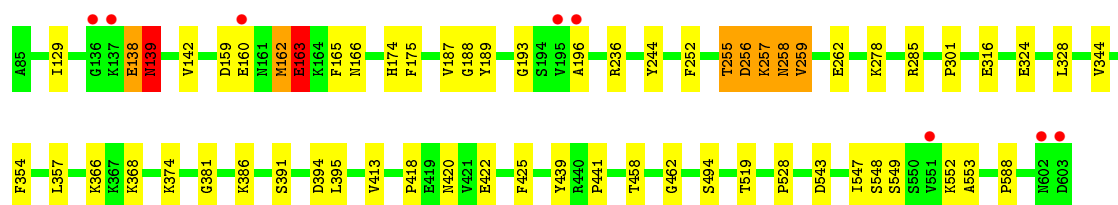


- Molecule 1: M17 leucyl aminopeptidase

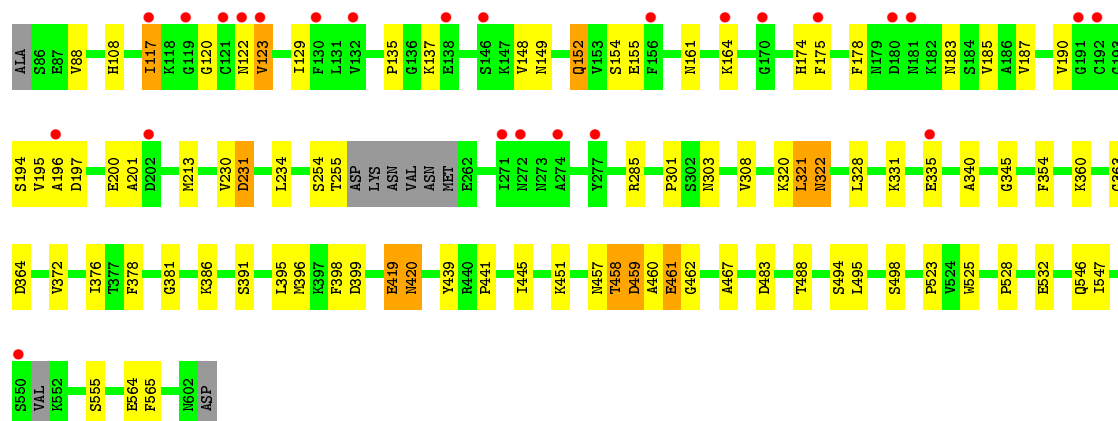
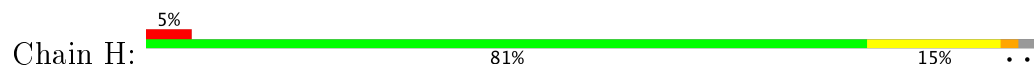


- Molecule 1: M17 leucyl aminopeptidase

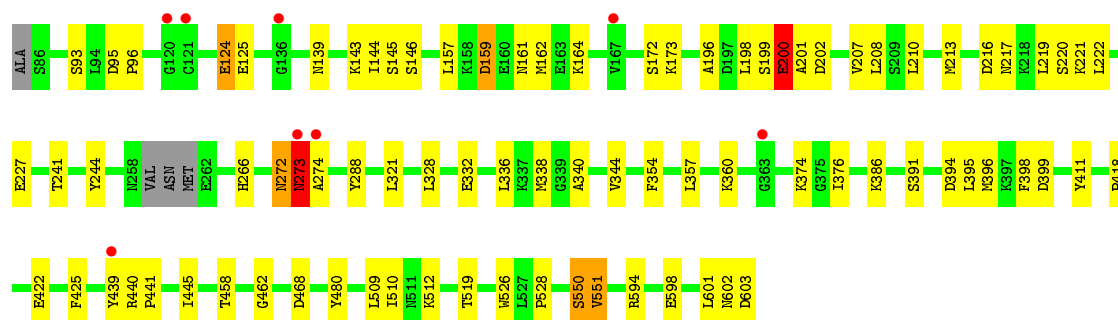
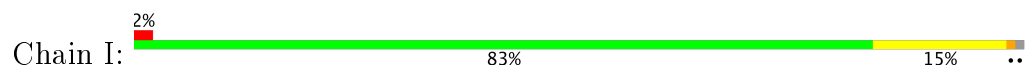




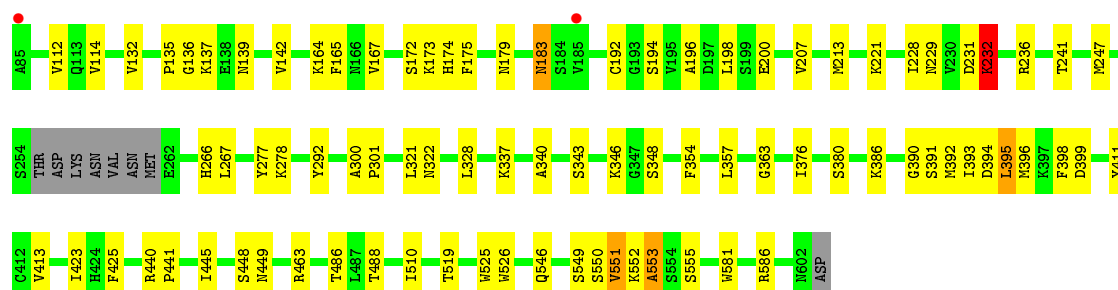
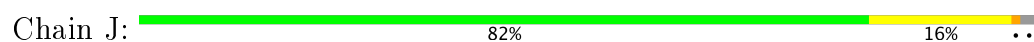
• Molecule 1: M17 leucyl aminopeptidase



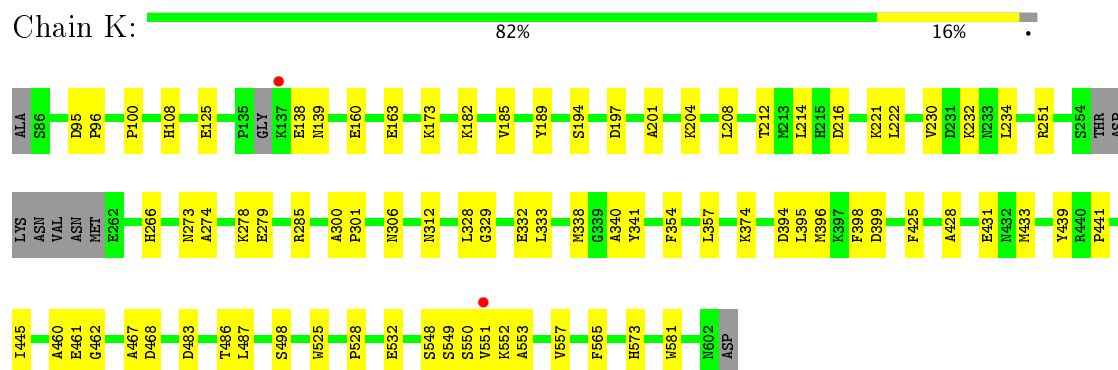
• Molecule 1: M17 leucyl aminopeptidase



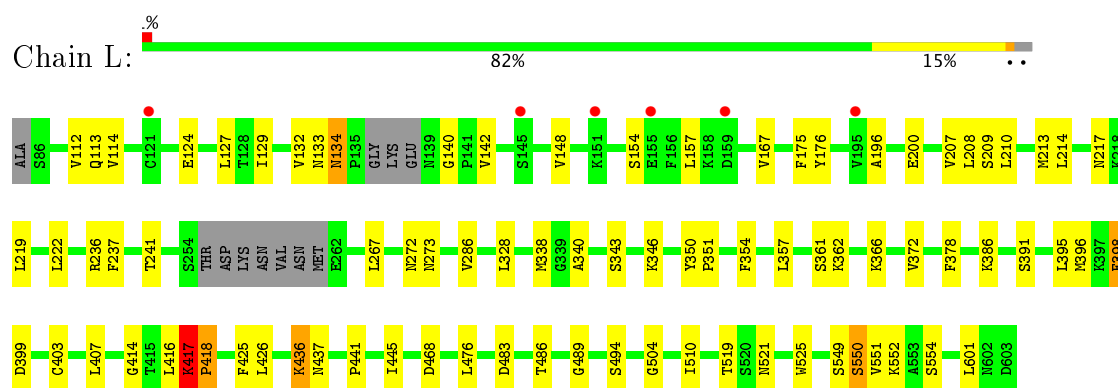
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.72Å 176.70Å 223.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.73 48.75 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.75-2.73) 94.1 (48.75-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.220 , 0.274 0.221 , 0.276	Depositor DCC
$R_{free}$ test set	8641 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 30.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2953e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CO3, ZN, TOD, 1PE

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	0.38	2/4007 (0.0%)	0.58	3/5440 (0.1%)
1	B	0.57	10/3913 (0.3%)	0.70	15/5316 (0.3%)
1	C	0.43	5/4019 (0.1%)	0.70	8/5453 (0.1%)
1	D	0.32	0/3976	0.58	2/5395 (0.0%)
1	E	0.32	0/3960	0.59	9/5375 (0.2%)
1	F	0.39	3/3835 (0.1%)	0.65	10/5222 (0.2%)
1	G	0.35	1/4057 (0.0%)	0.65	9/5505 (0.2%)
1	H	0.38	1/3931 (0.0%)	0.62	2/5340 (0.0%)
1	I	0.38	1/3989 (0.0%)	0.64	6/5414 (0.1%)
1	J	0.38	0/3952	0.63	3/5366 (0.1%)
1	K	0.42	2/3954 (0.1%)	0.55	1/5367 (0.0%)
1	L	0.41	1/3881 (0.0%)	0.63	3/5282 (0.1%)
All	All	0.40	26/47474 (0.1%)	0.63	71/64475 (0.1%)

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	B	0	9
1	C	0	5
1	D	0	2
1	E	0	2
1	F	0	6
1	G	0	3
1	H	0	3
1	I	0	4
1	J	0	3
1	K	0	1
1	L	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	43

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	TYR	CE2-CZ	-13.71	1.20	1.38
1	B	439	TYR	CG-CD1	-13.27	1.21	1.39
1	L	418	PRO	N-CD	11.39	1.63	1.47
1	B	549	SER	CB-OG	-10.96	1.27	1.42
1	F	488	THR	C-O	-10.84	1.02	1.23
1	C	398	PHE	C-O	-9.93	1.04	1.23
1	B	439	TYR	CD2-CE2	-8.13	1.27	1.39
1	B	439	TYR	CG-CD2	-7.89	1.28	1.39
1	C	398	PHE	CG-CD1	-7.31	1.27	1.38
1	C	398	PHE	CG-CD2	-6.96	1.28	1.38
1	B	439	TYR	CE1-CZ	-6.95	1.29	1.38
1	G	324	GLU	CB-CG	-6.94	1.39	1.52
1	K	461	GLU	CD-OE1	-6.68	1.18	1.25
1	B	549	SER	C-O	-6.54	1.10	1.23
1	A	418	PRO	N-CD	6.30	1.56	1.47
1	B	549	SER	CA-CB	-6.22	1.43	1.52
1	C	398	PHE	CD1-CE1	-6.15	1.26	1.39
1	F	488	THR	N-CA	-6.08	1.34	1.46
1	F	488	THR	CB-CG2	-5.97	1.32	1.52
1	H	461	GLU	CD-OE1	-5.90	1.19	1.25
1	A	288	TYR	CD1-CE1	-5.68	1.30	1.39
1	K	439	TYR	CE1-CZ	-5.63	1.31	1.38
1	B	439	TYR	CZ-OH	-5.33	1.28	1.37
1	I	159	ASP	N-CA	-5.19	1.35	1.46
1	B	439	TYR	C-O	-5.11	1.13	1.23
1	C	398	PHE	CD2-CE2	-5.01	1.29	1.39

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	GLU	O-C-N	-26.02	81.06	122.70
1	C	123	VAL	C-N-CA	-14.52	85.40	121.70
1	G	139	ASN	CA-C-N	-13.54	89.11	116.20
1	B	151	LYS	C-N-CA	-11.96	91.81	121.70
1	G	163	GLU	CA-C-N	-9.24	96.86	117.20
1	I	273	ASN	O-C-N	-9.22	107.95	122.70
1	B	273	ASN	CA-C-N	-9.06	97.26	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	111	LYS	O-C-N	-9.06	108.21	122.70
1	B	202	ASP	O-C-N	-8.80	108.61	122.70
1	C	334	GLU	C-N-CA	-8.59	100.22	121.70
1	I	159	ASP	N-CA-CB	-8.53	95.25	110.60
1	E	273	ASN	CA-C-N	-8.52	98.45	117.20
1	F	550	SER	CA-C-N	-8.52	98.46	117.20
1	B	152	GLN	O-C-N	-8.45	109.19	122.70
1	B	163	GLU	C-N-CA	7.74	141.06	121.70
1	J	232	LYS	O-C-N	-7.55	110.62	122.70
1	F	422	GLU	O-C-N	-7.54	110.63	122.70
1	G	418	PRO	C-N-CA	-6.93	104.37	121.70
1	D	322	ASN	O-C-N	-6.81	111.80	122.70
1	E	549	SER	C-N-CA	6.65	138.33	121.70
1	B	272	ASN	C-N-CA	6.65	138.32	121.70
1	E	274	ALA	N-CA-CB	6.62	119.36	110.10
1	J	395	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	B	164	LYS	CA-C-N	-6.47	102.95	117.20
1	F	488	THR	N-CA-CB	-6.43	98.08	110.30
1	C	330	VAL	C-N-CA	-6.38	105.75	121.70
1	F	335	GLU	CA-C-N	-6.38	103.17	117.20
1	B	418	PRO	C-N-CA	6.38	137.65	121.70
1	G	258	ASN	N-CA-C	-6.26	94.08	111.00
1	G	324	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	E	272	ASN	N-CA-C	-6.23	94.18	111.00
1	C	397	LYS	C-N-CA	6.17	137.12	121.70
1	B	201	ALA	C-N-CA	-6.09	106.47	121.70
1	E	272	ASN	C-N-CA	6.08	136.91	121.70
1	E	182	LYS	CA-C-N	-6.06	103.87	117.20
1	B	180	ASP	C-N-CA	6.03	136.78	121.70
1	E	550	SER	O-C-N	-5.95	113.18	122.70
1	I	274	ALA	N-CA-CB	-5.93	101.80	110.10
1	I	272	ASN	C-N-CA	-5.88	107.01	121.70
1	B	439	TYR	CG-CD2-CE2	5.78	125.92	121.30
1	C	233	ASN	O-C-N	-5.77	113.47	122.70
1	G	549	SER	O-C-N	-5.75	113.50	122.70
1	J	231	ASP	C-N-CA	-5.72	107.39	121.70
1	L	418	PRO	CA-N-CD	-5.71	103.50	111.50
1	A	125	GLU	N-CA-C	-5.63	95.78	111.00
1	F	334	GLU	C-N-CA	5.62	135.75	121.70
1	L	418	PRO	N-CA-CB	5.62	110.05	103.30
1	F	111	LYS	CA-C-N	5.57	129.45	117.20
1	B	439	TYR	CA-CB-CG	5.52	123.89	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	LEU	N-CA-C	-5.50	96.14	111.00
1	E	273	ASN	O-C-N	5.50	131.50	122.70
1	C	331	LYS	O-C-N	-5.49	113.91	122.70
1	F	550	SER	O-C-N	5.49	131.48	122.70
1	E	394	ASP	C-N-CA	5.44	135.30	121.70
1	F	110	ILE	C-N-CA	5.37	135.11	121.70
1	A	124	GLU	N-CA-C	5.31	125.35	111.00
1	H	231	ASP	CB-CG-OD1	5.27	123.04	118.30
1	I	200	GLU	CA-C-N	-5.26	105.62	117.20
1	K	197	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	145	SER	O-C-N	-5.24	114.31	122.70
1	A	123	VAL	C-N-CA	5.22	134.75	121.70
1	G	162	MET	C-N-CA	5.19	134.68	121.70
1	B	419	GLU	O-C-N	-5.18	114.40	122.70
1	G	138	GLU	C-N-CA	-5.17	108.77	121.70
1	H	322	ASN	CA-C-N	-5.16	105.84	117.20
1	F	328	LEU	CB-CG-CD2	-5.13	102.27	111.00
1	G	255	THR	N-CA-C	-5.13	97.15	111.00
1	C	232	LYS	C-N-CA	-5.13	108.88	121.70
1	I	124	GLU	C-N-CA	5.11	134.48	121.70
1	L	417	LYS	O-C-N	5.07	130.73	121.10
1	D	518	LYS	O-C-N	-5.02	114.67	122.70

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	SER	Mainchain
1	B	152	GLN	Mainchain
1	B	164	LYS	Mainchain
1	B	181	ASN	Mainchain
1	B	199	SER	Peptide
1	B	202	ASP	Mainchain
1	B	272	ASN	Peptide
1	B	273	ASN	Mainchain
1	B	549	SER	Peptide
1	C	124	GLU	Mainchain,Peptide
1	C	233	ASN	Mainchain
1	C	331	LYS	Mainchain
1	C	335	GLU	Mainchain
1	D	322	ASN	Mainchain
1	D	518	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	E	164	LYS	Mainchain
1	E	273	ASN	Mainchain
1	F	111	LYS	Mainchain
1	F	335	GLU	Mainchain
1	F	488	THR	Mainchain
1	F	549	SER	Peptide
1	F	550	SER	Mainchain,Peptide
1	G	138	GLU	Peptide
1	G	139	ASN	Mainchain
1	G	163	GLU	Mainchain
1	H	164	LYS	Mainchain
1	H	321	LEU	Peptide
1	H	420	ASN	Mainchain
1	I	145	SER	Mainchain
1	I	200	GLU	Mainchain
1	I	273	ASN	Mainchain
1	I	550	SER	Peptide
1	J	183	ASN	Sidechain
1	J	232	LYS	Mainchain
1	J	549	SER	Peptide
1	K	163	GLU	Mainchain
1	L	398	PHE	Mainchain
1	L	417	LYS	Mainchain
1	L	436	LYS	Mainchain
1	L	550	SER	Peptide
1	L	552	LYS	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3928	0	3824	47	1
1	B	3837	0	3716	63	0
1	C	3942	0	3864	90	0
1	D	3899	0	3817	65	0
1	E	3884	0	3789	64	0
1	F	3762	0	3570	76	0
1	G	3979	0	3890	46	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3855	0	3732	72	0
1	I	3912	0	3831	86	0
1	J	3875	0	3773	69	1
1	K	3878	0	3776	66	1
1	L	3806	0	3638	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	24	0	20	0	0
3	B	24	0	21	4	0
3	C	17	0	15	0	0
3	E	15	0	14	3	0
3	F	24	0	20	1	0
3	G	22	0	20	0	0
3	H	14	0	13	0	0
3	I	24	0	21	2	0
3	J	22	0	20	2	0
3	K	22	0	20	3	0
3	L	24	0	20	1	0
4	A	4	0	0	3	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	1	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	2	0
4	H	4	0	0	1	0
4	I	4	0	0	1	0
4	J	4	0	0	3	0
4	K	4	0	0	3	0
4	L	4	0	0	0	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	0	1	0
5	D	5	0	0	1	0
5	E	10	0	0	0	0
5	G	10	0	0	1	0
5	I	5	0	0	0	0
5	L	10	0	0	1	0
6	A	9	0	10	1	0
6	B	7	0	6	0	0
6	C	22	0	24	12	0
6	D	20	0	20	5	0
6	E	12	0	14	0	0
6	G	18	0	18	4	0
6	H	10	0	10	1	0
7	A	102	0	0	5	0
7	B	74	0	0	4	0
7	C	70	0	0	5	0
7	D	80	0	0	7	0
7	E	113	0	0	6	0
7	F	88	0	0	11	0
7	G	93	0	0	6	0
7	H	74	0	0	5	0
7	I	91	0	0	6	0
7	J	86	0	0	15	0
7	K	91	0	0	4	0
7	L	69	0	0	4	0
All	All	48055	0	45526	803	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (803) 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)
7:G:885:HOH:O	1:L:551:VAL:HG22	1.25	1.35
1:C:331:LYS:CG	1:C:334:GLU:OE1	1.75	1.34
1:C:331:LYS:HG3	1:C:334:GLU:OE1	1.16	1.29
1:J:278:LYS:HG3	7:J:865:HOH:O	1.29	1.27
1:D:320:LYS:NZ	6:D:706:1PE:H142	1.48	1.25
1:I:143:LYS:HD3	1:I:159:ASP:OD1	1.29	1.22
1:C:320:LYS:NZ	6:C:706:1PE:OH3	1.75	1.18
1:L:200:GLU:OE2	1:L:521:ASN:HB3	1.40	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:VAL:HA	1:D:439:TYR:CE2	1.79	1.17
1:I:396:MET:SD	1:I:398:PHE:HE2	1.69	1.15
1:I:272:ASN:O	1:I:273:ASN:HB2	1.32	1.12
1:B:142:VAL:HG12	1:B:167:VAL:HG12	1.25	1.12
1:C:320:LYS:HZ2	6:C:706:1PE:C12	1.62	1.12
1:L:396:MET:SD	1:L:398:PHE:HE2	1.71	1.11
1:I:144:ILE:HG13	1:I:157:LEU:HG	1.18	1.11
1:B:124:GLU:CB	1:B:125:GLU:OE1	2.00	1.09
1:J:278:LYS:CG	7:J:865:HOH:O	1.88	1.08
1:L:148:VAL:CG2	1:L:154:SER:HB2	1.83	1.08
1:L:200:GLU:OE2	1:L:521:ASN:CB	2.00	1.08
1:A:598:GLU:O	1:A:602:ASN:ND2	1.87	1.07
1:C:436:LYS:NZ	7:C:826:HOH:O	1.67	1.07
1:B:125:GLU:N	1:B:125:GLU:OE1	1.87	1.07
1:K:462:GLY:N	4:K:704:CO3:O2	1.87	1.07
1:I:519:THR:CG2	1:I:598:GLU:OE1	2.03	1.06
1:F:198:LEU:HD11	1:F:202:ASP:CB	1.86	1.05
1:F:320:LYS:NZ	7:F:877:HOH:O	1.88	1.05
1:D:320:LYS:HZ1	6:D:706:1PE:H142	0.90	1.04
1:E:124:GLU:OE1	7:E:801:HOH:O	1.75	1.03
1:I:272:ASN:O	1:I:273:ASN:CB	2.04	1.03
1:C:331:LYS:HG3	1:C:334:GLU:CD	1.78	1.03
1:B:199:SER:CB	1:B:202:ASP:H	1.71	1.02
1:D:540:LYS:NZ	7:D:877:HOH:O	1.92	1.02
1:G:462:GLY:N	4:G:704:CO3:O2	1.91	1.02
1:C:172:SER:O	1:C:173:LYS:HD2	1.59	1.01
1:L:200:GLU:OE2	1:L:521:ASN:CA	2.11	0.99
1:L:272:ASN:OD1	1:L:273:ASN:N	1.96	0.99
1:B:142:VAL:HG12	1:B:167:VAL:CG1	1.93	0.98
1:K:374:LYS:HE2	1:K:462:GLY:HA3	1.46	0.98
1:G:494:SER:OG	1:L:494:SER:HB3	1.65	0.97
1:F:198:LEU:HD11	1:F:202:ASP:HB3	1.47	0.97
1:L:414:GLY:O	7:L:864:HOH:O	1.79	0.97
1:I:519:THR:HG21	1:I:598:GLU:OE1	1.64	0.96
1:A:244:TYR:HA	1:A:288:TYR:HE1	1.27	0.96
1:I:396:MET:CE	1:I:398:PHE:CE2	2.47	0.96
1:B:386:LYS:HB2	1:B:393:ILE:HD13	1.44	0.96
1:C:398:PHE:HE1	1:C:580:SER:HB3	1.30	0.95
1:D:320:LYS:HZ1	6:D:706:1PE:C14	1.79	0.95
1:I:396:MET:SD	1:I:398:PHE:CE2	2.60	0.95
1:H:532:GLU:OE1	1:K:498:SER:OG	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LYS:HB2	1:A:393:ILE:HD13	1.46	0.94
1:L:200:GLU:OE2	1:L:521:ASN:C	2.05	0.94
1:B:125:GLU:CD	1:B:125:GLU:H	1.70	0.94
1:A:173:LYS:NZ	7:A:857:HOH:O	1.99	0.94
1:C:320:LYS:NZ	6:C:706:1PE:C12	2.29	0.94
1:I:396:MET:CE	1:I:398:PHE:HE2	1.81	0.94
1:I:144:ILE:HG13	1:I:157:LEU:CG	1.96	0.93
1:L:200:GLU:OE2	1:L:521:ASN:O	1.85	0.93
1:D:321:LEU:O	1:D:322:ASN:CB	2.15	0.93
1:F:419:GLU:OE1	1:F:419:GLU:HA	1.69	0.92
1:B:199:SER:OG	1:B:201:ALA:N	2.03	0.91
1:G:494:SER:OG	1:L:494:SER:CB	2.19	0.91
1:G:258:ASN:OD1	1:G:259:VAL:N	2.05	0.90
1:I:519:THR:HG22	1:I:598:GLU:OE1	1.70	0.90
1:I:144:ILE:CG1	1:I:157:LEU:HG	2.02	0.89
1:J:114:VAL:H	1:J:278:LYS:NZ	1.71	0.89
1:J:278:LYS:CD	7:J:865:HOH:O	2.10	0.89
1:C:316:GLU:CD	6:C:706:1PE:H231	1.95	0.87
1:F:173:LYS:N	1:F:189:TYR:CE2	2.42	0.87
1:L:148:VAL:HG21	1:L:154:SER:HB2	1.54	0.87
1:L:396:MET:SD	1:L:398:PHE:CE2	2.64	0.87
1:D:344:VAL:HA	1:D:439:TYR:HE2	1.36	0.87
1:F:480:TYR:OH	1:F:508:GLU:OE2	1.92	0.87
1:J:200:GLU:CG	7:J:863:HOH:O	2.22	0.86
1:F:322:ASN:ND2	1:K:160:GLU:OE2	2.09	0.86
1:H:419:GLU:O	1:H:420:ASN:HB2	1.75	0.86
1:J:463:ARG:HG3	4:J:704:CO3:O1	1.74	0.86
1:L:357:LEU:HB2	1:L:425:PHE:HB2	1.58	0.86
1:H:345:GLY:O	7:H:861:HOH:O	1.93	0.86
1:A:155:GLU:O	1:A:158:LYS:HG2	1.76	0.85
1:I:143:LYS:CD	1:I:159:ASP:OD1	2.22	0.85
1:L:396:MET:HA	1:L:398:PHE:HD2	1.41	0.85
1:J:278:LYS:CE	7:J:865:HOH:O	2.25	0.85
1:F:122:ASN:OD1	1:F:149:ASN:CB	2.25	0.85
1:L:200:GLU:CD	1:L:521:ASN:HB3	1.97	0.84
1:A:244:TYR:CA	1:A:288:TYR:HE1	1.91	0.83
1:J:463:ARG:NH1	1:J:546:GLN:O	2.10	0.83
1:H:458:THR:O	1:H:460:ALA:N	2.10	0.83
1:C:331:LYS:HG2	1:C:334:GLU:OE1	1.78	0.83
1:J:200:GLU:HG2	7:J:863:HOH:O	1.78	0.83
1:A:506:ASN:OD1	7:A:886:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396:MET:HA	1:I:398:PHE:CD2	2.14	0.82
1:C:316:GLU:OE2	6:C:706:1PE:OH4	1.96	0.82
1:J:114:VAL:H	1:J:278:LYS:HZ2	1.27	0.82
1:G:193:GLY:HA3	7:G:863:HOH:O	1.79	0.81
1:H:195:VAL:HG23	1:H:195:VAL:O	1.81	0.81
1:C:171:THR:HG23	1:C:173:LYS:NZ	1.96	0.81
1:L:396:MET:HA	1:L:398:PHE:CD2	2.16	0.81
1:F:142:VAL:HG23	1:F:162:MET:HB3	1.63	0.80
1:B:282:GLU:OE1	1:B:285:ARG:NH2	2.13	0.80
1:C:398:PHE:CE1	1:C:580:SER:HB3	2.16	0.80
1:B:199:SER:OG	1:B:200:GLU:C	2.19	0.80
1:B:199:SER:HB2	1:B:202:ASP:H	1.44	0.80
1:J:390:GLY:O	1:J:392:MET:N	2.12	0.80
1:I:418:PRO:HB3	1:I:601:LEU:HD11	1.64	0.79
1:J:396:MET:SD	1:J:398:PHE:HE2	2.06	0.79
1:H:152:GLN:HG2	1:H:178:PHE:O	1.83	0.79
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.64	0.78
1:I:344:VAL:HA	1:I:439:TYR:CE2	2.18	0.78
1:J:386:LYS:HB2	1:J:393:ILE:HD13	1.63	0.78
1:G:543:ASP:OD2	1:H:254:SER:OG	2.00	0.78
1:K:182:LYS:O	7:K:801:HOH:O	2.01	0.78
1:B:386:LYS:NZ	3:B:1004:TOD:O3	2.16	0.78
1:I:396:MET:HA	1:I:398:PHE:HD2	1.47	0.78
1:C:316:GLU:OE2	6:C:706:1PE:C23	2.32	0.77
1:L:148:VAL:HG23	1:L:154:SER:HB2	1.65	0.77
1:C:253:LYS:O	1:C:257:LYS:NZ	2.18	0.77
1:J:278:LYS:HE2	7:J:865:HOH:O	1.84	0.77
1:C:232:LYS:HD3	1:C:276:THR:O	1.85	0.76
1:B:199:SER:OG	1:B:200:GLU:N	2.08	0.76
1:C:320:LYS:NZ	6:C:706:1PE:C22	2.47	0.76
1:F:488:THR:HG22	1:F:575:ASP:OD2	1.85	0.76
1:L:200:GLU:HG2	1:L:237:PHE:CZ	2.19	0.76
1:A:244:TYR:HA	1:A:288:TYR:CE1	2.17	0.76
1:A:419:GLU:O	1:A:421:VAL:HG23	1.85	0.76
1:C:123:VAL:C	1:C:124:GLU:HG3	2.05	0.76
1:C:172:SER:C	1:C:173:LYS:HD2	2.04	0.76
1:F:443:ASP:OD2	7:F:849:HOH:O	2.04	0.75
1:B:199:SER:CB	1:B:202:ASP:N	2.46	0.75
1:L:200:GLU:CD	1:L:521:ASN:O	2.24	0.75
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.67	0.75
1:J:586:ARG:NH2	7:J:884:HOH:O	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLN:OE1	1:C:115:TYR:OH	2.06	0.74
1:J:114:VAL:HB	1:J:278:LYS:HD3	1.67	0.74
7:G:885:HOH:O	1:L:551:VAL:CG2	2.01	0.74
1:D:321:LEU:O	1:D:322:ASN:HB2	1.87	0.74
1:D:320:LYS:HZ2	6:D:706:1PE:H142	1.52	0.74
1:E:392:MET:O	1:E:395:LEU:HB3	1.87	0.73
1:I:216:ASP:CB	7:I:871:HOH:O	2.35	0.73
1:L:148:VAL:HG21	1:L:154:SER:CB	2.18	0.73
1:F:198:LEU:CD1	1:F:202:ASP:HB2	2.18	0.73
1:H:381:GLY:O	1:H:458:THR:OG1	2.05	0.73
1:C:316:GLU:OE2	6:C:706:1PE:H231	1.88	0.73
1:F:427:SER:O	7:F:812:HOH:O	2.07	0.73
1:I:396:MET:HE2	1:I:398:PHE:CE2	2.23	0.72
1:B:320:LYS:NZ	7:B:1174:HOH:O	2.11	0.72
1:B:471:VAL:HG12	1:B:475:LYS:HE3	1.72	0.72
1:J:386:LYS:HD2	1:J:393:ILE:HD12	1.70	0.72
1:F:198:LEU:HD11	1:F:202:ASP:HB2	1.70	0.72
1:F:137:LYS:CB	1:F:140:GLY:H	2.03	0.72
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.71	0.72
1:L:148:VAL:CG2	1:L:154:SER:CB	2.67	0.72
1:K:483:ASP:OD1	1:K:573:HIS:ND1	2.20	0.71
1:H:122:ASN:ND2	1:H:149:ASN:HB2	2.05	0.71
1:B:169:LEU:HD21	1:B:202:ASP:CB	2.20	0.71
1:F:198:LEU:CD1	1:F:202:ASP:CB	2.66	0.71
1:E:392:MET:O	1:E:395:LEU:CB	2.39	0.71
1:I:125:GLU:OE2	1:I:220:SER:OG	2.08	0.71
1:F:173:LYS:N	1:F:189:TYR:HE2	1.87	0.70
1:E:326:LYS:HE3	1:E:328:LEU:HD11	1.73	0.70
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.73	0.70
1:J:463:ARG:CG	4:J:704:CO3:O1	2.40	0.70
1:D:117:ILE:HD11	1:D:271:ILE:HA	1.74	0.70
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.74	0.70
1:D:321:LEU:O	1:D:322:ASN:HB3	1.92	0.69
1:K:332:GLU:CD	1:K:332:GLU:H	1.93	0.69
1:C:195:VAL:HG23	1:C:195:VAL:O	1.93	0.69
1:D:155:GLU:HA	1:D:155:GLU:OE1	1.89	0.69
1:C:254:SER:HA	1:C:257:LYS:NZ	2.08	0.69
1:H:462:GLY:N	4:H:704:CO3:O2	2.25	0.69
1:L:133:ASN:HA	1:L:167:VAL:HG11	1.74	0.69
1:H:419:GLU:O	1:H:420:ASN:CB	2.40	0.69
1:I:161:ASN:O	1:I:164:LYS:HE2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:361:SER:OG	1:L:366:LYS:NZ	2.26	0.69
1:I:418:PRO:HB3	1:I:601:LEU:CD1	2.23	0.69
1:C:301:PRO:HA	1:C:397:LYS:HD2	1.76	0.68
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.74	0.68
3:E:703:TOD:H5	3:E:703:TOD:O1	1.93	0.68
1:J:247:MET:CE	7:J:849:HOH:O	2.40	0.68
1:C:123:VAL:O	1:C:124:GLU:CG	2.42	0.68
1:E:436:LYS:NZ	7:E:827:HOH:O	2.26	0.68
1:F:221:LYS:HG3	1:F:266:HIS:HB2	1.74	0.68
1:I:551:VAL:HG12	1:I:551:VAL:O	1.94	0.68
1:C:398:PHE:HE1	1:C:580:SER:CB	2.04	0.67
1:C:522:GLU:OE2	7:C:848:HOH:O	2.13	0.67
1:D:396:MET:SD	1:D:398:PHE:HE2	2.17	0.67
1:H:331:LYS:O	1:H:335:GLU:HG3	1.95	0.67
1:E:326:LYS:CE	1:E:328:LEU:HD11	2.24	0.67
1:G:344:VAL:HA	1:G:439:TYR:CE2	2.29	0.67
1:I:146:SER:OG	1:I:227:GLU:OE2	2.06	0.67
1:C:171:THR:HG23	1:C:173:LYS:HZ2	1.58	0.67
3:J:703:TOD:O2	4:J:704:CO3:O2	2.13	0.67
1:G:163:GLU:C	1:G:165:PHE:N	2.47	0.66
1:J:449:ASN:O	7:J:874:HOH:O	2.13	0.66
1:B:199:SER:OG	1:B:202:ASP:N	2.28	0.66
1:C:395:LEU:O	1:C:398:PHE:HB3	1.95	0.66
1:D:144:ILE:HD13	1:D:157:LEU:HD22	1.76	0.66
1:D:217:ASN:HD21	1:D:219:LEU:HD12	1.61	0.66
1:D:232:LYS:NZ	1:D:280:GLU:OE2	2.29	0.66
1:B:176:TYR:HB3	1:F:177:MET:HG2	1.78	0.66
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.76	0.66
1:D:442:GLY:O	7:D:824:HOH:O	2.12	0.66
1:F:353:LYS:O	7:F:812:HOH:O	2.14	0.66
1:L:112:VAL:HG22	1:L:267:LEU:HB3	1.76	0.66
1:E:324:GLU:CG	1:E:358:THR:HB	2.26	0.66
1:J:200:GLU:HG3	7:J:863:HOH:O	1.86	0.65
1:H:175:PHE:N	1:H:187:VAL:O	2.25	0.65
1:E:324:GLU:OE2	1:E:358:THR:HB	1.96	0.65
1:A:533:TYR:O	1:A:536:THR:HG22	1.96	0.65
1:I:208:LEU:O	7:I:867:HOH:O	2.14	0.65
1:G:374:LYS:HE3	1:G:462:GLY:HA3	1.79	0.65
1:L:200:GLU:CG	1:L:521:ASN:HB3	2.27	0.65
1:K:357:LEU:HB2	1:K:425:PHE:HB2	1.77	0.65
7:D:847:HOH:O	1:F:454:GLU:OE2	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:PRO:O	7:B:1143:HOH:O	2.15	0.65
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.77	0.65
1:G:262:GLU:O	7:G:867:HOH:O	2.15	0.64
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.80	0.64
1:H:254:SER:OG	1:H:255:THR:N	2.31	0.64
1:H:460:ALA:HB3	1:H:546:GLN:NE2	2.13	0.64
1:I:143:LYS:NZ	1:I:159:ASP:HB3	2.12	0.64
1:I:374:LYS:HE3	1:I:462:GLY:HA3	1.79	0.64
1:F:331:LYS:O	1:F:335:GLU:HG3	1.97	0.64
1:D:205:ARG:NH1	7:D:836:HOH:O	2.30	0.64
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.79	0.63
1:C:439:TYR:CE1	1:C:458:THR:HG22	2.34	0.63
1:I:221:LYS:HD2	1:I:266:HIS:HB2	1.80	0.63
1:C:220:SER:OG	5:C:705:SO4:O2	2.16	0.63
1:G:547:ILE:HG12	1:G:548:SER:H	1.63	0.63
1:L:208:LEU:CD2	7:L:856:HOH:O	2.46	0.63
1:D:247:MET:HB2	1:D:288:TYR:OH	1.99	0.63
1:E:232:LYS:NZ	1:E:276:THR:O	2.32	0.63
1:F:326:LYS:HE3	1:F:328:LEU:HD21	1.79	0.63
1:F:142:VAL:HG22	1:F:162:MET:O	1.99	0.63
1:K:431:GLU:HG2	1:K:433:MET:HG2	1.79	0.63
1:K:551:VAL:O	1:K:553:ALA:N	2.32	0.63
1:I:418:PRO:CB	1:I:601:LEU:HD11	2.28	0.62
1:F:142:VAL:CG2	1:F:162:MET:HB3	2.29	0.62
1:F:322:ASN:HB2	1:K:160:GLU:OE2	1.99	0.62
1:H:122:ASN:HD21	1:H:149:ASN:HB2	1.64	0.62
1:I:125:GLU:OE1	1:I:221:LYS:HD3	1.98	0.62
1:D:244:TYR:HA	1:D:288:TYR:HE1	1.64	0.62
1:C:328:LEU:HG	1:C:332:GLU:CD	2.20	0.62
1:J:343:SER:HA	1:J:346:LYS:HD3	1.82	0.62
1:B:123:VAL:O	1:B:125:GLU:CD	2.38	0.61
1:F:117:ILE:CB	1:F:272:ASN:ND2	2.63	0.61
1:H:148:VAL:HG23	1:H:154:SER:OG	1.99	0.61
1:F:459:ASP:OD2	7:F:822:HOH:O	2.16	0.61
1:J:114:VAL:HB	1:J:278:LYS:CD	2.30	0.61
1:F:396:MET:SD	1:F:398:PHE:HE2	2.22	0.61
1:G:236:ARG:NH2	1:G:519:THR:O	2.32	0.61
1:K:329:GLY:O	1:K:332:GLU:OE1	2.17	0.61
1:I:551:VAL:O	1:I:551:VAL:CG1	2.47	0.61
1:E:324:GLU:CD	1:E:358:THR:HB	2.21	0.61
1:B:347:GLY:HA3	1:B:438:SER:OG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:386:LYS:HB3	1:L:391:SER:HB3	1.82	0.61
1:G:163:GLU:C	1:G:165:PHE:H	2.04	0.60
1:L:208:LEU:HD22	7:L:856:HOH:O	2.00	0.60
1:C:258:ASN:OD1	1:C:260:ASN:N	2.29	0.60
1:C:316:GLU:OE2	6:C:706:1PE:C13	2.50	0.60
1:E:230:VAL:HG12	1:E:234:LEU:HD23	1.82	0.60
1:B:199:SER:HG	1:B:200:GLU:C	2.05	0.60
1:E:273:ASN:O	1:E:276:THR:OG1	2.16	0.60
1:E:364:ASP:O	1:E:420:ASN:HA	2.02	0.60
1:L:436:LYS:HE3	5:L:705:SO4:O2	2.02	0.60
1:A:108:HIS:CD2	6:A:708:1PE:H221	2.36	0.60
1:L:362:LYS:N	1:L:362:LYS:HD3	2.16	0.60
3:I:703:TOD:O2	4:I:704:CO3:O2	2.19	0.60
1:C:328:LEU:HG	1:C:332:GLU:OE1	2.02	0.60
1:K:396:MET:CE	1:K:398:PHE:HE2	2.14	0.60
1:D:514:LEU:O	1:D:518:LYS:HG3	2.02	0.60
1:I:336:LEU:HD23	7:I:883:HOH:O	2.00	0.60
1:C:123:VAL:O	1:C:124:GLU:HG3	2.01	0.59
1:F:153:VAL:HB	1:F:177:MET:HE1	1.84	0.59
1:H:135:PRO:HA	1:H:194:SER:O	2.01	0.59
1:B:386:LYS:HB3	1:B:391:SER:HB3	1.84	0.59
1:F:532:GLU:OE1	7:F:847:HOH:O	2.15	0.59
1:H:200:GLU:OE1	1:H:523:PRO:HD3	2.02	0.59
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.85	0.59
1:A:244:TYR:CA	1:A:288:TYR:CE1	2.80	0.59
1:G:160:GLU:O	1:G:163:GLU:OE1	2.20	0.59
1:H:360:LYS:HD2	7:H:858:HOH:O	2.02	0.59
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.85	0.59
1:E:249:ASP:OD2	1:E:251:ARG:NH2	2.31	0.59
1:G:175:PHE:N	1:G:187:VAL:O	2.35	0.58
1:L:395:LEU:O	1:L:398:PHE:HB3	2.03	0.58
1:C:411:TYR:HE1	6:C:707:1PE:H232	1.66	0.58
1:B:123:VAL:HG23	1:B:124:GLU:H	1.67	0.58
1:K:221:LYS:HG3	1:K:266:HIS:HB2	1.84	0.58
1:G:494:SER:HG	1:L:494:SER:HB3	1.65	0.58
1:C:331:LYS:HE3	1:C:334:GLU:OE2	2.04	0.58
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.86	0.58
3:B:1004:TOD:N1	3:B:1004:TOD:H5	2.16	0.58
1:K:549:SER:N	1:K:550:SER:HA	2.18	0.58
1:F:440:ARG:NH2	7:F:849:HOH:O	2.36	0.58
1:G:381:GLY:O	1:G:458:THR:OG1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:418:PRO:HG3	1:I:601:LEU:CD1	2.33	0.57
1:H:396:MET:SD	1:H:398:PHE:HE2	2.26	0.57
1:G:494:SER:OG	1:L:494:SER:CA	2.53	0.57
1:C:238:PHE:HD2	1:C:239:LEU:HD12	1.69	0.57
1:E:160:GLU:N	1:E:160:GLU:OE1	2.35	0.57
1:C:171:THR:HG23	1:C:173:LYS:HZ3	1.70	0.57
1:I:144:ILE:HG13	1:I:157:LEU:CD2	2.34	0.57
1:E:273:ASN:O	1:E:277:TYR:CD2	2.58	0.57
1:F:332:GLU:HA	1:F:335:GLU:CD	2.25	0.57
1:D:324:GLU:HB2	1:D:358:THR:HB	1.87	0.57
1:K:312:ASN:CB	7:K:845:HOH:O	2.52	0.57
1:K:396:MET:SD	1:K:398:PHE:HE2	2.27	0.57
1:I:550:SER:OG	1:I:551:VAL:N	2.38	0.56
1:L:148:VAL:HG11	1:L:157:LEU:HD12	1.87	0.56
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.86	0.56
1:B:118:LYS:HE3	1:B:272:ASN:OD1	2.05	0.56
1:F:138:GLU:N	1:F:139:ASN:HA	2.20	0.56
1:J:337:LYS:HB3	1:J:448:SER:HA	1.87	0.56
1:C:171:THR:CG2	1:C:173:LYS:NZ	2.67	0.56
1:E:392:MET:HB3	1:E:395:LEU:HD22	1.87	0.56
1:I:143:LYS:CE	1:I:159:ASP:HB3	2.35	0.56
1:I:199:SER:HG	1:I:200:GLU:CD	2.08	0.56
1:J:348:SER:N	7:J:873:HOH:O	2.39	0.56
1:D:462:GLY:N	4:D:703:CO3:O2	2.35	0.56
1:I:418:PRO:CG	1:I:601:LEU:HD11	2.36	0.56
1:A:214:LEU:HD21	1:A:222:LEU:HD22	1.87	0.56
1:C:536:THR:HG21	1:C:551:VAL:CG2	2.36	0.56
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.87	0.56
1:I:418:PRO:HG3	1:I:601:LEU:HD11	1.87	0.56
1:L:148:VAL:HG23	1:L:148:VAL:O	2.05	0.56
1:C:411:TYR:OH	7:C:834:HOH:O	2.15	0.55
1:E:176:TYR:OH	1:E:217:ASN:OD1	2.16	0.55
1:C:376:ILE:HB	1:C:399:ASP:HB3	1.88	0.55
1:E:440:ARG:NH2	1:F:431:GLU:OE2	2.39	0.55
1:H:152:GLN:CG	1:H:178:PHE:O	2.52	0.55
1:H:395:LEU:O	1:H:398:PHE:CD2	2.59	0.55
1:D:184:SER:OG	5:D:704:SO4:O3	2.15	0.55
1:F:173:LYS:CB	1:F:189:TYR:HE2	2.19	0.55
1:L:127:LEU:HD11	1:L:129:ILE:HD11	1.89	0.55
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.89	0.55
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:GLU:CD	6:C:706:1PE:C23	2.69	0.55
1:E:227:GLU:OE1	7:E:850:HOH:O	2.18	0.54
1:E:392:MET:CB	1:E:395:LEU:HD22	2.37	0.54
1:I:244:TYR:HA	1:I:288:TYR:HE1	1.72	0.54
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.89	0.54
1:L:200:GLU:HG3	1:L:521:ASN:HB3	1.88	0.54
1:I:396:MET:HE1	1:I:398:PHE:CE2	2.40	0.54
1:F:198:LEU:HD12	1:F:199:SER:H	1.73	0.54
1:J:192:CYS:HB3	1:J:198:LEU:HD11	1.90	0.54
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.35	0.54
1:C:331:LYS:CD	1:C:334:GLU:OE1	2.52	0.54
1:C:456:GLY:HA3	1:C:547:ILE:HD11	1.89	0.54
5:G:706:SO4:O2	1:J:164:LYS:HE3	2.07	0.54
1:H:395:LEU:O	1:H:398:PHE:HD2	1.91	0.54
1:L:129:ILE:HG21	1:L:210:LEU:HD21	1.88	0.54
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.88	0.54
1:D:343:SER:O	1:D:439:TYR:HD2	1.90	0.54
1:K:395:LEU:O	1:K:398:PHE:CD2	2.61	0.54
1:F:498:SER:O	1:F:523:PRO:HG2	2.08	0.54
1:L:140:GLY:O	1:L:167:VAL:HG23	2.08	0.54
1:A:522:GLU:OE2	7:A:858:HOH:O	2.19	0.54
1:B:538:ASN:O	1:C:586:ARG:NH2	2.41	0.54
1:F:132:VAL:HG22	1:F:227:GLU:OE1	2.07	0.54
1:K:306:ASN:ND2	7:K:848:HOH:O	2.24	0.54
1:B:207:VAL:HG11	1:B:241:THR:HG22	1.89	0.53
1:C:273:ASN:O	1:C:276:THR:HG22	2.09	0.53
1:C:316:GLU:HG3	6:C:706:1PE:OH3	2.07	0.53
1:E:392:MET:O	1:E:395:LEU:HB2	2.07	0.53
1:L:148:VAL:HG21	1:L:154:SER:CA	2.39	0.53
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.89	0.53
1:J:386:LYS:HB2	1:J:393:ILE:CD1	2.36	0.53
1:G:494:SER:OG	1:L:494:SER:HA	2.09	0.53
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.90	0.53
1:F:386:LYS:HB3	1:F:391:SER:HB3	1.90	0.53
1:I:594:ARG:NH2	7:I:803:HOH:O	2.42	0.53
1:E:489:GLY:N	3:E:703:TOD:O4	2.30	0.53
1:K:395:LEU:O	1:K:398:PHE:HD2	1.92	0.53
1:F:117:ILE:CB	1:F:272:ASN:HD21	2.22	0.53
1:C:331:LYS:CE	1:C:334:GLU:OE1	2.56	0.53
1:K:138:GLU:HA	1:K:194:SER:OG	2.09	0.52
1:B:336:LEU:O	1:B:337:LYS:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:457:ASN:C	1:H:458:THR:O	2.46	0.52
1:I:210:LEU:HD21	1:I:222:LEU:HD21	1.91	0.52
1:I:217:ASN:OD1	1:I:219:LEU:HG	2.09	0.52
3:K:703:TOD:N1	4:K:704:CO3:O3	2.43	0.52
1:D:419:GLU:HG2	1:D:420:ASN:CG	2.29	0.52
1:E:214:LEU:HD11	1:E:222:LEU:HD22	1.90	0.52
1:B:244:TYR:OH	1:B:588:PRO:O	2.28	0.52
1:H:200:GLU:OE1	7:H:848:HOH:O	2.19	0.52
1:I:221:LYS:HD2	1:I:266:HIS:CB	2.40	0.52
1:A:463:ARG:NE	4:A:704:CO3:O1	2.29	0.52
1:C:171:THR:CG2	1:C:173:LYS:HZ3	2.21	0.52
1:L:200:GLU:HG2	1:L:237:PHE:CE2	2.44	0.52
1:A:244:TYR:N	1:A:288:TYR:CE1	2.77	0.52
1:E:386:LYS:HB3	1:E:391:SER:HB3	1.92	0.52
1:J:292:TYR:OH	7:J:850:HOH:O	2.10	0.52
1:B:198:LEU:O	1:B:199:SER:O	2.28	0.52
1:C:536:THR:HG21	1:C:551:VAL:HG21	1.91	0.52
1:D:343:SER:O	1:D:439:TYR:CD2	2.63	0.52
1:J:399:ASP:OD1	1:J:486:THR:OG1	2.28	0.52
1:L:217:ASN:HB3	1:L:219:LEU:HG	1.91	0.52
1:C:112:VAL:HG22	1:C:267:LEU:HB3	1.92	0.52
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.92	0.51
1:I:336:LEU:CD2	7:I:883:HOH:O	2.54	0.51
1:E:392:MET:CE	1:E:395:LEU:CD2	2.89	0.51
1:F:326:LYS:CE	1:F:328:LEU:HD21	2.39	0.51
1:I:198:LEU:HD22	1:I:202:ASP:HB3	1.92	0.51
1:A:431:GLU:OE2	1:C:440:ARG:NE	2.43	0.51
1:I:418:PRO:CB	1:I:601:LEU:CD1	2.86	0.51
1:K:100:PRO:O	1:K:251:ARG:NH1	2.36	0.51
1:C:150:ASP:OD1	1:C:179:ASN:HB2	2.10	0.51
1:G:368:LYS:HD3	1:G:422:GLU:HB3	1.92	0.51
1:H:195:VAL:CG2	1:H:195:VAL:O	2.54	0.51
1:H:321:LEU:O	1:H:322:ASN:HB3	2.09	0.51
1:I:439:TYR:CE1	1:I:458:THR:HB	2.46	0.51
1:K:332:GLU:N	1:K:332:GLU:CD	2.63	0.51
1:A:440:ARG:NH1	7:A:824:HOH:O	2.43	0.51
1:B:199:SER:OG	1:B:200:GLU:CA	2.59	0.51
1:J:135:PRO:HA	1:J:194:SER:O	2.10	0.51
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.93	0.51
1:K:374:LYS:HE3	1:K:487:LEU:HD12	1.92	0.51
1:F:488:THR:HG21	1:F:555:SER:OG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:MET:O	1:L:217:ASN:ND2	2.41	0.50
1:D:386:LYS:HB3	1:D:391:SER:HB3	1.92	0.50
1:D:397:LYS:NZ	7:D:847:HOH:O	2.03	0.50
1:E:507:GLU:O	1:E:511:ASN:ND2	2.37	0.50
1:F:551:VAL:O	1:F:553:ALA:N	2.44	0.50
1:I:199:SER:OG	1:I:200:GLU:OE1	2.26	0.50
1:D:117:ILE:HD12	1:D:272:ASN:N	2.27	0.50
1:E:324:GLU:OE2	1:E:358:THR:CG2	2.59	0.50
1:L:554:SER:HA	7:L:839:HOH:O	2.11	0.50
1:I:360:LYS:HD3	1:I:422:GLU:OE1	2.12	0.50
1:K:329:GLY:C	1:K:332:GLU:OE1	2.50	0.50
1:K:460:ALA:HA	3:K:703:TOD:H2	1.92	0.50
1:C:376:ILE:O	1:C:399:ASP:HB3	2.12	0.50
1:F:200:GLU:OE1	7:F:860:HOH:O	2.19	0.50
1:H:148:VAL:CG2	1:H:154:SER:OG	2.59	0.50
1:I:172:SER:HB2	1:I:213:MET:CE	2.41	0.50
1:H:129:ILE:CD1	1:H:213:MET:HE1	2.42	0.50
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.93	0.50
1:H:320:LYS:HB3	6:H:705:1PE:H141	1.94	0.50
1:B:168:LYS:O	1:B:171:THR:OG1	2.17	0.49
1:G:386:LYS:HB3	1:G:391:SER:HB3	1.94	0.49
1:H:376:ILE:HB	1:H:399:ASP:HB3	1.92	0.49
1:J:174:HIS:HB3	1:J:213:MET:HE2	1.94	0.49
1:J:440:ARG:NH1	7:J:812:HOH:O	2.41	0.49
1:B:113:GLN:OE1	1:B:115:TYR:OH	2.26	0.49
1:B:202:ASP:O	1:B:203:MET:C	2.50	0.49
1:H:108:HIS:HA	1:H:285:ARG:HH11	1.77	0.49
1:H:386:LYS:HB3	1:H:391:SER:HB3	1.94	0.49
1:I:510:ILE:HD13	1:I:526:TRP:NE1	2.27	0.49
1:B:216:ASP:HA	7:B:1148:HOH:O	2.11	0.49
1:D:155:GLU:OE2	1:D:158:LYS:HD3	2.12	0.49
1:E:213:MET:O	1:E:217:ASN:ND2	2.39	0.49
1:H:532:GLU:HG3	1:K:201:ALA:HB1	1.93	0.49
1:F:395:LEU:HD11	1:F:581:TRP:CE2	2.46	0.49
1:I:200:GLU:HG2	1:I:201:ALA:H	1.77	0.49
1:J:198:LEU:HD12	1:J:228:ILE:HD12	1.95	0.49
1:C:198:LEU:HD22	1:C:202:ASP:HB3	1.93	0.49
1:C:379:ASP:HB2	1:C:399:ASP:OD1	2.11	0.49
1:I:376:ILE:HB	1:I:399:ASP:HB3	1.94	0.49
1:A:332:GLU:HG3	7:A:874:HOH:O	2.13	0.49
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:549:SER:N	1:L:550:SER:HA	2.27	0.49
1:F:221:LYS:HG3	1:F:266:HIS:CB	2.41	0.49
1:F:332:GLU:O	1:F:335:GLU:HB2	2.13	0.49
1:G:316:GLU:HG3	6:G:708:1PE:C13	2.42	0.49
3:B:1004:TOD:C4	3:B:1004:TOD:N1	2.74	0.49
1:J:114:VAL:H	1:J:278:LYS:HZ3	1.53	0.49
1:C:254:SER:HA	1:C:257:LYS:HZ1	1.78	0.48
1:E:326:LYS:HE2	1:E:328:LEU:HD11	1.95	0.48
1:H:396:MET:HA	1:H:398:PHE:HD2	1.78	0.48
1:J:413:VAL:HG11	1:J:423:ILE:HD12	1.95	0.48
1:J:221:LYS:HG3	1:J:266:HIS:HB2	1.94	0.48
1:A:214:LEU:HD11	1:A:222:LEU:HD22	1.96	0.48
1:A:247:MET:HB2	1:A:288:TYR:OH	2.14	0.48
1:E:116:ASP:HA	1:E:271:ILE:O	2.13	0.48
1:L:176:TYR:OH	1:L:217:ASN:OD1	2.17	0.48
1:L:357:LEU:HD11	1:L:407:LEU:HD12	1.94	0.48
1:A:395:LEU:O	1:A:398:PHE:HD2	1.97	0.48
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.96	0.48
1:H:88:VAL:HG22	1:H:308:VAL:HB	1.95	0.48
1:A:328:LEU:HD22	1:A:332:GLU:OE1	2.14	0.48
1:K:332:GLU:N	1:K:332:GLU:OE1	2.38	0.48
1:A:195:VAL:O	1:A:197:ASP:N	2.44	0.48
1:D:204:LYS:O	1:D:208:LEU:HD13	2.14	0.48
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.96	0.48
1:I:173:LYS:NZ	1:K:216:ASP:O	2.42	0.48
1:E:439:TYR:HD1	7:E:891:HOH:O	1.97	0.48
1:K:312:ASN:HB2	7:K:845:HOH:O	2.12	0.48
1:L:504:GLY:HA3	1:L:510:ILE:HD11	1.95	0.48
1:F:169:LEU:HD23	1:F:192:CYS:HA	1.95	0.48
1:F:355:ILE:N	7:F:812:HOH:O	2.45	0.48
1:I:396:MET:HA	1:I:398:PHE:CE2	2.49	0.48
1:C:199:SER:HG	1:C:202:ASP:CG	2.17	0.47
1:F:213:MET:O	1:F:217:ASN:ND2	2.44	0.47
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.95	0.47
1:G:547:ILE:HG12	1:G:548:SER:N	2.26	0.47
1:C:124:GLU:HB3	1:C:179:ASN:ND2	2.29	0.47
1:C:199:SER:OG	1:C:202:ASP:CG	2.52	0.47
1:H:178:PHE:HA	1:H:183:ASN:O	2.14	0.47
1:H:488:THR:HG21	1:H:555:SER:HA	1.95	0.47
1:K:399:ASP:OD1	1:K:486:THR:OG1	2.32	0.47
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:395:LEU:HD21	1:J:581:TRP:CE2	2.50	0.47
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.95	0.47
1:D:117:ILE:HD12	1:D:271:ILE:C	2.35	0.47
1:I:396:MET:HE1	1:I:398:PHE:CZ	2.49	0.47
1:E:392:MET:HB2	1:E:395:LEU:HD23	1.97	0.47
1:J:395:LEU:O	1:J:398:PHE:CD2	2.67	0.47
1:K:462:GLY:CA	4:K:704:CO3:O2	2.62	0.47
1:A:155:GLU:CD	1:A:158:LYS:HD3	2.35	0.47
1:H:396:MET:HA	1:H:398:PHE:CD2	2.49	0.47
1:E:274:ALA:O	1:E:278:LYS:HG3	2.14	0.47
1:E:392:MET:CB	1:E:395:LEU:CD2	2.93	0.47
1:E:392:MET:HE3	1:E:395:LEU:CD2	2.45	0.47
1:L:214:LEU:HD11	1:L:222:LEU:HD22	1.96	0.47
1:E:271:ILE:HG12	1:E:272:ASN:O	2.16	0.46
1:K:341:TYR:CE1	1:K:428:ALA:HB1	2.50	0.46
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.97	0.46
1:C:123:VAL:O	1:C:124:GLU:CB	2.47	0.46
1:D:170:GLY:HA3	1:D:205:ARG:NH1	2.29	0.46
1:I:512:LYS:HD3	1:I:603:ASP:C	2.36	0.46
1:B:396:MET:SD	1:B:398:PHE:HE2	2.39	0.46
1:G:139:ASN:HB2	1:G:166:ASN:HB2	1.98	0.46
1:L:134:ASN:C	1:L:134:ASN:OD1	2.53	0.46
1:C:331:LYS:CE	1:C:334:GLU:OE2	2.63	0.46
1:D:497:THR:O	1:D:589:LYS:NZ	2.48	0.46
1:E:324:GLU:HG3	1:E:358:THR:HB	1.98	0.46
1:F:321:LEU:O	1:F:322:ASN:CB	2.63	0.46
1:H:459:ASP:C	1:H:461:GLU:H	2.17	0.46
1:J:179:ASN:OD1	1:J:183:ASN:N	2.29	0.46
1:E:459:ASP:O	3:E:703:TOD:O1	2.33	0.46
1:G:413:VAL:HG21	1:G:425:PHE:HZ	1.79	0.46
1:I:161:ASN:HA	1:I:164:LYS:NZ	2.30	0.46
1:I:172:SER:HB2	1:I:213:MET:HE1	1.97	0.46
1:C:205:ARG:HG2	7:C:839:HOH:O	2.14	0.46
1:C:205:ARG:O	7:C:839:HOH:O	2.21	0.46
1:D:533:TYR:O	1:D:536:THR:HG22	2.15	0.46
1:E:324:GLU:OE2	1:E:358:THR:CB	2.63	0.46
1:J:247:MET:HE2	7:J:849:HOH:O	2.11	0.46
1:B:142:VAL:HG11	1:B:189:TYR:CE2	2.51	0.46
1:I:143:LYS:HD3	1:I:159:ASP:CG	2.24	0.46
1:I:395:LEU:O	1:I:398:PHE:CD2	2.69	0.46
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:132:VAL:HG11	1:J:142:VAL:HG13	1.98	0.46
1:H:532:GLU:CD	1:K:498:SER:HG	2.03	0.46
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.97	0.46
1:I:207:VAL:HG11	1:I:241:THR:HG22	1.96	0.46
1:K:173:LYS:HB2	1:K:189:TYR:HE1	1.80	0.46
1:A:467:ALA:HB1	1:A:565:PHE:CE2	2.51	0.45
1:B:498:SER:O	1:B:523:PRO:HG2	2.16	0.45
1:E:338:MET:HE2	1:E:468:ASP:HB3	1.98	0.45
1:K:274:ALA:O	1:K:278:LYS:HG3	2.16	0.45
1:A:287:TYR:CD2	1:A:594:ARG:HG2	2.52	0.45
1:B:487:LEU:O	3:B:1004:TOD:N1	2.49	0.45
1:D:396:MET:HA	1:D:398:PHE:HD2	1.79	0.45
1:F:429:VAL:HG23	7:F:812:HOH:O	2.16	0.45
1:J:552:LYS:HB3	1:J:553:ALA:H	1.40	0.45
1:L:286:VAL:HG11	1:L:416:LEU:HG	1.98	0.45
1:H:525:TRP:CZ3	1:K:528:PRO:HB3	2.51	0.45
1:K:95:ASP:HA	1:K:96:PRO:HD3	1.73	0.45
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.99	0.45
1:C:344:VAL:HA	1:C:439:TYR:CE2	2.51	0.45
1:H:129:ILE:HD11	1:H:213:MET:HE1	1.99	0.45
1:J:510:ILE:HD13	1:J:526:TRP:NE1	2.32	0.45
1:L:112:VAL:O	1:L:113:GLN:HG3	2.17	0.45
1:L:399:ASP:OD1	1:L:486:THR:OG1	2.35	0.45
1:L:436:LYS:HG3	1:L:437:ASN:N	2.32	0.45
1:B:125:GLU:CG	1:B:221:LYS:HD3	2.47	0.45
1:K:204:LYS:O	1:K:208:LEU:HD13	2.17	0.45
1:A:467:ALA:HB1	1:A:565:PHE:CD2	2.51	0.45
1:B:419:GLU:CD	1:B:419:GLU:H	2.20	0.45
1:D:301:PRO:HA	1:D:397:LYS:HD2	1.98	0.45
1:E:217:ASN:HB3	1:E:219:LEU:HG	1.99	0.45
1:J:550:SER:CB	1:J:551:VAL:HA	2.47	0.45
1:L:127:LEU:HD21	1:L:213:MET:HE2	1.99	0.45
1:D:144:ILE:HD12	1:D:162:MET:HG3	1.98	0.44
1:F:236:ARG:NE	1:F:240:GLU:OE2	2.39	0.44
1:H:460:ALA:O	1:H:546:GLN:NE2	2.50	0.44
1:K:230:VAL:HG12	1:K:234:LEU:HD23	1.99	0.44
1:A:512:LYS:HD3	1:A:603:ASP:OD2	2.18	0.44
1:F:460:ALA:HB3	1:F:546:GLN:NE2	2.32	0.44
1:H:364:ASP:O	1:H:364:ASP:OD1	2.35	0.44
1:K:396:MET:HA	1:K:398:PHE:HD2	1.81	0.44
1:E:494:SER:HB3	7:E:903:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:498:SER:O	1:E:523:PRO:HG2	2.18	0.44
1:I:395:LEU:O	1:I:398:PHE:HD2	2.01	0.44
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.53	0.44
1:A:463:ARG:HE	4:A:704:CO3:C	2.25	0.44
1:G:244:TYR:OH	1:G:588:PRO:O	2.35	0.44
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.98	0.44
1:I:338:MET:CE	1:I:468:ASP:HB3	2.47	0.44
1:I:440:ARG:NH2	7:I:816:HOH:O	2.50	0.44
1:D:374:LYS:HB3	7:D:811:HOH:O	2.17	0.44
1:F:328:LEU:HA	1:F:328:LEU:HD23	1.83	0.44
1:I:519:THR:O	1:I:519:THR:HG22	2.17	0.44
1:J:165:PHE:CD2	1:J:173:LYS:HG3	2.53	0.44
1:A:380:SER:HA	1:A:393:ILE:HD11	1.99	0.44
1:E:150:ASP:OD1	1:E:179:ASN:HB2	2.17	0.44
1:F:138:GLU:N	1:F:139:ASN:CA	2.80	0.44
1:G:162:MET:O	1:G:165:PHE:CD2	2.71	0.44
1:H:129:ILE:HG21	1:H:190:VAL:HG23	2.00	0.44
1:I:157:LEU:HD12	1:I:162:MET:SD	2.58	0.44
1:K:108:HIS:HA	1:K:285:ARG:HH11	1.82	0.44
3:K:703:TOD:C7	3:K:703:TOD:H4	2.48	0.44
1:L:207:VAL:HG11	1:L:241:THR:HG22	2.00	0.44
1:D:338:MET:CE	1:D:468:ASP:HB3	2.48	0.44
1:G:255:THR:O	1:G:256:ASP:C	2.56	0.44
1:G:255:THR:O	1:G:257:LYS:N	2.50	0.44
1:E:392:MET:HE2	1:E:392:MET:HB2	1.79	0.44
1:F:111:LYS:HA	1:F:111:LYS:HD3	1.74	0.44
1:G:316:GLU:HG3	6:G:708:1PE:H132	2.00	0.44
1:D:247:MET:CB	1:D:288:TYR:OH	2.66	0.44
1:I:200:GLU:N	1:I:200:GLU:OE1	2.31	0.44
1:J:396:MET:SD	1:J:398:PHE:CE2	2.98	0.44
1:A:175:PHE:N	1:A:187:VAL:O	2.47	0.43
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.99	0.43
1:B:274:ALA:O	1:B:278:LYS:HG3	2.18	0.43
1:C:386:LYS:HB3	1:C:391:SER:HB2	2.00	0.43
1:F:326:LYS:HE3	1:F:328:LEU:CD2	2.46	0.43
1:G:328:LEU:HB2	1:G:354:PHE:HB3	2.00	0.43
1:K:232:LYS:NZ	1:K:279:GLU:OE2	2.38	0.43
1:E:376:ILE:HB	1:E:399:ASP:HB3	2.00	0.43
1:H:155:GLU:O	1:H:161:ASN:ND2	2.51	0.43
1:J:142:VAL:HG22	1:J:167:VAL:HG12	2.00	0.43
1:L:129:ILE:HD11	1:L:213:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:CD1	1:D:157:LEU:HD22	2.45	0.43
1:D:372:VAL:O	1:D:483:ASP:HA	2.18	0.43
1:I:396:MET:CA	1:I:398:PHE:HD2	2.26	0.43
7:H:874:HOH:O	1:K:532:GLU:CB	2.65	0.43
1:B:142:VAL:CG1	1:B:167:VAL:CG1	2.81	0.43
1:D:396:MET:HA	1:D:398:PHE:CD2	2.53	0.43
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.84	0.43
1:E:204:LYS:O	1:E:208:LEU:HD13	2.18	0.43
1:E:392:MET:HE3	1:E:395:LEU:HD21	1.99	0.43
1:G:462:GLY:CA	4:G:704:CO3:O2	2.64	0.43
1:I:161:ASN:O	1:I:164:LYS:CE	2.63	0.43
1:I:480:TYR:CD1	1:I:509:LEU:HD13	2.53	0.43
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.99	0.43
1:E:207:VAL:HG11	1:E:241:THR:HG22	2.00	0.43
1:H:451:LYS:NZ	1:H:564:GLU:HB3	2.33	0.43
3:I:703:TOD:H4	3:I:703:TOD:H9	2.00	0.43
1:L:343:SER:HA	1:L:346:LYS:HD3	1.99	0.43
1:L:236:ARG:NH2	1:L:519:THR:O	2.51	0.43
1:A:321:LEU:HD11	1:A:411:TYR:HA	2.00	0.43
1:B:199:SER:HG	1:B:203:MET:H	1.67	0.43
1:B:471:VAL:CG1	1:B:475:LYS:HE3	2.46	0.43
1:F:321:LEU:O	1:F:322:ASN:HB3	2.18	0.43
1:G:316:GLU:OE1	6:G:708:1PE:H241	2.19	0.43
1:H:498:SER:O	1:H:523:PRO:HG2	2.17	0.43
1:K:338:MET:HE2	1:K:468:ASP:HB3	2.01	0.43
1:A:243:PHE:C	1:A:288:TYR:CE1	2.92	0.43
1:C:509:LEU:O	1:C:513:ILE:HG12	2.19	0.43
1:D:107:ILE:HG21	1:D:288:TYR:CE2	2.53	0.43
1:E:198:LEU:HD22	1:E:202:ASP:HB3	2.00	0.43
1:G:366:LYS:HG2	1:G:420:ASN:HB3	2.00	0.43
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.99	0.43
1:B:117:ILE:CD1	1:B:272:ASN:N	2.82	0.43
1:B:481:ILE:O	1:B:571:TRP:HA	2.19	0.43
1:D:395:LEU:HD12	7:D:821:HOH:O	2.18	0.43
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.93	0.43
1:L:209:SER:O	1:L:213:MET:HG3	2.19	0.43
1:B:549:SER:O	7:B:1167:HOH:O	2.21	0.43
1:C:253:LYS:HB2	1:C:257:LYS:HG2	2.01	0.43
1:C:574:ILE:HD13	1:C:595:LEU:HD21	2.00	0.43
1:D:117:ILE:HD11	1:D:271:ILE:CA	2.47	0.43
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:236:ARG:NH2	1:J:519:THR:O	2.46	0.43
1:C:204:LYS:HG2	1:C:241:THR:HG21	2.00	0.43
1:D:544:ILE:HD12	1:D:564:GLU:HG3	2.01	0.43
1:G:285:ARG:HD3	7:G:858:HOH:O	2.18	0.43
1:I:95:ASP:HA	1:I:96:PRO:HD3	1.86	0.43
1:K:441:PRO:HD2	1:L:378:PHE:CZ	2.54	0.43
1:B:507:GLU:O	1:B:511:ASN:ND2	2.48	0.42
1:C:124:GLU:HB3	1:C:179:ASN:HD22	1.84	0.42
1:F:171:THR:HG22	1:F:189:TYR:OH	2.19	0.42
1:H:372:VAL:O	1:H:483:ASP:HA	2.19	0.42
1:J:232:LYS:HA	1:J:277:TYR:HE1	1.84	0.42
1:H:459:ASP:C	1:H:461:GLU:N	2.73	0.42
1:F:322:ASN:CB	1:K:160:GLU:OE2	2.67	0.42
1:K:173:LYS:HB2	1:K:189:TYR:CE1	2.52	0.42
1:K:329:GLY:O	1:K:333:LEU:HG	2.19	0.42
1:J:441:PRO:HB2	1:K:394:ASP:HA	2.01	0.42
1:G:252:PHE:CZ	1:G:301:PRO:HD2	2.54	0.42
7:G:891:HOH:O	1:J:164:LYS:HD3	2.19	0.42
1:K:329:GLY:N	1:K:332:GLU:OE1	2.52	0.42
1:A:463:ARG:HB3	4:A:704:CO3:O1	2.20	0.42
1:K:395:LEU:HD11	1:K:581:TRP:NE1	2.34	0.42
1:K:467:ALA:HB1	1:K:565:PHE:CE2	2.54	0.42
1:E:553:ALA:O	1:E:557:VAL:HG23	2.18	0.42
1:F:321:LEU:HA	1:F:321:LEU:HD23	1.77	0.42
1:H:458:THR:C	1:H:460:ALA:N	2.73	0.42
1:L:338:MET:CE	1:L:468:ASP:HB3	2.50	0.42
1:B:133:ASN:HB3	1:B:192:CYS:HB2	2.02	0.42
1:C:254:SER:HA	1:C:257:LYS:HZ2	1.83	0.42
1:D:214:LEU:HD11	1:D:222:LEU:HD22	2.02	0.42
1:J:380:SER:HA	1:J:393:ILE:HD11	2.00	0.42
1:L:426:LEU:HD11	1:L:476:LEU:HD11	2.01	0.42
1:A:395:LEU:HD11	1:A:581:TRP:CD1	2.55	0.42
1:B:125:GLU:HG2	1:B:221:LYS:HD3	2.02	0.42
1:B:244:TYR:HA	1:B:288:TYR:HE1	1.85	0.42
1:C:200:GLU:HG3	1:C:521:ASN:O	2.20	0.42
1:C:208:LEU:O	1:C:212:THR:HG23	2.20	0.42
1:D:419:GLU:HG2	1:D:420:ASN:ND2	2.35	0.42
1:E:95:ASP:HA	1:E:96:PRO:HD3	1.93	0.42
1:H:117:ILE:HG21	1:H:117:ILE:HD13	1.74	0.42
1:H:137:LYS:O	1:H:194:SER:OG	2.34	0.42
1:E:273:ASN:O	1:E:277:TYR:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:114:VAL:N	1:J:278:LYS:HZ2	2.06	0.42
1:J:300:ALA:HA	1:J:301:PRO:HD3	1.83	0.42
1:J:395:LEU:O	1:J:398:PHE:HD2	2.02	0.42
1:C:124:GLU:HG2	1:C:179:ASN:HD22	1.85	0.42
1:K:125:GLU:HA	1:K:185:VAL:HG12	2.01	0.42
1:L:418:PRO:HB3	1:L:601:LEU:HD12	2.02	0.42
1:A:326:LYS:HG3	1:A:328:LEU:HD23	2.02	0.42
1:B:124:GLU:O	1:B:185:VAL:HG12	2.19	0.42
1:D:198:LEU:HD12	1:D:202:ASP:HB3	2.01	0.42
1:L:129:ILE:HA	1:L:129:ILE:HD13	1.78	0.42
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.19	0.41
1:A:96:PRO:HG2	1:A:303:ASN:O	2.20	0.41
1:D:170:GLY:HA3	1:D:205:ARG:HH11	1.85	0.41
3:F:703:TOD:H19	3:F:703:TOD:C8	2.50	0.41
1:H:123:VAL:HG11	1:H:185:VAL:HG21	2.02	0.41
1:H:441:PRO:HB2	1:I:394:ASP:HA	2.02	0.41
1:J:488:THR:OG1	1:J:555:SER:OG	2.24	0.41
1:A:386:LYS:HB3	1:A:391:SER:HB3	2.01	0.41
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.55	0.41
1:H:255:THR:O	1:H:255:THR:OG1	2.35	0.41
1:L:328:LEU:HB2	1:L:354:PHE:HB3	2.02	0.41
1:C:331:LYS:HE2	1:C:334:GLU:OE1	2.20	0.41
1:F:168:LYS:HB3	1:F:171:THR:OG1	2.21	0.41
1:G:316:GLU:HG3	6:G:708:1PE:H131	2.02	0.41
1:G:528:PRO:HB3	1:L:525:TRP:CZ3	2.55	0.41
1:H:200:GLU:CG	1:H:201:ALA:N	2.83	0.41
1:H:494:SER:OG	1:H:495:LEU:N	2.52	0.41
1:J:207:VAL:HG11	1:J:241:THR:HG22	2.01	0.41
3:J:703:TOD:C8	3:J:703:TOD:H19	2.49	0.41
1:L:489:GLY:N	3:L:703:TOD:O4	2.33	0.41
1:B:106:PRO:HD2	1:B:247:MET:SD	2.61	0.41
1:F:484:ILE:HD11	1:F:576:ILE:HG21	2.02	0.41
1:F:95:ASP:HA	1:F:96:PRO:HD3	1.91	0.41
1:H:467:ALA:HB1	1:H:565:PHE:CD2	2.54	0.41
1:J:376:ILE:HB	1:J:399:ASP:HB3	2.02	0.41
1:K:212:THR:HG22	1:K:216:ASP:OD2	2.21	0.41
1:L:403:CYS:O	1:L:407:LEU:HD22	2.20	0.41
1:C:346:LYS:HB3	1:C:437:ASN:O	2.20	0.41
1:F:355:ILE:HG13	7:F:812:HOH:O	2.20	0.41
1:H:546:GLN:HG3	1:H:547:ILE:HG23	2.01	0.41
1:K:338:MET:CE	1:K:468:ASP:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:548:SER:HB2	1:K:557:VAL:HG11	2.02	0.41
1:A:195:VAL:O	1:A:195:VAL:HG12	2.21	0.41
1:A:369:ILE:HB	1:A:423:ILE:HD13	2.02	0.41
1:C:168:LYS:HB3	1:C:171:THR:OG1	2.20	0.41
1:C:444:ILE:HA	1:C:453:ILE:O	2.20	0.41
1:G:142:VAL:HG21	1:G:189:TYR:CE2	2.56	0.41
1:G:395:LEU:HA	1:G:395:LEU:HD23	1.85	0.41
1:E:460:ALA:O	1:E:546:GLN:NE2	2.53	0.41
1:H:301:PRO:HB2	1:H:303:ASN:OD1	2.21	0.41
1:I:338:MET:HE2	1:I:468:ASP:HB3	2.01	0.41
1:J:112:VAL:HG22	1:J:267:LEU:HB3	2.03	0.41
1:K:396:MET:HA	1:K:398:PHE:CD2	2.55	0.41
1:B:375:GLY:O	1:B:429:VAL:HA	2.20	0.41
1:D:121:CYS:HB2	1:D:148:VAL:HG12	2.02	0.41
1:D:285:ARG:O	1:D:288:TYR:HB3	2.21	0.41
1:D:346:LYS:HB3	1:D:437:ASN:O	2.21	0.41
1:B:394:ASP:OD1	1:B:395:LEU:HG	2.21	0.41
1:C:419:GLU:N	1:C:419:GLU:OE1	2.52	0.41
1:I:418:PRO:CG	1:I:601:LEU:CD1	2.98	0.41
1:D:338:MET:HE2	1:D:468:ASP:HB3	2.03	0.41
1:F:372:VAL:HG22	1:F:426:LEU:HD12	2.03	0.41
1:H:195:VAL:O	1:H:197:ASP:N	2.54	0.41
1:H:528:PRO:HD3	1:K:525:TRP:CE2	2.55	0.41
1:H:451:LYS:HZ3	1:H:564:GLU:HB3	1.85	0.41
7:H:866:HOH:O	1:K:551:VAL:CB	2.68	0.41
1:L:350:TYR:HA	1:L:351:PRO:HD3	1.93	0.41
1:A:159:ASP:HA	1:A:162:MET:HB2	2.03	0.41
1:E:392:MET:SD	1:E:395:LEU:HD22	2.60	0.41
1:I:328:LEU:HA	1:I:332:GLU:OE1	2.21	0.41
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.56	0.41
1:D:103:TYR:HB3	6:D:705:1PE:H241	2.03	0.40
1:D:210:LEU:HD12	1:D:213:MET:HE3	2.03	0.40
1:D:244:TYR:HA	1:D:288:TYR:CE1	2.49	0.40
1:E:494:SER:CB	7:E:903:HOH:O	2.70	0.40
1:F:424:HIS:CG	1:F:476:LEU:HD13	2.56	0.40
1:L:372:VAL:O	1:L:483:ASP:HA	2.21	0.40
1:C:229:ASN:OD1	1:C:230:VAL:N	2.53	0.40
1:E:520:SER:HB3	1:E:598:GLU:HG3	2.03	0.40
1:F:116:ASP:HA	1:F:271:ILE:O	2.21	0.40
1:C:536:THR:HG21	1:C:551:VAL:HG23	2.04	0.40
1:D:378:PHE:CZ	1:F:441:PRO:HD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ASP:O	1:G:163:GLU:HG3	2.21	0.40
1:G:129:ILE:HA	1:G:188:GLY:O	2.21	0.40
1:B:174:HIS:CE1	1:B:213:MET:HG2	2.57	0.40
1:F:483:ASP:OD2	1:F:571:TRP:NE1	2.48	0.40
1:G:441:PRO:HD2	1:H:378:PHE:CZ	2.57	0.40
1:H:120:GLY:HA3	1:H:149:ASN:OD1	2.22	0.40
1:I:386:LYS:HB3	1:I:391:SER:HB3	2.03	0.40
1:J:172:SER:HB2	1:J:213:MET:HE1	2.02	0.40
1:L:112:VAL:HA	1:L:267:LEU:O	2.22	0.40
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.96	0.40
1:E:392:MET:HB2	1:E:395:LEU:CD2	2.50	0.40
1:F:153:VAL:HB	1:F:177:MET:CE	2.49	0.40
1:I:321:LEU:HD11	1:I:411:TYR:HA	2.03	0.40
1:J:321:LEU:O	1:J:322:ASN:HB2	2.21	0.40
1:K:396:MET:CE	1:K:398:PHE:CE2	3.01	0.40
1:K:431:GLU:HG2	1:K:433:MET:CG	2.48	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:OD1	1:G:278:LYS:NZ[2_564]	1.65	0.55
1:J:229:ASN:ND2	1:K:273:ASN:ND2[4_456]	2.12	0.08

## 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	511/519 (98%)	492 (96%)	16 (3%)	3 (1%)	28 55
1	B	504/519 (97%)	479 (95%)	19 (4%)	6 (1%)	15 36
1	C	513/519 (99%)	499 (97%)	12 (2%)	2 (0%)	38 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	507/519 (98%)	490 (97%)	11 (2%)	6 (1%)	15	36
1	E	503/519 (97%)	489 (97%)	10 (2%)	4 (1%)	22	48
1	F	501/519 (96%)	478 (95%)	19 (4%)	4 (1%)	22	48
1	G	517/519 (100%)	491 (95%)	19 (4%)	7 (1%)	13	31
1	H	504/519 (97%)	480 (95%)	18 (4%)	6 (1%)	15	36
1	I	511/519 (98%)	489 (96%)	17 (3%)	5 (1%)	18	41
1	J	507/519 (98%)	486 (96%)	13 (3%)	8 (2%)	11	27
1	K	503/519 (97%)	486 (97%)	15 (3%)	2 (0%)	38	65
1	L	502/519 (97%)	484 (96%)	15 (3%)	3 (1%)	28	55
All	All	6083/6228 (98%)	5843 (96%)	184 (3%)	56 (1%)	20	45

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	GLU
1	A	139	ASN
1	B	196	ALA
1	B	199	SER
1	C	196	ALA
1	D	322	ASN
1	D	553	ALA
1	E	139	ASN
1	F	124	GLU
1	F	322	ASN
1	F	552	LYS
1	G	163	GLU
1	G	196	ALA
1	G	256	ASP
1	G	257	LYS
1	H	196	ALA
1	H	231	ASP
1	I	124	GLU
1	I	139	ASN
1	I	196	ALA
1	I	551	VAL
1	J	137	LYS
1	J	139	ASN
1	J	196	ALA
1	J	391	SER

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Mol	Chain	Res	Type
1	K	139	ASN
1	K	552	LYS
1	L	196	ALA
1	B	273	ASN
1	C	552	LYS
1	D	124	GLU
1	D	139	ASN
1	E	124	GLU
1	E	273	ASN
1	G	259	VAL
1	H	363	GLY
1	I	602	ASN
1	L	124	GLU
1	B	124	GLU
1	D	196	ALA
1	G	552	LYS
1	G	553	ALA
1	H	458	THR
1	H	459	ASP
1	E	182	LYS
1	H	123	VAL
1	J	553	ALA
1	B	119	GLY
1	F	551	VAL
1	J	551	VAL
1	L	417	LYS
1	B	363	GLY
1	D	551	VAL
1	J	136	GLY
1	J	363	GLY
1	A	363	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	414/447 (93%)	414 (100%)	0	100	100
1	B	396/447 (89%)	394 (100%)	2 (0%)	91	97
1	C	417/447 (93%)	416 (100%)	1 (0%)	94	98
1	D	411/447 (92%)	410 (100%)	1 (0%)	94	98
1	E	411/447 (92%)	411 (100%)	0	100	100
1	F	379/447 (85%)	377 (100%)	2 (0%)	91	97
1	G	424/447 (95%)	424 (100%)	0	100	100
1	H	402/447 (90%)	398 (99%)	4 (1%)	80	93
1	I	412/447 (92%)	411 (100%)	1 (0%)	94	98
1	J	402/447 (90%)	402 (100%)	0	100	100
1	K	409/447 (92%)	409 (100%)	0	100	100
1	L	391/447 (88%)	389 (100%)	2 (0%)	91	97
All	All	4868/5364 (91%)	4855 (100%)	13 (0%)	94	98

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	GLU
1	B	419	GLU
1	C	204	LYS
1	D	104	ASN
1	F	332	GLU
1	F	439	TYR
1	H	117	ILE
1	H	152	GLN
1	H	419	GLU
1	H	439	TYR
1	I	93	SER
1	L	114	VAL
1	L	134	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	ASN

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Mol	Chain	Res	Type
1	E	567	GLN
1	F	272	ASN
1	H	122	ASN
1	H	139	ASN
1	H	152	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 70 ligands modelled in this entry, 24 are monoatomic - leaving 46 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	$\# Z  > 2$
3	TOD	A	703	2	21,24,24	2.37	2 (9%)	22,32,32	1.15	3 (13%)
4	CO3	A	704	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	A	705	-	4,4,4	0.18	0	6,6,6	0.10	0
5	SO4	A	706	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	A	707	-	4,4,4	0.16	0	6,6,6	0.08	0
6	1PE	A	708	-	8,8,15	0.52	0	7,7,14	0.25	0
4	CO3	B	1001	-	0,3,3	0.00	-	0,3,3	0.00	-
3	TOD	B	1004	2	21,24,24	2.72	3 (14%)	22,32,32	1.63	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	1005	-	4,4,4	0.12	0	6,6,6	0.11	0
6	1PE	B	1006	-	6,6,15	0.45	0	5,5,14	0.65	0
3	TOD	C	703	2	16,16,24	2.17	2 (12%)	15,21,32	1.46	1 (6%)
4	CO3	C	704	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	C	705	-	4,4,4	0.15	0	6,6,6	0.08	0
6	1PE	C	706	-	12,12,15	0.56	0	11,11,14	0.49	0
6	1PE	C	707	-	8,8,15	0.54	0	7,7,14	0.41	0
4	CO3	D	703	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	D	704	-	4,4,4	0.14	0	6,6,6	0.08	0
6	1PE	D	705	-	9,9,15	0.47	0	8,8,14	0.29	0
6	1PE	D	706	-	9,9,15	0.74	0	8,8,14	0.79	0
3	TOD	E	703	2	14,14,24	1.17	1 (7%)	12,18,32	0.56	0
4	CO3	E	704	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	E	705	-	4,4,4	0.12	0	6,6,6	0.14	0
5	SO4	E	706	-	4,4,4	1.01	0	6,6,6	1.58	1 (16%)
6	1PE	E	707	-	11,11,15	0.39	0	10,10,14	0.53	0
3	TOD	F	703	2	21,24,24	2.42	4 (19%)	22,32,32	1.90	4 (18%)
4	CO3	F	704	-	0,3,3	0.00	-	0,3,3	0.00	-
3	TOD	G	703	2	22,22,24	1.17	2 (9%)	23,29,32	1.48	6 (26%)
4	CO3	G	704	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	G	705	-	4,4,4	0.16	0	6,6,6	0.08	0
5	SO4	G	706	-	4,4,4	0.11	0	6,6,6	0.26	0
6	1PE	G	707	-	8,8,15	0.57	0	7,7,14	0.36	0
6	1PE	G	708	-	8,8,15	0.72	0	7,7,14	0.64	0
3	TOD	H	703	2	12,13,24	0.90	1 (8%)	10,17,32	0.67	0
4	CO3	H	704	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	H	705	-	9,9,15	0.52	0	8,8,14	0.56	0
3	TOD	I	703	2	21,24,24	2.40	2 (9%)	22,32,32	1.17	3 (13%)
4	CO3	I	704	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	I	705	-	4,4,4	0.14	0	6,6,6	0.15	0
3	TOD	J	703	2	22,22,24	1.56	2 (9%)	23,29,32	1.62	3 (13%)
4	CO3	J	704	-	0,3,3	0.00	-	0,3,3	0.00	-
3	TOD	K	703	2	22,22,24	1.20	1 (4%)	23,29,32	1.47	2 (8%)
4	CO3	K	704	-	0,3,3	0.00	-	0,3,3	0.00	-
3	TOD	L	703	2	21,24,24	2.24	2 (9%)	22,32,32	1.33	4 (18%)
4	CO3	L	704	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	L	705	-	4,4,4	0.19	0	6,6,6	0.09	0
5	SO4	L	706	-	4,4,4	0.16	0	6,6,6	0.09	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
3	TOD	A	703	2	-	0/26/30/30	0/1/1/1
4	CO3	A	704	-	-	0/0/0/0	0/0/0/0
5	SO4	A	705	-	-	0/0/0/0	0/0/0/0
5	SO4	A	706	-	-	0/0/0/0	0/0/0/0
5	SO4	A	707	-	-	0/0/0/0	0/0/0/0
6	1PE	A	708	-	-	0/6/6/13	0/0/0/0
4	CO3	B	1001	-	-	0/0/0/0	0/0/0/0
3	TOD	B	1004	2	-	0/26/30/30	0/1/1/1
5	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
6	1PE	B	1006	-	-	0/4/4/13	0/0/0/0
3	TOD	C	703	2	-	0/22/22/30	0/0/0/1
4	CO3	C	704	-	-	0/0/0/0	0/0/0/0
5	SO4	C	705	-	-	0/0/0/0	0/0/0/0
6	1PE	C	706	-	-	0/10/10/13	0/0/0/0
6	1PE	C	707	-	-	0/6/6/13	0/0/0/0
4	CO3	D	703	-	-	0/0/0/0	0/0/0/0
5	SO4	D	704	-	-	0/0/0/0	0/0/0/0
6	1PE	D	705	-	-	0/7/7/13	0/0/0/0
6	1PE	D	706	-	-	0/7/7/13	0/0/0/0
3	TOD	E	703	2	-	0/20/20/30	0/0/0/1
4	CO3	E	704	-	-	0/0/0/0	0/0/0/0
5	SO4	E	705	-	-	0/0/0/0	0/0/0/0
5	SO4	E	706	-	-	0/0/0/0	0/0/0/0
6	1PE	E	707	-	-	0/9/9/13	0/0/0/0
3	TOD	F	703	2	-	1/26/30/30	0/1/1/1
4	CO3	F	704	-	-	0/0/0/0	0/0/0/0
3	TOD	G	703	2	-	0/26/26/30	0/1/1/1
4	CO3	G	704	-	-	0/0/0/0	0/0/0/0
5	SO4	G	705	-	-	0/0/0/0	0/0/0/0
5	SO4	G	706	-	-	0/0/0/0	0/0/0/0
6	1PE	G	707	-	-	0/6/6/13	0/0/0/0
6	1PE	G	708	-	-	0/6/6/13	0/0/0/0
3	TOD	H	703	2	-	0/18/18/30	0/0/0/1
4	CO3	H	704	-	-	0/0/0/0	0/0/0/0
6	1PE	H	705	-	-	0/7/7/13	0/0/0/0
3	TOD	I	703	2	-	0/26/30/30	0/1/1/1
4	CO3	I	704	-	-	0/0/0/0	0/0/0/0
5	SO4	I	705	-	-	0/0/0/0	0/0/0/0
3	TOD	J	703	2	-	0/26/26/30	0/1/1/1
4	CO3	J	704	-	-	0/0/0/0	0/0/0/0
3	TOD	K	703	2	-	0/26/26/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CO3	K	704	-	-	0/0/0/0	0/0/0/0
3	TOD	L	703	2	-	0/26/30/30	0/1/1/1
4	CO3	L	704	-	-	0/0/0/0	0/0/0/0
5	SO4	L	705	-	-	0/0/0/0	0/0/0/0
5	SO4	L	706	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	TOD	C10-C9	-10.03	1.39	1.52
3	L	703	TOD	C10-C9	-9.75	1.39	1.52
3	B	1004	TOD	C10-C9	-8.87	1.41	1.52
3	F	703	TOD	C10-C9	-8.84	1.41	1.52
3	I	703	TOD	C10-C9	-8.72	1.41	1.52
3	K	703	TOD	C10-C9	-4.84	1.39	1.52
3	J	703	TOD	C10-C9	-4.54	1.40	1.52
3	G	703	TOD	C10-C9	-4.52	1.40	1.52
3	C	703	TOD	C10-C9	-4.41	1.39	1.51
3	L	703	TOD	C5-C6	-2.34	1.51	1.54
3	G	703	TOD	O2-N1	2.26	1.43	1.39
3	H	703	TOD	O2-N1	2.28	1.43	1.39
3	A	703	TOD	O2-N1	2.30	1.43	1.39
3	F	703	TOD	C9-N2	2.41	1.50	1.46
3	F	703	TOD	C5-C8	2.52	1.56	1.51
3	B	1004	TOD	C9-N2	2.53	1.50	1.46
3	E	703	TOD	O2-N1	3.78	1.46	1.39
3	J	703	TOD	O2-N1	5.19	1.48	1.39
3	F	703	TOD	O2-N1	5.24	1.49	1.39
3	I	703	TOD	O2-N1	6.06	1.50	1.39
3	C	703	TOD	O2-N1	7.21	1.52	1.39
3	B	1004	TOD	O2-N1	7.85	1.53	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	703	TOD	C5-C8-N2	-5.62	109.17	116.05
3	J	703	TOD	C5-C8-N2	-5.01	109.91	116.05
3	C	703	TOD	C5-C8-N2	-4.35	110.72	116.05
3	F	703	TOD	C5-C8-N2	-4.13	110.99	116.05
3	B	1004	TOD	O3-C6-C7	-3.70	102.44	110.59
3	B	1004	TOD	O4-C8-C5	-3.49	117.47	121.64
3	L	703	TOD	O4-C8-C5	-2.67	118.45	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	TOD	O4-C8-C5	-2.59	118.55	121.64
3	A	703	TOD	C16-C9-C10	-2.48	109.13	112.89
3	G	703	TOD	C16-C9-N2	-2.28	105.41	109.06
3	G	703	TOD	C5-C8-N2	-2.27	113.26	116.05
3	G	703	TOD	C16-C9-C10	-2.26	107.23	112.23
3	B	1004	TOD	C15-C10-C9	-2.24	116.91	120.75
3	L	703	TOD	C10-C9-N2	-2.20	106.91	111.09
3	I	703	TOD	O4-C8-C5	-2.11	119.11	121.64
3	F	703	TOD	C16-C9-C10	-2.04	109.81	112.89
3	G	703	TOD	C9-N2-C8	2.10	125.94	123.00
3	G	703	TOD	C6-C7-N1	2.16	119.22	116.28
3	I	703	TOD	C9-N2-C8	2.18	125.83	121.27
3	L	703	TOD	C3-C2-C4	2.24	119.42	111.09
3	A	703	TOD	C3-C2-C4	2.29	119.61	111.09
3	J	703	TOD	O4-C8-N2	2.39	127.40	122.90
3	B	1004	TOD	C9-N2-C8	2.46	126.43	121.27
3	L	703	TOD	C5-C8-N2	2.51	119.12	116.05
3	I	703	TOD	C3-C2-C4	2.57	120.65	111.09
3	K	703	TOD	O4-C8-N2	2.93	128.43	122.90
3	J	703	TOD	C10-C9-N2	3.12	117.92	111.36
5	E	706	SO4	O4-S-O3	3.65	125.39	108.96
3	G	703	TOD	C10-C9-N2	3.70	119.13	111.36
3	F	703	TOD	C9-N2-C8	4.50	130.69	121.27
3	F	703	TOD	C10-C9-N2	4.68	120.02	111.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	703	TOD	C10-C9-N2-C8

There are no ring outliers.

25 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	704	CO3	3	0
6	A	708	1PE	1	0
3	B	1004	TOD	4	0
5	C	705	SO4	1	0
6	C	706	1PE	11	0
6	C	707	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	703	CO3	1	0
5	D	704	SO4	1	0
6	D	705	1PE	1	0
6	D	706	1PE	4	0
3	E	703	TOD	3	0
3	F	703	TOD	1	0
4	G	704	CO3	2	0
5	G	706	SO4	1	0
6	G	708	1PE	4	0
4	H	704	CO3	1	0
6	H	705	1PE	1	0
3	I	703	TOD	2	0
4	I	704	CO3	1	0
3	J	703	TOD	2	0
4	J	704	CO3	3	0
3	K	703	TOD	3	0
4	K	704	CO3	3	0
3	L	703	TOD	1	0
5	L	705	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	516/519 (99%)	-0.12	7 (1%) 75 76	20, 28, 50, 96	0
1	B	510/519 (98%)	0.15	15 (2%) 52 52	19, 29, 61, 79	0
1	C	517/519 (99%)	-0.11	2 (0%) 92 93	18, 27, 50, 82	0
1	D	511/519 (98%)	-0.14	3 (0%) 89 90	15, 24, 46, 70	0
1	E	509/519 (98%)	-0.24	2 (0%) 92 93	14, 25, 42, 63	0
1	F	509/519 (98%)	0.03	15 (2%) 52 52	15, 31, 59, 73	0
1	G	519/519 (100%)	-0.02	8 (1%) 74 75	22, 30, 53, 94	0
1	H	510/519 (98%)	0.21	25 (4%) 30 29	20, 32, 63, 78	1 (0%)
1	I	515/519 (99%)	-0.04	8 (1%) 72 74	18, 28, 53, 80	0
1	J	511/519 (98%)	-0.15	2 (0%) 92 93	15, 27, 46, 65	0
1	K	509/519 (98%)	-0.17	2 (0%) 92 93	17, 26, 44, 78	5 (0%)
1	L	508/519 (97%)	-0.04	6 (1%) 79 80	18, 31, 54, 70	2 (0%)
All	All	6144/6228 (98%)	-0.05	95 (1%) 74 75	14, 28, 54, 96	8 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	GLY	6.7
1	A	603	ASP	4.9
1	B	196	ALA	4.8
1	G	603	ASP	4.8
1	L	145	SER	4.1
1	H	122	ASN	4.1
1	D	136	GLY	4.0
1	I	274	ALA	3.8
1	H	170	GLY	3.7
1	K	137	LYS	3.6
1	F	121	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	121	CYS	3.5
1	A	551	VAL	3.5
1	H	117	ILE	3.5
1	E	273	ASN	3.5
1	H	180	ASP	3.4
1	I	439	TYR	3.3
1	B	167	VAL	3.3
1	G	551	VAL	3.3
1	H	181	ASN	3.2
1	G	160	GLU	3.2
1	A	136	GLY	3.2
1	H	130	PHE	3.1
1	I	120	GLY	3.1
1	A	363	GLY	3.1
1	B	192	CYS	3.1
1	H	271	ILE	3.1
1	B	124	GLU	3.0
1	B	185	VAL	2.9
1	A	602	ASN	2.8
1	H	191	GLY	2.8
1	E	550	SER	2.8
1	I	273	ASN	2.8
1	H	277	TYR	2.8
1	H	196	ALA	2.8
1	B	197	ASP	2.8
1	H	138	GLU	2.7
1	F	141	PRO	2.7
1	G	195	VAL	2.7
1	B	125	GLU	2.7
1	A	362	LYS	2.6
1	B	195	VAL	2.6
1	G	602	ASN	2.6
1	G	136	GLY	2.6
1	H	335	GLU	2.6
1	D	439	TYR	2.6
1	H	274	ALA	2.6
1	F	157	LEU	2.6
1	B	262	GLU	2.5
1	D	145	SER	2.5
1	H	119	GLY	2.5
1	I	136	GLY	2.5
1	F	551	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	167	VAL	2.5
1	G	137	LYS	2.5
1	F	129	ILE	2.5
1	F	196	ALA	2.4
1	G	196	ALA	2.4
1	H	175	PHE	2.4
1	L	151	LYS	2.4
1	B	117	ILE	2.4
1	B	228	ILE	2.4
1	H	272	ASN	2.4
1	H	121	CYS	2.4
1	A	159	ASP	2.3
1	H	550	SER	2.3
1	H	156	PHE	2.3
1	K	551	VAL	2.3
1	B	194	SER	2.3
1	J	85	ALA	2.3
1	H	123	VAL	2.3
1	H	146	SER	2.3
1	C	551	VAL	2.3
1	C	229	ASN	2.3
1	F	231	ASP	2.3
1	F	138	GLU	2.2
1	L	121	CYS	2.2
1	F	148	VAL	2.2
1	F	139	ASN	2.2
1	F	161	ASN	2.2
1	F	118	LYS	2.2
1	H	202	ASP	2.2
1	B	225	VAL	2.2
1	J	185	VAL	2.2
1	H	132	VAL	2.1
1	I	363	GLY	2.1
1	L	195	VAL	2.1
1	H	164	LYS	2.1
1	B	229	ASN	2.1
1	F	144	ILE	2.1
1	F	123	VAL	2.0
1	L	155	GLU	2.0
1	F	154	SER	2.0
1	L	159	ASP	2.0
1	H	192	CYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CO3	I	704	4/4	0.84	0.33	11.09	28,34,37,41	0
6	1PE	A	708	9/16	0.83	0.30	6.89	38,43,54,58	0
6	1PE	B	1006	7/16	0.83	0.32	6.19	44,48,55,58	0
4	CO3	A	704	4/4	0.94	0.21	5.66	19,20,20,20	0
6	1PE	H	705	10/16	0.82	0.28	5.08	47,52,55,56	0
6	1PE	G	707	9/16	0.85	0.25	4.71	31,35,47,48	0
4	CO3	J	704	4/4	0.86	0.28	4.47	33,38,42,43	0
4	CO3	E	704	4/4	0.86	0.25	4.06	30,31,33,38	0
4	CO3	G	704	4/4	0.92	0.24	3.53	35,36,38,40	0
5	SO4	E	706	5/5	0.93	0.29	2.98	71,72,77,78	0
3	TOD	I	703	24/24	0.91	0.22	2.93	23,35,43,55	0
3	TOD	A	703	24/24	0.93	0.20	2.41	25,49,58,61	0
6	1PE	D	705	10/16	0.83	0.24	2.27	34,46,52,52	0
5	SO4	D	704	5/5	0.96	0.27	2.24	44,50,51,62	0
4	CO3	L	704	4/4	0.95	0.20	1.96	27,35,37,37	0
5	SO4	G	706	5/5	0.90	0.23	1.79	52,57,66,70	0
5	SO4	A	706	5/5	0.97	0.18	1.75	37,44,49,62	0
3	TOD	J	703	22/24	0.93	0.20	1.49	27,35,42,51	0
3	TOD	B	1004	24/24	0.90	0.22	1.43	27,37,52,63	0
3	TOD	E	703	15/24	0.94	0.18	1.38	26,41,51,51	0
5	SO4	C	705	5/5	0.89	0.20	1.31	79,80,81,82	0
4	CO3	H	704	4/4	0.97	0.18	1.24	20,20,20,27	0
3	TOD	F	703	24/24	0.94	0.19	1.14	33,46,59,64	0
6	1PE	E	707	12/16	0.90	0.22	1.12	30,40,51,53	0
3	TOD	K	703	22/24	0.95	0.20	1.03	32,44,54,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TOD	C	703	17/24	0.92	0.18	1.00	20,29,39,46	0
4	CO3	F	704	4/4	0.96	0.18	0.88	15,16,24,29	0
3	TOD	H	703	14/24	0.95	0.16	0.62	20,33,39,43	0
4	CO3	B	1001	4/4	0.95	0.18	0.59	18,19,20,29	0
3	TOD	L	703	24/24	0.93	0.17	0.50	19,38,46,48	0
3	TOD	G	703	22/24	0.95	0.16	-0.01	21,28,36,40	0
4	CO3	K	704	4/4	0.95	0.16	-0.06	17,22,23,30	0
2	ZN	J	702	1/1	0.99	0.14	-0.16	51,51,51,51	0
4	CO3	C	704	4/4	0.97	0.14	-0.27	25,27,27,30	0
6	1PE	C	707	9/16	0.90	0.16	-0.28	29,34,42,51	0
4	CO3	D	703	4/4	0.98	0.13	-0.64	15,19,20,23	0
2	ZN	K	702	1/1	0.98	0.09	-1.73	32,32,32,32	0
2	ZN	D	701	1/1	0.98	0.10	-1.78	26,26,26,26	0
5	SO4	L	705	5/5	0.98	0.10	-2.00	21,26,32,36	0
2	ZN	K	701	1/1	1.00	0.06	-2.56	19,19,19,19	0
2	ZN	B	1003	1/1	0.99	0.07	-2.68	29,29,29,29	0
5	SO4	E	705	5/5	0.98	0.09	-2.70	12,22,26,33	0
2	ZN	F	702	1/1	0.99	0.06	-2.72	32,32,32,32	0
5	SO4	B	1005	5/5	0.99	0.11	-2.72	21,21,21,25	0
2	ZN	D	702	1/1	0.99	0.06	-2.84	23,23,23,23	0
2	ZN	F	701	1/1	0.99	0.04	-2.92	14,14,14,14	0
2	ZN	C	701	1/1	1.00	0.06	-2.94	23,23,23,23	0
2	ZN	J	701	1/1	0.98	0.07	-2.99	30,30,30,30	0
5	SO4	I	705	5/5	0.99	0.11	-3.52	23,23,23,28	0
2	ZN	E	701	1/1	0.98	0.06	-3.67	30,30,30,30	0
2	ZN	C	702	1/1	1.00	0.04	-4.02	27,27,27,27	0
2	ZN	B	1002	1/1	0.97	0.04	-4.24	19,19,19,19	0
2	ZN	G	701	1/1	0.99	0.04	-4.35	23,23,23,23	0
2	ZN	L	701	1/1	0.98	0.04	-4.50	21,21,21,21	0
2	ZN	H	702	1/1	0.99	0.05	-4.82	21,21,21,21	0
2	ZN	H	701	1/1	0.99	0.03	-5.35	27,27,27,27	0
2	ZN	I	702	1/1	0.97	0.05	-5.84	27,27,27,27	0
2	ZN	I	701	1/1	0.99	0.05	-5.94	19,19,19,19	0
2	ZN	L	702	1/1	0.98	0.06	-6.31	24,24,24,24	0
2	ZN	E	702	1/1	0.98	0.04	-6.39	30,30,30,30	0
2	ZN	A	702	1/1	0.98	0.07	-6.86	27,27,27,27	0
2	ZN	A	701	1/1	0.99	0.06	-8.19	19,19,19,19	0
2	ZN	G	702	1/1	0.99	0.08	-8.42	23,23,23,23	0
6	1PE	C	706	13/16	0.81	0.26	-	35,48,54,58	0
6	1PE	G	708	9/16	0.83	0.24	-	39,48,57,57	0
5	SO4	L	706	5/5	0.94	0.18	-	53,60,63,65	0
5	SO4	A	705	5/5	0.88	0.19	-	57,59,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	707	5/5	0.94	0.29	-	65,66,72,77	0
5	SO4	G	705	5/5	0.93	0.16	-	61,63,66,68	0
6	1PE	D	706	10/16	0.88	0.22	-	40,49,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.