



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:33 am GMT

PDB ID : 3KR5
Title : Structure of a protease 4
Authors : McGowan, S.; Whisstock, J.C.
Deposited on : 2009-11-17
Resolution : 2.56 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

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

with specific help available everywhere you see the ⓘ symbol.

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 : trunk28620
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) : recalc28949

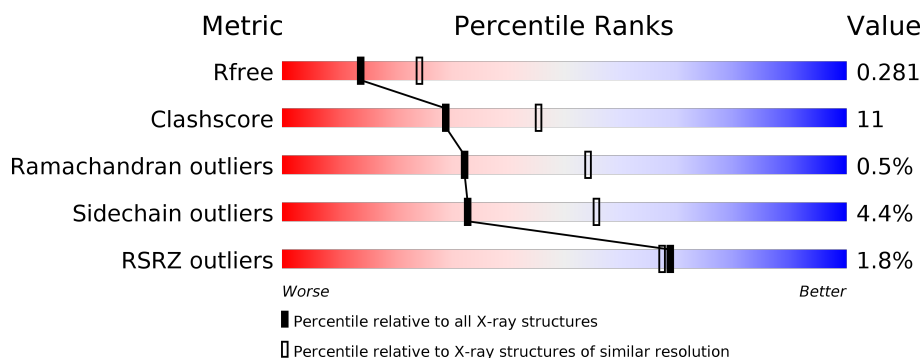
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

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 ≥ 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	528	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>••</div> </div> </div>
1	B	528	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>••</div> </div> </div>
1	C	528	<div> <div></div> <div> <div></div> <div>76%</div> <div>21%</div> <div>••</div> </div> </div>
1	D	528	<div> <div>0%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>••</div> </div> </div>
1	E	528	<div> <div>0%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>••</div> </div> </div>
1	F	528	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	528	
1	H	528	
1	I	528	
1	J	528	
1	K	528	
1	L	528	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	D	1002	-	-	X	-
2	CO3	J	1002	-	-	-	X
2	CO3	K	1002	-	-	X	-
5	SO4	E	7	-	-	X	-
5	SO4	G	26	-	-	-	X
6	1PE	A	20	-	-	-	X
6	1PE	B	60	-	-	-	X
6	1PE	D	44	-	-	-	X
6	1PE	D	67	-	-	-	X
6	1PE	F	31	-	-	-	X
6	1PE	F	33	-	-	-	X
6	1PE	G	58	-	-	-	X
6	1PE	H	64	-	-	-	X
6	1PE	K	50	-	-	-	X
6	1PE	L	612	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50444 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	518	Total	C	N	O	S	0	0	0
			3980	2556	639	765	20			
1	B	518	Total	C	N	O	S	0	0	0
			3929	2527	635	747	20			
1	C	518	Total	C	N	O	S	0	0	0
			3953	2544	637	752	20			
1	D	513	Total	C	N	O	S	0	0	0
			3928	2531	633	744	20			
1	E	510	Total	C	N	O	S	0	0	0
			3897	2509	626	743	19			
1	F	510	Total	C	N	O	S	0	0	0
			3873	2492	624	738	19			
1	G	516	Total	C	N	O	S	0	0	0
			3989	2560	650	760	19			
1	H	509	Total	C	N	O	S	0	0	0
			3938	2531	640	748	19			
1	I	518	Total	C	N	O	S	0	0	0
			4006	2569	651	766	20			
1	J	513	Total	C	N	O	S	0	0	0
			3954	2539	639	756	20			
1	K	509	Total	C	N	O	S	0	0	0
			3930	2525	637	749	19			
1	L	513	Total	C	N	O	S	0	0	0
			3932	2526	634	753	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	ENGINEERED	UNP Q8IL11
A	515	GLN	ASN	ENGINEERED	UNP Q8IL11
A	546	GLN	ASN	ENGINEERED	UNP Q8IL11
A	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	607	HIS	-	EXPRESSION TAG	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	152	GLN	ASN	ENGINEERED	UNP Q8IL11
B	515	GLN	ASN	ENGINEERED	UNP Q8IL11
B	546	GLN	ASN	ENGINEERED	UNP Q8IL11
B	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	152	GLN	ASN	ENGINEERED	UNP Q8IL11
C	515	GLN	ASN	ENGINEERED	UNP Q8IL11
C	546	GLN	ASN	ENGINEERED	UNP Q8IL11
C	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	152	GLN	ASN	ENGINEERED	UNP Q8IL11
D	515	GLN	ASN	ENGINEERED	UNP Q8IL11
D	546	GLN	ASN	ENGINEERED	UNP Q8IL11
D	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	152	GLN	ASN	ENGINEERED	UNP Q8IL11
E	515	GLN	ASN	ENGINEERED	UNP Q8IL11
E	546	GLN	ASN	ENGINEERED	UNP Q8IL11
E	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	152	GLN	ASN	ENGINEERED	UNP Q8IL11
F	515	GLN	ASN	ENGINEERED	UNP Q8IL11

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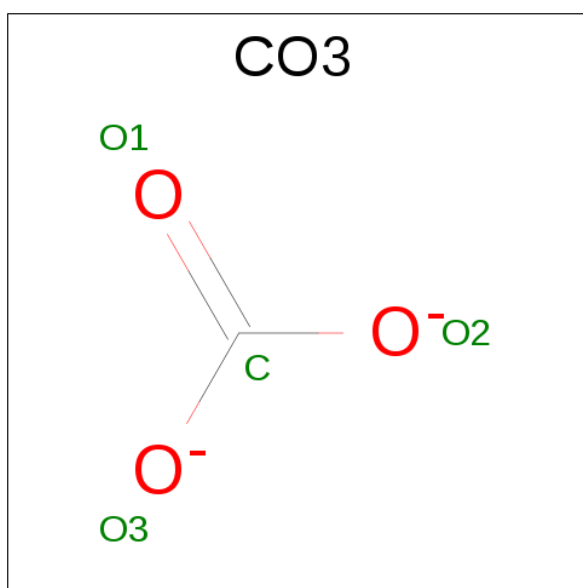
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	ENGINEERED	UNP Q8IL11
F	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	152	GLN	ASN	ENGINEERED	UNP Q8IL11
G	515	GLN	ASN	ENGINEERED	UNP Q8IL11
G	546	GLN	ASN	ENGINEERED	UNP Q8IL11
G	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	152	GLN	ASN	ENGINEERED	UNP Q8IL11
H	515	GLN	ASN	ENGINEERED	UNP Q8IL11
H	546	GLN	ASN	ENGINEERED	UNP Q8IL11
H	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	152	GLN	ASN	ENGINEERED	UNP Q8IL11
I	515	GLN	ASN	ENGINEERED	UNP Q8IL11
I	546	GLN	ASN	ENGINEERED	UNP Q8IL11
I	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	152	GLN	ASN	ENGINEERED	UNP Q8IL11
J	515	GLN	ASN	ENGINEERED	UNP Q8IL11
J	546	GLN	ASN	ENGINEERED	UNP Q8IL11
J	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	610	HIS	-	EXPRESSION TAG	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	152	GLN	ASN	ENGINEERED	UNP Q8IL11
K	515	GLN	ASN	ENGINEERED	UNP Q8IL11
K	546	GLN	ASN	ENGINEERED	UNP Q8IL11
K	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	152	GLN	ASN	ENGINEERED	UNP Q8IL11
L	515	GLN	ASN	ENGINEERED	UNP Q8IL11
L	546	GLN	ASN	ENGINEERED	UNP Q8IL11
L	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	611	HIS	-	EXPRESSION TAG	UNP Q8IL11

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



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

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

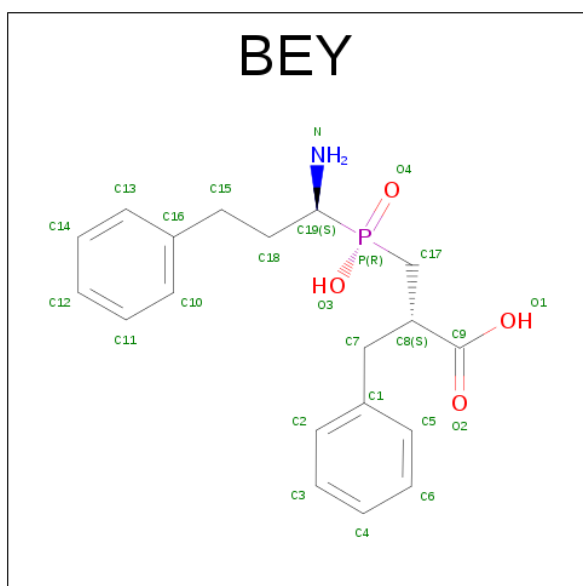
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	L	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (2S)-3-[(R)-[(1S)-1-AMINO-3-PHENYLPROPYL](HYDROXY)PHOSPHORYL]-2-BENZYLPROPANOIC ACID (three-letter code: BEY) (formula: C₁₉H₂₄NO₄P).



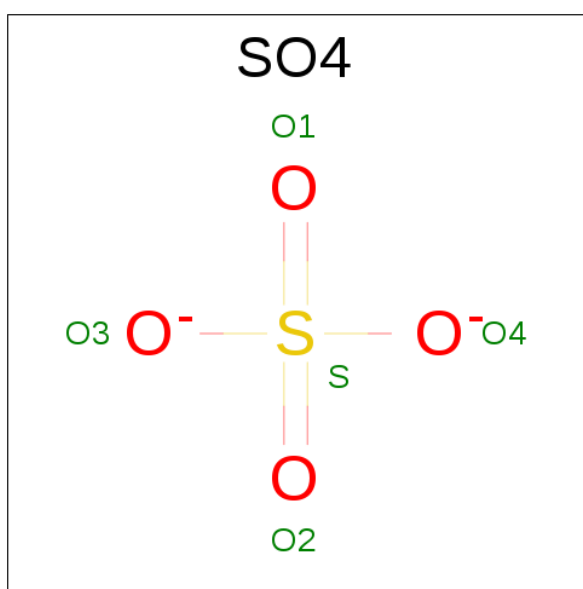
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			25	19	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	I	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	J	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			25	19	1	4	1		
4	L	1	Total	C	N	O	P	0	0
			25	19	1	4	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



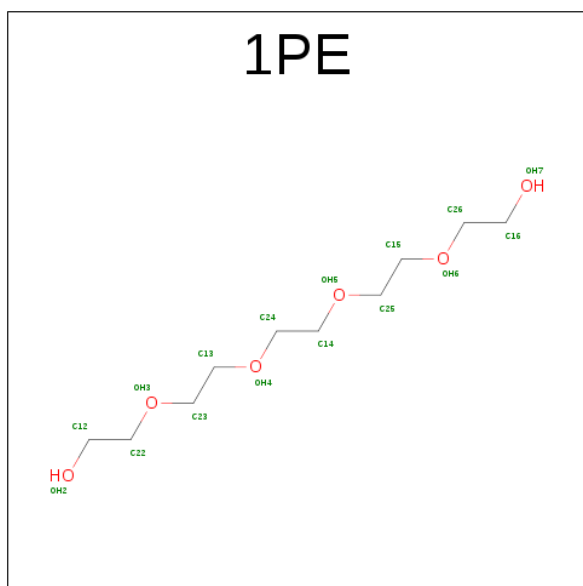
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 6 3	0	0
6	A	1	Total C O 12 8 4	0	0
6	B	1	Total C O 10 7 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		
6	C	1	Total	C	O	0	0
			13	9	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			11	8	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			7	5	2		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			8	5	3		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			7	4	3		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			15	10	5		
6	H	1	Total	C	O	0	0
			10	7	3		
6	H	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			15	10	5		
6	I	1	Total	C	O	0	0
			11	8	3		
6	I	1	Total	C	O	0	0
			7	5	2		
6	J	1	Total	C	O	0	0
			11	7	4		
6	J	1	Total	C	O	0	0
			10	6	4		
6	J	1	Total	C	O	0	0
			10	7	3		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			11	7	4		
6	K	1	Total	C	O	0	0
			6	4	2		
6	L	1	Total	C	O	0	0
			10	6	4		
6	L	1	Total	C	O	0	0
			12	8	4		
6	L	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	217	Total	O	0	0
			217	217		
7	B	158	Total	O	0	0
			158	158		
7	C	188	Total	O	0	0
			188	188		
7	D	182	Total	O	0	0
			182	182		
7	E	203	Total	O	0	0
			203	203		
7	F	165	Total	O	0	0
			165	165		

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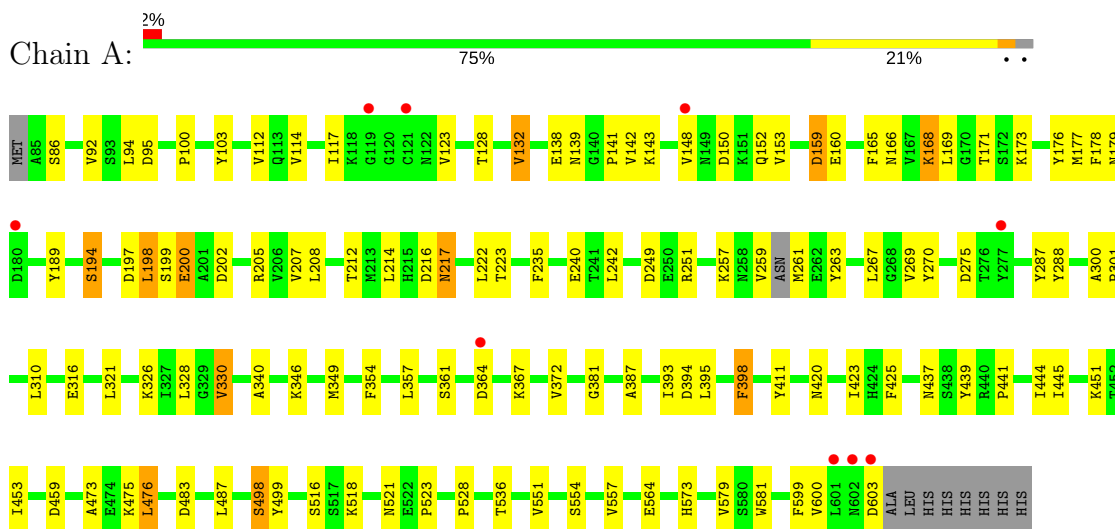
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	204	Total 204	O 204	0	0
7	H	203	Total 203	O 203	0	0
7	I	207	Total 207	O 207	0	0
7	J	207	Total 207	O 207	0	0
7	K	222	Total 222	O 222	0	0
7	L	158	Total 158	O 158	0	0

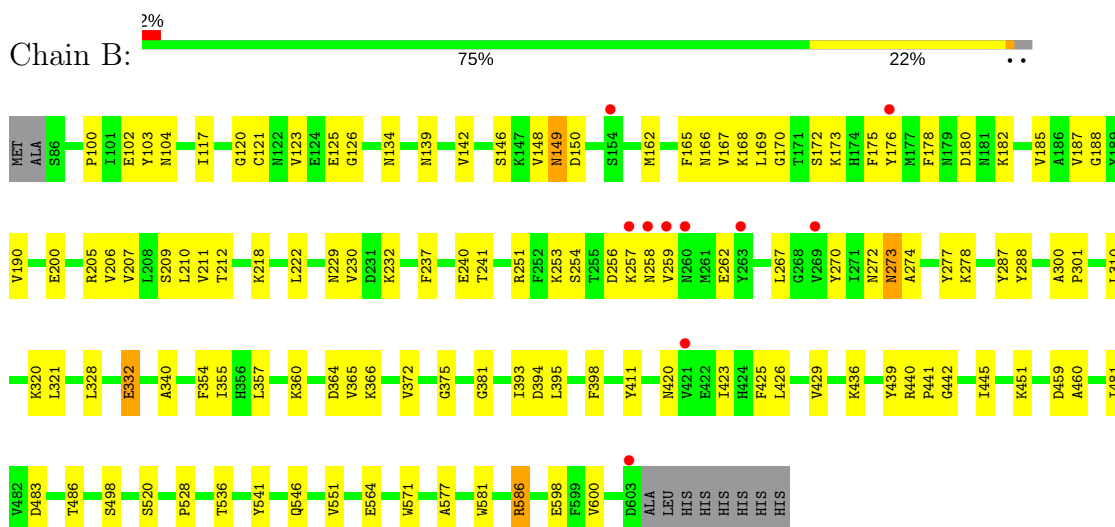
3 Residue-property plots

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

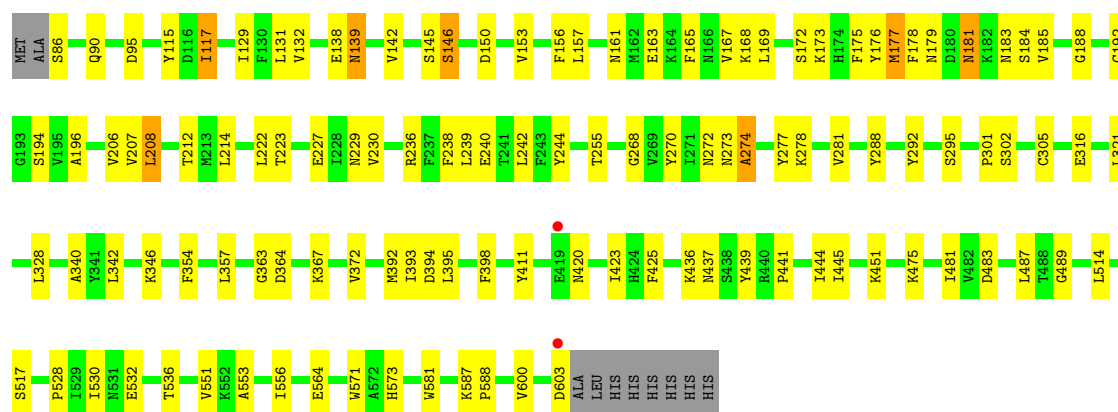


• Molecule 1: M17 leucyl aminopeptidase

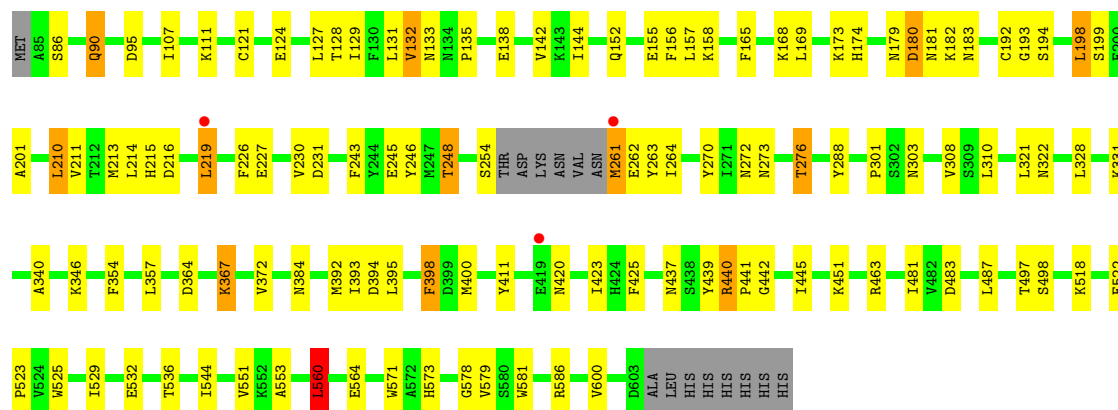
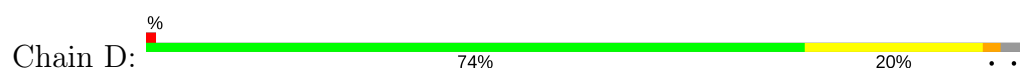


• Molecule 1: M17 leucyl aminopeptidase

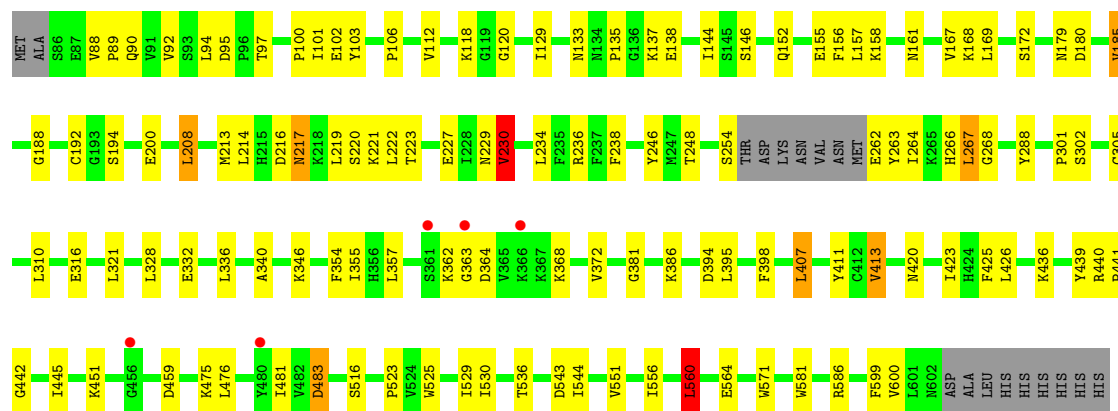
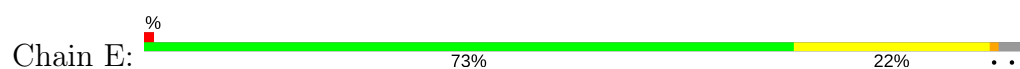




• Molecule 1: M17 leucyl aminopeptidase

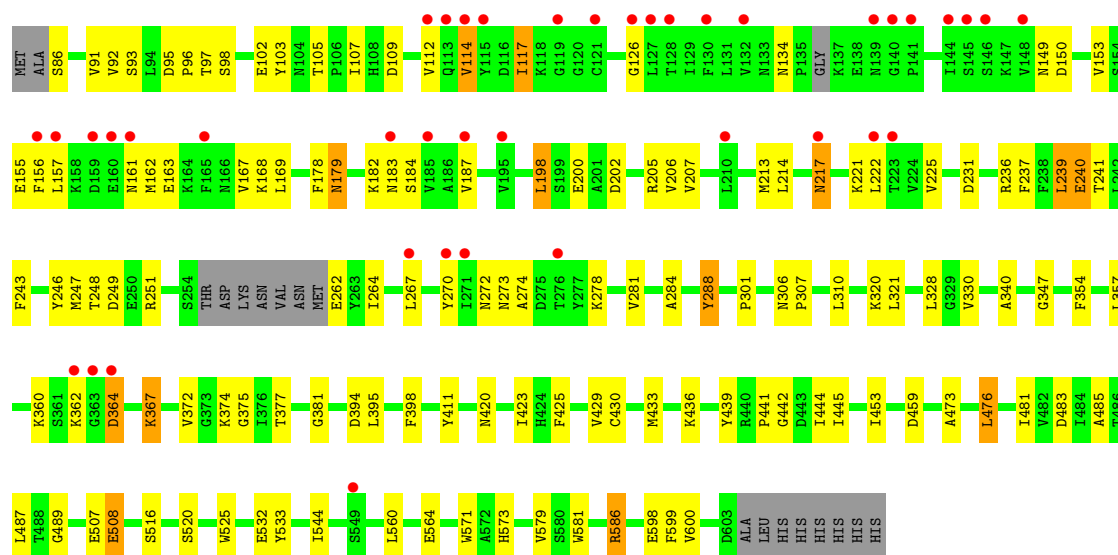


• Molecule 1: M17 leucyl aminopeptidase

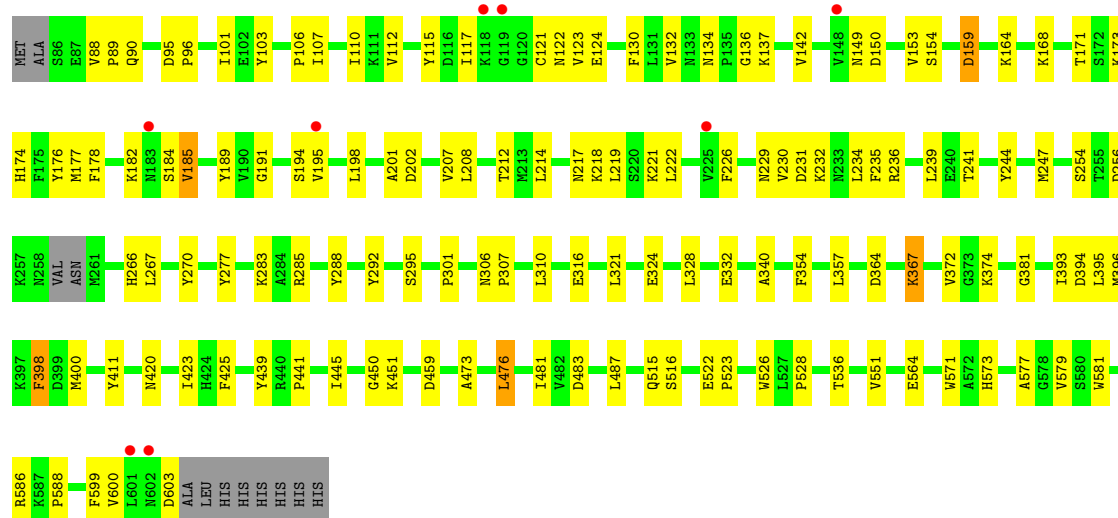


• Molecule 1: M17 leucyl aminopeptidase



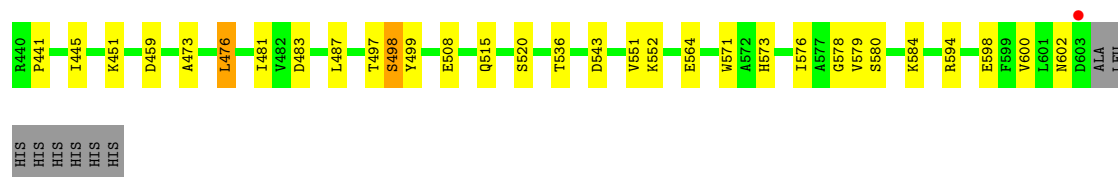


• Molecule 1: M17 leucyl aminopeptidase

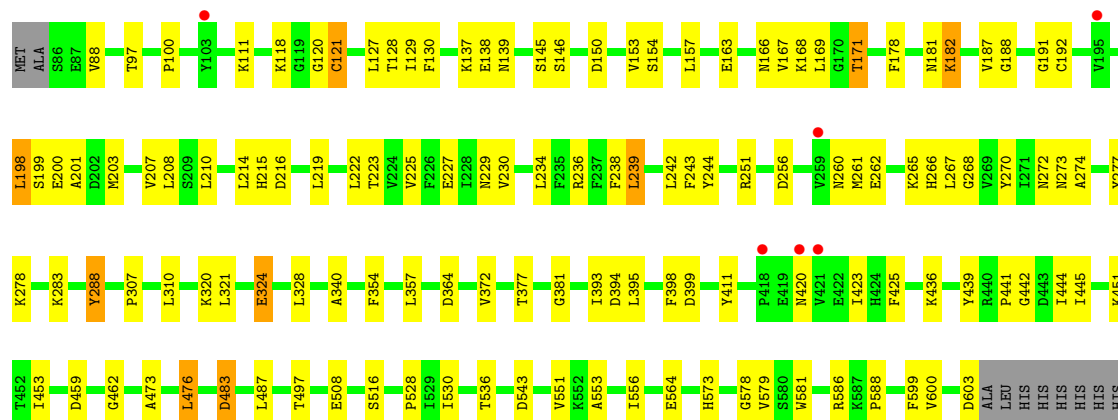


• Molecule 1: M17 leucyl aminopeptidase

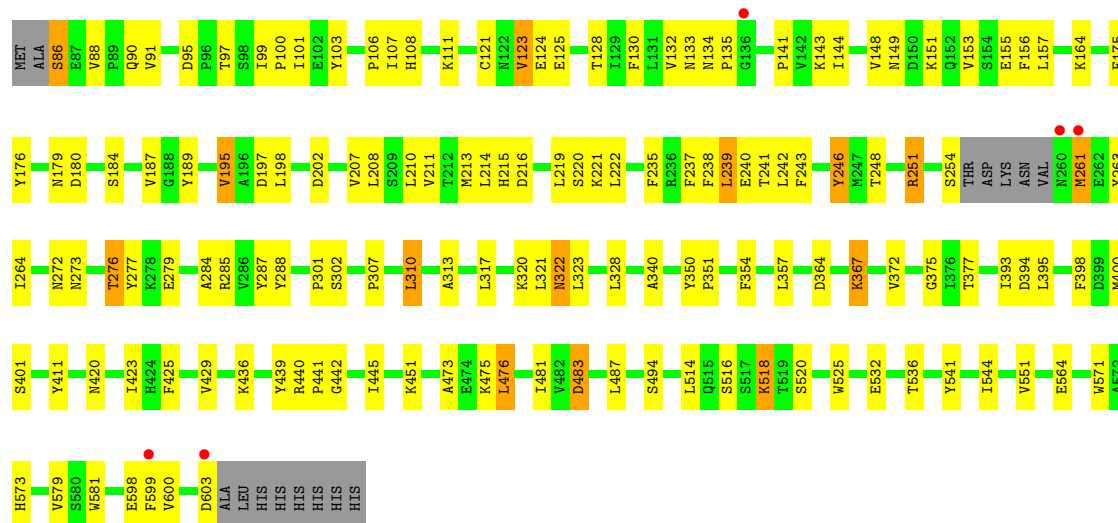




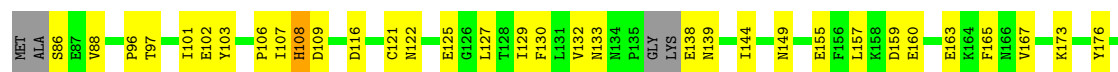
• Molecule 1: M17 leucyl aminopeptidase

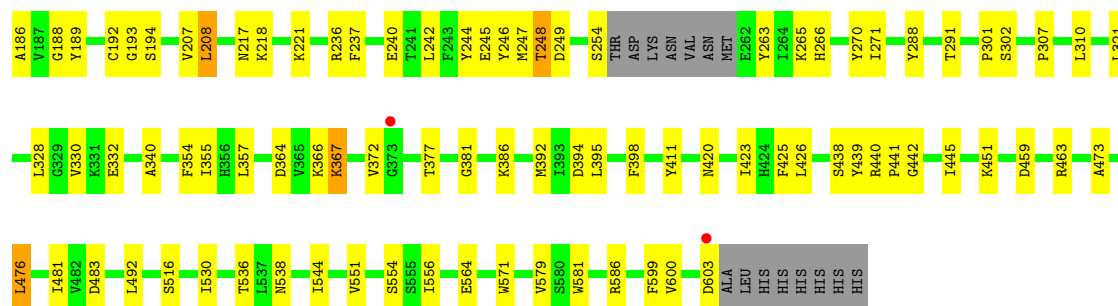


• Molecule 1: M17 leucyl aminopeptidase

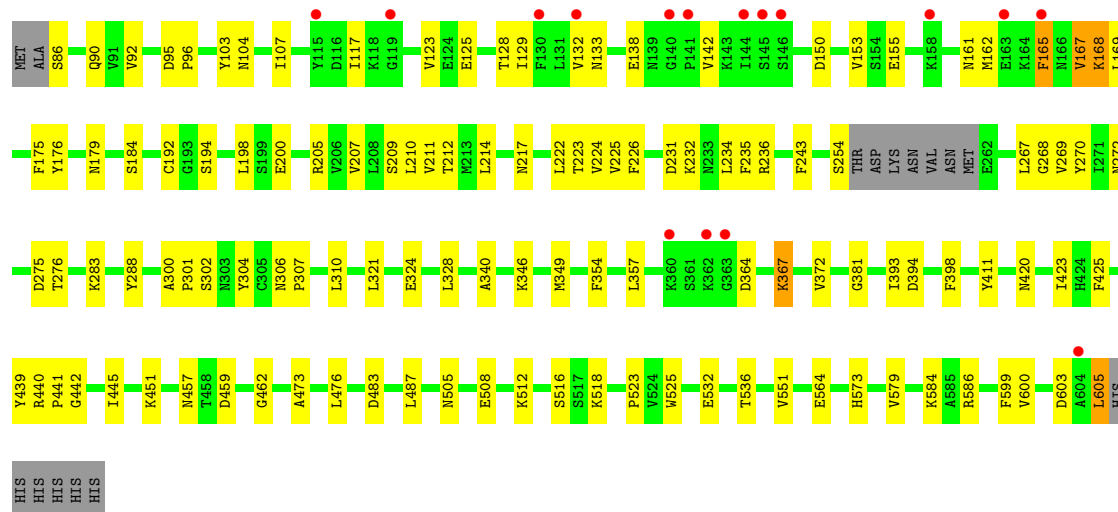
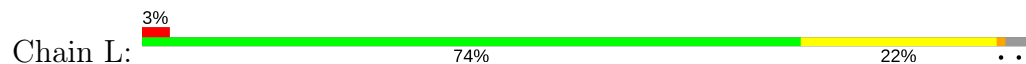


• Molecule 1: M17 leucyl aminopeptidase





• 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, α , β , γ	172.08Å 174.16Å 227.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.70 – 2.56 77.70 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.8 (77.70-2.56) 98.8 (77.70-2.56)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.220 , 0.278 0.224 , 0.281	Depositor DCC
R_{free} test set	10903 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	50444	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 47.88 % 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 9.3151e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CO3, BEY, ZN, 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	0.67	0/4057	0.71	1/5500 (0.0%)
1	B	0.63	0/4007	0.69	2/5442 (0.0%)
1	C	0.67	1/4031 (0.0%)	0.71	0/5469
1	D	0.69	0/4005	0.74	6/5429 (0.1%)
1	E	0.71	1/3974 (0.0%)	0.76	6/5393 (0.1%)
1	F	0.64	1/3949 (0.0%)	0.76	3/5364 (0.1%)
1	G	0.69	0/4066	0.71	1/5505 (0.0%)
1	H	0.66	0/4014	0.68	0/5434
1	I	0.68	0/4084	0.79	3/5531 (0.1%)
1	J	0.70	0/4031	0.72	0/5461
1	K	0.72	0/4006	0.75	1/5427 (0.0%)
1	L	0.66	0/4009	0.69	1/5440 (0.0%)
All	All	0.68	3/48233 (0.0%)	0.72	24/65395 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	305	CYS	CB-SG	-5.60	1.72	1.81
1	C	305	CYS	CB-SG	-5.25	1.73	1.81
1	F	430	CYS	CB-SG	-5.20	1.73	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	586	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	I	586	ARG	NE-CZ-NH1	-17.07	111.76	120.30
1	F	586	ARG	NE-CZ-NH2	16.73	128.66	120.30
1	F	586	ARG	NE-CZ-NH1	-16.10	112.25	120.30
1	F	586	ARG	CD-NE-CZ	8.03	134.84	123.60
1	I	586	ARG	CD-NE-CZ	7.90	134.65	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	560	LEU	CB-CG-CD1	6.85	122.64	111.00
1	K	586	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	D	210	LEU	CA-CB-CG	5.94	128.96	115.30
1	E	560	LEU	CA-CB-CG	5.93	128.95	115.30
1	E	407	LEU	CB-CG-CD1	5.88	120.99	111.00
1	D	586	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	E	407	LEU	CB-CG-CD2	5.75	120.78	111.00
1	E	560	LEU	CB-CG-CD1	5.65	120.61	111.00
1	E	586	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	560	LEU	CA-CB-CG	5.54	128.03	115.30
1	E	413	VAL	CG1-CB-CG2	5.49	119.69	110.90
1	G	586	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	330	VAL	CG1-CB-CG2	5.38	119.51	110.90
1	D	463	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	586	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	L	586	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	440	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	586	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3980	0	3912	93	0
1	B	3929	0	3828	87	1
1	C	3953	0	3882	89	0
1	D	3928	0	3876	102	0
1	E	3897	0	3822	92	0
1	F	3873	0	3772	98	0
1	G	3989	0	3976	95	0
1	H	3938	0	3931	84	0
1	I	4006	0	3986	93	0
1	J	3954	0	3923	120	0
1	K	3930	0	3901	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3932	0	3862	86	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	2	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	1	0
2	I	4	0	0	1	0
2	J	4	0	0	1	0
2	K	4	0	0	2	0
2	L	4	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	25	0	21	4	0
4	B	25	0	22	2	0
4	C	25	0	21	5	0
4	D	25	0	22	6	0
4	E	25	0	22	2	0
4	F	25	0	21	2	0
4	G	25	0	21	2	0
4	H	25	0	22	7	0
4	I	25	0	22	2	0
4	J	25	0	22	3	0
4	K	25	0	22	4	0
4	L	25	0	22	2	0
5	A	15	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	0	0
5	E	10	0	0	3	0
5	F	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	10	0	0	0	0
5	I	5	0	0	1	0
5	J	10	0	0	2	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
6	A	21	0	22	2	0
6	B	30	0	30	3	0
6	C	22	0	24	1	0
6	D	38	0	38	5	0
6	E	32	0	36	3	0
6	F	30	0	39	1	0
6	G	43	0	47	4	0
6	H	20	0	20	1	0
6	I	33	0	37	5	0
6	J	31	0	36	9	0
6	K	41	0	44	8	0
6	L	33	0	40	5	0
7	A	217	0	0	12	0
7	B	158	0	0	7	0
7	C	188	0	0	6	0
7	D	182	0	0	5	1
7	E	203	0	0	15	0
7	F	165	0	0	14	0
7	G	204	0	0	11	0
7	H	203	0	0	6	0
7	I	207	0	0	6	0
7	J	207	0	0	18	0
7	K	222	0	0	7	0
7	L	158	0	0	11	0
All	All	50444	0	47344	1043	1

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 11.

All (1043) 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:H:436:LYS:HE2	7:I:3958:HOH:O	1.43	1.15
1:B:257:LYS:HA	1:B:258:ASN:HB3	1.34	1.09
1:J:518:LYS:HE2	7:J:2650:HOH:O	1.52	1.08
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:GLY:HA3	1:G:137:LYS:CB	1.86	1.02
1:J:320:LYS:NZ	6:J:3:1PE:H142	1.74	1.02
1:B:436:LYS:HE2	7:C:3093:HOH:O	1.59	0.99
1:J:254:SER:HB2	7:L:2793:HOH:O	1.61	0.99
1:B:586:ARG:HA	7:B:1076:HOH:O	1.62	0.98
1:A:361:SER:HB3	7:A:755:HOH:O	1.63	0.98
1:E:230:VAL:HG22	1:E:234:LEU:HB3	1.47	0.96
1:A:259:VAL:O	1:A:261:MET:N	2.00	0.94
1:K:133:ASN:HA	1:K:167:VAL:HG11	1.48	0.94
1:C:230:VAL:O	1:C:277:TYR:OH	1.86	0.93
1:A:173:LYS:NZ	1:D:216:ASP:OD2	2.01	0.92
1:I:230:VAL:O	1:I:277:TYR:OH	1.89	0.89
1:B:274:ALA:O	1:B:278:LYS:HG3	1.76	0.86
1:K:96:PRO:HA	6:K:50:1PE:H142	1.58	0.86
1:D:254:SER:HB2	7:F:1110:HOH:O	1.75	0.86
1:J:320:LYS:HZ3	6:J:3:1PE:H142	1.40	0.86
1:B:178:PHE:HZ	1:F:155:GLU:HG2	1.42	0.83
1:J:411:TYR:HE1	6:J:2:1PE:H151	1.44	0.82
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.61	0.82
1:I:121:CYS:SG	1:I:225:VAL:HG21	2.19	0.82
1:F:231:ASP:HB2	7:F:3092:HOH:O	1.79	0.82
1:D:127:LEU:HD11	1:D:129:ILE:HD11	1.60	0.82
1:E:229:ASN:O	1:E:230:VAL:HB	1.79	0.81
1:F:117:ILE:HG13	1:F:270:TYR:HB3	1.60	0.81
1:L:90:GLN:NE2	1:L:95:ASP:O	2.13	0.81
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.45	0.81
1:J:401:SER:HB3	7:J:748:HOH:O	1.81	0.80
1:B:175:PHE:CD2	1:B:188:GLY:HA2	2.17	0.80
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.62	0.79
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.64	0.79
1:G:367:LYS:HG2	1:G:603:ASP:OD1	1.83	0.79
1:F:114:VAL:HG21	1:F:278:LYS:HG2	1.63	0.79
1:C:532:GLU:OE1	1:D:498:SER:OG	1.99	0.79
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.66	0.77
1:A:216:ASP:O	1:D:173:LYS:HE3	1.85	0.77
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.65	0.77
1:K:538:ASN:HB2	7:K:5283:HOH:O	1.83	0.77
1:K:173:LYS:HA	7:K:1921:HOH:O	1.84	0.77
1:L:349:MET:HB2	7:L:2456:HOH:O	1.84	0.77
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.65	0.76
1:B:175:PHE:HD2	1:B:188:GLY:HA2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.68	0.76
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.66	0.75
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.68	0.75
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.66	0.75
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.68	0.75
1:D:90:GLN:HB3	1:D:95:ASP:HB2	1.66	0.74
1:E:230:VAL:HG23	1:E:234:LEU:HD23	1.67	0.74
1:J:164:LYS:HE2	7:J:944:HOH:O	1.86	0.74
1:E:103:TYR:HB2	5:E:22:SO4:O3	1.88	0.74
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.68	0.74
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.69	0.74
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.70	0.74
6:J:45:1PE:H242	7:J:3061:HOH:O	1.88	0.74
1:G:168:LYS:O	1:G:171:THR:HG22	1.87	0.74
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.71	0.73
1:H:192:CYS:HB3	1:H:198:LEU:HD11	1.71	0.72
1:J:207:VAL:HG11	1:J:241:THR:HG22	1.71	0.72
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.23	0.72
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.71	0.72
1:A:178:PHE:HZ	1:D:155:GLU:CG	2.02	0.72
1:C:363:GLY:HA3	7:C:4562:HOH:O	1.90	0.72
1:D:219:LEU:H	1:D:219:LEU:HD13	1.54	0.72
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.71	0.72
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.69	0.72
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.71	0.72
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.72	0.72
1:C:172:SER:O	1:C:173:LYS:HD2	1.90	0.72
1:C:274:ALA:O	1:C:278:LYS:HG3	1.89	0.71
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.72	0.71
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.72	0.71
1:E:475:LYS:HD3	7:E:4546:HOH:O	1.89	0.71
1:I:215:HIS:O	1:I:216:ASP:HB2	1.88	0.71
1:J:237:PHE:HA	1:J:240:GLU:OE1	1.91	0.71
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.72	0.71
1:L:176:TYR:OH	1:L:217:ASN:OD1	2.04	0.71
1:F:117:ILE:HD11	1:F:225:VAL:HG13	1.72	0.71
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.56	0.71
1:B:253:LYS:HD2	1:B:256:ASP:HB3	1.73	0.71
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.73	0.71
1:K:451:LYS:HD3	6:K:42:1PE:H231	1.73	0.71
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:VAL:HG21	1:C:142:VAL:HG13	1.73	0.70
1:J:321:LEU:O	1:J:322:ASN:HB2	1.90	0.70
1:D:179:ASN:OD1	1:D:183:ASN:HB2	1.92	0.70
1:I:128:THR:HB	1:I:187:VAL:HG13	1.73	0.70
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.71	0.70
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.74	0.70
1:H:392:MET:CE	4:H:1003:BEY:H12	2.22	0.70
1:A:173:LYS:CE	1:D:216:ASP:OD2	2.40	0.70
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.72	0.70
1:K:321:LEU:HD11	1:K:411:TYR:HA	1.74	0.70
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.74	0.70
1:K:386:LYS:NZ	4:K:1003:BEY:O3	2.23	0.69
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.73	0.69
1:C:173:LYS:NZ	1:E:217:ASN:OD1	2.25	0.69
1:J:151:LYS:N	1:J:180:ASP:OD2	2.24	0.69
1:L:104:ASN:OD1	6:L:1:1PE:H141	1.92	0.69
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.74	0.69
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.73	0.69
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.75	0.69
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.74	0.69
1:B:257:LYS:HA	1:B:258:ASN:CB	2.18	0.69
1:E:100:PRO:O	1:E:101:ILE:HD13	1.92	0.69
1:H:240:GLU:OE2	1:H:287:TYR:HD2	1.75	0.69
1:J:320:LYS:HZ1	6:J:3:1PE:H142	1.58	0.69
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.76	0.68
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.75	0.68
1:I:244:TYR:OH	1:I:588:PRO:O	2.12	0.68
1:H:232:LYS:HE3	1:H:276:THR:HB	1.74	0.68
1:D:174:HIS:CE1	1:D:213:MET:HG2	2.29	0.68
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.75	0.68
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.76	0.68
1:K:133:ASN:HB2	1:K:193:GLY:O	1.94	0.68
1:K:133:ASN:CA	1:K:167:VAL:HG11	2.23	0.68
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.76	0.68
1:H:392:MET:HE1	4:H:1003:BEY:H12	1.75	0.68
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.75	0.67
6:D:63:1PE:C25	7:D:3204:HOH:O	2.42	0.67
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.58	0.67
1:G:117:ILE:HD11	1:G:226:PHE:O	1.95	0.67
1:J:219:LEU:HD11	7:J:3193:HOH:O	1.94	0.67
1:F:107:ILE:HG21	1:F:243:PHE:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLU:HB3	7:B:675:HOH:O	1.93	0.67
1:A:208:LEU:O	1:A:212:THR:HG23	1.94	0.67
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.75	0.67
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.76	0.67
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.75	0.67
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.76	0.66
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.76	0.66
1:I:169:LEU:HA	1:I:191:GLY:O	1.94	0.66
1:F:156:PHE:O	1:F:162:MET:HE3	1.95	0.66
1:I:274:ALA:O	1:I:278:LYS:HG3	1.95	0.66
1:G:173:LYS:HD2	1:J:176:TYR:HE1	1.61	0.66
1:C:274:ALA:HB1	1:C:278:LYS:HE3	1.78	0.65
1:L:462:GLY:N	2:L:1002:CO3:O2	2.27	0.65
1:J:215:HIS:O	1:J:261:MET:HB3	1.96	0.65
1:B:230:VAL:O	1:B:277:TYR:OH	2.09	0.65
1:L:107:ILE:HG21	1:L:243:PHE:HB3	1.78	0.65
1:B:102:GLU:CG	7:B:4121:HOH:O	2.45	0.65
1:C:173:LYS:HE3	1:E:217:ASN:OD1	1.97	0.65
1:B:139:ASN:O	1:B:166:ASN:HB2	1.97	0.65
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.77	0.65
1:B:218:LYS:HG2	1:B:262:GLU:CD	2.18	0.64
2:D:1002:CO3:O2	4:D:1003:BEY:H7A	1.97	0.64
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.78	0.64
1:C:153:VAL:HG12	1:C:157:LEU:CD1	2.27	0.64
1:I:129:ILE:HA	1:I:188:GLY:O	1.97	0.64
1:B:232:LYS:HB2	7:B:4536:HOH:O	1.96	0.64
1:I:230:VAL:HG22	1:I:234:LEU:HB3	1.79	0.64
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.80	0.64
1:H:274:ALA:O	1:H:278:LYS:HG3	1.97	0.64
1:H:240:GLU:OE2	1:H:287:TYR:CD2	2.51	0.64
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.80	0.63
1:D:451:LYS:HE2	6:D:44:1PE:H151	1.79	0.63
1:G:136:GLY:CA	1:G:137:LYS:CB	2.72	0.63
1:H:150:ASP:OD2	1:H:153:VAL:HG23	1.98	0.63
1:D:423:ILE:HD11	1:D:600:VAL:HG13	1.80	0.63
1:J:123:VAL:O	1:J:123:VAL:HG23	1.96	0.63
1:K:176:TYR:OH	1:K:217:ASN:OD1	2.14	0.63
1:J:321:LEU:O	1:J:322:ASN:CB	2.43	0.63
1:D:331:LYS:CD	1:D:331:LYS:H	2.09	0.63
1:J:88:VAL:HG11	1:J:97:THR:O	1.98	0.63
1:A:372:VAL:O	1:A:483:ASP:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:LYS:HE3	7:I:4080:HOH:O	1.98	0.63
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.81	0.63
1:D:192:CYS:HB3	1:D:198:LEU:HD21	1.79	0.63
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.64	0.63
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.33	0.63
1:L:231:ASP:HB3	1:L:234:LEU:H	1.64	0.62
1:A:498:SER:OG	1:F:532:GLU:OE1	2.17	0.62
1:D:124:GLU:HA	1:D:179:ASN:ND2	2.14	0.62
1:D:273:ASN:O	1:D:276:THR:HG23	2.00	0.62
1:I:238:PHE:HD2	1:I:239:LEU:HD13	1.63	0.62
1:K:236:ARG:NE	1:K:240:GLU:OE2	2.27	0.62
1:C:146:SER:OG	1:C:227:GLU:OE2	2.16	0.62
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.81	0.62
1:H:167:VAL:O	1:H:168:LYS:C	2.36	0.62
1:A:523:PRO:HA	7:A:1372:HOH:O	1.98	0.62
1:J:198:LEU:HD22	1:J:202:ASP:HB3	1.82	0.62
1:L:367:LYS:HG2	1:L:603:ASP:OD2	1.99	0.62
1:L:451:LYS:HE2	6:L:612:1PE:H241	1.82	0.62
1:A:499:TYR:CZ	1:A:523:PRO:HB3	2.35	0.62
1:L:138:GLU:HA	1:L:194:SER:OG	1.99	0.62
1:B:148:VAL:O	1:B:150:ASP:N	2.28	0.62
1:A:499:TYR:CD2	1:A:523:PRO:HB2	2.34	0.62
1:C:153:VAL:HG12	1:C:157:LEU:HD11	1.80	0.62
1:L:523:PRO:HD3	7:L:644:HOH:O	1.99	0.62
1:H:192:CYS:O	1:H:198:LEU:HD21	1.99	0.61
1:K:554:SER:HB3	7:K:3921:HOH:O	1.99	0.61
1:A:518:LYS:HB2	7:A:3052:HOH:O	2.00	0.61
1:C:173:LYS:CE	1:E:217:ASN:OD1	2.49	0.61
1:F:213:MET:O	1:F:217:ASN:HB2	1.99	0.61
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.35	0.61
1:D:124:GLU:HA	1:D:179:ASN:HD22	1.66	0.61
1:J:423:ILE:HD11	1:J:600:VAL:HG13	1.81	0.61
1:K:451:LYS:HE3	1:K:564:GLU:O	2.00	0.61
1:J:123:VAL:HG21	1:J:153:VAL:HG21	1.83	0.61
1:G:372:VAL:O	1:G:483:ASP:HA	2.01	0.61
1:B:320:LYS:NZ	6:B:61:1PE:H241	2.15	0.61
1:C:223:THR:HA	1:C:268:GLY:O	2.01	0.60
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.82	0.60
1:E:436:LYS:HG2	5:E:7:SO4:O4	2.00	0.60
1:G:132:VAL:HG21	1:G:142:VAL:HG13	1.83	0.60
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:ILE:CG2	1:D:560:LEU:HD13	2.31	0.60
1:G:201:ALA:HB1	1:L:532:GLU:OE1	2.01	0.60
1:H:106:PRO:HD2	1:H:247:MET:SD	2.42	0.60
1:I:230:VAL:HG23	1:I:234:LEU:HD23	1.83	0.60
1:H:174:HIS:HB3	1:L:175:PHE:CE1	2.36	0.60
1:D:301:PRO:HB3	1:F:442:GLY:O	2.01	0.60
1:B:176:TYR:OH	1:F:155:GLU:HG3	2.02	0.60
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.83	0.60
2:K:1002:CO3:O2	4:K:1003:BEY:H17A	2.02	0.60
1:A:387:ALA:HB1	7:A:5072:HOH:O	2.01	0.60
1:F:237:PHE:HA	1:F:240:GLU:OE1	2.01	0.60
1:L:209:SER:O	1:L:212:THR:HB	2.01	0.60
1:D:155:GLU:O	1:D:158:LYS:HG2	2.02	0.60
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.82	0.60
1:E:451:LYS:HE3	1:E:564:GLU:O	2.02	0.59
1:L:451:LYS:HG3	6:L:612:1PE:H131	1.85	0.59
1:A:398:PHE:HZ	4:A:1003:BEY:H13	1.67	0.59
1:G:473:ALA:O	1:G:476:LEU:HB2	2.03	0.59
1:J:123:VAL:CG2	1:J:153:VAL:HG21	2.32	0.59
1:D:219:LEU:HD23	1:D:264:ILE:HG22	1.83	0.59
1:E:152:GLN:HG2	1:E:180:ASP:OD1	2.03	0.59
1:K:122:ASN:OD1	1:K:149:ASN:HB2	2.02	0.59
1:L:605:LEU:HD21	7:L:5436:HOH:O	2.01	0.59
1:C:138:GLU:O	1:C:139:ASN:HB2	2.03	0.59
1:B:451:LYS:HE3	1:B:564:GLU:O	2.03	0.58
1:L:169:LEU:HD23	1:L:205:ARG:HH21	1.69	0.58
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.85	0.58
1:E:230:VAL:CG2	1:E:234:LEU:HB3	2.27	0.58
1:H:117:ILE:HG23	1:H:118:LYS:N	2.18	0.58
1:J:240:GLU:OE2	1:J:287:TYR:HD2	1.86	0.58
1:D:423:ILE:HD11	1:D:600:VAL:CG1	2.34	0.58
1:F:372:VAL:O	1:F:483:ASP:HA	2.03	0.58
1:H:170:GLY:O	1:H:209:SER:OG	2.21	0.58
1:E:372:VAL:O	1:E:483:ASP:HA	2.03	0.58
1:G:208:LEU:O	1:G:212:THR:HG23	2.03	0.58
1:L:423:ILE:HD11	1:L:600:VAL:HG13	1.85	0.58
1:A:441:PRO:HG2	1:B:393:ILE:HG12	1.84	0.58
1:B:486:THR:O	4:B:1003:BEY:N	2.37	0.58
1:D:107:ILE:HG21	1:D:243:PHE:HB3	1.85	0.58
1:E:386:LYS:NZ	4:E:1003:BEY:O3	2.34	0.57
1:I:138:GLU:O	1:I:139:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:473:ALA:O	1:K:476:LEU:HB2	2.04	0.57
1:A:554:SER:HB3	7:A:2697:HOH:O	2.04	0.57
1:A:117:ILE:HG13	1:A:270:TYR:HB3	1.85	0.57
1:F:179:ASN:OD1	1:F:183:ASN:HB2	2.04	0.57
1:K:125:GLU:HG3	1:K:221:LYS:HD2	1.85	0.57
1:B:123:VAL:HG12	1:B:185:VAL:HG21	1.86	0.57
1:B:207:VAL:HG11	1:B:241:THR:HG22	1.85	0.57
1:B:218:LYS:HG2	1:B:262:GLU:OE2	2.04	0.57
1:F:249:ASP:OD2	1:F:251:ARG:NH2	2.29	0.57
1:F:489:GLY:N	4:F:1003:BEY:O1	2.33	0.57
1:G:324:GLU:HG3	7:G:3727:HOH:O	2.05	0.57
1:J:440:ARG:NH2	7:J:635:HOH:O	2.37	0.57
1:A:321:LEU:CD1	1:A:411:TYR:HA	2.35	0.57
1:C:475:LYS:HD3	7:C:3447:HOH:O	2.04	0.57
1:D:138:GLU:HA	1:D:194:SER:OG	2.05	0.57
1:G:136:GLY:N	7:G:3954:HOH:O	2.38	0.57
1:I:320:LYS:NZ	6:I:21:1PE:OH7	2.37	0.57
1:J:411:TYR:CE1	6:J:2:1PE:H151	2.33	0.57
1:A:487:LEU:O	4:A:1003:BEY:H17A	2.05	0.57
1:J:301:PRO:HB3	1:L:442:GLY:O	2.04	0.57
1:D:215:HIS:C	1:D:261:MET:HB3	2.26	0.56
1:C:244:TYR:OH	1:C:588:PRO:O	2.23	0.56
1:D:215:HIS:O	1:D:261:MET:HB3	2.05	0.56
1:E:213:MET:HG3	7:E:1714:HOH:O	2.04	0.56
1:L:473:ALA:O	1:L:476:LEU:HB2	2.05	0.56
1:A:381:GLY:HA2	1:A:459:ASP:OD1	2.05	0.56
1:D:248:THR:HG23	1:D:263:TYR:OH	2.06	0.56
1:F:347:GLY:N	7:F:618:HOH:O	2.38	0.56
1:L:381:GLY:HA2	1:L:459:ASP:OD1	2.05	0.56
1:A:103:TYR:CD1	6:A:20:1PE:H251	2.41	0.56
1:F:179:ASN:CG	1:F:183:ASN:HB2	2.26	0.56
1:F:381:GLY:HA2	1:F:459:ASP:OD1	2.05	0.56
1:E:332:GLU:HG3	7:E:4802:HOH:O	2.04	0.56
1:F:423:ILE:HD11	1:F:600:VAL:HG13	1.87	0.56
1:J:254:SER:CB	7:L:2793:HOH:O	2.35	0.56
1:K:133:ASN:HA	1:K:167:VAL:CG1	2.29	0.56
1:J:322:ASN:HA	7:J:3618:HOH:O	2.06	0.56
1:B:240:GLU:OE2	1:B:287:TYR:HD2	1.88	0.56
1:E:423:ILE:HD11	1:E:600:VAL:HG13	1.88	0.56
1:D:372:VAL:O	1:D:483:ASP:HA	2.05	0.56
1:I:436:LYS:HG2	5:I:17:SO4:O3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:LEU:O	1:L:267:LEU:HA	2.06	0.56
1:F:320:LYS:HD3	6:F:31:1PE:H141	1.88	0.56
1:J:211:VAL:HG12	7:J:5351:HOH:O	2.04	0.56
1:L:372:VAL:O	1:L:483:ASP:HA	2.06	0.56
1:J:123:VAL:CG2	1:J:123:VAL:O	2.53	0.55
1:D:451:LYS:HE3	1:D:564:GLU:O	2.06	0.55
1:G:451:LYS:HE3	1:G:564:GLU:O	2.05	0.55
1:K:463:ARG:NE	2:K:1002:CO3:O1	2.27	0.55
1:K:372:VAL:O	1:K:483:ASP:HA	2.06	0.55
1:C:117:ILE:HG22	1:C:272:ASN:HA	1.89	0.55
1:H:145:SER:N	1:H:227:GLU:OE1	2.38	0.55
1:I:127:LEU:HB2	1:I:219:LEU:HD22	1.87	0.55
1:G:487:LEU:O	4:G:1003:BEY:H17A	2.06	0.55
1:G:236:ARG:HD3	1:G:283:LYS:HD3	1.88	0.55
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.88	0.55
1:H:179:ASN:OD1	1:H:183:ASN:HB2	2.06	0.55
2:J:1002:CO3:O1	4:J:1003:BEY:H7A	2.06	0.55
1:L:133:ASN:HB3	1:L:192:CYS:HB2	1.87	0.55
1:B:121:CYS:HA	1:B:270:TYR:CE2	2.41	0.55
1:F:473:ALA:O	1:F:476:LEU:HB2	2.07	0.55
1:A:216:ASP:O	1:A:217:ASN:HB2	2.06	0.55
1:B:272:ASN:O	1:B:273:ASN:C	2.45	0.55
1:C:146:SER:N	1:C:227:GLU:OE2	2.21	0.55
1:F:117:ILE:HD11	1:F:225:VAL:CG1	2.37	0.55
1:F:214:LEU:HB3	1:F:246:TYR:CE1	2.41	0.55
1:I:178:PHE:CZ	1:K:155:GLU:HG2	2.41	0.55
1:J:215:HIS:C	1:J:261:MET:HB3	2.26	0.55
1:K:330:VAL:HG21	7:K:5424:HOH:O	2.07	0.55
1:E:146:SER:OG	1:E:227:GLU:OE2	2.11	0.55
1:E:336:LEU:HD21	7:E:4649:HOH:O	2.05	0.55
1:F:114:VAL:HG23	1:F:278:LYS:HE2	1.89	0.55
1:E:321:LEU:CD1	1:E:411:TYR:HA	2.37	0.55
1:G:423:ILE:HD11	1:G:600:VAL:HG13	1.88	0.55
1:F:433:MET:HG3	7:F:615:HOH:O	2.07	0.55
1:G:168:LYS:O	1:G:171:THR:CG2	2.55	0.55
1:H:117:ILE:HG23	1:H:118:LYS:H	1.70	0.55
1:E:386:LYS:HA	7:E:623:HOH:O	2.06	0.54
1:J:132:VAL:HG11	1:J:144:ILE:HD13	1.89	0.54
1:B:207:VAL:HG21	1:B:241:THR:HB	1.88	0.54
1:H:372:VAL:O	1:H:483:ASP:HA	2.08	0.54
1:B:222:LEU:HD23	1:B:267:LEU:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:SER:CB	7:F:1110:HOH:O	2.44	0.54
1:G:90:GLN:NE2	1:G:95:ASP:O	2.40	0.54
1:K:423:ILE:HD11	1:K:600:VAL:HG13	1.90	0.54
1:D:152:GLN:HG2	1:D:180:ASP:OD1	2.07	0.54
1:G:176:TYR:CE2	1:J:156:PHE:HB2	2.42	0.54
1:G:171:THR:HG22	1:G:191:GLY:HA3	1.89	0.54
1:D:131:LEU:O	1:D:227:GLU:HB2	2.08	0.54
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.90	0.54
1:A:100:PRO:HA	7:A:4912:HOH:O	2.07	0.54
1:H:316:GLU:HG3	6:H:65:1PE:H142	1.89	0.54
1:J:442:GLY:O	1:K:301:PRO:HB3	2.08	0.54
1:A:451:LYS:HE3	1:A:564:GLU:O	2.07	0.53
1:C:156:PHE:O	1:C:161:ASN:HB2	2.08	0.53
1:C:167:VAL:O	1:C:168:LYS:C	2.46	0.53
1:I:127:LEU:HB2	1:I:219:LEU:CD2	2.38	0.53
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.36	0.53
7:J:3061:HOH:O	1:K:254:SER:C	2.46	0.53
1:B:117:ILE:HD11	1:B:146:SER:OG	2.08	0.53
1:I:201:ALA:HB1	1:J:532:GLU:OE2	2.07	0.53
1:J:451:LYS:HG2	6:J:45:1PE:H241	1.89	0.53
1:K:116:ASP:HA	1:K:271:ILE:O	2.08	0.53
1:C:169:LEU:HD11	1:C:206:VAL:HG23	1.91	0.53
1:L:487:LEU:O	4:L:1003:BEY:H17A	2.08	0.53
1:C:372:VAL:O	1:C:483:ASP:HA	2.09	0.53
1:C:530:ILE:HD12	1:C:556:ILE:HD13	1.89	0.53
1:E:221:LYS:HG3	1:E:266:HIS:HB2	1.90	0.53
1:E:451:LYS:HG2	6:E:43:1PE:H141	1.89	0.53
1:F:236:ARG:O	1:F:240:GLU:HG3	2.08	0.53
1:G:381:GLY:HA2	1:G:459:ASP:OD1	2.09	0.53
1:H:222:LEU:HD23	1:H:267:LEU:CD1	2.39	0.53
1:I:150:ASP:OD2	1:I:153:VAL:HG23	2.09	0.53
1:I:230:VAL:HG23	1:I:234:LEU:CG	2.38	0.53
1:G:173:LYS:HE2	1:J:216:ASP:OD2	2.09	0.53
1:A:168:LYS:O	1:A:171:THR:HG22	2.09	0.53
1:A:173:LYS:HE2	1:D:216:ASP:OD2	2.08	0.53
1:I:372:VAL:O	1:I:483:ASP:HA	2.09	0.53
1:K:108:HIS:CD2	6:K:5:1PE:H131	2.43	0.53
1:A:240:GLU:OE2	1:A:287:TYR:HD2	1.92	0.53
1:C:451:LYS:HE3	1:C:564:GLU:O	2.09	0.53
1:E:102:GLU:HB3	7:E:2665:HOH:O	2.08	0.53
1:F:360:LYS:CD	7:F:2922:HOH:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:457:ASN:ND2	4:L:1003:BEY:H3	2.24	0.53
1:A:473:ALA:O	1:A:476:LEU:HB2	2.09	0.53
1:I:238:PHE:CD2	1:I:239:LEU:HD13	2.43	0.53
1:D:179:ASN:O	1:D:181:ASN:N	2.42	0.53
1:F:362:LYS:CB	1:K:163:GLU:OE1	2.57	0.53
1:L:125:GLU:N	7:L:2009:HOH:O	2.35	0.53
1:A:257:LYS:HG3	7:A:3234:HOH:O	2.08	0.53
1:D:321:LEU:CD1	1:D:411:TYR:HA	2.37	0.53
1:E:90:GLN:NE2	1:E:95:ASP:O	2.41	0.53
1:C:272:ASN:O	1:C:273:ASN:HB2	2.09	0.53
1:B:103:TYR:HB3	6:B:60:1PE:H242	1.91	0.52
1:F:508:GLU:OE2	1:F:508:GLU:HA	2.08	0.52
1:L:225:VAL:HG22	1:L:270:TYR:HB2	1.91	0.52
1:B:372:VAL:O	1:B:483:ASP:HA	2.10	0.52
1:B:423:ILE:HD11	1:B:600:VAL:HG13	1.91	0.52
1:C:165:PHE:CD2	1:C:173:LYS:HG2	2.45	0.52
1:C:184:SER:CB	7:C:2540:HOH:O	2.57	0.52
1:E:262:GLU:N	7:E:5300:HOH:O	2.42	0.52
1:J:130:PHE:O	1:J:189:TYR:HA	2.10	0.52
1:L:451:LYS:HE3	1:L:564:GLU:O	2.10	0.52
1:J:215:HIS:ND1	7:J:5351:HOH:O	2.33	0.52
1:K:321:LEU:CD1	1:K:411:TYR:HA	2.40	0.52
1:L:357:LEU:HB2	1:L:425:PHE:HB2	1.90	0.52
1:G:244:TYR:OH	1:G:588:PRO:O	2.28	0.52
1:I:230:VAL:CG2	1:I:234:LEU:HB3	2.38	0.52
1:J:121:CYS:HB2	1:J:148:VAL:HG12	1.91	0.52
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.91	0.52
1:G:441:PRO:HG2	1:H:393:ILE:HG12	1.91	0.52
1:H:169:LEU:HD23	7:H:3248:HOH:O	2.08	0.52
1:J:451:LYS:HE3	1:J:564:GLU:O	2.09	0.52
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.92	0.52
1:E:529:ILE:CG2	1:E:560:LEU:HD13	2.39	0.52
1:H:576:ILE:HD12	1:H:580:SER:HB2	1.91	0.52
1:J:207:VAL:O	1:J:211:VAL:HG23	2.09	0.52
1:A:178:PHE:HZ	1:D:155:GLU:HG3	1.73	0.52
1:I:320:LYS:CE	6:I:21:1PE:H131	2.39	0.52
2:H:1002:CO3:O3	4:H:1003:BEY:H17A	2.10	0.52
1:I:451:LYS:HE3	1:I:564:GLU:O	2.10	0.52
1:J:423:ILE:HD11	1:J:600:VAL:CG1	2.40	0.52
1:D:214:LEU:HB3	1:D:246:TYR:CE1	2.45	0.52
1:B:120:GLY:HA3	1:B:149:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:LEU:HB2	1:D:425:PHE:HB2	1.91	0.51
1:D:384:ASN:HB3	7:D:1189:HOH:O	2.10	0.51
1:H:176:TYR:OH	1:L:155:GLU:HG3	2.10	0.51
1:J:106:PRO:HG2	1:J:263:TYR:CE2	2.45	0.51
1:F:169:LEU:HD21	1:F:202:ASP:HA	1.90	0.51
1:G:231:ASP:OD1	1:G:234:LEU:N	2.26	0.51
1:K:442:GLY:O	1:L:301:PRO:HB3	2.10	0.51
1:A:139:ASN:HD21	1:A:168:LYS:HG3	1.75	0.51
1:F:169:LEU:HD23	1:F:205:ARG:HE	1.75	0.51
1:L:321:LEU:CD1	1:L:411:TYR:HA	2.39	0.51
1:C:423:ILE:HD11	1:C:600:VAL:HG13	1.92	0.51
1:E:112:VAL:HG13	1:E:267:LEU:HG	1.91	0.51
1:H:487:LEU:O	4:H:1003:BEY:C17	2.58	0.51
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.92	0.51
1:H:473:ALA:O	1:H:476:LEU:HB2	2.10	0.51
1:B:172:SER:O	1:B:173:LYS:HD2	2.11	0.51
1:B:321:LEU:CD1	1:B:411:TYR:HA	2.40	0.51
1:D:392:MET:HE1	4:D:1003:BEY:H12	1.93	0.51
1:G:221:LYS:HG3	1:G:266:HIS:HB2	1.92	0.51
1:D:442:GLY:O	1:E:301:PRO:HB3	2.10	0.51
1:E:423:ILE:HD11	1:E:600:VAL:CG1	2.40	0.51
1:G:364:ASP:O	1:G:420:ASN:HA	2.10	0.51
1:I:230:VAL:HG23	1:I:234:LEU:CD2	2.41	0.51
1:L:487:LEU:HD22	1:L:573:HIS:CE1	2.46	0.51
1:A:150:ASP:OD1	1:A:179:ASN:HB2	2.10	0.51
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.92	0.51
1:D:392:MET:CE	4:D:1003:BEY:H12	2.40	0.51
1:F:179:ASN:ND2	1:F:183:ASN:HB2	2.25	0.51
1:F:157:LEU:HD21	1:F:187:VAL:HG11	1.93	0.51
1:I:153:VAL:O	1:I:157:LEU:HG	2.10	0.51
1:F:114:VAL:CG2	1:F:278:LYS:HG2	2.37	0.51
1:I:423:ILE:HD11	1:I:600:VAL:HG13	1.93	0.51
1:J:473:ALA:O	1:J:476:LEU:HB2	2.11	0.51
1:B:180:ASP:C	1:B:182:LYS:H	2.15	0.51
1:C:489:GLY:N	4:C:1003:BEY:O1	2.37	0.51
1:H:392:MET:HE3	4:H:1003:BEY:H12	1.93	0.51
1:H:423:ILE:HD11	1:H:600:VAL:HG13	1.93	0.51
1:K:357:LEU:HB2	1:K:425:PHE:HB2	1.91	0.51
1:C:238:PHE:HD2	1:C:239:LEU:HD12	1.76	0.50
1:C:392:MET:CE	4:C:1003:BEY:H12	2.40	0.50
1:F:112:VAL:HG22	1:F:267:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:ASP:O	1:F:420:ASN:HA	2.11	0.50
1:G:235:PHE:CE2	1:G:277:TYR:HB3	2.46	0.50
1:K:129:ILE:HA	1:K:188:GLY:O	2.11	0.50
1:A:240:GLU:OE2	1:A:287:TYR:CD2	2.65	0.50
1:C:176:TYR:CE2	1:E:156:PHE:HB2	2.45	0.50
1:D:219:LEU:HD22	7:D:2082:HOH:O	2.12	0.50
1:B:176:TYR:CE2	1:F:156:PHE:HB2	2.46	0.50
1:H:230:VAL:O	1:H:230:VAL:HG23	2.11	0.50
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.92	0.50
1:H:135:PRO:HA	1:H:196:ALA:HB2	1.93	0.50
1:K:411:TYR:CE1	6:K:5:1PE:H142	2.46	0.50
1:A:150:ASP:OD2	1:A:152:GLN:HB2	2.11	0.50
1:A:476:LEU:CD1	7:A:645:HOH:O	2.59	0.50
1:E:92:VAL:HG23	1:E:94:LEU:H	1.77	0.50
1:F:247:MET:HG2	1:F:288:TYR:OH	2.11	0.50
1:E:179:ASN:HB3	1:E:185:VAL:HG21	1.94	0.50
1:F:262:GLU:HA	7:F:645:HOH:O	2.11	0.50
1:I:121:CYS:SG	1:I:225:VAL:CG2	2.96	0.50
1:B:240:GLU:OE2	1:B:287:TYR:CD2	2.65	0.50
1:C:321:LEU:CD1	1:C:411:TYR:HA	2.41	0.50
1:E:138:GLU:HA	1:E:194:SER:OG	2.11	0.50
1:E:442:GLY:O	1:F:301:PRO:HB3	2.12	0.50
1:A:528:PRO:HB3	1:F:525:TRP:CZ3	2.47	0.50
1:J:372:VAL:O	1:J:483:ASP:HA	2.11	0.50
1:L:423:ILE:HD11	1:L:600:VAL:CG1	2.42	0.50
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.93	0.50
1:H:230:VAL:O	1:H:231:ASP:O	2.30	0.50
1:I:192:CYS:HB3	1:I:198:LEU:HD21	1.93	0.50
1:C:90:GLN:NE2	1:C:95:ASP:O	2.33	0.49
1:D:211:VAL:HG21	1:D:245:GLU:HB2	1.93	0.49
1:H:150:ASP:HB3	1:H:153:VAL:HB	1.94	0.49
1:I:320:LYS:HE2	6:I:21:1PE:H131	1.93	0.49
1:J:214:LEU:HD21	1:J:222:LEU:HD22	1.94	0.49
1:K:423:ILE:HD11	1:K:600:VAL:CG1	2.42	0.49
1:D:536:THR:HG21	1:D:551:VAL:HG23	1.94	0.49
1:F:321:LEU:CD1	1:F:411:TYR:HA	2.41	0.49
1:A:94:LEU:HD12	1:C:342:LEU:HD12	1.94	0.49
1:B:320:LYS:HZ1	6:B:61:1PE:H241	1.77	0.49
1:C:156:PHE:O	1:C:161:ASN:CB	2.60	0.49
1:G:130:PHE:O	1:G:189:TYR:HA	2.12	0.49
1:H:321:LEU:CD1	1:H:411:TYR:HA	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:487:LEU:HD23	7:J:783:HOH:O	2.12	0.49
1:L:129:ILE:HG21	1:L:210:LEU:CD1	2.43	0.49
1:D:133:ASN:HB2	1:D:193:GLY:O	2.13	0.49
1:D:226:PHE:CD2	1:D:230:VAL:HG11	2.47	0.49
1:E:214:LEU:HB3	1:E:246:TYR:CE1	2.47	0.49
1:H:481:ILE:O	1:H:571:TRP:HA	2.13	0.49
1:I:146:SER:OG	1:I:227:GLU:OE2	2.25	0.49
1:A:153:VAL:HG22	1:A:177:MET:SD	2.53	0.49
1:D:529:ILE:HG22	1:D:560:LEU:HD13	1.94	0.49
1:E:346:LYS:HE3	1:F:91:VAL:HG21	1.94	0.49
1:G:321:LEU:CD1	1:G:411:TYR:HA	2.39	0.49
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.94	0.49
1:G:526:TRP:CZ3	6:G:30:1PE:H151	2.47	0.49
1:B:100:PRO:O	1:B:251:ARG:HD2	2.12	0.49
1:I:364:ASP:O	1:I:420:ASN:HA	2.13	0.49
1:L:117:ILE:HG22	1:L:272:ASN:OD1	2.13	0.49
1:L:95:ASP:HB3	7:L:4971:HOH:O	2.13	0.49
1:A:199:SER:O	1:A:200:GLU:C	2.51	0.49
1:A:487:LEU:HD22	1:A:573:HIS:CE1	2.48	0.49
1:E:346:LYS:HE3	1:F:91:VAL:CG2	2.43	0.49
1:I:236:ARG:HD3	1:I:283:LYS:HD3	1.94	0.49
1:K:88:VAL:HG21	1:K:97:THR:O	2.13	0.49
1:B:237:PHE:HA	1:B:240:GLU:OE1	2.13	0.49
1:G:117:ILE:CD1	1:G:226:PHE:O	2.61	0.49
1:H:584:LYS:HB2	7:H:4904:HOH:O	2.12	0.49
1:L:226:PHE:HE1	1:L:269:VAL:HG13	1.77	0.49
1:C:236:ARG:NE	1:C:240:GLU:OE2	2.38	0.48
1:D:395:LEU:HD11	1:D:581:TRP:CG	2.48	0.48
1:E:88:VAL:HG21	1:E:97:THR:O	2.13	0.48
1:F:487:LEU:HD22	1:F:573:HIS:CE1	2.48	0.48
1:C:196:ALA:HB1	7:C:2678:HOH:O	2.12	0.48
1:L:226:PHE:CE1	1:L:269:VAL:HG13	2.48	0.48
1:A:207:VAL:HG11	1:A:242:LEU:HA	1.94	0.48
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.95	0.48
1:C:367:LYS:HG2	1:C:603:ASP:OD1	2.14	0.48
1:D:273:ASN:HB3	1:D:276:THR:HG23	1.94	0.48
1:B:142:VAL:HG13	1:B:165:PHE:O	2.13	0.48
1:D:364:ASP:O	1:D:420:ASN:HA	2.13	0.48
1:J:133:ASN:OD1	1:J:135:PRO:HD3	2.13	0.48
1:J:134:ASN:ND2	1:J:141:PRO:HD2	2.28	0.48
1:J:124:GLU:HA	1:J:179:ASN:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:440:ARG:NH2	7:L:4845:HOH:O	2.46	0.48
1:G:107:ILE:HA	1:G:110:ILE:HD12	1.96	0.48
1:H:487:LEU:HD22	1:H:573:HIS:CE1	2.48	0.48
1:H:451:LYS:HE3	1:H:564:GLU:O	2.13	0.48
1:I:272:ASN:O	1:I:273:ASN:HB2	2.14	0.48
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.96	0.48
1:D:121:CYS:HA	1:D:270:TYR:CE2	2.48	0.48
1:F:508:GLU:HB3	7:F:1215:HOH:O	2.13	0.48
1:G:177:MET:HG2	1:G:185:VAL:HG23	1.96	0.48
1:C:364:ASP:O	1:C:420:ASN:HA	2.14	0.48
1:E:364:ASP:O	1:E:420:ASN:HA	2.14	0.48
1:A:528:PRO:HD3	1:F:525:TRP:CE2	2.49	0.48
1:H:160:GLU:O	1:H:163:GLU:HG2	2.14	0.48
1:I:321:LEU:CD1	1:I:411:TYR:HA	2.42	0.48
1:I:516:SER:OG	1:I:599:PHE:HA	2.14	0.48
1:J:487:LEU:O	4:J:1003:BEY:H17A	2.13	0.48
1:J:214:LEU:HB3	1:J:246:TYR:CE1	2.49	0.48
1:A:423:ILE:HD11	1:A:600:VAL:HG13	1.96	0.48
1:B:207:VAL:O	1:B:211:VAL:HG23	2.14	0.48
1:E:316:GLU:HG3	6:E:612:1PE:H252	1.95	0.48
1:F:423:ILE:HD11	1:F:600:VAL:CG1	2.44	0.48
1:A:207:VAL:CG1	1:A:242:LEU:HA	2.43	0.47
1:A:316:GLU:HG3	6:A:20:1PE:H231	1.96	0.47
1:B:222:LEU:HD23	1:B:267:LEU:HD13	1.94	0.47
1:D:199:SER:HB2	7:D:2343:HOH:O	2.13	0.47
1:D:423:ILE:HD13	1:D:600:VAL:HG11	1.94	0.47
1:E:133:ASN:OD1	1:E:135:PRO:HD3	2.14	0.47
1:E:167:VAL:O	1:E:168:LYS:C	2.52	0.47
1:G:122:ASN:HD22	6:G:47:1PE:H142	1.78	0.47
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.96	0.47
1:J:272:ASN:O	1:J:273:ASN:HB2	2.14	0.47
1:J:99:ILE:HD11	1:J:310:LEU:HA	1.96	0.47
1:A:275:ASP:HB2	7:A:3251:HOH:O	2.14	0.47
1:D:165:PHE:CD2	1:D:173:LYS:HG3	2.50	0.47
1:E:516:SER:OG	1:E:599:PHE:HA	2.14	0.47
1:F:364:ASP:HB3	7:I:2655:HOH:O	2.14	0.47
1:G:577:ALA:HB1	4:G:1003:BEY:H13	1.96	0.47
1:G:395:LEU:HD11	1:G:581:TRP:CG	2.49	0.47
1:J:487:LEU:O	4:J:1003:BEY:C17	2.63	0.47
1:J:395:LEU:HD11	1:J:581:TRP:CG	2.50	0.47
1:L:306:ASN:HB2	1:L:307:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:ARG:NH2	7:G:633:HOH:O	2.45	0.47
1:G:450:GLY:HA2	7:G:3308:HOH:O	2.13	0.47
1:I:551:VAL:HG12	1:I:553:ALA:H	1.79	0.47
1:A:139:ASN:ND2	1:A:168:LYS:HG3	2.29	0.47
1:A:499:TYR:CE2	1:A:523:PRO:CB	2.97	0.47
1:A:557:VAL:HG11	7:A:37:HOH:O	2.14	0.47
1:B:257:LYS:CB	1:B:259:VAL:N	2.77	0.47
1:C:423:ILE:HD11	1:C:600:VAL:CG1	2.45	0.47
1:D:423:ILE:CD1	1:D:600:VAL:HG11	2.44	0.47
1:I:230:VAL:HG23	1:I:234:LEU:HG	1.95	0.47
1:I:395:LEU:HD11	1:I:581:TRP:CG	2.50	0.47
1:L:236:ARG:HD3	1:L:283:LYS:HD3	1.96	0.47
1:C:131:LEU:HB3	1:C:192:CYS:SG	2.54	0.47
1:D:86:SER:HB2	1:D:308:VAL:HG13	1.95	0.47
6:I:22:1PE:H231	7:I:624:HOH:O	2.15	0.47
1:D:440:ARG:CD	1:E:302:SER:HB2	2.44	0.47
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.15	0.47
1:G:423:ILE:HD11	1:G:600:VAL:CG1	2.44	0.47
1:H:142:VAL:CG2	1:H:162:MET:HB3	2.44	0.47
1:K:367:LYS:HD3	1:K:367:LYS:HA	1.75	0.47
1:K:108:HIS:NE2	6:K:5:1PE:H131	2.29	0.47
1:G:536:THR:HG21	1:G:551:VAL:HG23	1.97	0.47
1:B:209:SER:O	1:B:212:THR:HB	2.15	0.47
1:C:150:ASP:OD1	1:C:179:ASN:HB2	2.14	0.47
1:D:133:ASN:OD1	1:D:135:PRO:HD3	2.15	0.47
1:G:150:ASP:OD2	1:G:153:VAL:N	2.43	0.47
1:H:203:MET:SD	1:H:238:PHE:HD1	2.38	0.47
1:H:497:THR:HA	1:H:578:GLY:O	2.14	0.47
1:I:473:ALA:O	1:I:476:LEU:HB2	2.15	0.47
1:A:499:TYR:CG	1:A:523:PRO:HB2	2.50	0.47
1:B:257:LYS:CA	1:B:258:ASN:HB3	2.25	0.47
1:C:436:LYS:HG2	5:C:3:SO4:O3	2.14	0.47
1:F:374:LYS:HB3	7:F:622:HOH:O	2.14	0.47
1:J:235:PHE:O	1:J:238:PHE:HB3	2.14	0.47
1:J:364:ASP:O	1:J:420:ASN:HA	2.15	0.47
1:L:169:LEU:HD23	1:L:205:ARG:NH2	2.29	0.47
1:B:355:ILE:O	1:B:426:LEU:HA	2.14	0.47
1:E:529:ILE:HG22	1:E:560:LEU:HD13	1.97	0.47
1:K:364:ASP:O	1:K:420:ASN:HA	2.15	0.47
1:A:148:VAL:HG11	1:A:153:VAL:HG12	1.97	0.46
1:D:423:ILE:CD1	1:D:600:VAL:CG1	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLU:OE1	1:E:523:PRO:HG3	2.14	0.46
1:G:256:ASP:CG	1:G:256:ASP:O	2.53	0.46
1:H:215:HIS:O	1:H:216:ASP:HB2	2.15	0.46
1:H:236:ARG:HB2	1:H:280:GLU:HB3	1.97	0.46
1:J:100:PRO:O	1:J:251:ARG:HD2	2.14	0.46
1:B:170:GLY:O	1:B:209:SER:OG	2.20	0.46
1:D:216:ASP:O	1:D:216:ASP:CG	2.53	0.46
1:F:272:ASN:O	1:F:273:ASN:HB2	2.14	0.46
1:F:347:GLY:CA	7:F:618:HOH:O	2.63	0.46
1:G:124:GLU:O	1:G:185:VAL:HG12	2.15	0.46
1:J:246:TYR:CE2	1:J:264:ILE:HG12	2.50	0.46
1:J:261:MET:HG2	7:J:2991:HOH:O	2.14	0.46
1:J:451:LYS:HD3	7:J:3214:HOH:O	2.15	0.46
4:I:1003:BEY:H10	4:I:1003:BEY:H18A	1.74	0.46
1:K:221:LYS:HD3	7:K:1354:HOH:O	2.16	0.46
1:C:273:ASN:O	1:C:274:ALA:C	2.54	0.46
1:D:487:LEU:O	4:D:1003:BEY:C17	2.64	0.46
1:E:169:LEU:HB3	7:E:5009:HOH:O	2.15	0.46
1:H:134:ASN:HA	1:H:135:PRO:HD2	1.62	0.46
1:I:536:THR:HG21	1:I:551:VAL:HG23	1.98	0.46
1:A:128:THR:HG23	1:A:223:THR:HB	1.96	0.46
1:B:395:LEU:HD11	1:B:581:TRP:CG	2.50	0.46
1:E:476:LEU:HD23	7:E:1550:HOH:O	2.16	0.46
1:F:239:LEU:HB3	1:F:284:ALA:HB1	1.97	0.46
1:G:103:TYR:CD1	6:G:58:1PE:H151	2.51	0.46
1:I:128:THR:O	1:I:188:GLY:N	2.47	0.46
1:I:222:LEU:O	1:I:267:LEU:HA	2.14	0.46
1:K:138:GLU:HA	1:K:194:SER:OG	2.16	0.46
1:B:257:LYS:CB	1:B:259:VAL:H	2.28	0.46
1:D:487:LEU:O	4:D:1003:BEY:H17A	2.15	0.46
1:G:254:SER:HB3	1:I:543:ASP:OD2	2.16	0.46
1:G:232:LYS:HB2	7:G:903:HOH:O	2.16	0.46
1:A:364:ASP:O	1:A:420:ASN:HA	2.16	0.46
1:G:307:PRO:HG2	7:G:622:HOH:O	2.15	0.46
1:A:169:LEU:HG	1:A:205:ARG:HD2	1.97	0.46
2:D:1002:CO3:O2	4:D:1003:BEY:H17A	2.16	0.46
1:F:516:SER:OG	1:F:599:PHE:HA	2.16	0.46
1:H:138:GLU:HA	7:H:1925:HOH:O	2.15	0.46
1:H:140:GLY:O	1:H:166:ASN:HA	2.16	0.46
1:I:167:VAL:O	1:I:168:LYS:C	2.53	0.46
1:J:246:TYR:HE2	1:J:264:ILE:HG12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:273:ASN:HB3	1:J:276:THR:HG23	1.98	0.46
1:K:101:ILE:HG21	1:K:103:TYR:CE2	2.51	0.46
1:L:516:SER:OG	1:L:599:PHE:HA	2.16	0.46
1:C:177:MET:O	1:C:184:SER:HA	2.16	0.46
1:G:121:CYS:HA	1:G:270:TYR:CZ	2.51	0.46
1:H:602:ASN:HB2	7:H:2166:HOH:O	2.16	0.46
1:K:167:VAL:HG12	1:K:192:CYS:H	1.81	0.46
1:L:224:VAL:N	1:L:268:GLY:O	2.42	0.46
1:F:207:VAL:HG12	1:F:207:VAL:O	2.17	0.45
1:G:106:PRO:HD2	1:G:247:MET:SD	2.56	0.45
1:I:230:VAL:O	1:I:277:TYR:CZ	2.68	0.45
1:J:125:GLU:CG	1:J:221:LYS:HD2	2.46	0.45
1:J:128:THR:O	1:J:187:VAL:HA	2.16	0.45
1:J:436:LYS:HG2	5:J:18:SO4:O2	2.17	0.45
1:B:577:ALA:HB1	4:B:1003:BEY:H13	1.98	0.45
1:G:217:ASN:OD1	1:G:219:LEU:HG	2.16	0.45
1:H:217:ASN:ND2	1:L:165:PHE:HE2	2.14	0.45
1:I:130:PHE:CD2	1:I:225:VAL:HB	2.50	0.45
1:C:115:TYR:HB2	1:C:270:TYR:CD2	2.52	0.45
1:D:367:LYS:HD3	1:D:367:LYS:HA	1.66	0.45
1:D:451:LYS:HG3	6:D:44:1PE:H151	1.98	0.45
1:F:306:ASN:HB2	1:F:307:PRO:HD2	1.98	0.45
1:K:530:ILE:HD12	1:K:556:ILE:HD13	1.99	0.45
1:E:530:ILE:HD12	1:E:556:ILE:HD13	1.98	0.45
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.98	0.45
1:F:487:LEU:HD23	7:F:617:HOH:O	2.17	0.45
1:G:230:VAL:O	1:G:277:TYR:OH	2.28	0.45
1:J:320:LYS:HZ3	6:J:3:1PE:C14	2.22	0.45
1:A:143:LYS:HG2	1:A:159:ASP:OD2	2.17	0.45
1:B:375:GLY:O	1:B:429:VAL:HA	2.17	0.45
1:B:451:LYS:HG2	1:C:255:THR:OG1	2.16	0.45
1:D:398:PHE:CD2	1:D:398:PHE:C	2.89	0.45
1:K:481:ILE:O	1:K:571:TRP:HA	2.17	0.45
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.99	0.45
1:H:207:VAL:HG11	1:H:241:THR:HG22	1.99	0.45
1:K:244:TYR:CE1	1:K:291:THR:HG22	2.52	0.45
1:A:141:PRO:HA	1:A:165:PHE:O	2.17	0.45
1:A:216:ASP:O	1:D:173:LYS:CE	2.60	0.45
1:B:142:VAL:CG2	1:B:162:MET:HB3	2.44	0.45
1:C:129:ILE:HA	1:C:188:GLY:O	2.16	0.45
1:D:551:VAL:HG12	1:D:553:ALA:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:PHE:CD2	1:K:173:LYS:HG3	2.52	0.45
1:L:167:VAL:O	1:L:168:LYS:C	2.53	0.45
1:A:249:ASP:CG	1:A:251:ARG:HE	2.20	0.45
1:C:153:VAL:HG12	1:C:157:LEU:HD12	1.96	0.45
1:C:536:THR:HG21	1:C:551:VAL:HG23	1.99	0.45
1:D:497:THR:HA	1:D:578:GLY:O	2.17	0.45
4:E:1003:BEY:H18A	4:E:1003:BEY:H10	1.76	0.45
1:F:487:LEU:O	4:F:1003:BEY:H17A	2.16	0.45
1:H:128:THR:HG23	1:H:223:THR:HB	1.99	0.45
1:I:260:ASN:O	1:I:262:GLU:N	2.50	0.45
1:J:164:LYS:HB2	1:J:164:LYS:HE3	1.65	0.45
1:J:367:LYS:HD3	1:J:367:LYS:HA	1.68	0.45
1:K:130:PHE:O	1:K:189:TYR:HA	2.17	0.45
1:F:107:ILE:O	1:F:107:ILE:HG22	2.17	0.45
5:E:7:SO4:O2	1:F:436:LYS:HG2	2.17	0.45
1:J:107:ILE:HG21	1:J:243:PHE:HB3	1.97	0.45
1:J:536:THR:HG21	1:J:551:VAL:HG23	1.99	0.45
1:K:332:GLU:HG3	1:K:332:GLU:H	1.45	0.45
1:K:355:ILE:O	1:K:426:LEU:HA	2.17	0.45
1:C:528:PRO:HB3	1:D:525:TRP:CZ3	2.52	0.45
1:H:487:LEU:O	4:H:1003:BEY:H17	2.17	0.45
1:L:324:GLU:HA	7:L:970:HOH:O	2.16	0.45
1:E:229:ASN:O	1:E:230:VAL:CB	2.57	0.44
1:G:332:GLU:HB2	7:G:5439:HOH:O	2.16	0.44
1:K:381:GLY:HA2	1:K:459:ASP:OD1	2.16	0.44
1:A:444:ILE:HA	1:A:453:ILE:O	2.17	0.44
1:B:586:ARG:HB3	7:B:2591:HOH:O	2.17	0.44
1:D:481:ILE:O	1:D:571:TRP:HA	2.16	0.44
1:H:180:ASP:C	1:H:182:LYS:H	2.21	0.44
1:J:100:PRO:O	1:J:101:ILE:HD13	2.18	0.44
1:J:487:LEU:HD22	1:J:573:HIS:CE1	2.53	0.44
1:B:187:VAL:HG12	1:B:188:GLY:N	2.31	0.44
1:F:202:ASP:O	1:F:206:VAL:HG23	2.17	0.44
1:K:516:SER:OG	1:K:599:PHE:HA	2.17	0.44
1:L:232:LYS:HB2	7:L:5173:HOH:O	2.17	0.44
1:B:481:ILE:O	1:B:571:TRP:HA	2.16	0.44
1:C:514:LEU:O	1:C:517:SER:HB3	2.17	0.44
1:H:307:PRO:HD3	1:H:377:THR:OG1	2.16	0.44
1:I:210:LEU:HD23	1:I:242:LEU:HD13	1.98	0.44
1:J:210:LEU:HA	1:J:213:MET:HE3	1.98	0.44
1:D:152:GLN:O	1:D:155:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ASN:HB2	1:F:167:VAL:HG11	1.99	0.44
1:I:100:PRO:O	1:I:251:ARG:HD2	2.18	0.44
1:I:307:PRO:HD3	1:I:377:THR:OG1	2.18	0.44
1:K:103:TYR:CD1	6:K:4:1PE:H132	2.53	0.44
7:B:2359:HOH:O	1:E:551:VAL:HG13	2.16	0.44
1:E:395:LEU:HD11	1:E:581:TRP:CG	2.53	0.44
1:F:97:THR:O	1:F:98:SER:HB3	2.17	0.44
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.52	0.44
1:L:128:THR:HG23	1:L:223:THR:HB	2.00	0.44
1:L:198:LEU:HD23	1:L:198:LEU:HA	1.60	0.44
1:K:441:PRO:HG2	1:L:393:ILE:HG12	1.99	0.44
1:A:138:GLU:HA	1:A:194:SER:CB	2.47	0.44
1:D:451:LYS:HE2	6:D:44:1PE:H261	1.99	0.44
1:E:368:LYS:CE	7:E:2241:HOH:O	2.65	0.44
1:F:586:ARG:NH2	7:F:2842:HOH:O	2.36	0.44
1:H:375:GLY:O	1:H:429:VAL:HA	2.18	0.44
1:I:243:PHE:HB3	1:I:288:TYR:CD1	2.53	0.44
1:I:497:THR:HA	1:I:578:GLY:O	2.18	0.44
1:B:300:ALA:HA	1:B:301:PRO:HD3	1.88	0.44
1:H:335:GLU:CB	7:H:2588:HOH:O	2.65	0.44
1:I:118:LYS:C	1:I:120:GLY:H	2.21	0.44
1:I:128:THR:HG23	1:I:223:THR:HB	2.00	0.44
1:J:302:SER:HB3	7:J:1429:HOH:O	2.18	0.44
1:J:544:ILE:CD1	1:J:564:GLU:HG3	2.47	0.44
1:K:451:LYS:CD	6:K:42:1PE:H231	2.43	0.44
1:K:438:SER:HA	7:K:17:HOH:O	2.18	0.44
1:B:218:LYS:HG2	1:B:262:GLU:CG	2.48	0.44
1:D:198:LEU:HA	1:D:198:LEU:HD12	1.86	0.44
1:C:532:GLU:HG3	1:D:201:ALA:HB1	1.99	0.44
1:L:451:LYS:CG	6:L:612:1PE:H131	2.47	0.44
1:A:123:VAL:HG21	1:A:153:VAL:HG11	1.99	0.43
1:C:392:MET:HE3	4:C:1003:BEY:H12	2.00	0.43
1:D:219:LEU:N	1:D:219:LEU:HD22	2.33	0.43
1:E:135:PRO:HA	1:E:194:SER:O	2.18	0.43
1:E:223:THR:HA	1:E:268:GLY:O	2.18	0.43
1:E:368:LYS:HE3	7:E:2241:HOH:O	2.17	0.43
1:F:395:LEU:HD11	1:F:581:TRP:CG	2.53	0.43
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.99	0.43
1:J:86:SER:HB2	7:J:1689:HOH:O	2.18	0.43
1:K:208:LEU:HD13	1:K:245:GLU:HG3	2.00	0.43
4:A:1003:BEY:H18A	4:A:1003:BEY:H10	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LYS:HG2	1:A:328:LEU:HD12	2.00	0.43
1:C:156:PHE:CE2	1:C:175:PHE:HB3	2.54	0.43
1:C:207:VAL:CG1	1:C:242:LEU:HA	2.48	0.43
1:G:198:LEU:HD22	1:G:202:ASP:HB2	1.99	0.43
1:H:355:ILE:O	1:H:426:LEU:HA	2.18	0.43
1:I:462:GLY:N	2:I:1002:CO3:O1	2.52	0.43
1:J:541:TYR:HE1	1:K:249:ASP:HB3	1.83	0.43
1:L:300:ALA:HA	1:L:301:PRO:HD3	1.84	0.43
1:B:180:ASP:C	1:B:182:LYS:N	2.72	0.43
1:B:423:ILE:HD11	1:B:600:VAL:CG1	2.48	0.43
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.99	0.43
1:H:594:ARG:HG3	7:H:781:HOH:O	2.17	0.43
1:J:99:ILE:HD12	1:J:313:ALA:HB2	1.99	0.43
1:G:528:PRO:HD3	1:L:525:TRP:CE2	2.53	0.43
1:B:440:ARG:HD2	1:C:302:SER:HB2	2.00	0.43
1:E:216:ASP:C	1:E:217:ASN:ND2	2.71	0.43
1:E:355:ILE:O	1:E:426:LEU:HA	2.18	0.43
1:F:150:ASP:HB3	1:F:153:VAL:HB	2.00	0.43
1:D:393:ILE:HG12	1:F:441:PRO:HG2	2.01	0.43
1:J:516:SER:OG	1:J:599:PHE:HA	2.18	0.43
1:K:392:MET:HE1	4:K:1003:BEY:H12	2.00	0.43
1:K:395:LEU:HD11	1:K:581:TRP:CG	2.54	0.43
1:A:214:LEU:HD11	1:A:222:LEU:HD22	1.99	0.43
1:B:364:ASP:O	1:B:420:ASN:HA	2.17	0.43
1:G:232:LYS:N	7:G:903:HOH:O	2.51	0.43
1:I:381:GLY:HA2	1:I:459:ASP:OD1	2.18	0.43
1:J:221:LYS:HE2	7:J:633:HOH:O	2.17	0.43
1:J:520:SER:HB3	1:J:598:GLU:HG3	2.01	0.43
1:E:157:LEU:HD23	1:E:157:LEU:HA	1.87	0.43
1:G:222:LEU:O	1:G:267:LEU:HD12	2.17	0.43
1:I:182:LYS:HD3	1:I:182:LYS:N	2.29	0.43
1:I:320:LYS:NZ	6:I:21:1PE:H131	2.34	0.43
1:L:254:SER:OG	1:L:254:SER:O	2.36	0.43
1:A:536:THR:HG21	1:A:551:VAL:HG23	2.01	0.43
1:F:481:ILE:O	1:F:571:TRP:HA	2.19	0.43
1:K:536:THR:HG21	1:K:551:VAL:HG23	2.00	0.43
1:E:106:PRO:HG2	1:E:263:TYR:CE2	2.54	0.43
1:G:396:MET:HE3	7:G:2070:HOH:O	2.19	0.43
1:G:516:SER:OG	1:G:599:PHE:HA	2.18	0.43
1:J:108:HIS:HA	1:J:285:ARG:HD2	2.00	0.43
1:L:150:ASP:HB3	1:L:153:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LEU:O	1:C:212:THR:HG23	2.19	0.43
1:D:179:ASN:C	1:D:181:ASN:H	2.22	0.43
1:D:394:ASP:HB3	7:F:3100:HOH:O	2.19	0.43
1:E:543:ASP:CG	6:E:43:1PE:H142	2.39	0.43
1:F:423:ILE:HD13	1:F:600:VAL:HG11	2.01	0.43
1:I:168:LYS:O	1:I:171:THR:HB	2.19	0.43
1:I:530:ILE:HD12	1:I:556:ILE:HD13	2.01	0.43
1:K:159:ASP:O	1:K:160:GLU:C	2.53	0.43
1:K:246:TYR:CE2	1:K:263:TYR:HD1	2.37	0.43
1:F:103:TYR:HB2	5:F:21:SO4:O4	2.19	0.43
1:G:112:VAL:HG22	1:G:267:LEU:HB3	2.00	0.43
1:G:292:TYR:O	1:G:295:SER:HB3	2.18	0.43
1:G:423:ILE:HD13	1:G:600:VAL:HG11	2.01	0.43
1:G:95:ASP:HA	1:G:96:PRO:HD2	1.90	0.43
1:H:202:ASP:O	1:H:206:VAL:HG23	2.19	0.43
1:H:131:LEU:O	1:H:228:ILE:HG23	2.19	0.43
1:H:364:ASP:O	1:H:420:ASN:HA	2.18	0.43
1:I:324:GLU:H	1:I:324:GLU:HG2	1.68	0.43
1:A:475:LYS:HD3	7:A:2808:HOH:O	2.19	0.42
1:G:306:ASN:HB2	1:G:307:PRO:HD2	2.01	0.42
1:H:498:SER:HB3	1:H:499:TYR:HD2	1.84	0.42
1:J:423:ILE:HD13	1:J:600:VAL:HG11	2.01	0.42
1:K:451:LYS:NZ	6:K:42:1PE:H231	2.34	0.42
1:L:512:LYS:HD3	1:L:603:ASP:OD1	2.19	0.42
1:B:134:ASN:HB3	1:B:167:VAL:HG21	2.00	0.42
1:B:229:ASN:ND2	7:B:2947:HOH:O	2.52	0.42
4:C:1003:BEY:H8	4:C:1003:BEY:H2	1.66	0.42
1:J:103:TYR:HB2	5:J:20:SO4:O1	2.19	0.42
1:E:88:VAL:HA	1:E:89:PRO:HD2	1.79	0.42
1:F:109:ASP:HB2	7:F:1094:HOH:O	2.19	0.42
1:F:222:LEU:HB3	1:F:264:ILE:HD13	2.01	0.42
1:G:123:VAL:HG12	1:G:185:VAL:HG11	2.01	0.42
1:G:316:GLU:HG3	6:G:58:1PE:H131	2.01	0.42
1:K:106:PRO:HD2	1:K:247:MET:SD	2.59	0.42
1:B:169:LEU:HD21	1:B:205:ARG:HD3	2.02	0.42
1:C:139:ASN:ND2	1:C:168:LYS:HB2	2.34	0.42
6:D:44:1PE:H141	1:E:254:SER:C	2.39	0.42
1:E:544:ILE:CD1	1:E:564:GLU:HG3	2.49	0.42
1:F:306:ASN:HB2	1:F:307:PRO:CD	2.48	0.42
1:K:392:MET:CE	4:K:1003:BEY:H12	2.49	0.42
1:L:96:PRO:HB3	1:L:304:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HA	1:A:269:VAL:O	2.20	0.42
1:E:363:GLY:HA3	7:E:1962:HOH:O	2.19	0.42
1:F:374:LYS:HB2	1:F:485:ALA:CB	2.49	0.42
1:F:95:ASP:O	1:F:96:PRO:C	2.56	0.42
1:H:181:ASN:ND2	1:H:183:ASN:ND2	2.67	0.42
1:H:543:ASP:HA	1:I:256:ASP:HB3	2.00	0.42
1:I:137:LYS:CB	7:I:5069:HOH:O	2.66	0.42
1:J:239:LEU:HB3	1:J:284:ALA:HB1	2.01	0.42
1:K:107:ILE:O	1:K:109:ASP:N	2.52	0.42
1:K:248:THR:HG23	7:K:2935:HOH:O	2.19	0.42
1:G:528:PRO:HD3	1:L:525:TRP:NE1	2.35	0.42
1:D:219:LEU:N	1:D:219:LEU:HD13	2.26	0.42
1:E:362:LYS:N	7:E:1815:HOH:O	2.52	0.42
1:F:544:ILE:CD1	1:F:564:GLU:HG3	2.49	0.42
1:H:423:ILE:HD11	1:H:600:VAL:CG1	2.49	0.42
1:J:317:LEU:HG	1:J:321:LEU:HD12	2.02	0.42
1:J:440:ARG:CD	1:K:302:SER:HB2	2.49	0.42
1:A:112:VAL:HA	1:A:267:LEU:O	2.19	0.42
1:C:395:LEU:HD11	1:C:581:TRP:CG	2.55	0.42
1:E:440:ARG:NH2	7:E:663:HOH:O	2.52	0.42
1:F:444:ILE:HA	1:F:453:ILE:O	2.18	0.42
1:I:423:ILE:HD11	1:I:600:VAL:CG1	2.50	0.42
1:J:273:ASN:HB2	1:J:277:TYR:HE2	1.83	0.42
1:J:321:LEU:CD1	1:J:411:TYR:HA	2.47	0.42
1:K:121:CYS:HA	1:K:270:TYR:CE2	2.54	0.42
1:A:92:VAL:O	1:A:95:ASP:HB2	2.19	0.42
1:C:316:GLU:HG3	6:C:17:1PE:H221	2.02	0.42
1:E:169:LEU:HD12	1:E:192:CYS:HA	2.01	0.42
1:F:134:ASN:CB	1:F:167:VAL:HG11	2.50	0.42
1:G:398:PHE:CD2	1:G:398:PHE:C	2.93	0.42
1:G:445:ILE:HA	7:G:866:HOH:O	2.19	0.42
1:J:207:VAL:HG13	1:J:242:LEU:HA	2.00	0.42
1:J:320:LYS:CE	6:J:3:1PE:H142	2.49	0.42
1:J:393:ILE:HG12	1:L:441:PRO:HG2	2.02	0.42
1:J:423:ILE:CD1	1:J:600:VAL:CG1	2.98	0.42
1:C:392:MET:HE1	4:C:1003:BEY:H12	2.01	0.42
1:C:168:LYS:O	1:C:169:LEU:C	2.57	0.42
1:D:133:ASN:C	1:D:133:ASN:OD1	2.57	0.42
1:D:179:ASN:O	1:D:182:LYS:N	2.51	0.42
1:D:272:ASN:O	1:D:273:ASN:HB2	2.20	0.42
1:E:129:ILE:HA	1:E:188:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:GLU:HG3	1:F:240:GLU:H	1.60	0.42
1:F:533:TYR:HB2	1:F:560:LEU:CD1	2.49	0.42
1:L:150:ASP:OD1	1:L:179:ASN:HB2	2.19	0.42
1:E:222:LEU:O	1:E:267:LEU:HA	2.19	0.42
1:G:134:ASN:O	1:G:194:SER:HB2	2.20	0.42
1:H:381:GLY:HA2	1:H:459:ASP:OD1	2.19	0.42
1:J:195:VAL:HG12	1:J:195:VAL:O	2.20	0.42
1:K:207:VAL:CG1	1:K:242:LEU:HA	2.50	0.42
1:A:395:LEU:HD11	1:A:581:TRP:CG	2.54	0.41
1:E:118:LYS:C	1:E:120:GLY:H	2.23	0.41
1:A:528:PRO:HD3	1:F:525:TRP:NE1	2.35	0.41
1:I:444:ILE:HA	1:I:453:ILE:O	2.20	0.41
1:A:346:LYS:HB3	1:A:437:ASN:O	2.19	0.41
1:A:516:SER:OG	1:A:599:PHE:HA	2.20	0.41
1:B:381:GLY:HA2	1:B:459:ASP:OD1	2.19	0.41
1:D:544:ILE:CD1	1:D:564:GLU:HG3	2.50	0.41
1:F:178:PHE:HD1	1:F:182:LYS:O	2.03	0.41
1:F:198:LEU:HD12	1:F:198:LEU:HA	1.84	0.41
1:F:239:LEU:HD23	1:F:281:VAL:HA	2.01	0.41
1:G:234:LEU:HD12	1:G:234:LEU:O	2.20	0.41
1:J:307:PRO:HD3	1:J:377:THR:OG1	2.20	0.41
1:J:350:TYR:HE1	1:L:440:ARG:HH21	1.68	0.41
1:L:162:MET:CE	1:L:165:PHE:HE1	2.32	0.41
1:L:214:LEU:HD21	1:L:222:LEU:HD22	2.02	0.41
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.87	0.41
1:B:520:SER:HB3	1:B:598:GLU:HG3	2.01	0.41
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.54	0.41
1:C:532:GLU:HB2	7:D:4750:HOH:O	2.20	0.41
1:D:346:LYS:HB3	1:D:437:ASN:O	2.19	0.41
1:E:158:LYS:O	1:E:161:ASN:HB3	2.20	0.41
1:E:161:ASN:ND2	7:E:1724:HOH:O	2.53	0.41
1:E:208:LEU:HA	1:E:208:LEU:HD12	1.90	0.41
1:F:375:GLY:O	1:F:429:VAL:HA	2.19	0.41
1:J:91:VAL:HB	1:L:346:LYS:HE3	2.02	0.41
1:J:90:GLN:NE2	1:J:95:ASP:O	2.53	0.41
1:L:142:VAL:HG23	1:L:165:PHE:O	2.20	0.41
1:L:235:PHE:HE1	1:L:269:VAL:HG11	1.86	0.41
1:A:142:VAL:HG21	1:A:189:TYR:CZ	2.56	0.41
1:C:181:ASN:ND2	1:C:183:ASN:ND2	2.67	0.41
1:D:168:LYS:O	1:D:169:LEU:C	2.57	0.41
1:F:307:PRO:HD3	1:F:377:THR:OG1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.56	0.41
1:G:487:LEU:HD22	1:G:573:HIS:CE1	2.56	0.41
1:I:225:VAL:HG22	1:I:270:TYR:HB2	2.01	0.41
1:J:494:SER:HB3	7:J:1288:HOH:O	2.19	0.41
1:K:307:PRO:HD3	1:K:377:THR:OG1	2.20	0.41
1:B:541:TYR:OH	1:C:587:LYS:HB2	2.21	0.41
1:F:207:VAL:HG11	1:F:241:THR:HG22	2.03	0.41
1:J:323:LEU:HD23	1:J:323:LEU:HA	1.78	0.41
1:J:514:LEU:O	1:J:518:LYS:HG2	2.21	0.41
1:K:221:LYS:HG3	1:K:266:HIS:HB2	2.03	0.41
1:K:237:PHE:O	1:K:240:GLU:HB2	2.20	0.41
1:C:481:ILE:O	1:C:571:TRP:HA	2.20	0.41
1:E:219:LEU:O	1:E:264:ILE:HG22	2.20	0.41
1:H:487:LEU:O	4:H:1003:BEY:H17A	2.19	0.41
1:I:207:VAL:HG11	1:I:242:LEU:N	2.36	0.41
1:I:497:THR:HB	7:I:4920:HOH:O	2.20	0.41
1:L:232:LYS:HE2	1:L:276:THR:O	2.20	0.41
1:B:441:PRO:HG2	1:C:393:ILE:HG12	2.03	0.41
1:C:346:LYS:HB3	1:C:437:ASN:O	2.20	0.41
1:G:88:VAL:HA	1:G:89:PRO:HD2	1.88	0.41
1:H:178:PHE:HZ	1:L:155:GLU:HG2	1.84	0.41
1:I:111:LYS:HE2	1:I:266:HIS:NE2	2.36	0.41
1:I:230:VAL:CG2	1:I:234:LEU:HG	2.51	0.41
1:A:176:TYR:CE2	1:D:156:PHE:HB2	2.55	0.41
1:B:167:VAL:O	1:B:168:LYS:C	2.59	0.41
1:A:301:PRO:CG	1:C:444:ILE:HD12	2.50	0.41
1:C:487:LEU:HD22	1:C:573:HIS:CE1	2.56	0.41
1:D:440:ARG:HD3	1:E:302:SER:HB2	2.01	0.41
1:E:481:ILE:O	1:E:571:TRP:HA	2.20	0.41
1:G:522:GLU:HA	1:G:523:PRO:HD3	1.92	0.41
1:G:528:PRO:HD3	1:L:525:TRP:CD1	2.56	0.41
1:H:520:SER:HB3	1:H:598:GLU:HG3	2.02	0.41
1:J:481:ILE:O	1:J:571:TRP:HA	2.20	0.41
1:L:364:ASP:O	1:L:420:ASN:HA	2.21	0.41
1:L:536:THR:HG21	1:L:551:VAL:HG23	2.02	0.41
1:A:263:TYR:N	7:A:2776:HOH:O	2.43	0.41
1:C:551:VAL:HG12	1:C:553:ALA:H	1.86	0.41
1:D:487:LEU:HD22	1:D:573:HIS:CE1	2.56	0.41
1:F:105:THR:C	1:F:107:ILE:N	2.74	0.41
1:F:126:GLY:HA3	1:F:221:LYS:O	2.20	0.41
1:H:156:PHE:CD2	1:H:156:PHE:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:219:LEU:O	1:H:264:ILE:HG22	2.21	0.41
1:H:552:LYS:HE3	1:K:492:LEU:HD13	2.03	0.41
1:I:203:MET:O	1:I:207:VAL:HG23	2.21	0.41
1:I:487:LEU:HD12	1:I:487:LEU:HA	1.95	0.41
1:J:219:LEU:HB3	1:J:220:SER:H	1.62	0.41
1:K:544:ILE:CD1	1:K:564:GLU:HG3	2.51	0.41
1:L:103:TYR:HB3	6:L:1:1PE:H252	2.03	0.41
4:A:1003:BEY:H17	4:A:1003:BEY:H18	1.78	0.41
1:A:393:ILE:HG12	1:C:441:PRO:HG2	2.03	0.41
1:B:360:LYS:HE3	1:B:365:VAL:HG21	2.03	0.41
1:F:367:LYS:HA	1:F:367:LYS:HD3	1.83	0.41
1:G:177:MET:O	1:G:184:SER:HA	2.21	0.41
1:G:374:LYS:HB3	7:G:636:HOH:O	2.20	0.41
1:I:139:ASN:O	1:I:166:ASN:HB2	2.21	0.41
1:L:207:VAL:O	1:L:211:VAL:HG23	2.20	0.41
1:A:198:LEU:HB3	1:A:202:ASP:HB2	2.03	0.40
1:A:235:PHE:HE1	1:A:269:VAL:HG11	1.84	0.40
1:E:129:ILE:HA	1:E:129:ILE:HD13	1.84	0.40
1:G:481:ILE:O	1:G:571:TRP:HA	2.21	0.40
1:I:265:LYS:HA	1:I:265:LYS:HE2	2.03	0.40
1:J:375:GLY:O	1:J:429:VAL:HA	2.21	0.40
1:K:440:ARG:CD	1:L:302:SER:HB2	2.51	0.40
1:A:349:MET:HG2	7:C:1438:HOH:O	2.21	0.40
1:B:442:GLY:O	1:C:301:PRO:HB3	2.21	0.40
1:C:239:LEU:HD21	1:C:281:VAL:HG22	2.03	0.40
1:C:292:TYR:O	1:C:295:SER:HB3	2.22	0.40
1:D:128:THR:O	1:D:129:ILE:HD13	2.21	0.40
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.21	0.40
1:H:138:GLU:O	1:H:140:GLY:N	2.50	0.40
1:H:441:PRO:HG2	1:I:393:ILE:HG12	2.03	0.40
1:G:301:PRO:HB3	1:I:442:GLY:O	2.20	0.40
1:J:475:LYS:HB3	7:J:4358:HOH:O	2.21	0.40
1:K:366:LYS:HG3	1:K:420:ASN:HB3	2.03	0.40
1:B:190:VAL:HG11	1:B:206:VAL:HG13	2.02	0.40
1:C:176:TYR:CE1	1:C:184:SER:HB2	2.56	0.40
1:D:522:GLU:HA	1:D:523:PRO:HD3	1.94	0.40
1:I:487:LEU:HD22	1:I:573:HIS:CE1	2.56	0.40
1:I:88:VAL:HG21	1:I:97:THR:O	2.21	0.40
1:J:350:TYR:HA	1:J:351:PRO:HD3	1.97	0.40
1:L:505:ASN:HA	7:L:2672:HOH:O	2.21	0.40
1:A:326:LYS:HG2	1:A:328:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLU:HB2	1:A:521:ASN:OD1	2.21	0.40
1:B:125:GLU:HG2	1:B:126:GLY:N	2.36	0.40
1:B:460:ALA:O	1:B:546:GLN:NE2	2.54	0.40
1:C:178:PHE:CZ	1:E:155:GLU:HG2	2.52	0.40
1:I:223:THR:HA	1:I:268:GLY:O	2.22	0.40
1:G:393:ILE:HG12	1:I:441:PRO:HG2	2.03	0.40
1:K:127:LEU:HA	1:K:186:ALA:O	2.20	0.40
1:C:156:PHE:CZ	1:C:175:PHE:HB3	2.56	0.40
1:G:159:ASP:N	1:G:159:ASP:OD1	2.55	0.40
1:G:239:LEU:HD23	1:G:239:LEU:HA	1.86	0.40
1:G:115:TYR:O	1:G:270:TYR:HA	2.21	0.40
1:I:399:ASP:OD1	4:I:1003:BEY:N	2.55	0.40
1:K:157:LEU:HA	1:K:157:LEU:HD23	1.88	0.40
1:L:123:VAL:HG11	1:L:153:VAL:HG21	2.04	0.40

All (1) 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:B:366:LYS:NZ	7:D:3762:HOH:O[4_555]	1.84	0.36

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	514/528 (97%)	493 (96%)	19 (4%)	2 (0%)	38 59
1	B	516/528 (98%)	488 (95%)	25 (5%)	3 (1%)	28 49
1	C	516/528 (98%)	495 (96%)	18 (4%)	3 (1%)	28 49
1	D	509/528 (96%)	492 (97%)	16 (3%)	1 (0%)	51 72
1	E	506/528 (96%)	487 (96%)	17 (3%)	2 (0%)	38 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	504/528 (96%)	484 (96%)	14 (3%)	6 (1%)	15	29
1	G	512/528 (97%)	483 (94%)	27 (5%)	2 (0%)	38	59
1	H	503/528 (95%)	477 (95%)	21 (4%)	5 (1%)	18	34
1	I	516/528 (98%)	493 (96%)	22 (4%)	1 (0%)	51	72
1	J	509/528 (96%)	483 (95%)	24 (5%)	2 (0%)	38	59
1	K	503/528 (95%)	479 (95%)	22 (4%)	2 (0%)	38	59
1	L	509/528 (96%)	484 (95%)	24 (5%)	1 (0%)	51	72
All	All	6117/6336 (96%)	5838 (95%)	249 (4%)	30 (0%)	32	54

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	B	149	ASN
1	E	230	VAL
1	H	139	ASN
1	B	273	ASN
1	C	274	ALA
1	E	137	LYS
1	H	231	ASP
1	I	261	MET
1	K	108	HIS
1	D	180	ASP
1	F	163	GLU
1	F	184	SER
1	F	274	ALA
1	J	149	ASN
1	C	139	ASN
1	F	149	ASN
1	F	179	ASN
1	G	149	ASN
1	J	251	ARG
1	K	139	ASN
1	L	168	LYS
1	A	200	GLU
1	B	254	SER
1	F	168	LYS
1	G	218	LYS
1	H	117	ILE
1	H	181	ASN

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Mol	Chain	Res	Type
1	C	117	ILE
1	H	195	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/455 (94%)	407 (96%)	19 (4%)	32	54
1	B	412/455 (90%)	403 (98%)	9 (2%)	57	79
1	C	419/455 (92%)	406 (97%)	13 (3%)	45	69
1	D	417/455 (92%)	395 (95%)	22 (5%)	26	46
1	E	414/455 (91%)	396 (96%)	18 (4%)	33	57
1	F	409/455 (90%)	385 (94%)	24 (6%)	23	41
1	G	435/455 (96%)	418 (96%)	17 (4%)	37	61
1	H	430/455 (94%)	412 (96%)	18 (4%)	34	58
1	I	437/455 (96%)	414 (95%)	23 (5%)	26	46
1	J	430/455 (94%)	404 (94%)	26 (6%)	22	40
1	K	427/455 (94%)	412 (96%)	15 (4%)	41	65
1	L	421/455 (92%)	403 (96%)	18 (4%)	33	57
All	All	5077/5460 (93%)	4855 (96%)	222 (4%)	33	56

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	132	VAL
1	A	159	ASP
1	A	160	GLU
1	A	166	ASN
1	A	168	LYS
1	A	194	SER
1	A	197	ASP

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Mol	Chain	Res	Type
1	A	198	LEU
1	A	288	TYR
1	A	310	LEU
1	A	330	VAL
1	A	367	LYS
1	A	398	PHE
1	A	439	TYR
1	A	476	LEU
1	A	498	SER
1	A	579	VAL
1	A	603	ASP
1	B	104	ASN
1	B	200	GLU
1	B	210	LEU
1	B	288	TYR
1	B	310	LEU
1	B	332	GLU
1	B	398	PHE
1	B	439	TYR
1	B	498	SER
1	C	86	SER
1	C	145	SER
1	C	146	SER
1	C	163	GLU
1	C	177	MET
1	C	181	ASN
1	C	185	VAL
1	C	194	SER
1	C	208	LEU
1	C	229	ASN
1	C	288	TYR
1	C	398	PHE
1	C	439	TYR
1	D	90	GLN
1	D	111	LYS
1	D	132	VAL
1	D	198	LEU
1	D	210	LEU
1	D	219	LEU
1	D	231	ASP
1	D	248	THR
1	D	261	MET

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Mol	Chain	Res	Type
1	D	262	GLU
1	D	276	THR
1	D	288	TYR
1	D	310	LEU
1	D	322	ASN
1	D	367	LYS
1	D	398	PHE
1	D	400	MET
1	D	439	TYR
1	D	518	LYS
1	D	532	GLU
1	D	560	LEU
1	D	579	VAL
1	E	172	SER
1	E	185	VAL
1	E	208	LEU
1	E	217	ASN
1	E	220	SER
1	E	230	VAL
1	E	236	ARG
1	E	238	PHE
1	E	248	THR
1	E	267	LEU
1	E	288	TYR
1	E	310	LEU
1	E	398	PHE
1	E	407	LEU
1	E	413	VAL
1	E	439	TYR
1	E	483	ASP
1	E	560	LEU
1	F	86	SER
1	F	92	VAL
1	F	93	SER
1	F	102	GLU
1	F	114	VAL
1	F	117	ILE
1	F	161	ASN
1	F	198	LEU
1	F	200	GLU
1	F	217	ASN
1	F	239	LEU

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Mol	Chain	Res	Type
1	F	240	GLU
1	F	248	THR
1	F	288	TYR
1	F	310	LEU
1	F	330	VAL
1	F	364	ASP
1	F	367	LYS
1	F	398	PHE
1	F	439	TYR
1	F	476	LEU
1	F	507	GLU
1	F	508	GLU
1	F	579	VAL
1	G	101	ILE
1	G	154	SER
1	G	159	ASP
1	G	164	LYS
1	G	182	LYS
1	G	185	VAL
1	G	195	VAL
1	G	229	ASN
1	G	288	TYR
1	G	310	LEU
1	G	367	LYS
1	G	398	PHE
1	G	400	MET
1	G	439	TYR
1	G	476	LEU
1	G	515	GLN
1	G	579	VAL
1	H	155	GLU
1	H	158	LYS
1	H	173	LYS
1	H	200	GLU
1	H	212	THR
1	H	213	MET
1	H	276	THR
1	H	279	GLU
1	H	288	TYR
1	H	310	LEU
1	H	331	LYS
1	H	398	PHE

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Mol	Chain	Res	Type
1	H	439	TYR
1	H	476	LEU
1	H	498	SER
1	H	508	GLU
1	H	515	GLN
1	H	579	VAL
1	I	121	CYS
1	I	145	SER
1	I	154	SER
1	I	163	GLU
1	I	171	THR
1	I	181	ASN
1	I	182	LYS
1	I	198	LEU
1	I	199	SER
1	I	200	GLU
1	I	208	LEU
1	I	229	ASN
1	I	239	LEU
1	I	288	TYR
1	I	310	LEU
1	I	324	GLU
1	I	398	PHE
1	I	439	TYR
1	I	476	LEU
1	I	483	ASP
1	I	508	GLU
1	I	579	VAL
1	I	603	ASP
1	J	86	SER
1	J	111	LYS
1	J	123	VAL
1	J	143	LYS
1	J	184	SER
1	J	195	VAL
1	J	197	ASP
1	J	208	LEU
1	J	239	LEU
1	J	246	TYR
1	J	248	THR
1	J	261	MET
1	J	276	THR

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Mol	Chain	Res	Type
1	J	279	GLU
1	J	288	TYR
1	J	310	LEU
1	J	322	ASN
1	J	367	LYS
1	J	398	PHE
1	J	400	MET
1	J	439	TYR
1	J	476	LEU
1	J	483	ASP
1	J	518	LYS
1	J	579	VAL
1	J	603	ASP
1	K	86	SER
1	K	102	GLU
1	K	132	VAL
1	K	208	LEU
1	K	218	LYS
1	K	248	THR
1	K	265	LYS
1	K	288	TYR
1	K	310	LEU
1	K	367	LYS
1	K	398	PHE
1	K	439	TYR
1	K	476	LEU
1	K	579	VAL
1	K	603	ASP
1	L	86	SER
1	L	92	VAL
1	L	161	ASN
1	L	165	PHE
1	L	167	VAL
1	L	184	SER
1	L	200	GLU
1	L	275	ASP
1	L	288	TYR
1	L	310	LEU
1	L	367	LYS
1	L	398	PHE
1	L	439	TYR
1	L	508	GLU

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Mol	Chain	Res	Type
1	L	518	LYS
1	L	579	VAL
1	L	584	LYS
1	L	605	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	113	GLN
1	B	181	ASN
1	B	229	ASN
1	C	181	ASN
1	C	215	HIS
1	E	161	ASN
1	E	181	ASN
1	E	272	ASN
1	E	531	ASN
1	F	217	ASN
1	G	122	ASN
1	G	567	GLN
1	H	183	ASN
1	H	511	ASN
1	I	139	ASN
1	I	166	ASN
1	I	602	ASN
1	K	181	ASN
1	K	322	ASN
1	K	602	ASN
1	L	420	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 24 are monoatomic - leaving 76 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	$\# Z > 2$
5	SO4	A	1	-	4,4,4	0.18	0	6,6,6	0.29	0
2	CO3	A	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	A	1003	3	20,26,26	0.82	0	20,35,35	1.18	2 (10%)
6	1PE	A	19	-	8,8,15	0.61	0	7,7,14	0.20	0
5	SO4	A	2	-	4,4,4	0.25	0	6,6,6	0.56	0
6	1PE	A	20	-	11,11,15	0.63	0	10,10,14	0.34	0
5	SO4	A	24	-	4,4,4	0.23	0	6,6,6	0.32	0
2	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	B	1003	3	20,26,26	0.89	0	20,35,35	0.89	0
6	1PE	B	60	-	9,9,15	0.54	0	8,8,14	0.29	0
6	1PE	B	61	-	9,9,15	0.71	0	8,8,14	0.91	0
6	1PE	B	62	-	9,9,15	0.68	0	8,8,14	0.43	0
2	CO3	C	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	C	1003	3	20,26,26	1.18	1 (5%)	20,35,35	1.44	3 (15%)
6	1PE	C	17	-	12,12,15	0.91	0	11,11,14	1.03	1 (9%)
6	1PE	C	18	-	8,8,15	0.59	0	7,7,14	0.38	0
5	SO4	C	3	-	4,4,4	0.12	0	6,6,6	0.37	0
2	CO3	D	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	D	1003	3	20,26,26	0.99	1 (5%)	20,35,35	1.16	2 (10%)
6	1PE	D	44	-	10,10,15	0.70	0	9,9,14	0.44	0
5	SO4	D	5	-	4,4,4	0.15	0	6,6,6	0.15	0
6	1PE	D	63	-	9,9,15	0.70	0	8,8,14	0.42	0
6	1PE	D	67	-	6,6,15	0.73	0	5,5,14	0.36	0
6	1PE	D	9	-	9,9,15	0.61	0	8,8,14	0.58	0
2	CO3	E	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	E	1003	3	20,26,26	0.76	0	20,35,35	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	E	22	-	4,4,4	0.23	0	6,6,6	0.28	0
6	1PE	E	43	-	7,7,15	0.47	0	6,6,14	0.49	0
6	1PE	E	612	-	11,11,15	0.60	0	10,10,14	0.42	0
5	SO4	E	7	-	4,4,4	0.09	0	6,6,6	0.39	0
6	1PE	E	8	-	11,11,15	0.53	0	10,10,14	0.44	0
2	CO3	F	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	F	1003	3	20,26,26	1.11	1 (5%)	20,35,35	0.95	0
5	SO4	F	21	-	4,4,4	0.22	0	6,6,6	0.23	0
6	1PE	F	31	-	9,9,15	0.50	0	8,8,14	0.52	0
6	1PE	F	32	-	9,9,15	0.67	0	8,8,14	0.43	0
6	1PE	F	33	-	9,9,15	0.62	0	8,8,14	0.27	0
2	CO3	G	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	G	1003	3	20,26,26	0.96	0	20,35,35	1.11	0
6	1PE	G	12	-	8,8,15	0.49	0	7,7,14	0.20	0
5	SO4	G	23	-	4,4,4	0.14	0	6,6,6	0.20	0
5	SO4	G	26	-	4,4,4	0.14	0	6,6,6	0.06	0
6	1PE	G	30	-	6,6,15	0.56	0	5,5,14	0.43	0
6	1PE	G	47	-	5,5,15	0.41	0	4,4,14	0.25	0
6	1PE	G	48	-	5,5,15	0.65	0	4,4,14	0.79	0
6	1PE	G	58	-	14,14,15	0.73	0	13,13,14	0.53	0
2	CO3	H	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	H	1003	3	20,26,26	0.79	0	20,35,35	0.94	0
6	1PE	H	64	-	9,9,15	0.62	0	8,8,14	0.25	0
6	1PE	H	65	-	9,9,15	0.59	0	8,8,14	0.23	0
2	CO3	I	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	I	1003	3	20,26,26	0.78	1 (5%)	20,35,35	1.63	2 (10%)
5	SO4	I	17	-	4,4,4	0.10	0	6,6,6	0.16	0
6	1PE	I	21	-	14,14,15	0.73	0	13,13,14	0.50	0
6	1PE	I	22	-	10,10,15	0.57	0	9,9,14	0.52	0
6	1PE	I	66	-	6,6,15	0.61	0	5,5,14	0.55	0
2	CO3	J	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	J	1003	3	20,26,26	0.86	0	20,35,35	0.62	0
5	SO4	J	18	-	4,4,4	0.19	0	6,6,6	0.30	0
6	1PE	J	2	-	10,10,15	0.61	0	9,9,14	0.36	0
5	SO4	J	20	-	4,4,4	0.11	0	6,6,6	0.29	0
6	1PE	J	3	-	9,9,15	0.59	0	8,8,14	0.53	0
6	1PE	J	45	-	9,9,15	0.67	0	8,8,14	0.52	0
2	CO3	K	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	K	1003	3	20,26,26	0.70	0	20,35,35	1.83	3 (15%)
5	SO4	K	19	-	4,4,4	0.18	0	6,6,6	0.20	0
6	1PE	K	4	-	11,11,15	0.73	0	10,10,14	0.64	0
6	1PE	K	42	-	10,10,15	0.59	0	9,9,14	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	K	5	-	11,11,15	0.51	0	10,10,14	0.41	0
6	1PE	K	50	-	5,5,15	0.68	0	4,4,14	0.50	0
6	1PE	L	1	-	9,9,15	0.52	0	8,8,14	0.37	0
2	CO3	L	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BEY	L	1003	3	20,26,26	0.85	1 (5%)	20,35,35	0.97	1 (5%)
5	SO4	L	25	-	4,4,4	0.18	0	6,6,6	0.33	0
6	1PE	L	56	-	10,10,15	0.78	0	9,9,14	0.48	0
6	1PE	L	612	-	11,11,15	0.65	0	10,10,14	0.33	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
5	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	CO3	A	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	A	1003	3	-	0/14/24/24	0/2/2/2
6	1PE	A	19	-	-	0/6/6/13	0/0/0/0
5	SO4	A	2	-	-	0/0/0/0	0/0/0/0
6	1PE	A	20	-	-	0/9/9/13	0/0/0/0
5	SO4	A	24	-	-	0/0/0/0	0/0/0/0
2	CO3	B	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	B	1003	3	-	0/14/24/24	0/2/2/2
6	1PE	B	60	-	-	0/7/7/13	0/0/0/0
6	1PE	B	61	-	-	0/7/7/13	0/0/0/0
6	1PE	B	62	-	-	0/7/7/13	0/0/0/0
2	CO3	C	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	C	1003	3	-	0/14/24/24	0/2/2/2
6	1PE	C	17	-	-	0/10/10/13	0/0/0/0
6	1PE	C	18	-	-	0/6/6/13	0/0/0/0
5	SO4	C	3	-	-	0/0/0/0	0/0/0/0
2	CO3	D	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	D	1003	3	-	0/14/24/24	0/2/2/2
6	1PE	D	44	-	-	0/8/8/13	0/0/0/0
5	SO4	D	5	-	-	0/0/0/0	0/0/0/0
6	1PE	D	63	-	-	0/7/7/13	0/0/0/0
6	1PE	D	67	-	-	0/4/4/13	0/0/0/0
6	1PE	D	9	-	-	0/7/7/13	0/0/0/0
2	CO3	E	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	E	1003	3	-	0/14/24/24	0/2/2/2
5	SO4	E	22	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	E	43	-	-	0/5/5/13	0/0/0/0
6	1PE	E	612	-	-	0/9/9/13	0/0/0/0
5	SO4	E	7	-	-	0/0/0/0	0/0/0/0
6	1PE	E	8	-	-	0/9/9/13	0/0/0/0
2	CO3	F	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	F	1003	3	-	0/14/24/24	0/2/2/2
5	SO4	F	21	-	-	0/0/0/0	0/0/0/0
6	1PE	F	31	-	-	0/7/7/13	0/0/0/0
6	1PE	F	32	-	-	0/7/7/13	0/0/0/0
6	1PE	F	33	-	-	0/7/7/13	0/0/0/0
2	CO3	G	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	G	1003	3	-	0/14/24/24	0/2/2/2
6	1PE	G	12	-	-	0/6/6/13	0/0/0/0
5	SO4	G	23	-	-	0/0/0/0	0/0/0/0
5	SO4	G	26	-	-	0/0/0/0	0/0/0/0
6	1PE	G	30	-	-	0/4/4/13	0/0/0/0
6	1PE	G	47	-	-	0/3/3/13	0/0/0/0
6	1PE	G	48	-	-	0/3/3/13	0/0/0/0
6	1PE	G	58	-	-	0/12/12/13	0/0/0/0
2	CO3	H	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	H	1003	3	-	0/14/24/24	0/2/2/2
6	1PE	H	64	-	-	0/7/7/13	0/0/0/0
6	1PE	H	65	-	-	0/7/7/13	0/0/0/0
2	CO3	I	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	I	1003	3	-	0/14/24/24	0/2/2/2
5	SO4	I	17	-	-	0/0/0/0	0/0/0/0
6	1PE	I	21	-	-	0/12/12/13	0/0/0/0
6	1PE	I	22	-	-	0/8/8/13	0/0/0/0
6	1PE	I	66	-	-	0/4/4/13	0/0/0/0
2	CO3	J	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	J	1003	3	-	0/14/24/24	0/2/2/2
5	SO4	J	18	-	-	0/0/0/0	0/0/0/0
6	1PE	J	2	-	-	0/8/8/13	0/0/0/0
5	SO4	J	20	-	-	0/0/0/0	0/0/0/0
6	1PE	J	3	-	-	0/7/7/13	0/0/0/0
6	1PE	J	45	-	-	0/7/7/13	0/0/0/0
2	CO3	K	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	K	1003	3	-	0/14/24/24	0/2/2/2
5	SO4	K	19	-	-	0/0/0/0	0/0/0/0
6	1PE	K	4	-	-	0/9/9/13	0/0/0/0
6	1PE	K	42	-	-	0/8/8/13	0/0/0/0
6	1PE	K	5	-	-	0/9/9/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	K	50	-	-	0/3/3/13	0/0/0/0
6	1PE	L	1	-	-	0/7/7/13	0/0/0/0
2	CO3	L	1002	-	-	0/0/0/0	0/0/0/0
4	BEY	L	1003	3	-	0/14/24/24	0/2/2/2
5	SO4	L	25	-	-	0/0/0/0	0/0/0/0
6	1PE	L	56	-	-	0/8/8/13	0/0/0/0
6	1PE	L	612	-	-	0/9/9/13	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1003	BEY	P-C17	2.21	1.81	1.79
4	L	1003	BEY	P-C17	2.43	1.82	1.79
4	F	1003	BEY	P-C17	2.69	1.82	1.79
4	D	1003	BEY	P-C17	2.86	1.82	1.79
4	C	1003	BEY	P-C17	3.97	1.83	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1003	BEY	C7-C8-C9	-4.27	102.27	111.08
4	K	1003	BEY	O3-P-C19	-3.79	99.15	107.08
4	A	1003	BEY	O3-P-C19	-3.06	100.67	107.08
4	D	1003	BEY	O3-P-C19	-2.98	100.84	107.08
4	C	1003	BEY	C1-C7-C8	-2.98	109.58	113.82
4	D	1003	BEY	C1-C7-C8	-2.10	110.83	113.82
4	E	1003	BEY	C7-C8-C9	2.00	115.21	111.08
4	C	1003	BEY	C5-C1-C2	2.00	121.34	118.16
6	C	17	1PE	OH4-C24-C14	2.01	119.64	110.41
4	L	1003	BEY	C1-C7-C8	2.12	116.83	113.82
4	A	1003	BEY	C13-C16-C10	2.14	121.55	118.16
4	I	1003	BEY	C7-C8-C9	3.08	117.44	111.08
4	K	1003	BEY	C7-C8-C9	4.22	119.79	111.08
4	K	1003	BEY	C1-C7-C8	4.59	120.36	113.82
4	I	1003	BEY	C1-C7-C8	5.53	121.69	113.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

49 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	BEY	4	0
6	A	20	1PE	2	0
4	B	1003	BEY	2	0
6	B	60	1PE	1	0
6	B	61	1PE	2	0
4	C	1003	BEY	5	0
6	C	17	1PE	1	0
5	C	3	SO4	1	0
2	D	1002	CO3	2	0
4	D	1003	BEY	6	0
6	D	44	1PE	4	0
6	D	63	1PE	1	0
4	E	1003	BEY	2	0
5	E	22	SO4	1	0
6	E	43	1PE	2	0
6	E	612	1PE	1	0
5	E	7	SO4	2	0
4	F	1003	BEY	2	0
5	F	21	SO4	1	0
6	F	31	1PE	1	0
4	G	1003	BEY	2	0
6	G	30	1PE	1	0
6	G	47	1PE	1	0
6	G	58	1PE	2	0
2	H	1002	CO3	1	0
4	H	1003	BEY	7	0
6	H	65	1PE	1	0
2	I	1002	CO3	1	0
4	I	1003	BEY	2	0
5	I	17	SO4	1	0
6	I	21	1PE	4	0
6	I	22	1PE	1	0
2	J	1002	CO3	1	0
4	J	1003	BEY	3	0
5	J	18	SO4	1	0
6	J	2	1PE	2	0
5	J	20	SO4	1	0
6	J	3	1PE	5	0
6	J	45	1PE	2	0
2	K	1002	CO3	2	0
4	K	1003	BEY	4	0
6	K	4	1PE	1	0
6	K	42	1PE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	5	1PE	3	0
6	K	50	1PE	1	0
6	L	1	1PE	2	0
2	L	1002	CO3	1	0
4	L	1003	BEY	2	0
6	L	612	1PE	3	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	518/528 (98%)	0.11	9 (1%) 70 69	13, 25, 45, 61	1 (0%)
1	B	518/528 (98%)	0.16	10 (1%) 67 65	13, 29, 64, 77	0
1	C	518/528 (98%)	0.11	2 (0%) 92 92	11, 26, 49, 59	0
1	D	513/528 (97%)	-0.05	3 (0%) 89 89	15, 25, 45, 66	0
1	E	510/528 (96%)	-0.01	5 (0%) 82 81	11, 24, 40, 59	0
1	F	510/528 (96%)	0.46	40 (7%) 14 12	18, 30, 60, 72	0
1	G	516/528 (97%)	0.17	8 (1%) 72 71	13, 25, 44, 62	0
1	H	509/528 (96%)	0.10	5 (0%) 82 81	14, 28, 60, 72	0
1	I	518/528 (98%)	0.14	6 (1%) 79 78	15, 26, 52, 64	0
1	J	513/528 (97%)	0.01	5 (0%) 82 81	12, 25, 46, 69	0
1	K	509/528 (96%)	-0.03	2 (0%) 92 92	13, 24, 42, 58	0
1	L	513/528 (97%)	0.26	16 (3%) 49 46	16, 28, 55, 63	0
All	All	6165/6336 (97%)	0.12	111 (1%) 69 67	11, 26, 53, 77	1 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	363	GLY	5.6
1	F	362	LYS	5.5
1	F	156	PHE	4.6
1	B	259	VAL	4.6
1	F	140	GLY	4.6
1	F	113	GLN	4.4
1	J	260	ASN	4.2
1	B	257	LYS	4.0
1	L	145	SER	4.0
1	F	165	PHE	3.9
1	F	126	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	267	LEU	3.6
1	F	364	ASP	3.5
1	B	258	ASN	3.5
1	L	165	PHE	3.4
1	F	132	VAL	3.4
1	F	121	CYS	3.3
1	L	132	VAL	3.3
1	A	364	ASP	3.3
1	F	222	LEU	3.3
1	F	270	TYR	3.3
1	B	260	ASN	3.2
1	L	163	GLU	3.2
1	F	276	THR	3.2
1	G	183	ASN	3.1
1	F	157	LEU	3.1
1	F	148	VAL	3.1
1	G	602	ASN	3.1
1	F	127	LEU	3.1
1	G	148	VAL	3.0
1	L	141	PRO	3.0
1	F	223	THR	3.0
1	F	187	VAL	3.0
1	K	603	ASP	2.9
1	F	114	VAL	2.9
1	A	121	CYS	2.9
1	G	119	GLY	2.9
1	A	601	LEU	2.9
1	H	603	ASP	2.8
1	L	604	ALA	2.8
1	F	185	VAL	2.8
1	F	139	ASN	2.8
1	L	119	GLY	2.8
1	F	159	ASP	2.8
1	F	161	ASN	2.7
1	L	115	TYR	2.7
1	D	219	LEU	2.7
1	F	160	GLU	2.7
1	F	128	THR	2.7
1	L	144	ILE	2.6
1	A	603	ASP	2.6
1	B	603	ASP	2.6
1	F	271	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	141	PRO	2.6
1	J	261	MET	2.6
1	B	421	VAL	2.6
1	F	115	TYR	2.6
1	F	119	GLY	2.5
1	J	603	ASP	2.5
1	F	130	PHE	2.5
1	L	130	PHE	2.5
1	I	103	TYR	2.4
1	L	360	LYS	2.4
1	F	549	SER	2.4
1	B	176	TYR	2.4
1	L	140	GLY	2.4
1	H	196	ALA	2.4
1	A	277	TYR	2.4
1	F	183	ASN	2.4
1	E	456	GLY	2.4
1	L	363	GLY	2.4
1	J	599	PHE	2.4
1	A	119	GLY	2.3
1	F	145	SER	2.3
1	D	419	GLU	2.3
1	F	146	SER	2.3
1	E	366	LYS	2.3
1	I	421	VAL	2.3
1	I	259	VAL	2.2
1	F	210	LEU	2.2
1	E	361	SER	2.2
1	L	362	LYS	2.2
1	B	269	VAL	2.2
1	D	261	MET	2.2
1	L	146	SER	2.2
1	C	419	GLU	2.2
1	H	178	PHE	2.2
1	I	418	PRO	2.2
1	J	136	GLY	2.2
1	F	144	ILE	2.2
1	H	175	PHE	2.2
1	F	112	VAL	2.2
1	A	180	ASP	2.2
1	C	603	ASP	2.2
1	E	363	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	195	VAL	2.1
1	F	217	ASN	2.1
1	I	195	VAL	2.1
1	G	601	LEU	2.1
1	A	148	VAL	2.1
1	G	195	VAL	2.1
1	G	225	VAL	2.1
1	K	373	GLY	2.1
1	E	480	TYR	2.1
1	B	154	SER	2.1
1	I	420	ASN	2.1
1	L	158	LYS	2.1
1	A	602	ASN	2.0
1	G	118	LYS	2.0
1	B	263	TYR	2.0
1	H	163	GLU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	1PE	D	67	7/16	0.82	0.29	7.10	30,41,53,54	0
6	1PE	L	612	12/16	0.85	0.28	6.51	41,59,63,64	0
6	1PE	F	33	10/16	0.86	0.23	5.51	33,61,63,64	0
5	SO4	G	26	5/5	0.93	0.41	5.34	30,30,30,30	0
6	1PE	D	44	11/16	0.80	0.26	4.99	37,51,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CO3	J	1002	4/4	0.98	0.18	3.82	27,27,29,31	0
6	1PE	K	50	6/16	0.88	0.21	3.48	11,25,55,55	0
6	1PE	B	60	10/16	0.90	0.25	3.32	33,48,74,75	0
6	1PE	F	31	10/16	0.86	0.22	2.94	36,44,74,74	0
6	1PE	G	58	15/16	0.88	0.21	2.51	43,47,56,56	0
6	1PE	A	20	12/16	0.88	0.21	2.31	49,54,58,58	0
6	1PE	H	64	10/16	0.88	0.23	2.05	43,47,52,53	0
6	1PE	G	47	6/16	0.96	0.27	1.91	15,22,28,39	0
4	BEY	A	1003	25/25	0.94	0.19	1.68	17,33,63,65	0
2	CO3	F	1002	4/4	0.98	0.18	1.66	35,38,39,44	0
4	BEY	L	1003	25/25	0.92	0.20	1.62	36,57,69,71	0
5	SO4	A	2	5/5	0.84	0.19	1.33	60,62,74,74	0
2	CO3	L	1002	4/4	0.97	0.18	1.29	27,27,28,33	0
2	CO3	A	1002	4/4	0.95	0.16	1.19	39,42,43,46	0
6	1PE	J	2	11/16	0.94	0.21	1.08	12,25,44,48	0
4	BEY	K	1003	25/25	0.95	0.18	1.05	19,30,45,54	0
4	BEY	I	1003	25/25	0.94	0.17	1.03	21,33,40,50	0
2	CO3	B	1002	4/4	0.97	0.18	1.02	11,14,16,19	0
4	BEY	F	1003	25/25	0.92	0.18	0.95	23,35,51,55	0
2	CO3	H	1002	4/4	0.96	0.17	0.93	15,23,23,28	0
4	BEY	H	1003	25/25	0.90	0.18	0.91	26,38,46,50	0
2	CO3	E	1002	4/4	0.96	0.16	0.87	31,33,34,34	0
2	CO3	G	1002	4/4	0.97	0.17	0.80	19,20,22,26	0
6	1PE	E	43	8/16	0.86	0.22	0.76	43,45,55,55	0
4	BEY	J	1003	25/25	0.93	0.17	0.59	28,42,55,57	0
2	CO3	K	1002	4/4	0.95	0.17	0.58	25,30,31,37	0
4	BEY	D	1003	25/25	0.93	0.17	0.53	20,40,59,61	0
4	BEY	E	1003	25/25	0.94	0.17	0.45	22,42,59,61	0
4	BEY	C	1003	25/25	0.94	0.17	0.31	16,33,43,47	0
5	SO4	J	18	5/5	0.99	0.17	0.22	22,28,36,37	0
4	BEY	G	1003	25/25	0.94	0.16	0.12	13,29,59,61	0
4	BEY	B	1003	25/25	0.94	0.15	0.04	26,38,48,50	0
6	1PE	I	22	11/16	0.91	0.21	0.03	30,47,62,67	0
6	1PE	K	42	11/16	0.87	0.16	-0.12	30,44,49,51	0
6	1PE	D	9	10/16	0.91	0.17	-0.16	27,38,45,48	0
5	SO4	A	24	5/5	0.94	0.16	-0.31	53,57,63,64	0
6	1PE	E	8	12/16	0.93	0.15	-0.33	18,34,63,63	0
6	1PE	K	5	12/16	0.92	0.16	-0.48	23,35,52,53	0
2	CO3	C	1002	4/4	0.96	0.15	-0.65	13,21,22,28	0
6	1PE	A	19	9/16	0.93	0.14	-0.76	20,25,34,41	0
6	1PE	I	66	7/16	0.91	0.17	-0.79	26,35,44,46	0
5	SO4	C	3	5/5	0.99	0.14	-0.86	17,18,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CO3	D	1002	4/4	0.97	0.14	-1.00	22,24,25,27	0
6	1PE	L	1	10/16	0.95	0.13	-1.10	15,23,33,35	0
5	SO4	E	7	5/5	0.99	0.12	-1.45	16,24,35,37	0
6	1PE	G	12	9/16	0.94	0.14	-1.46	20,25,41,44	0
6	1PE	G	48	6/16	0.95	0.16	-2.09	16,22,26,26	0
5	SO4	I	17	5/5	0.99	0.10	-2.14	8,10,15,22	0
2	CO3	I	1002	4/4	0.98	0.12	-2.41	18,19,22,23	0
3	ZN	E	1001	1/1	0.99	0.06	-2.46	30,30,30,30	0
3	ZN	F	1001	1/1	0.99	0.08	-2.49	29,29,29,29	0
3	ZN	E	1004	1/1	0.99	0.04	-3.07	45,45,45,45	0
3	ZN	H	1001	1/1	0.99	0.07	-3.29	39,39,39,39	0
3	ZN	J	1004	1/1	0.99	0.05	-3.79	46,46,46,46	0
3	ZN	G	1004	1/1	0.98	0.08	-3.80	35,35,35,35	0
3	ZN	K	1001	1/1	1.00	0.05	-3.85	23,23,23,23	0
3	ZN	B	1001	1/1	0.99	0.06	-3.99	35,35,35,35	0
3	ZN	L	1001	1/1	0.99	0.08	-4.27	29,29,29,29	0
3	ZN	C	1001	1/1	0.99	0.07	-4.28	26,26,26,26	0
6	1PE	C	18	9/16	0.92	0.13	-4.31	27,36,38,45	0
3	ZN	G	1001	1/1	1.00	0.06	-4.36	28,28,28,28	0
3	ZN	C	1004	1/1	0.97	0.05	-4.40	42,42,42,42	0
3	ZN	D	1004	1/1	0.99	0.06	-4.48	39,39,39,39	0
3	ZN	H	1004	1/1	0.98	0.04	-4.59	32,32,32,32	0
3	ZN	B	1004	1/1	0.97	0.05	-4.65	36,36,36,36	0
3	ZN	K	1004	1/1	0.96	0.04	-4.65	39,39,39,39	0
3	ZN	A	1004	1/1	0.99	0.06	-4.75	37,37,37,37	0
3	ZN	F	1004	1/1	0.99	0.05	-4.88	37,37,37,37	0
3	ZN	J	1001	1/1	0.98	0.06	-5.15	39,39,39,39	0
3	ZN	A	1001	1/1	0.99	0.07	-5.76	30,30,30,30	0
3	ZN	L	1004	1/1	0.99	0.05	-6.22	39,39,39,39	0
3	ZN	I	1004	1/1	0.99	0.06	-6.69	35,35,35,35	0
3	ZN	I	1001	1/1	0.99	0.07	-7.30	26,26,26,26	0
3	ZN	D	1001	1/1	0.97	0.05	-7.38	41,41,41,41	0
5	SO4	K	19	5/5	0.97	0.33	-	71,71,76,77	0
5	SO4	G	23	5/5	0.97	0.20	-	45,45,49,50	0
5	SO4	E	22	5/5	0.89	0.36	-	90,90,94,97	0
6	1PE	I	21	15/16	0.91	0.20	-	25,34,53,54	0
6	1PE	C	17	13/16	0.90	0.20	-	15,36,43,43	0
6	1PE	B	62	10/16	0.44	0.47	-	74,89,91,92	0
5	SO4	A	1	5/5	0.94	0.18	-	61,62,66,66	0
6	1PE	L	56	11/16	0.82	0.19	-	30,44,50,50	0
6	1PE	E	612	12/16	0.88	0.26	-	31,46,54,55	0
6	1PE	H	65	10/16	0.90	0.20	-	42,49,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	L	25	5/5	0.93	0.15	-	68,71,75,76	0
6	1PE	B	61	10/16	0.86	0.21	-	34,46,48,51	0
6	1PE	J	45	10/16	0.66	0.35	-	50,68,73,75	0
6	1PE	G	30	7/16	0.94	0.16	-	24,39,53,57	0
6	1PE	F	32	10/16	0.92	0.14	-	33,42,45,46	0
6	1PE	J	3	10/16	0.89	0.30	-	33,50,53,54	0
6	1PE	K	4	12/16	0.82	0.21	-	27,44,55,55	0
5	SO4	D	5	5/5	0.94	0.30	-	92,94,97,97	0
5	SO4	F	21	5/5	0.95	0.17	-	69,70,71,75	0
6	1PE	D	63	10/16	0.88	0.19	-	37,42,46,53	0
5	SO4	J	20	5/5	0.93	0.41	-	72,74,78,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.