



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:00 AM GMT

PDB ID : 3KFE
Title : Crystal structures of a group II chaperonin from *Methanococcus maripaludis*
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.; Meyer, D.; Knee, K.M.; Goulet, D.R.; King, J.A.; Frydman, J.; Adams, P.D.
Deposited on : 2009-10-27
Resolution : 3.50 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

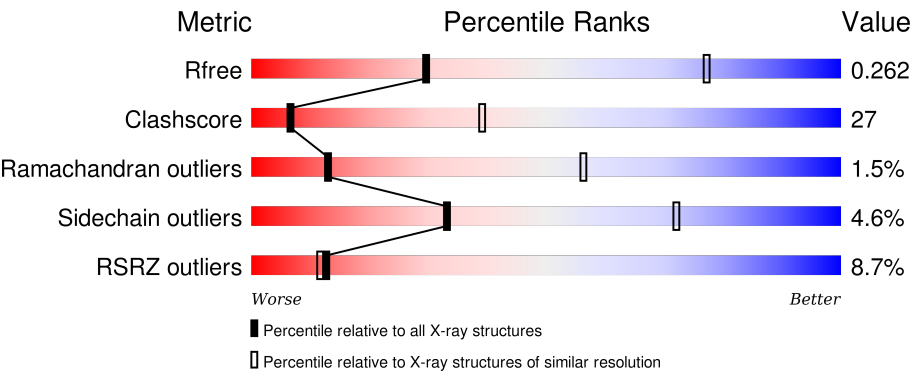
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	521	<div><div>8%</div><div>51%39%7%</div></div>
1	B	521	<div><div>2%</div><div>51%39%7%</div></div>
1	C	521	<div><div>8%</div><div>51%40%7%</div></div>
1	D	521	<div><div>9%</div><div>51%39%7%</div></div>
1	E	521	<div><div>11%</div><div>50%40%7%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	521	
1	G	521	
1	H	521	

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	MG	B	544	-	-	-	X
2	MG	F	544	-	-	-	X
2	MG	H	544	-	-	-	X
4	SO4	A	546	-	-	X	-
4	SO4	B	546	-	-	X	-
4	SO4	C	546	-	-	X	-
4	SO4	D	546	-	-	X	-
4	SO4	E	546	-	-	X	-
4	SO4	F	546	-	-	X	-
4	SO4	G	546	-	-	X	-
4	SO4	H	546	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29296 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	B	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	C	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	D	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	E	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	F	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	G	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	H	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	DELETION	UNP Q877G8
A	?	-	LYS	DELETION	UNP Q877G8
A	?	-	GLU	DELETION	UNP Q877G8
A	?	-	THR	DELETION	UNP Q877G8
A	?	-	ASP	DELETION	UNP Q877G8
A	?	-	ALA	DELETION	UNP Q877G8
A	?	-	GLU	DELETION	UNP Q877G8
A	?	-	ILE	DELETION	UNP Q877G8
A	?	-	ARG	DELETION	UNP Q877G8
A	?	-	ILE	DELETION	UNP Q877G8
A	?	-	THR	DELETION	UNP Q877G8
A	?	-	ASP	DELETION	UNP Q877G8
A	?	-	PRO	DELETION	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP Q877G8
A	?	-	LEU	DELETION	UNP Q877G8
A	?	-	MET	DELETION	UNP Q877G8
A	?	-	GLU	DELETION	UNP Q877G8
A	?	-	PHE	DELETION	UNP Q877G8
A	?	-	ILE	DELETION	UNP Q877G8
A	264	THR	GLN	ENGINEERED	UNP Q877G8
A	265	ALA	GLU	ENGINEERED	UNP Q877G8
A	266	SER	GLU	ENGINEERED	UNP Q877G8
A	267	GLU	LYS	ENGINEERED	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	?	-	LYS	DELETION	UNP Q877G8
B	?	-	GLU	DELETION	UNP Q877G8
B	?	-	THR	DELETION	UNP Q877G8
B	?	-	ASP	DELETION	UNP Q877G8
B	?	-	ALA	DELETION	UNP Q877G8
B	?	-	GLU	DELETION	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	?	-	ARG	DELETION	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	?	-	THR	DELETION	UNP Q877G8
B	?	-	ASP	DELETION	UNP Q877G8
B	?	-	PRO	DELETION	UNP Q877G8
B	?	-	LYS	DELETION	UNP Q877G8
B	?	-	LEU	DELETION	UNP Q877G8
B	?	-	MET	DELETION	UNP Q877G8
B	?	-	GLU	DELETION	UNP Q877G8
B	?	-	PHE	DELETION	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	264	THR	GLN	ENGINEERED	UNP Q877G8
B	265	ALA	GLU	ENGINEERED	UNP Q877G8
B	266	SER	GLU	ENGINEERED	UNP Q877G8
B	267	GLU	LYS	ENGINEERED	UNP Q877G8
C	?	-	ILE	DELETION	UNP Q877G8
C	?	-	LYS	DELETION	UNP Q877G8
C	?	-	GLU	DELETION	UNP Q877G8
C	?	-	THR	DELETION	UNP Q877G8
C	?	-	ASP	DELETION	UNP Q877G8
C	?	-	ALA	DELETION	UNP Q877G8
C	?	-	GLU	DELETION	UNP Q877G8
C	?	-	ILE	DELETION	UNP Q877G8
C	?	-	ARG	DELETION	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ILE	DELETION	UNP Q877G8
C	?	-	THR	DELETION	UNP Q877G8
C	?	-	ASP	DELETION	UNP Q877G8
C	?	-	PRO	DELETION	UNP Q877G8
C	?	-	LYS	DELETION	UNP Q877G8
C	?	-	LEU	DELETION	UNP Q877G8
C	?	-	MET	DELETION	UNP Q877G8
C	?	-	GLU	DELETION	UNP Q877G8
C	?	-	PHE	DELETION	UNP Q877G8
C	?	-	ILE	DELETION	UNP Q877G8
C	264	THR	GLN	ENGINEERED	UNP Q877G8
C	265	ALA	GLU	ENGINEERED	UNP Q877G8
C	266	SER	GLU	ENGINEERED	UNP Q877G8
C	267	GLU	LYS	ENGINEERED	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	?	-	LYS	DELETION	UNP Q877G8
D	?	-	GLU	DELETION	UNP Q877G8
D	?	-	THR	DELETION	UNP Q877G8
D	?	-	ASP	DELETION	UNP Q877G8
D	?	-	ALA	DELETION	UNP Q877G8
D	?	-	GLU	DELETION	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	?	-	ARG	DELETION	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	?	-	THR	DELETION	UNP Q877G8
D	?	-	ASP	DELETION	UNP Q877G8
D	?	-	PRO	DELETION	UNP Q877G8
D	?	-	LYS	DELETION	UNP Q877G8
D	?	-	LEU	DELETION	UNP Q877G8
D	?	-	MET	DELETION	UNP Q877G8
D	?	-	GLU	DELETION	UNP Q877G8
D	?	-	PHE	DELETION	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	264	THR	GLN	ENGINEERED	UNP Q877G8
D	265	ALA	GLU	ENGINEERED	UNP Q877G8
D	266	SER	GLU	ENGINEERED	UNP Q877G8
D	267	GLU	LYS	ENGINEERED	UNP Q877G8
E	?	-	ILE	DELETION	UNP Q877G8
E	?	-	LYS	DELETION	UNP Q877G8
E	?	-	GLU	DELETION	UNP Q877G8
E	?	-	THR	DELETION	UNP Q877G8
E	?	-	ASP	DELETION	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ALA	DELETION	UNP Q877G8
E	?	-	GLU	DELETION	UNP Q877G8
E	?	-	ILE	DELETION	UNP Q877G8
E	?	-	ARG	DELETION	UNP Q877G8
E	?	-	ILE	DELETION	UNP Q877G8
E	?	-	THR	DELETION	UNP Q877G8
E	?	-	ASP	DELETION	UNP Q877G8
E	?	-	PRO	DELETION	UNP Q877G8
E	?	-	LYS	DELETION	UNP Q877G8
E	?	-	LEU	DELETION	UNP Q877G8
E	?	-	MET	DELETION	UNP Q877G8
E	?	-	GLU	DELETION	UNP Q877G8
E	?	-	PHE	DELETION	UNP Q877G8
E	?	-	ILE	DELETION	UNP Q877G8
E	264	THR	GLN	ENGINEERED	UNP Q877G8
E	265	ALA	GLU	ENGINEERED	UNP Q877G8
E	266	SER	GLU	ENGINEERED	UNP Q877G8
E	267	GLU	LYS	ENGINEERED	UNP Q877G8
F	?	-	ILE	DELETION	UNP Q877G8
F	?	-	LYS	DELETION	UNP Q877G8
F	?	-	GLU	DELETION	UNP Q877G8
F	?	-	THR	DELETION	UNP Q877G8
F	?	-	ASP	DELETION	UNP Q877G8
F	?	-	ALA	DELETION	UNP Q877G8
F	?	-	GLU	DELETION	UNP Q877G8
F	?	-	ILE	DELETION	UNP Q877G8
F	?	-	ARG	DELETION	UNP Q877G8
F	?	-	ILE	DELETION	UNP Q877G8
F	?	-	THR	DELETION	UNP Q877G8
F	?	-	ASP	DELETION	UNP Q877G8
F	?	-	PRO	DELETION	UNP Q877G8
F	?	-	LYS	DELETION	UNP Q877G8
F	?	-	LEU	DELETION	UNP Q877G8
F	?	-	MET	DELETION	UNP Q877G8
F	?	-	GLU	DELETION	UNP Q877G8
F	?	-	PHE	DELETION	UNP Q877G8
F	?	-	ILE	DELETION	UNP Q877G8
F	264	THR	GLN	ENGINEERED	UNP Q877G8
F	265	ALA	GLU	ENGINEERED	UNP Q877G8
F	266	SER	GLU	ENGINEERED	UNP Q877G8
F	267	GLU	LYS	ENGINEERED	UNP Q877G8
G	?	-	ILE	DELETION	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	DELETION	UNP Q877G8
G	?	-	GLU	DELETION	UNP Q877G8
G	?	-	THR	DELETION	UNP Q877G8
G	?	-	ASP	DELETION	UNP Q877G8
G	?	-	ALA	DELETION	UNP Q877G8
G	?	-	GLU	DELETION	UNP Q877G8
G	?	-	ILE	DELETION	UNP Q877G8
G	?	-	ARG	DELETION	UNP Q877G8
G	?	-	ILE	DELETION	UNP Q877G8
G	?	-	THR	DELETION	UNP Q877G8
G	?	-	ASP	DELETION	UNP Q877G8
G	?	-	PRO	DELETION	UNP Q877G8
G	?	-	LYS	DELETION	UNP Q877G8
G	?	-	LEU	DELETION	UNP Q877G8
G	?	-	MET	DELETION	UNP Q877G8
G	?	-	GLU	DELETION	UNP Q877G8
G	?	-	PHE	DELETION	UNP Q877G8
G	?	-	ILE	DELETION	UNP Q877G8
G	264	THR	GLN	ENGINEERED	UNP Q877G8
G	265	ALA	GLU	ENGINEERED	UNP Q877G8
G	266	SER	GLU	ENGINEERED	UNP Q877G8
G	267	GLU	LYS	ENGINEERED	UNP Q877G8
H	?	-	ILE	DELETION	UNP Q877G8
H	?	-	LYS	DELETION	UNP Q877G8
H	?	-	GLU	DELETION	UNP Q877G8
H	?	-	THR	DELETION	UNP Q877G8
H	?	-	ASP	DELETION	UNP Q877G8
H	?	-	ALA	DELETION	UNP Q877G8
H	?	-	GLU	DELETION	UNP Q877G8
H	?	-	ILE	DELETION	UNP Q877G8
H	?	-	ARG	DELETION	UNP Q877G8
H	?	-	ILE	DELETION	UNP Q877G8
H	?	-	THR	DELETION	UNP Q877G8
H	?	-	ASP	DELETION	UNP Q877G8
H	?	-	PRO	DELETION	UNP Q877G8
H	?	-	LYS	DELETION	UNP Q877G8
H	?	-	LEU	DELETION	UNP Q877G8
H	?	-	MET	DELETION	UNP Q877G8
H	?	-	GLU	DELETION	UNP Q877G8
H	?	-	PHE	DELETION	UNP Q877G8
H	?	-	ILE	DELETION	UNP Q877G8
H	264	THR	GLN	ENGINEERED	UNP Q877G8

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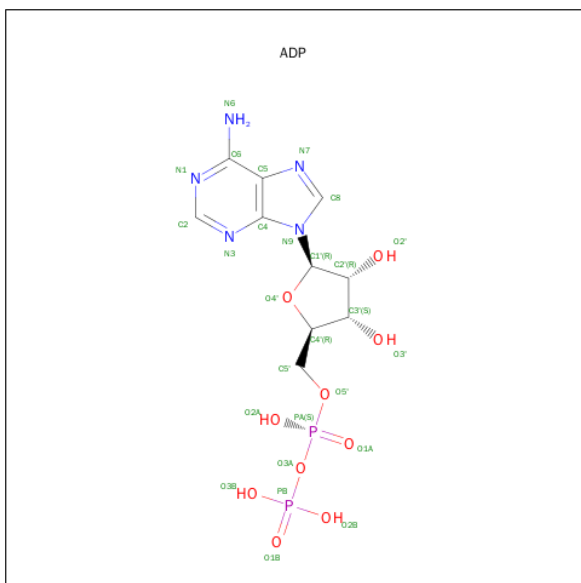
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Chain	Residue	Modelled	Actual	Comment	Reference
H	265	ALA	GLU	ENGINEERED	UNP Q877G8
H	266	SER	GLU	ENGINEERED	UNP Q877G8
H	267	GLU	LYS	ENGINEERED	UNP Q877G8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

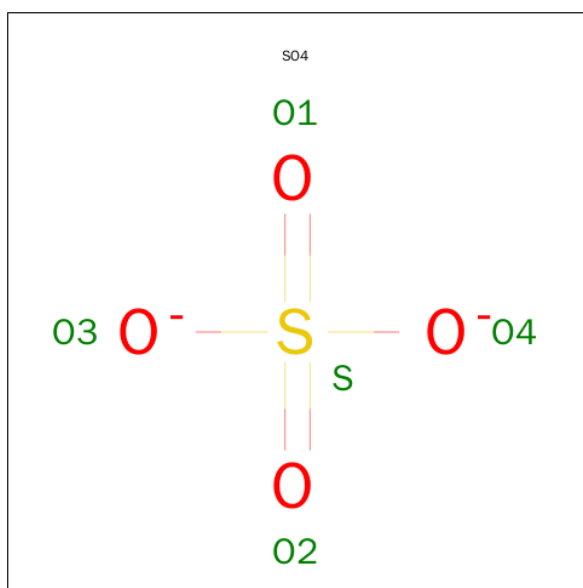
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

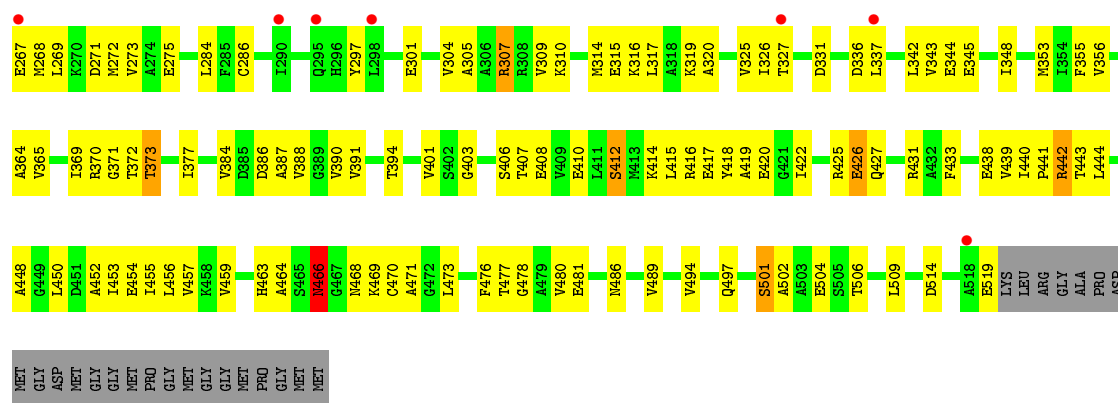


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S	0	0
			5 4 1			
4	B	1	Total	O S	0	0
			5 4 1			
4	C	1	Total	O S	0	0
			5 4 1			
4	D	1	Total	O S	0	0
			5 4 1			

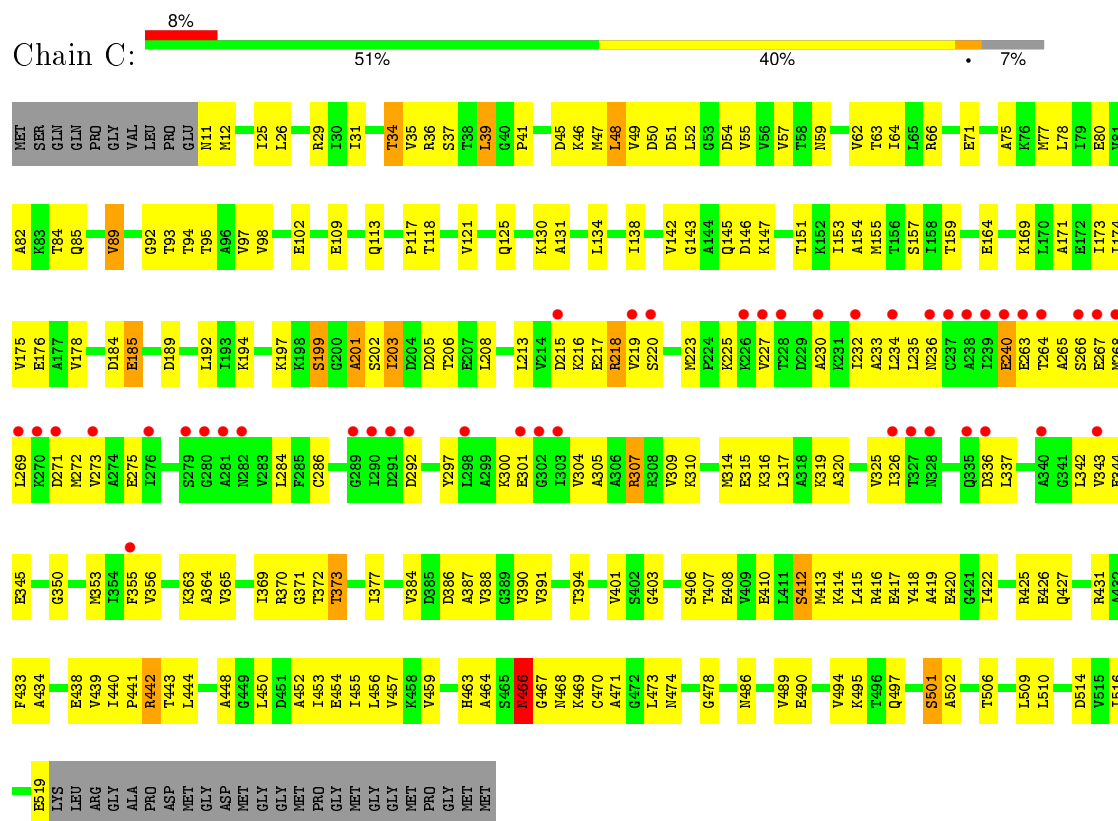
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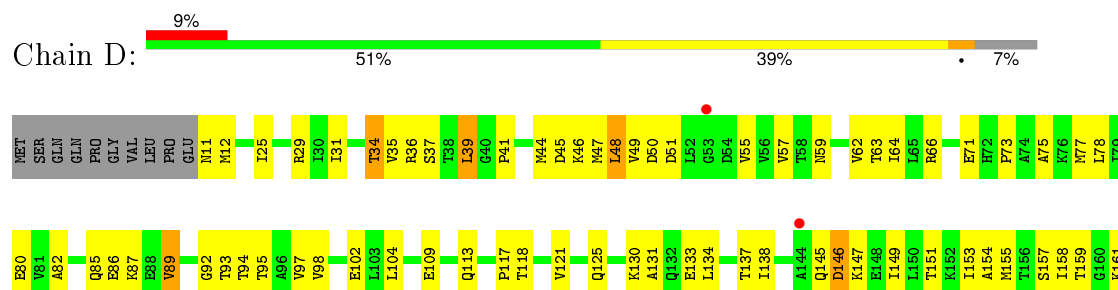
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

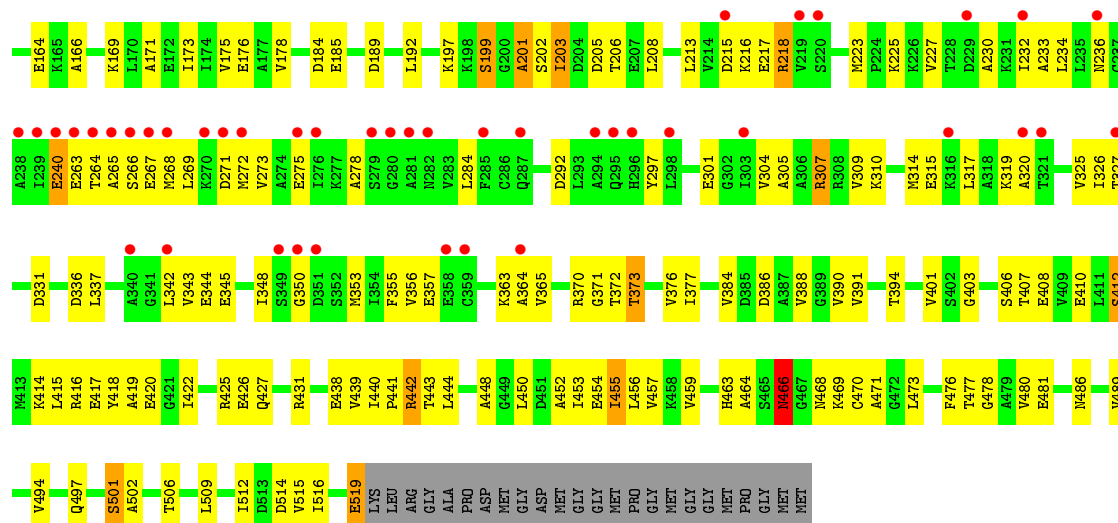


• Molecule 1: Chaperonin

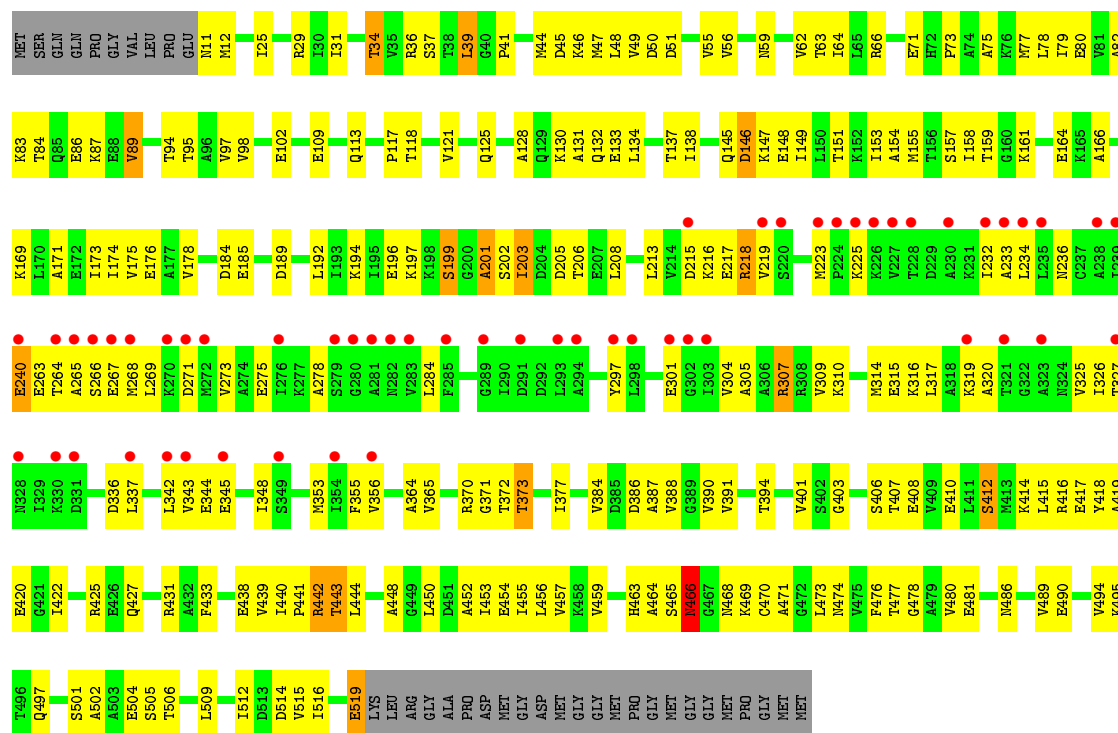


• Molecule 1: Chaperonin

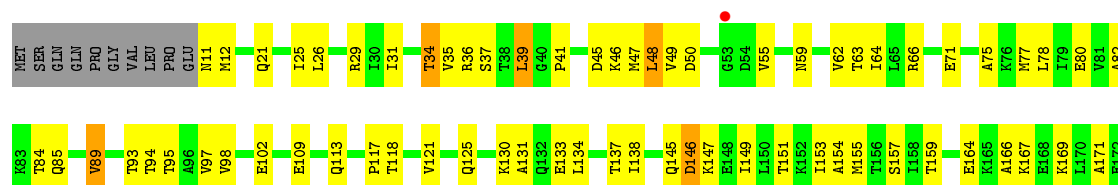


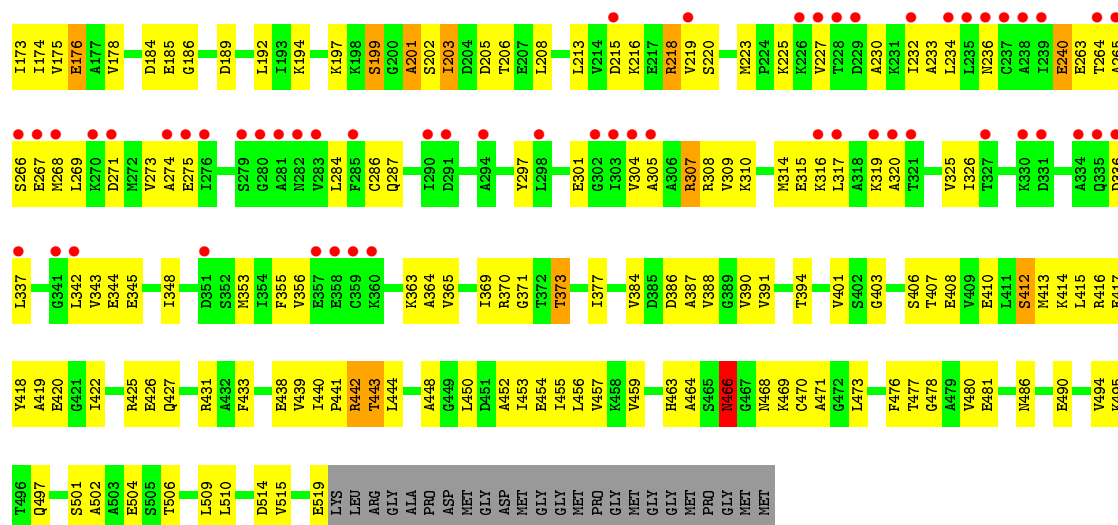


• Molecule 1: Chaperonin

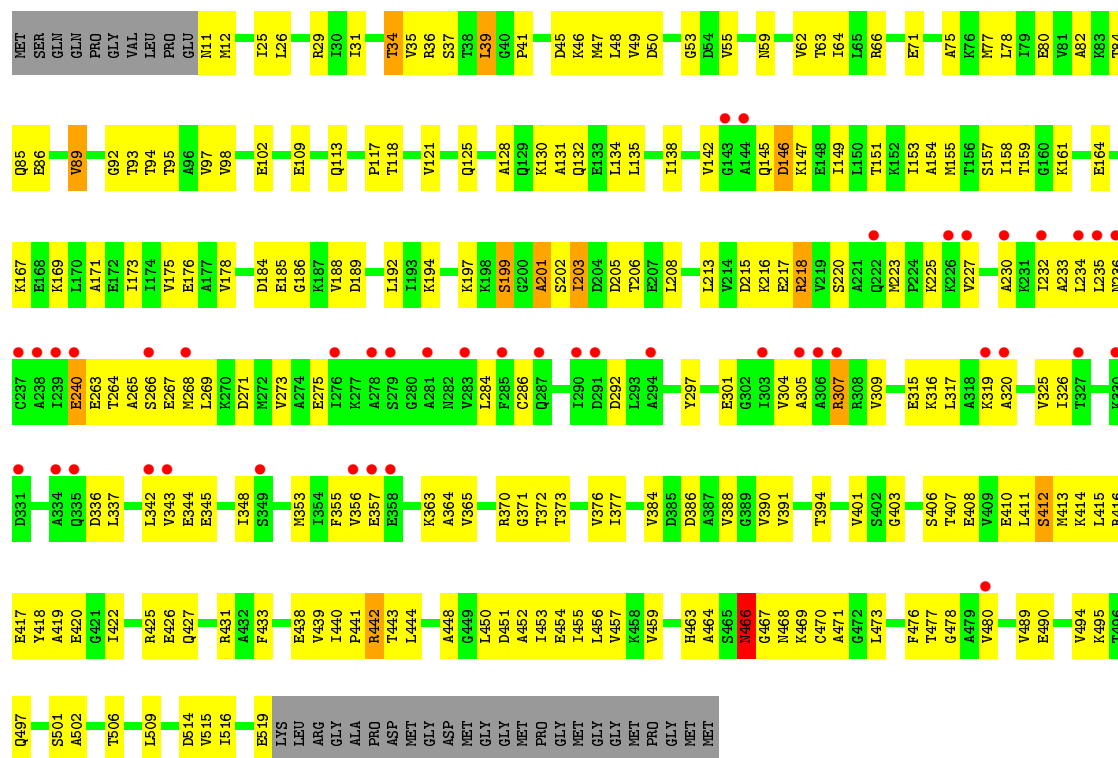


• Molecule 1: Chaperonin

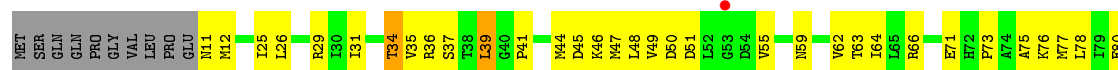




• Molecule 1: Chaperonin



• Molecule 1: Chaperonin





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.45Å 161.92Å 147.37Å 90.00° 124.12° 90.00°	Depositor
Resolution (Å)	54.49 – 3.50 54.49 – 3.50	Depositor EDS
% Data completeness (in resolution range)	77.1 (54.49-3.50) 86.5 (54.49-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.232 , 0.269 0.235 , 0.262	Depositor DCC
R_{free} test set	2797 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.0	EDS
Estimated twinning fraction	0.053 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 55394 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29296	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, SO4, ADP

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	0.49	0/3649	0.64	0/4911
1	B	0.50	1/3649 (0.0%)	0.63	0/4911
1	C	0.50	0/3649	0.63	0/4911
1	D	0.48	0/3649	0.62	0/4911
1	E	0.50	0/3649	0.63	0/4911
1	F	0.48	0/3649	0.62	0/4911
1	G	0.46	0/3649	0.62	0/4911
1	H	0.45	0/3649	0.62	0/4911
All	All	0.48	1/29192 (0.0%)	0.63	0/39288

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	HIS	CG-CD2	7.38	1.48	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ALA	Peptide
1	A	202	SER	Peptide
1	B	201	ALA	Peptide
1	C	201	ALA	Peptide
1	D	201	ALA	Peptide
1	E	201	ALA	Peptide
1	F	201	ALA	Peptide
1	G	201	ALA	Peptide
1	H	201	ALA	Peptide

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	3629	0	3762	198	5
1	B	3629	0	3762	202	1
1	C	3629	0	3762	217	3
1	D	3629	0	3762	232	0
1	E	3629	0	3762	221	3
1	F	3629	0	3762	199	3
1	G	3629	0	3762	206	4
1	H	3629	0	3762	212	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	12	5	0
3	B	27	0	12	6	0
3	C	27	0	12	7	0
3	D	27	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	27	0	12	6	0
3	F	27	0	12	6	0
3	G	27	0	12	6	0
3	H	27	0	12	6	0
4	A	5	0	0	3	0
4	B	5	0	0	4	0
4	C	5	0	0	5	0
4	D	5	0	0	4	0
4	E	5	0	0	4	0
4	F	5	0	0	4	0
4	G	5	0	0	4	0
4	H	5	0	0	4	0
All	All	29296	0	30192	1616	10

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 27.

All (1616) 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:39:LEU:HD23	1:H:444:LEU:CD2	1.71	1.21
1:G:39:LEU:HD23	1:G:444:LEU:CD2	1.73	1.18
1:D:39:LEU:HD23	1:D:444:LEU:CD2	1.74	1.17
1:F:39:LEU:HD23	1:F:444:LEU:CD2	1.71	1.17
1:C:39:LEU:HD23	1:C:444:LEU:CD2	1.74	1.16
1:E:39:LEU:HD23	1:E:444:LEU:CD2	1.76	1.16
1:A:39:LEU:HD23	1:A:444:LEU:CD2	1.76	1.16
1:B:39:LEU:HD23	1:B:444:LEU:CD2	1.73	1.15
1:C:206:THR:HG22	1:C:370:ARG:H	1.09	1.11
1:H:39:LEU:HD23	1:H:444:LEU:HD23	1.30	1.10
1:F:206:THR:HG22	1:F:370:ARG:H	1.07	1.10
1:D:206:THR:HG22	1:D:370:ARG:H	1.13	1.10
1:D:39:LEU:HD23	1:D:444:LEU:HD23	1.32	1.09
1:C:39:LEU:HD23	1:C:444:LEU:HD23	1.36	1.08
1:A:201:ALA:HB2	1:B:497:GLN:OE1	1.54	1.08
1:G:206:THR:HG22	1:G:370:ARG:H	1.11	1.07
1:B:39:LEU:HD23	1:B:444:LEU:HD23	1.33	1.07
1:E:206:THR:HG22	1:E:370:ARG:H	1.14	1.07
1:H:206:THR:HG22	1:H:370:ARG:H	1.09	1.06
1:G:39:LEU:HD23	1:G:444:LEU:HD23	1.32	1.06
1:E:39:LEU:HD23	1:E:444:LEU:HD23	1.34	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD23	1:A:444:LEU:HD23	1.34	1.04
1:F:39:LEU:HD23	1:F:444:LEU:HD23	1.34	1.03
1:A:206:THR:HG22	1:A:370:ARG:H	1.15	1.03
1:B:201:ALA:HB2	1:C:497:GLN:OE1	1.59	1.02
1:B:206:THR:HG22	1:B:370:ARG:H	1.19	1.00
1:A:372:THR:HB	1:B:501:SER:HB3	1.43	0.98
1:E:442:ARG:HG2	1:E:442:ARG:HH11	1.28	0.96
1:F:206:THR:HG22	1:F:370:ARG:N	1.81	0.96
1:C:46:LYS:HD3	1:D:514:ASP:HB3	1.48	0.94
1:C:39:LEU:HD23	1:C:444:LEU:HD21	1.49	0.94
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.31	0.94
1:D:372:THR:HB	1:E:501:SER:HB3	1.48	0.94
1:C:442:ARG:HH11	1:C:442:ARG:HG2	1.28	0.94
1:B:442:ARG:HG2	1:B:442:ARG:HH11	1.33	0.94
1:H:39:LEU:CD2	1:H:444:LEU:CD2	2.47	0.93
1:C:206:THR:HG22	1:C:370:ARG:N	1.82	0.93
1:F:39:LEU:HD23	1:F:444:LEU:HD21	1.47	0.93
1:H:206:THR:HG22	1:H:370:ARG:N	1.85	0.92
1:G:39:LEU:HD23	1:G:444:LEU:HD21	1.51	0.92
1:G:206:THR:HG22	1:G:370:ARG:N	1.85	0.92
1:D:442:ARG:HH11	1:D:442:ARG:HG2	1.34	0.92
1:B:39:LEU:CD2	1:B:444:LEU:CD2	2.49	0.91
1:B:130:LYS:HG3	1:B:134:LEU:HD12	1.51	0.91
1:D:39:LEU:CD2	1:D:444:LEU:CD2	2.49	0.91
1:F:442:ARG:HH11	1:F:442:ARG:HG2	1.35	0.91
1:H:39:LEU:HD23	1:H:444:LEU:HD21	1.50	0.90
1:G:39:LEU:CD2	1:G:444:LEU:CD2	2.48	0.90
1:E:45:ASP:OD1	1:E:59:ASN:HB2	1.70	0.90
1:F:39:LEU:CD2	1:F:444:LEU:CD2	2.49	0.90
1:C:201:ALA:HB2	1:D:497:GLN:OE1	1.72	0.90
1:B:39:LEU:HD23	1:B:444:LEU:HD21	1.51	0.90
1:E:206:THR:HG22	1:E:370:ARG:N	1.87	0.89
1:D:46:LYS:HD3	1:E:514:ASP:HB3	1.53	0.89
1:G:442:ARG:HH11	1:G:442:ARG:HG2	1.35	0.89
1:C:39:LEU:CD2	1:C:444:LEU:CD2	2.50	0.89
1:A:45:ASP:OD1	1:A:59:ASN:HB2	1.73	0.88
1:H:45:ASP:OD1	1:H:59:ASN:HB2	1.73	0.88
1:D:206:THR:HG22	1:D:370:ARG:N	1.88	0.88
1:F:45:ASP:OD1	1:F:59:ASN:HB2	1.73	0.88
1:B:45:ASP:OD1	1:B:59:ASN:HB2	1.74	0.88
1:D:39:LEU:HD23	1:D:444:LEU:HD21	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD23	1:A:444:LEU:HD21	1.55	0.87
1:A:514:ASP:HB3	1:H:46:LYS:HD3	1.53	0.87
1:B:373:THR:HB	1:C:80:GLU:HB3	1.56	0.87
1:E:39:LEU:HD23	1:E:444:LEU:HD21	1.55	0.87
1:A:164:GLU:HB2	1:B:125:GLN:OE1	1.75	0.86
1:D:45:ASP:OD1	1:D:59:ASN:HB2	1.75	0.86
1:E:39:LEU:CD2	1:E:444:LEU:CD2	2.51	0.86
1:A:39:LEU:CD2	1:A:444:LEU:CD2	2.52	0.86
1:D:46:LYS:HG3	1:D:64:ILE:HD13	1.57	0.86
1:F:439:VAL:O	1:F:443:THR:HG23	1.75	0.86
1:G:45:ASP:OD1	1:G:59:ASN:HB2	1.75	0.86
1:B:455:ILE:HG21	1:B:473:LEU:HD22	1.58	0.86
1:C:372:THR:HB	1:D:501:SER:HB3	1.55	0.86
1:B:268:MET:O	1:B:269:LEU:HD13	1.76	0.85
1:B:206:THR:HG22	1:B:370:ARG:N	1.91	0.85
1:G:39:LEU:CD2	1:G:444:LEU:HD21	2.07	0.85
1:A:206:THR:HG22	1:A:370:ARG:N	1.89	0.85
1:D:268:MET:O	1:D:269:LEU:HD13	1.76	0.85
1:H:442:ARG:HG2	1:H:442:ARG:HH11	1.39	0.85
1:C:45:ASP:OD1	1:C:59:ASN:HB2	1.75	0.85
1:F:39:LEU:CD2	1:F:444:LEU:HD21	2.06	0.85
1:H:268:MET:O	1:H:269:LEU:HD13	1.76	0.84
1:B:39:LEU:CD2	1:B:444:LEU:HD21	2.07	0.84
1:H:39:LEU:CD2	1:H:444:LEU:HD21	2.04	0.84
1:G:268:MET:O	1:G:269:LEU:HD13	1.76	0.84
1:A:218:ARG:HG3	1:A:345:GLU:OE1	1.78	0.84
1:A:31:ILE:HD13	1:A:75:ALA:HB1	1.60	0.84
1:G:31:ILE:HD13	1:G:75:ALA:HB1	1.57	0.84
1:A:125:GLN:OE1	1:H:164:GLU:HB2	1.78	0.84
1:E:218:ARG:HG3	1:E:345:GLU:OE1	1.77	0.84
1:C:439:VAL:O	1:C:443:THR:HG23	1.77	0.84
1:E:263:GLU:HA	1:E:269:LEU:HD21	1.58	0.83
1:G:46:LYS:HG3	1:G:64:ILE:HD13	1.58	0.83
1:G:130:LYS:HG3	1:G:134:LEU:HD12	1.59	0.83
1:A:46:LYS:HG3	1:A:64:ILE:HD13	1.61	0.83
1:E:439:VAL:O	1:E:443:THR:HG23	1.77	0.83
1:D:39:LEU:CD2	1:D:444:LEU:HD21	2.08	0.83
1:H:130:LYS:HG3	1:H:134:LEU:HD12	1.60	0.83
1:C:39:LEU:CD2	1:C:444:LEU:HD21	2.07	0.83
1:C:130:LYS:HG3	1:C:134:LEU:HD12	1.59	0.82
1:H:218:ARG:NH2	1:H:223:MET:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ARG:HG3	1:G:345:GLU:OE1	1.79	0.82
1:A:268:MET:O	1:A:269:LEU:HD13	1.80	0.82
1:F:130:LYS:HG3	1:F:134:LEU:HD12	1.60	0.82
1:D:51:ASP:HB2	1:E:519:GLU:HB2	1.61	0.82
1:H:31:ILE:HD13	1:H:75:ALA:HB1	1.61	0.82
1:D:31:ILE:HD13	1:D:75:ALA:HB1	1.60	0.82
1:B:31:ILE:HD13	1:B:75:ALA:HB1	1.62	0.82
1:H:46:LYS:HG3	1:H:64:ILE:HD13	1.60	0.82
1:E:268:MET:O	1:E:269:LEU:HD13	1.80	0.81
1:E:39:LEU:CD2	1:E:444:LEU:HD21	2.10	0.81
1:B:218:ARG:HG3	1:B:345:GLU:OE1	1.81	0.81
1:C:373:THR:HB	1:D:80:GLU:HB3	1.63	0.81
1:H:218:ARG:HG3	1:H:345:GLU:OE1	1.81	0.81
1:F:46:LYS:HG3	1:F:64:ILE:HD13	1.60	0.81
1:B:439:VAL:O	1:B:443:THR:HG23	1.81	0.81
1:D:263:GLU:HA	1:D:269:LEU:HD21	1.62	0.81
1:F:263:GLU:HA	1:F:269:LEU:HD21	1.62	0.81
1:C:268:MET:O	1:C:269:LEU:HD13	1.80	0.81
1:C:46:LYS:HG3	1:C:64:ILE:HD13	1.60	0.81
1:F:206:THR:CG2	1:F:370:ARG:H	1.92	0.80
1:F:268:MET:O	1:F:269:LEU:HD13	1.81	0.80
1:D:439:VAL:O	1:D:443:THR:HG23	1.79	0.80
1:D:218:ARG:NH2	1:D:223:MET:O	2.13	0.80
1:E:31:ILE:HD13	1:E:75:ALA:HB1	1.62	0.80
1:C:218:ARG:HG3	1:C:345:GLU:OE1	1.82	0.80
1:H:439:VAL:O	1:H:443:THR:HG23	1.81	0.80
1:F:199:SER:HA	1:F:377:ILE:HD11	1.63	0.80
1:E:218:ARG:CG	1:E:345:GLU:OE1	2.29	0.80
1:A:130:LYS:HG3	1:A:134:LEU:HD12	1.63	0.80
1:A:263:GLU:HA	1:A:269:LEU:HD21	1.62	0.80
1:H:455:ILE:HG21	1:H:473:LEU:HD22	1.64	0.80
1:C:218:ARG:NH2	1:C:223:MET:O	2.13	0.80
1:B:11:ASN:HA	1:B:12:MET:CG	2.12	0.80
1:F:218:ARG:HG3	1:F:345:GLU:OE1	1.81	0.80
1:A:218:ARG:CG	1:A:345:GLU:OE1	2.30	0.80
1:H:263:GLU:HA	1:H:269:LEU:HD21	1.64	0.79
1:E:46:LYS:HD3	1:F:514:ASP:HB3	1.63	0.79
1:C:11:ASN:HA	1:C:12:MET:CG	2.11	0.79
1:D:164:GLU:HB2	1:E:125:GLN:OE1	1.82	0.79
1:F:201:ALA:HB2	1:G:497:GLN:OE1	1.82	0.79
1:C:263:GLU:HA	1:C:269:LEU:HD21	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:SER:HA	1:D:377:ILE:HD11	1.65	0.79
1:B:468:ASN:HB2	1:B:471:ALA:HB2	1.65	0.79
1:D:11:ASN:HA	1:D:12:MET:CG	2.13	0.79
1:F:11:ASN:HA	1:F:12:MET:CG	2.12	0.79
1:A:455:ILE:HG21	1:A:473:LEU:HD22	1.64	0.79
1:E:201:ALA:HB2	1:F:497:GLN:OE1	1.83	0.79
1:G:218:ARG:CG	1:G:345:GLU:OE1	2.31	0.79
1:C:468:ASN:HB2	1:C:471:ALA:HB2	1.65	0.79
1:D:218:ARG:HG3	1:D:345:GLU:OE1	1.81	0.79
1:E:218:ARG:NH2	1:E:223:MET:O	2.14	0.79
1:A:39:LEU:CD2	1:A:444:LEU:HD21	2.11	0.78
1:B:263:GLU:HA	1:B:269:LEU:HD21	1.63	0.78
1:G:263:GLU:HA	1:G:269:LEU:HD21	1.63	0.78
1:F:218:ARG:CG	1:F:345:GLU:OE1	2.32	0.78
1:D:468:ASN:HB2	1:D:471:ALA:HB2	1.64	0.78
1:C:31:ILE:HD13	1:C:75:ALA:HB1	1.64	0.78
1:A:11:ASN:HA	1:A:12:MET:CG	2.12	0.78
1:H:11:ASN:HA	1:H:12:MET:CG	2.14	0.78
1:A:199:SER:HA	1:A:377:ILE:HD11	1.66	0.78
1:G:439:VAL:O	1:G:443:THR:HG23	1.83	0.78
1:A:218:ARG:NH2	1:A:223:MET:O	2.15	0.78
1:E:46:LYS:HG3	1:E:64:ILE:HD13	1.64	0.78
1:B:218:ARG:NH2	1:B:223:MET:O	2.13	0.78
1:G:11:ASN:HA	1:G:12:MET:CG	2.14	0.78
1:A:497:GLN:OE1	1:H:201:ALA:HB2	1.84	0.77
1:H:218:ARG:CG	1:H:345:GLU:OE1	2.32	0.77
1:B:11:ASN:HA	1:B:12:MET:HG2	1.65	0.77
1:G:218:ARG:NH2	1:G:223:MET:O	2.14	0.77
1:E:455:ILE:HG21	1:E:473:LEU:HD22	1.67	0.77
1:H:199:SER:HA	1:H:377:ILE:HD11	1.66	0.77
1:E:11:ASN:HA	1:E:12:MET:CG	2.15	0.77
1:D:130:LYS:HG3	1:D:134:LEU:HD12	1.67	0.77
1:B:46:LYS:HG3	1:B:64:ILE:HD13	1.64	0.77
1:H:320:ALA:HB2	1:H:364:ALA:HB3	1.66	0.77
1:B:218:ARG:CG	1:B:345:GLU:OE1	2.33	0.77
1:H:11:ASN:HA	1:H:12:MET:HG2	1.67	0.77
1:B:199:SER:HA	1:B:377:ILE:HD11	1.65	0.77
1:D:320:ALA:HB2	1:D:364:ALA:HB3	1.66	0.77
1:C:206:THR:CG2	1:C:370:ARG:H	1.94	0.77
1:E:320:ALA:HB2	1:E:364:ALA:HB3	1.67	0.77
1:D:455:ILE:HG21	1:D:473:LEU:HD22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:SER:HB3	1:H:372:THR:HB	1.65	0.77
1:A:11:ASN:HA	1:A:12:MET:HG2	1.66	0.77
1:F:31:ILE:HD13	1:F:75:ALA:HB1	1.65	0.77
1:E:442:ARG:HG2	1:E:442:ARG:NH1	2.00	0.76
1:G:455:ILE:HG21	1:G:473:LEU:HD22	1.65	0.76
1:F:455:ILE:HG21	1:F:473:LEU:HD22	1.68	0.76
3:C:545:ADP:O1B	4:C:546:SO4:O2	2.03	0.76
1:B:372:THR:HB	1:C:501:SER:HB3	1.65	0.76
1:E:372:THR:HB	1:F:501:SER:HB3	1.66	0.76
1:A:439:VAL:O	1:A:443:THR:HG23	1.84	0.76
1:C:218:ARG:CG	1:C:345:GLU:OE1	2.33	0.76
1:G:468:ASN:HB2	1:G:471:ALA:HB2	1.67	0.76
1:G:199:SER:HA	1:G:377:ILE:HD11	1.65	0.76
1:C:455:ILE:HG21	1:C:473:LEU:HD22	1.66	0.76
1:D:373:THR:HG21	1:E:505:SER:HB3	1.68	0.76
1:D:218:ARG:CG	1:D:345:GLU:OE1	2.34	0.75
1:C:11:ASN:HA	1:C:12:MET:HG2	1.68	0.75
1:A:320:ALA:HB2	1:A:364:ALA:HB3	1.69	0.75
1:F:320:ALA:HB2	1:F:364:ALA:HB3	1.66	0.75
1:B:164:GLU:HB2	1:C:125:GLN:OE1	1.85	0.75
1:D:11:ASN:HA	1:D:12:MET:HG2	1.67	0.75
1:A:468:ASN:HB2	1:A:471:ALA:HB2	1.67	0.75
1:C:199:SER:HA	1:C:377:ILE:HD11	1.66	0.75
1:G:63:THR:HG22	1:G:66:ARG:HH22	1.52	0.75
1:E:130:LYS:HG3	1:E:134:LEU:HD12	1.69	0.74
1:H:63:THR:HG22	1:H:66:ARG:HH22	1.52	0.74
1:F:218:ARG:NH2	1:F:223:MET:O	2.14	0.74
1:F:11:ASN:HA	1:F:12:MET:HG2	1.69	0.74
1:H:63:THR:HG22	1:H:66:ARG:NH2	2.03	0.74
1:H:468:ASN:HB2	1:H:471:ALA:HB2	1.70	0.73
1:C:320:ALA:HB2	1:C:364:ALA:HB3	1.69	0.73
1:C:442:ARG:HG2	1:C:442:ARG:NH1	2.03	0.73
1:G:11:ASN:HA	1:G:12:MET:HG2	1.70	0.73
1:F:468:ASN:HB2	1:F:471:ALA:HB2	1.70	0.73
1:G:46:LYS:HD3	1:H:514:ASP:HB3	1.71	0.73
1:E:199:SER:HA	1:E:377:ILE:HD11	1.70	0.73
1:E:468:ASN:HB2	1:E:471:ALA:HB2	1.70	0.73
1:A:372:THR:CB	1:B:501:SER:HB3	2.17	0.72
1:D:47:MET:HB2	1:E:512:ILE:HD13	1.72	0.72
1:E:11:ASN:HA	1:E:12:MET:HG2	1.69	0.72
1:E:63:THR:HG22	1:E:66:ARG:HH22	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASP:HB3	1:B:327:THR:HG21	1.70	0.72
1:D:206:THR:CG2	1:D:370:ARG:H	1.99	0.72
1:G:164:GLU:HB2	1:H:125:GLN:OE1	1.90	0.72
1:A:442:ARG:NH1	1:A:442:ARG:HG2	2.02	0.72
1:B:320:ALA:HB2	1:B:364:ALA:HB3	1.72	0.72
1:E:206:THR:CG2	1:E:370:ARG:H	1.98	0.71
1:F:63:THR:HG22	1:F:66:ARG:HH22	1.55	0.71
1:G:63:THR:HG22	1:G:66:ARG:NH2	2.04	0.71
1:D:47:MET:O	1:E:515:VAL:HA	1.89	0.71
1:C:292:ASP:O	1:D:327:THR:HG21	1.91	0.71
1:F:46:LYS:HD3	1:G:514:ASP:HB3	1.73	0.71
1:A:373:THR:HB	1:B:80:GLU:HB3	1.71	0.71
1:E:131:ALA:HB2	1:E:415:LEU:HD11	1.73	0.71
1:G:53:GLY:O	1:H:76:LYS:HE2	1.90	0.71
3:B:545:ADP:O1B	4:B:546:SO4:O2	2.08	0.70
1:F:502:ALA:O	1:F:506:THR:HG23	1.92	0.70
1:D:448:ALA:HB3	1:D:450:LEU:HD12	1.73	0.70
1:H:206:THR:CG2	1:H:370:ARG:H	1.95	0.70
1:F:416:ARG:O	1:F:419:ALA:HB3	1.92	0.70
1:G:206:THR:CG2	1:G:370:ARG:H	1.96	0.70
1:G:320:ALA:HB2	1:G:364:ALA:HB3	1.72	0.70
1:H:208:LEU:HD11	1:H:365:VAL:CG1	2.21	0.70
1:E:448:ALA:HB3	1:E:450:LEU:HD12	1.73	0.69
1:A:448:ALA:HB3	1:A:450:LEU:HD12	1.73	0.69
1:G:372:THR:HB	1:H:501:SER:HB3	1.73	0.69
1:F:131:ALA:HB2	1:F:415:LEU:HD11	1.74	0.69
3:G:545:ADP:O1B	4:G:546:SO4:O2	2.11	0.69
1:C:448:ALA:HB3	1:C:450:LEU:HD12	1.73	0.69
1:F:63:THR:HG22	1:F:66:ARG:NH2	2.07	0.69
1:G:208:LEU:HD11	1:G:365:VAL:CG1	2.22	0.69
1:F:442:ARG:NH1	1:F:442:ARG:HG2	2.08	0.69
1:H:448:ALA:HB3	1:H:450:LEU:HD12	1.74	0.69
1:D:51:ASP:CB	1:E:519:GLU:HB2	2.22	0.69
1:D:49:VAL:HG21	1:E:73:PRO:HG3	1.75	0.69
1:D:178:VAL:HG11	1:D:391:VAL:HG12	1.73	0.69
1:A:63:THR:HG22	1:A:66:ARG:HH22	1.58	0.68
1:B:208:LEU:HD11	1:B:365:VAL:CG1	2.23	0.68
1:E:502:ALA:O	1:E:506:THR:HG23	1.94	0.68
1:G:39:LEU:CD2	1:G:444:LEU:HD23	2.18	0.68
1:E:63:THR:HG22	1:E:66:ARG:NH2	2.09	0.68
1:D:63:THR:HG22	1:D:66:ARG:HH22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:448:ALA:HB3	1:F:450:LEU:HD12	1.76	0.67
1:G:442:ARG:NH1	1:G:442:ARG:HG2	2.08	0.67
1:H:189:ASP:HB3	1:H:192:LEU:HG	1.76	0.67
1:E:442:ARG:CG	1:E:442:ARG:HH11	2.05	0.67
1:G:502:ALA:O	1:G:506:THR:HG23	1.93	0.67
1:F:208:LEU:HD11	1:F:365:VAL:CG1	2.24	0.67
1:H:202:SER:OG	1:H:205:ASP:HB2	1.94	0.67
1:E:401:VAL:HB	1:E:407:THR:HG21	1.77	0.67
1:H:131:ALA:HB2	1:H:415:LEU:HD11	1.75	0.67
1:F:39:LEU:HD11	1:F:95:THR:HG22	1.76	0.67
1:D:350:GLY:HA3	1:E:87:LYS:HE2	1.77	0.67
1:F:401:VAL:HB	1:F:407:THR:HG21	1.77	0.67
1:H:89:VAL:HG11	1:H:494:VAL:HG22	1.76	0.67
1:B:448:ALA:HB3	1:B:450:LEU:HD12	1.75	0.67
1:C:63:THR:HG22	1:C:66:ARG:HH22	1.59	0.67
1:G:178:VAL:HG11	1:G:391:VAL:HG12	1.77	0.67
1:B:206:THR:CG2	1:B:370:ARG:H	2.04	0.66
1:H:442:ARG:HG2	1:H:442:ARG:NH1	2.10	0.66
1:H:502:ALA:O	1:H:506:THR:HG23	1.94	0.66
1:B:502:ALA:O	1:B:506:THR:HG23	1.94	0.66
1:E:39:LEU:HD11	1:E:95:THR:HG22	1.78	0.66
1:F:164:GLU:HB2	1:G:125:GLN:OE1	1.95	0.66
1:D:63:THR:HG22	1:D:66:ARG:NH2	2.10	0.66
1:H:39:LEU:CD2	1:H:444:LEU:HD23	2.17	0.66
1:G:440:ILE:O	1:G:444:LEU:HG	1.96	0.66
1:E:271:ASP:O	1:E:275:GLU:HG3	1.96	0.66
1:G:401:VAL:HB	1:G:407:THR:HG21	1.77	0.66
1:D:468:ASN:O	1:D:469:LYS:HG2	1.95	0.66
1:G:420:GLU:HG2	1:G:431:ARG:HH22	1.61	0.66
1:H:271:ASP:O	1:H:275:GLU:HG3	1.95	0.66
1:F:373:THR:HB	1:G:80:GLU:HB3	1.77	0.66
1:G:448:ALA:HB3	1:G:450:LEU:HD12	1.77	0.66
1:E:178:VAL:HG11	1:E:391:VAL:HG12	1.78	0.66
1:C:51:ASP:CB	1:D:519:GLU:HB2	2.26	0.66
1:F:440:ILE:O	1:F:444:LEU:HG	1.95	0.65
1:E:173:ILE:HG23	1:E:208:LEU:HB2	1.78	0.65
1:D:502:ALA:O	1:D:506:THR:HG23	1.95	0.65
1:D:202:SER:OG	1:D:205:ASP:HB2	1.96	0.65
1:D:442:ARG:HG2	1:D:442:ARG:NH1	2.06	0.65
1:G:131:ALA:HB2	1:G:415:LEU:HD11	1.78	0.65
3:C:545:ADP:PB	4:C:546:SO4:O2	2.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LEU:CD2	1:B:444:LEU:HD23	2.19	0.65
1:G:376:VAL:HG11	1:H:504:GLU:OE1	1.96	0.65
1:D:131:ALA:HB2	1:D:415:LEU:HD11	1.79	0.65
1:H:173:ILE:HG23	1:H:208:LEU:HB2	1.77	0.65
1:H:39:LEU:HD11	1:H:95:THR:HG22	1.79	0.65
1:B:440:ILE:O	1:B:444:LEU:HG	1.97	0.65
1:A:356:VAL:HG12	1:A:356:VAL:O	1.97	0.65
1:B:63:THR:HG22	1:B:66:ARG:HH22	1.61	0.65
1:D:208:LEU:HD11	1:D:365:VAL:CG1	2.25	0.65
3:F:545:ADP:O1B	4:F:546:SO4:O2	2.15	0.65
1:B:178:VAL:HG11	1:B:391:VAL:HG12	1.78	0.65
1:C:208:LEU:HD11	1:C:365:VAL:CG1	2.27	0.64
1:F:233:ALA:O	1:F:284:LEU:HD12	1.97	0.64
1:H:440:ILE:O	1:H:444:LEU:HG	1.96	0.64
1:F:468:ASN:O	1:F:469:LYS:HG2	1.98	0.64
1:B:401:VAL:HB	1:B:407:THR:HG21	1.77	0.64
1:G:31:ILE:HD13	1:G:75:ALA:CB	2.27	0.64
1:A:63:THR:HG22	1:A:66:ARG:NH2	2.12	0.64
1:C:63:THR:HG22	1:C:66:ARG:NH2	2.12	0.64
1:F:189:ASP:HB3	1:F:192:LEU:HG	1.78	0.64
1:C:202:SER:OG	1:C:205:ASP:HB2	1.98	0.64
1:E:440:ILE:O	1:E:444:LEU:HG	1.98	0.64
1:B:46:LYS:HD3	1:C:514:ASP:HB3	1.79	0.64
1:G:468:ASN:O	1:G:469:LYS:HG2	1.97	0.64
1:E:164:GLU:HB2	1:F:125:GLN:OE1	1.97	0.64
1:A:401:VAL:HB	1:A:407:THR:HG21	1.80	0.64
1:H:468:ASN:O	1:H:469:LYS:HG2	1.97	0.64
1:A:202:SER:OG	1:A:205:ASP:HB2	1.98	0.64
1:A:416:ARG:O	1:A:419:ALA:HB3	1.97	0.64
1:E:420:GLU:HG2	1:E:431:ARG:HH22	1.62	0.64
1:G:202:SER:OG	1:G:205:ASP:HB2	1.98	0.64
1:A:502:ALA:O	1:A:506:THR:HG23	1.98	0.64
1:A:173:ILE:HG23	1:A:208:LEU:HB2	1.80	0.64
1:F:178:VAL:HG11	1:F:391:VAL:HG12	1.80	0.64
1:C:502:ALA:O	1:C:506:THR:HG23	1.97	0.63
1:C:233:ALA:O	1:C:284:LEU:HD12	1.98	0.63
1:A:189:ASP:HB3	1:A:192:LEU:HG	1.80	0.63
1:C:440:ILE:O	1:C:444:LEU:HG	1.98	0.63
1:C:189:ASP:HB3	1:C:192:LEU:HG	1.80	0.63
1:A:420:GLU:HG2	1:A:431:ARG:HH22	1.63	0.63
1:G:89:VAL:HG11	1:G:494:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ARG:HG2	1:B:442:ARG:NH1	2.05	0.63
1:C:178:VAL:HG11	1:C:391:VAL:HG12	1.79	0.63
1:E:373:THR:HB	1:F:80:GLU:HB3	1.80	0.63
1:D:233:ALA:O	1:D:284:LEU:HD12	1.99	0.63
1:F:271:ASP:O	1:F:275:GLU:HG3	1.99	0.63
1:E:94:THR:O	1:E:98:VAL:HG23	1.99	0.63
1:E:95:THR:HG23	3:E:545:ADP:O2B	1.99	0.63
1:D:89:VAL:HG11	1:D:494:VAL:HG22	1.81	0.63
1:B:271:ASP:O	1:B:275:GLU:HG3	1.98	0.62
1:F:62:VAL:HG13	1:F:63:THR:N	2.14	0.62
1:H:77:MET:HA	1:H:80:GLU:HG2	1.81	0.62
1:G:189:ASP:HB3	1:G:192:LEU:HG	1.81	0.62
1:F:420:GLU:HG2	1:F:431:ARG:HH22	1.63	0.62
1:H:203:ILE:HA	1:H:370:ARG:O	2.00	0.62
1:E:189:ASP:HB3	1:E:192:LEU:HG	1.80	0.62
1:D:44:MET:HE1	1:E:118:THR:HG23	1.80	0.62
1:D:271:ASP:O	1:D:275:GLU:HG3	1.99	0.62
1:A:206:THR:CG2	1:A:370:ARG:H	2.00	0.62
1:A:131:ALA:HB2	1:A:415:LEU:HD11	1.80	0.62
1:B:233:ALA:O	1:B:284:LEU:HD12	2.00	0.62
3:G:545:ADP:PB	4:G:546:SO4:O2	2.58	0.62
1:B:63:THR:HG22	1:B:66:ARG:NH2	2.14	0.62
1:D:173:ILE:HG23	1:D:208:LEU:HB2	1.80	0.62
1:H:401:VAL:HB	1:H:407:THR:HG21	1.81	0.62
1:B:131:ALA:HB2	1:B:415:LEU:HD11	1.81	0.62
1:A:440:ILE:O	1:A:444:LEU:HG	1.99	0.62
1:G:271:ASP:O	1:G:275:GLU:HG3	2.00	0.62
1:F:202:SER:OG	1:F:205:ASP:HB2	1.99	0.62
1:E:468:ASN:O	1:E:469:LYS:HG2	2.00	0.62
1:H:408:GLU:O	1:H:412:SER:HB3	1.99	0.62
1:C:408:GLU:O	1:C:412:SER:HB3	2.00	0.62
1:E:416:ARG:O	1:E:419:ALA:HB3	1.99	0.62
1:C:271:ASP:O	1:C:275:GLU:HG3	2.00	0.62
1:B:39:LEU:HD11	1:B:95:THR:HG22	1.82	0.61
1:D:31:ILE:HD13	1:D:75:ALA:CB	2.30	0.61
1:G:77:MET:CE	1:G:509:LEU:HD21	2.30	0.61
1:D:189:ASP:HB3	1:D:192:LEU:HG	1.82	0.61
1:H:151:THR:OG1	1:H:175:VAL:HG21	2.00	0.61
1:G:416:ARG:O	1:G:419:ALA:HB3	2.00	0.61
1:E:202:SER:OG	1:E:205:ASP:HB2	2.00	0.61
1:B:31:ILE:HD11	1:B:78:LEU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:ASN:O	1:C:469:LYS:HG2	2.00	0.61
1:H:178:VAL:HG11	1:H:391:VAL:HG12	1.81	0.61
1:G:425:ARG:O	1:G:427:GLN:N	2.33	0.61
1:E:203:ILE:HA	1:E:370:ARG:O	2.01	0.61
1:A:468:ASN:O	1:A:469:LYS:HG2	2.00	0.61
1:C:401:VAL:HB	1:C:407:THR:HG21	1.81	0.61
1:D:440:ILE:O	1:D:444:LEU:HG	2.01	0.61
1:H:202:SER:CB	1:H:205:ASP:HB2	2.31	0.61
1:B:356:VAL:O	1:B:356:VAL:HG12	2.00	0.61
1:E:31:ILE:HD13	1:E:75:ALA:CB	2.30	0.61
1:F:31:ILE:HD11	1:F:78:LEU:HB2	1.82	0.61
1:A:271:ASP:O	1:A:275:GLU:HG3	1.99	0.61
1:C:47:MET:O	1:D:515:VAL:HA	2.00	0.61
1:E:208:LEU:HD11	1:E:365:VAL:CG1	2.29	0.61
1:E:153:ILE:HD13	1:E:394:THR:OG1	2.01	0.61
1:B:189:ASP:HB3	1:B:192:LEU:HG	1.83	0.61
1:D:372:THR:HB	1:E:501:SER:CB	2.27	0.61
1:B:468:ASN:O	1:B:469:LYS:HG2	2.01	0.61
1:H:233:ALA:O	1:H:284:LEU:HD12	2.01	0.61
1:B:315:GLU:O	1:B:319:LYS:HG3	2.01	0.61
1:E:386:ASP:O	1:E:390:VAL:HG22	2.01	0.61
1:E:418:TYR:CE2	1:E:422:ILE:HD11	2.35	0.60
1:H:82:ALA:HB2	1:H:97:VAL:CG2	2.31	0.60
1:A:408:GLU:O	1:A:412:SER:HB3	2.01	0.60
1:C:31:ILE:HD11	1:C:78:LEU:HB2	1.83	0.60
1:G:173:ILE:HG23	1:G:208:LEU:HB2	1.82	0.60
1:B:416:ARG:O	1:B:419:ALA:HB3	2.01	0.60
1:C:420:GLU:HG2	1:C:431:ARG:HH22	1.65	0.60
1:D:420:GLU:HG2	1:D:431:ARG:HH22	1.66	0.60
1:A:39:LEU:CD2	1:A:444:LEU:HD23	2.22	0.60
3:A:545:ADP:O1B	4:A:546:SO4:O2	2.20	0.60
1:G:37:SER:OG	1:G:46:LYS:NZ	2.33	0.60
1:B:173:ILE:HG23	1:B:208:LEU:HB2	1.80	0.60
1:C:173:ILE:HG23	1:C:208:LEU:HB2	1.83	0.60
1:G:408:GLU:O	1:G:412:SER:HB3	2.01	0.60
3:G:545:ADP:O3B	4:G:546:SO4:S	2.59	0.60
1:H:416:ARG:O	1:H:419:ALA:HB3	2.00	0.60
1:B:408:GLU:O	1:B:412:SER:HB3	2.01	0.60
1:D:201:ALA:HB2	1:E:497:GLN:OE1	2.01	0.60
1:D:401:VAL:HB	1:D:407:THR:HG21	1.82	0.60
3:E:545:ADP:O1B	4:E:546:SO4:O2	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:VAL:HG11	1:C:297:TYR:HB3	1.83	0.60
1:H:342:LEU:HD21	1:H:344:GLU:HB2	1.83	0.60
1:B:31:ILE:HD13	1:B:75:ALA:CB	2.30	0.60
1:C:49:VAL:HG21	1:D:73:PRO:HG3	1.84	0.60
1:D:273:VAL:HG11	1:D:297:TYR:HB3	1.82	0.60
1:E:218:ARG:HG2	1:E:345:GLU:OE1	2.02	0.60
1:F:273:VAL:HG11	1:F:297:TYR:HB3	1.84	0.60
1:F:203:ILE:HA	1:F:370:ARG:O	2.02	0.60
1:D:31:ILE:HD11	1:D:78:LEU:HB2	1.84	0.60
1:G:342:LEU:HD21	1:G:344:GLU:HB2	1.84	0.60
3:D:545:ADP:O1B	3:D:545:ADP:O2A	2.19	0.60
1:A:31:ILE:HD13	1:A:75:ALA:CB	2.31	0.60
1:E:77:MET:CE	1:E:509:LEU:HD21	2.31	0.60
1:G:233:ALA:O	1:G:284:LEU:HD12	2.01	0.60
1:F:89:VAL:HG11	1:F:494:VAL:HG22	1.84	0.60
1:G:31:ILE:HD11	1:G:78:LEU:HB2	1.83	0.60
1:E:273:VAL:HG11	1:E:297:TYR:HB3	1.84	0.60
1:C:31:ILE:HD13	1:C:75:ALA:CB	2.32	0.60
1:H:94:THR:O	1:H:98:VAL:HG23	2.02	0.60
1:C:416:ARG:O	1:C:419:ALA:HB3	2.01	0.60
1:C:164:GLU:HB2	1:D:125:GLN:OE1	2.02	0.60
1:G:384:VAL:O	1:G:388:VAL:HG23	2.02	0.60
1:F:315:GLU:O	1:F:319:LYS:HG3	2.01	0.60
1:H:31:ILE:HD13	1:H:75:ALA:CB	2.30	0.59
1:D:77:MET:CE	1:D:509:LEU:HD21	2.32	0.59
1:A:208:LEU:HD11	1:A:365:VAL:CG1	2.31	0.59
1:A:233:ALA:O	1:A:284:LEU:HD12	2.02	0.59
1:H:420:GLU:HG2	1:H:431:ARG:HH22	1.66	0.59
1:D:356:VAL:O	1:D:356:VAL:HG12	2.02	0.59
1:H:31:ILE:HD11	1:H:78:LEU:HB2	1.84	0.59
1:H:77:MET:CE	1:H:509:LEU:HD21	2.32	0.59
1:C:131:ALA:HB2	1:C:415:LEU:HD11	1.83	0.59
1:D:145:GLN:O	1:D:147:LYS:N	2.34	0.59
1:G:82:ALA:HB2	1:G:97:VAL:CG2	2.33	0.59
1:B:273:VAL:HG11	1:B:297:TYR:HB3	1.84	0.59
1:E:25:ILE:O	1:E:29:ARG:HG3	2.02	0.59
1:H:157:SER:HB2	1:H:390:VAL:HG21	1.84	0.59
1:B:420:GLU:HG2	1:B:431:ARG:HH22	1.66	0.59
1:D:408:GLU:O	1:D:412:SER:HB3	2.02	0.59
1:G:273:VAL:HG11	1:G:297:TYR:HB3	1.84	0.59
1:E:233:ALA:O	1:E:284:LEU:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:GLU:O	1:E:319:LYS:HG3	2.02	0.59
1:D:203:ILE:HA	1:D:370:ARG:O	2.02	0.59
1:G:315:GLU:O	1:G:319:LYS:HG3	2.03	0.59
1:F:356:VAL:HG12	1:F:356:VAL:O	2.03	0.59
1:D:450:LEU:HD22	1:D:455:ILE:HD11	1.85	0.59
1:G:77:MET:HA	1:G:80:GLU:HG2	1.84	0.59
1:D:315:GLU:O	1:D:319:LYS:HG3	2.03	0.59
1:C:203:ILE:HA	1:C:370:ARG:O	2.03	0.59
1:F:173:ILE:HG23	1:F:208:LEU:HB2	1.83	0.58
1:B:418:TYR:CE2	1:B:422:ILE:HD11	2.37	0.58
1:H:315:GLU:O	1:H:319:LYS:HG3	2.02	0.58
3:C:545:ADP:O1B	3:C:545:ADP:O2A	2.20	0.58
1:F:95:THR:HG23	3:F:545:ADP:O2B	2.02	0.58
1:A:273:VAL:HG11	1:A:297:TYR:HB3	1.85	0.58
3:D:545:ADP:O1B	4:D:546:SO4:O2	2.21	0.58
1:H:273:VAL:HG11	1:H:297:TYR:HB3	1.86	0.58
1:E:408:GLU:O	1:E:412:SER:HB3	2.02	0.58
1:A:178:VAL:HG11	1:A:391:VAL:HG12	1.86	0.58
1:D:62:VAL:HG13	1:D:63:THR:N	2.18	0.58
1:C:89:VAL:HG11	1:C:494:VAL:HG22	1.85	0.58
1:H:145:GLN:O	1:H:147:LYS:N	2.36	0.58
1:E:89:VAL:HG11	1:E:494:VAL:HG22	1.85	0.58
1:F:425:ARG:O	1:F:427:GLN:N	2.37	0.58
1:D:94:THR:O	1:D:98:VAL:HG23	2.04	0.58
3:G:545:ADP:O2A	3:G:545:ADP:O1B	2.22	0.58
1:A:218:ARG:HG2	1:A:345:GLU:OE1	2.03	0.58
1:F:418:TYR:CE2	1:F:422:ILE:HD11	2.39	0.58
1:H:418:TYR:CE2	1:H:422:ILE:HD11	2.38	0.58
1:G:203:ILE:HA	1:G:370:ARG:O	2.03	0.58
1:A:145:GLN:O	1:A:147:LYS:N	2.36	0.58
1:A:77:MET:CE	1:A:509:LEU:HD21	2.34	0.58
1:F:31:ILE:HD13	1:F:75:ALA:CB	2.34	0.58
1:C:356:VAL:HG12	1:C:356:VAL:O	2.04	0.58
1:E:342:LEU:HD21	1:E:344:GLU:HB2	1.85	0.58
1:G:218:ARG:HG2	1:G:345:GLU:OE1	2.03	0.58
1:E:138:ILE:HD12	1:E:410:GLU:HG2	1.86	0.58
3:B:545:ADP:PB	4:B:546:SO4:O2	2.62	0.57
1:C:425:ARG:O	1:C:427:GLN:N	2.36	0.57
1:F:153:ILE:HD13	1:F:394:THR:OG1	2.04	0.57
3:C:545:ADP:O3B	4:C:546:SO4:S	2.62	0.57
1:F:218:ARG:HG2	1:F:345:GLU:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:425:ARG:O	1:H:427:GLN:N	2.37	0.57
1:H:138:ILE:HD12	1:H:410:GLU:HG2	1.86	0.57
1:B:145:GLN:O	1:B:147:LYS:N	2.37	0.57
1:A:89:VAL:HG11	1:A:494:VAL:HG22	1.85	0.57
1:B:442:ARG:CG	1:B:442:ARG:HH11	2.10	0.57
1:D:44:MET:CE	1:E:118:THR:HG23	2.34	0.57
1:C:218:ARG:HG2	1:C:345:GLU:OE1	2.04	0.57
1:D:384:VAL:O	1:D:388:VAL:HG23	2.04	0.57
1:D:153:ILE:HD13	1:D:394:THR:OG1	2.03	0.57
1:E:39:LEU:CD2	1:E:444:LEU:HD23	2.21	0.57
3:B:545:ADP:O2A	3:B:545:ADP:O1B	2.21	0.57
1:D:372:THR:CB	1:E:501:SER:HA	2.35	0.57
1:D:47:MET:HB2	1:E:512:ILE:CD1	2.34	0.57
1:G:267:GLU:C	1:G:269:LEU:H	2.07	0.57
1:E:425:ARG:O	1:E:427:GLN:N	2.37	0.57
1:A:94:THR:O	1:A:98:VAL:HG23	2.05	0.57
1:A:216:LYS:HE2	1:A:307:ARG:O	2.05	0.57
3:H:545:ADP:O1B	4:H:546:SO4:O2	2.23	0.57
1:D:202:SER:CB	1:D:205:ASP:HB2	2.35	0.57
1:E:31:ILE:HD11	1:E:78:LEU:HB2	1.86	0.57
1:E:47:MET:O	1:F:515:VAL:HA	2.04	0.57
1:A:376:VAL:HG11	1:B:504:GLU:OE1	2.05	0.57
1:D:342:LEU:HD21	1:D:344:GLU:HB2	1.87	0.57
1:D:39:LEU:CD2	1:D:444:LEU:HD23	2.18	0.57
1:D:77:MET:HA	1:D:80:GLU:HG2	1.86	0.57
1:A:425:ARG:O	1:A:427:GLN:N	2.37	0.57
1:H:356:VAL:O	1:H:356:VAL:HG12	2.05	0.57
1:E:464:ALA:O	1:E:466:ASN:OD1	2.23	0.57
1:D:95:THR:HG23	3:D:545:ADP:O2B	2.05	0.57
1:B:202:SER:OG	1:B:205:ASP:HB2	2.04	0.57
1:A:31:ILE:HD11	1:A:78:LEU:HB2	1.86	0.57
1:F:267:GLU:C	1:F:269:LEU:H	2.09	0.57
1:C:153:ILE:HD13	1:C:394:THR:OG1	2.05	0.57
1:D:82:ALA:HB2	1:D:97:VAL:CG2	2.35	0.57
1:C:62:VAL:HG13	1:C:63:THR:N	2.21	0.56
1:D:267:GLU:C	1:D:269:LEU:H	2.09	0.56
1:F:342:LEU:HD21	1:F:344:GLU:HB2	1.86	0.56
1:F:408:GLU:O	1:F:412:SER:HB3	2.05	0.56
1:E:145:GLN:O	1:E:147:LYS:N	2.38	0.56
1:D:372:THR:OG1	1:E:504:GLU:HB2	2.04	0.56
1:A:267:GLU:C	1:A:269:LEU:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:ARG:NH2	1:G:443:THR:HG22	2.19	0.56
1:B:77:MET:HA	1:B:80:GLU:HG2	1.87	0.56
1:C:216:LYS:HE2	1:C:307:ARG:O	2.04	0.56
1:B:153:ILE:HD13	1:B:394:THR:OG1	2.06	0.56
1:E:216:LYS:HE2	1:E:307:ARG:O	2.06	0.56
1:F:145:GLN:O	1:F:147:LYS:N	2.38	0.56
1:F:326:ILE:HD11	1:F:336:ASP:OD1	2.06	0.56
1:A:202:SER:CB	1:A:205:ASP:HB2	2.36	0.56
1:B:267:GLU:C	1:B:269:LEU:H	2.07	0.56
1:A:342:LEU:HD21	1:A:344:GLU:HB2	1.87	0.56
1:B:425:ARG:O	1:B:427:GLN:N	2.38	0.56
1:C:342:LEU:HD21	1:C:344:GLU:HB2	1.87	0.56
1:B:94:THR:O	1:B:98:VAL:HG23	2.05	0.56
1:A:117:PRO:O	1:A:121:VAL:HG12	2.06	0.56
1:B:203:ILE:HA	1:B:370:ARG:O	2.04	0.56
1:A:36:ARG:NH2	1:A:443:THR:HG22	2.20	0.56
1:E:151:THR:OG1	1:E:175:VAL:HG21	2.06	0.56
1:G:154:ALA:HB2	1:G:391:VAL:CG2	2.35	0.56
1:A:418:TYR:CE2	1:A:422:ILE:HD11	2.41	0.56
1:G:82:ALA:HB2	1:G:97:VAL:HG23	1.87	0.56
1:C:202:SER:CB	1:C:205:ASP:HB2	2.36	0.56
1:C:315:GLU:O	1:C:319:LYS:HG3	2.05	0.56
1:H:95:THR:HG23	3:H:545:ADP:O2B	2.06	0.56
1:D:151:THR:OG1	1:D:175:VAL:HG21	2.05	0.56
3:B:545:ADP:O3B	4:B:546:SO4:S	2.64	0.56
1:H:267:GLU:C	1:H:269:LEU:H	2.09	0.56
1:C:267:GLU:C	1:C:269:LEU:H	2.08	0.56
1:D:218:ARG:HG2	1:D:345:GLU:OE1	2.06	0.56
1:B:372:THR:CB	1:C:501:SER:HB3	2.35	0.56
1:F:77:MET:HA	1:F:80:GLU:HG2	1.87	0.56
1:H:386:ASP:O	1:H:390:VAL:HG22	2.05	0.56
1:F:25:ILE:O	1:F:29:ARG:HG3	2.05	0.56
1:G:138:ILE:HD12	1:G:410:GLU:HG2	1.87	0.56
1:G:94:THR:O	1:G:98:VAL:HG23	2.05	0.56
1:B:218:ARG:HG2	1:B:345:GLU:OE1	2.05	0.56
1:A:77:MET:HA	1:A:80:GLU:HG2	1.88	0.55
1:G:153:ILE:HD13	1:G:394:THR:OG1	2.05	0.55
1:D:138:ILE:HD12	1:D:410:GLU:HG2	1.88	0.55
1:E:267:GLU:C	1:E:269:LEU:H	2.09	0.55
1:D:51:ASP:HB2	1:E:519:GLU:CB	2.36	0.55
1:H:268:MET:C	1:H:269:LEU:HD13	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HA	1:A:370:ARG:O	2.05	0.55
1:H:218:ARG:HG2	1:H:345:GLU:OE1	2.04	0.55
1:F:94:THR:O	1:F:98:VAL:HG23	2.06	0.55
1:D:425:ARG:O	1:D:427:GLN:N	2.40	0.55
1:F:39:LEU:CD2	1:F:444:LEU:HD23	2.21	0.55
1:H:197:LYS:HB3	1:H:377:ILE:HG21	1.88	0.55
1:H:384:VAL:O	1:H:388:VAL:HG23	2.06	0.55
1:D:117:PRO:O	1:D:121:VAL:HG12	2.06	0.55
3:H:545:ADP:O1B	3:H:545:ADP:O2A	2.24	0.55
3:E:545:ADP:O3B	4:E:546:SO4:S	2.65	0.55
1:A:39:LEU:HD11	1:A:95:THR:HG22	1.89	0.55
1:G:268:MET:C	1:G:269:LEU:HD13	2.27	0.55
1:G:157:SER:HB2	1:G:390:VAL:HG21	1.88	0.55
1:H:39:LEU:HD21	1:H:444:LEU:HD21	1.87	0.55
1:H:197:LYS:HB3	1:H:377:ILE:CG2	2.37	0.55
1:H:82:ALA:HB2	1:H:97:VAL:HG23	1.89	0.55
3:H:545:ADP:PB	4:H:546:SO4:O2	2.65	0.55
1:D:268:MET:C	1:D:269:LEU:HD13	2.27	0.55
1:A:384:VAL:O	1:A:388:VAL:HG23	2.06	0.55
1:H:153:ILE:HD13	1:H:394:THR:OG1	2.07	0.55
1:B:157:SER:HB2	1:B:390:VAL:HG21	1.89	0.55
1:D:39:LEU:HD11	1:D:95:THR:HG22	1.88	0.54
1:B:62:VAL:HG13	1:B:63:THR:N	2.21	0.54
1:D:39:LEU:HD21	1:D:444:LEU:HD21	1.90	0.54
1:C:77:MET:HA	1:C:80:GLU:HG2	1.90	0.54
1:F:266:SER:HB3	1:F:268:MET:CE	2.37	0.54
1:G:356:VAL:HG12	1:G:356:VAL:O	2.06	0.54
1:A:95:THR:HG23	3:A:545:ADP:O2B	2.08	0.54
1:H:203:ILE:H	1:H:371:GLY:HA2	1.71	0.54
1:A:442:ARG:NH1	1:A:442:ARG:CG	2.67	0.54
1:B:450:LEU:HD22	1:B:455:ILE:HD11	1.89	0.54
1:B:268:MET:C	1:B:269:LEU:HD13	2.27	0.54
3:F:545:ADP:PB	4:F:546:SO4:O2	2.65	0.54
1:A:80:GLU:HB3	1:H:373:THR:HB	1.90	0.54
1:D:416:ARG:O	1:D:419:ALA:HB3	2.08	0.54
1:E:384:VAL:O	1:E:388:VAL:HG23	2.08	0.54
1:F:442:ARG:CG	1:F:442:ARG:HH11	2.12	0.54
1:D:197:LYS:HB3	1:D:377:ILE:HG21	1.90	0.54
1:B:118:THR:HA	1:B:121:VAL:CG1	2.38	0.54
1:F:151:THR:OG1	1:F:175:VAL:HG21	2.08	0.54
1:A:215:ASP:HA	1:A:353:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLN:O	1:C:147:LYS:N	2.40	0.54
1:A:62:VAL:HG13	1:A:63:THR:N	2.23	0.54
1:D:464:ALA:O	1:D:466:ASN:OD1	2.26	0.54
1:G:216:LYS:HE2	1:G:307:ARG:O	2.07	0.54
1:C:51:ASP:HB2	1:D:519:GLU:HB2	1.89	0.54
1:D:157:SER:HB2	1:D:390:VAL:HG21	1.90	0.54
1:A:464:ALA:O	1:A:466:ASN:OD1	2.25	0.54
1:D:215:ASP:HA	1:D:353:MET:HG2	1.90	0.54
1:F:203:ILE:H	1:F:371:GLY:HA2	1.72	0.54
1:F:37:SER:OG	1:F:46:LYS:NZ	2.40	0.54
1:E:46:LYS:HG3	1:E:64:ILE:CD1	2.36	0.54
1:A:315:GLU:O	1:A:319:LYS:HG3	2.06	0.54
1:G:39:LEU:HD11	1:G:95:THR:HG22	1.88	0.54
1:B:197:LYS:HB3	1:B:377:ILE:HG21	1.90	0.54
1:B:89:VAL:HG11	1:B:494:VAL:HG22	1.90	0.54
1:G:440:ILE:HB	1:G:441:PRO:HD3	1.90	0.54
3:F:545:ADP:O3B	4:F:546:SO4:S	2.66	0.54
1:E:202:SER:CB	1:E:205:ASP:HB2	2.38	0.54
1:H:450:LEU:HD22	1:H:455:ILE:HD11	1.89	0.54
1:C:197:LYS:HB3	1:C:377:ILE:HG21	1.90	0.53
1:F:208:LEU:HD11	1:F:365:VAL:HG11	1.89	0.53
1:G:420:GLU:C	1:G:422:ILE:H	2.10	0.53
1:B:216:LYS:HE2	1:B:307:ARG:O	2.08	0.53
3:F:545:ADP:O2A	3:F:545:ADP:O1B	2.26	0.53
3:A:545:ADP:PB	4:A:546:SO4:O2	2.66	0.53
1:B:95:THR:HG23	3:B:545:ADP:O2B	2.08	0.53
1:H:36:ARG:NH2	1:H:443:THR:HG22	2.23	0.53
1:G:62:VAL:HG13	1:G:63:THR:N	2.23	0.53
1:F:154:ALA:HB2	1:F:391:VAL:CG2	2.38	0.53
1:G:145:GLN:O	1:G:147:LYS:N	2.41	0.53
1:F:440:ILE:HB	1:F:441:PRO:HD3	1.90	0.53
1:C:440:ILE:HB	1:C:441:PRO:HD3	1.89	0.53
1:H:202:SER:HB2	1:H:205:ASP:HB2	1.90	0.53
1:C:77:MET:CE	1:C:509:LEU:HD21	2.38	0.53
1:A:268:MET:C	1:A:269:LEU:HD13	2.28	0.53
1:F:11:ASN:HA	1:F:12:MET:HG3	1.90	0.53
1:F:450:LEU:HD22	1:F:455:ILE:HD11	1.90	0.53
1:B:117:PRO:O	1:B:121:VAL:HG12	2.08	0.53
1:H:37:SER:OG	1:H:46:LYS:NZ	2.38	0.53
1:H:464:ALA:O	1:H:466:ASN:OD1	2.25	0.53
3:E:545:ADP:O1B	3:E:545:ADP:O2A	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:448:ALA:CB	1:H:450:LEU:HD12	2.39	0.53
1:C:11:ASN:HA	1:C:12:MET:HG3	1.91	0.53
1:B:284:LEU:O	1:B:305:ALA:HA	2.09	0.53
1:E:203:ILE:H	1:E:371:GLY:HA2	1.74	0.53
1:A:515:VAL:HA	1:H:47:MET:O	2.09	0.53
1:H:62:VAL:HG13	1:H:63:THR:N	2.24	0.53
1:D:154:ALA:HB2	1:D:391:VAL:CG2	2.39	0.53
1:E:356:VAL:O	1:E:356:VAL:HG12	2.07	0.53
1:H:109:GLU:O	1:H:113:GLN:HG3	2.09	0.53
1:D:202:SER:OG	1:D:203:ILE:N	2.42	0.53
1:B:442:ARG:CG	1:B:442:ARG:NH1	2.69	0.53
1:G:59:ASN:OD1	1:G:59:ASN:O	2.27	0.53
1:G:418:TYR:CE2	1:G:422:ILE:HD11	2.44	0.53
1:A:146:ASP:OD1	1:A:149:ILE:HD12	2.08	0.53
1:B:464:ALA:O	1:B:466:ASN:OD1	2.26	0.53
1:C:442:ARG:CG	1:C:442:ARG:NH1	2.68	0.53
1:G:442:ARG:CG	1:G:442:ARG:NH1	2.70	0.53
1:B:151:THR:OG1	1:B:175:VAL:HG21	2.09	0.53
1:H:41:PRO:HG3	1:H:159:THR:HG22	1.91	0.53
1:F:138:ILE:HD12	1:F:410:GLU:HG2	1.90	0.53
1:B:202:SER:CB	1:B:205:ASP:HB2	2.39	0.53
1:C:138:ILE:HD12	1:C:410:GLU:HG2	1.89	0.53
1:B:342:LEU:HD21	1:B:344:GLU:HB2	1.89	0.53
1:G:49:VAL:HG22	1:H:73:PRO:HB3	1.90	0.53
1:E:82:ALA:HB2	1:E:97:VAL:CG2	2.38	0.53
1:F:216:LYS:HE2	1:F:307:ARG:O	2.09	0.53
3:D:545:ADP:PB	4:D:546:SO4:O2	2.67	0.53
1:G:203:ILE:H	1:G:371:GLY:HA2	1.73	0.53
1:B:268:MET:C	1:B:269:LEU:HD22	2.29	0.53
1:E:268:MET:C	1:E:269:LEU:HD13	2.29	0.53
1:E:284:LEU:O	1:E:305:ALA:HA	2.09	0.53
1:B:82:ALA:HB2	1:B:97:VAL:CG2	2.39	0.53
1:C:48:LEU:HG	1:D:516:ILE:HB	1.90	0.53
1:C:450:LEU:HD22	1:C:455:ILE:HD11	1.91	0.52
1:E:77:MET:HA	1:E:80:GLU:HG2	1.90	0.52
1:C:464:ALA:O	1:C:466:ASN:OD1	2.27	0.52
1:E:215:ASP:HA	1:E:353:MET:HG2	1.90	0.52
1:G:118:THR:HA	1:G:121:VAL:CG1	2.40	0.52
1:C:203:ILE:H	1:C:371:GLY:HA2	1.73	0.52
1:G:386:ASP:O	1:G:390:VAL:HG22	2.09	0.52
1:F:215:ASP:HA	1:F:353:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LYS:HB3	1:D:377:ILE:CG2	2.39	0.52
1:H:117:PRO:O	1:H:121:VAL:HG12	2.10	0.52
1:F:77:MET:CE	1:F:509:LEU:HD21	2.38	0.52
1:B:138:ILE:HD12	1:B:410:GLU:HG2	1.92	0.52
1:A:197:LYS:HB3	1:A:377:ILE:HG21	1.90	0.52
1:B:197:LYS:HB3	1:B:377:ILE:CG2	2.39	0.52
1:B:208:LEU:HD11	1:B:365:VAL:HG11	1.91	0.52
1:D:418:TYR:CE2	1:D:422:ILE:HD11	2.45	0.52
1:A:386:ASP:O	1:A:390:VAL:HG22	2.10	0.52
1:F:157:SER:HB2	1:F:390:VAL:HG21	1.90	0.52
1:C:153:ILE:HG13	1:C:489:VAL:HG23	1.92	0.52
1:E:216:LYS:HG3	1:E:309:VAL:HG22	1.92	0.52
1:C:25:ILE:O	1:C:29:ARG:HG3	2.09	0.52
1:F:202:SER:CB	1:F:205:ASP:HB2	2.40	0.52
1:E:263:GLU:HA	1:E:269:LEU:CD2	2.34	0.52
1:C:448:ALA:CB	1:C:450:LEU:HD12	2.39	0.52
1:G:208:LEU:HD11	1:G:365:VAL:HG11	1.90	0.52
1:F:284:LEU:O	1:F:305:ALA:HA	2.10	0.52
1:F:384:VAL:O	1:F:388:VAL:HG23	2.10	0.52
1:F:118:THR:HA	1:F:121:VAL:HG12	1.91	0.52
3:D:545:ADP:O3B	4:D:546:SO4:S	2.68	0.52
1:G:202:SER:CB	1:G:205:ASP:HB2	2.40	0.52
1:D:37:SER:OG	1:D:46:LYS:NZ	2.39	0.52
1:F:268:MET:C	1:F:269:LEU:HD13	2.29	0.52
1:F:169:LYS:O	1:F:173:ILE:HG13	2.10	0.52
1:B:118:THR:HA	1:B:121:VAL:HG12	1.91	0.52
1:E:326:ILE:HD11	1:E:336:ASP:OD1	2.08	0.52
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.92	0.52
1:F:273:VAL:HG21	1:F:297:TYR:HB2	1.92	0.52
1:E:62:VAL:HG13	1:E:63:THR:N	2.25	0.52
1:A:419:ALA:O	1:A:427:GLN:HG3	2.10	0.52
1:G:118:THR:HA	1:G:121:VAL:HG12	1.90	0.52
1:C:350:GLY:HA3	1:D:87:LYS:HE2	1.92	0.52
1:E:372:THR:OG1	1:F:504:GLU:HB2	2.10	0.52
1:D:216:LYS:HE2	1:D:307:ARG:O	2.09	0.52
1:A:273:VAL:HG21	1:A:297:TYR:HB2	1.93	0.51
1:C:268:MET:C	1:C:269:LEU:HD13	2.31	0.51
1:A:208:LEU:HD11	1:A:365:VAL:HG11	1.92	0.51
1:H:419:ALA:O	1:H:427:GLN:HG3	2.09	0.51
1:H:155:MET:HE3	1:H:171:ALA:HB2	1.92	0.51
1:F:109:GLU:O	1:F:113:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:GLU:HA	1:F:269:LEU:CD2	2.37	0.51
1:A:448:ALA:CB	1:A:450:LEU:HD12	2.40	0.51
1:C:384:VAL:O	1:C:388:VAL:HG23	2.10	0.51
1:H:154:ALA:HB2	1:H:391:VAL:CG2	2.40	0.51
1:D:41:PRO:HG3	1:D:159:THR:HG22	1.93	0.51
1:A:73:PRO:HG3	1:H:49:VAL:HG21	1.91	0.51
3:E:545:ADP:PB	4:E:546:SO4:O2	2.68	0.51
1:B:130:LYS:HG3	1:B:134:LEU:CD1	2.34	0.51
1:F:266:SER:HB3	1:F:268:MET:HE3	1.91	0.51
1:G:197:LYS:HB3	1:G:377:ILE:CG2	2.40	0.51
1:G:197:LYS:HB3	1:G:377:ILE:HG21	1.92	0.51
1:H:118:THR:HA	1:H:121:VAL:HG12	1.93	0.51
1:C:157:SER:HB2	1:C:390:VAL:HG21	1.91	0.51
1:D:442:ARG:CG	1:D:442:ARG:NH1	2.68	0.51
1:D:273:VAL:HG21	1:D:297:TYR:HB2	1.92	0.51
1:B:419:ALA:O	1:B:427:GLN:HG3	2.10	0.51
1:H:454:GLU:O	1:H:457:VAL:N	2.43	0.51
1:D:263:GLU:HA	1:D:269:LEU:CD2	2.37	0.51
1:F:80:GLU:O	1:F:84:THR:HG23	2.10	0.51
1:H:216:LYS:HE2	1:H:307:ARG:O	2.10	0.51
1:G:215:ASP:HA	1:G:353:MET:HG2	1.92	0.51
1:D:326:ILE:HD11	1:D:336:ASP:OD1	2.11	0.51
1:E:236:ASN:HB2	1:E:325:VAL:CG1	2.41	0.51
1:E:39:LEU:HD21	1:E:444:LEU:HD21	1.92	0.51
1:B:39:LEU:HD21	1:B:444:LEU:HD21	1.90	0.51
1:E:273:VAL:HG21	1:E:297:TYR:HB2	1.92	0.51
1:G:46:LYS:HG3	1:G:64:ILE:CD1	2.34	0.51
1:F:46:LYS:HG3	1:F:64:ILE:CD1	2.34	0.51
1:C:386:ASP:O	1:C:390:VAL:HG22	2.11	0.51
1:F:464:ALA:O	1:F:466:ASN:OD1	2.28	0.51
1:D:454:GLU:O	1:D:457:VAL:N	2.44	0.51
1:F:268:MET:C	1:F:269:LEU:HD22	2.31	0.51
1:H:440:ILE:HB	1:H:441:PRO:HD3	1.92	0.51
1:H:442:ARG:HG3	1:H:452:ALA:HB1	1.92	0.51
1:F:442:ARG:HG3	1:F:452:ALA:HB1	1.93	0.51
1:E:450:LEU:HD22	1:E:455:ILE:HD11	1.91	0.51
1:E:82:ALA:HB2	1:E:97:VAL:HG23	1.92	0.51
1:A:82:ALA:HB2	1:A:97:VAL:CG2	2.40	0.51
1:F:438:GLU:C	1:F:441:PRO:HD2	2.31	0.51
1:B:273:VAL:HG21	1:B:297:TYR:HB2	1.91	0.51
1:C:36:ARG:NH2	1:C:443:THR:HG22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ASN:C	1:B:470:CYS:H	2.13	0.51
1:F:468:ASN:C	1:F:470:CYS:H	2.14	0.51
1:C:208:LEU:HD11	1:C:365:VAL:HG11	1.92	0.51
1:G:419:ALA:O	1:G:427:GLN:HG3	2.11	0.51
1:E:155:MET:HE3	1:E:171:ALA:HB2	1.93	0.51
3:H:545:ADP:O3B	4:H:546:SO4:S	2.68	0.51
1:E:154:ALA:HB2	1:E:391:VAL:CG2	2.41	0.51
1:C:49:VAL:CG2	1:D:73:PRO:HG3	2.41	0.51
1:A:326:ILE:HD11	1:A:336:ASP:OD1	2.10	0.51
1:B:438:GLU:C	1:B:441:PRO:HD2	2.32	0.50
1:C:118:THR:HA	1:C:121:VAL:CG1	2.41	0.50
1:B:227:VAL:CG1	1:B:230:ALA:HB2	2.41	0.50
1:C:215:ASP:HA	1:C:353:MET:HG2	1.93	0.50
1:D:442:ARG:HG3	1:D:452:ALA:HB1	1.93	0.50
1:D:268:MET:C	1:D:269:LEU:HD22	2.31	0.50
1:B:403:GLY:O	1:B:406:SER:HB2	2.11	0.50
1:H:236:ASN:HB2	1:H:325:VAL:CG1	2.40	0.50
1:A:512:ILE:HA	1:H:45:ASP:O	2.11	0.50
1:A:420:GLU:C	1:A:422:ILE:H	2.15	0.50
1:H:420:GLU:C	1:H:422:ILE:H	2.15	0.50
1:H:215:ASP:HA	1:H:353:MET:HG2	1.93	0.50
1:C:109:GLU:O	1:C:113:GLN:HG3	2.11	0.50
1:C:94:THR:O	1:C:98:VAL:HG23	2.12	0.50
1:H:268:MET:C	1:H:269:LEU:HD22	2.31	0.50
1:A:450:LEU:HD22	1:A:455:ILE:HD11	1.93	0.50
1:C:197:LYS:HB3	1:C:377:ILE:CG2	2.41	0.50
1:G:425:ARG:C	1:G:427:GLN:N	2.64	0.50
1:C:216:LYS:HG3	1:C:309:VAL:HG22	1.92	0.50
1:G:151:THR:OG1	1:G:175:VAL:HG21	2.11	0.50
1:D:236:ASN:HB2	1:D:325:VAL:CG1	2.42	0.50
1:D:440:ILE:HB	1:D:441:PRO:HD3	1.94	0.50
1:C:39:LEU:CD2	1:C:444:LEU:HD23	2.21	0.50
1:C:273:VAL:HG21	1:C:297:TYR:HB2	1.92	0.50
1:F:197:LYS:HB3	1:F:377:ILE:HG21	1.92	0.50
1:D:11:ASN:HA	1:D:12:MET:HG3	1.94	0.50
1:E:448:ALA:CB	1:E:450:LEU:HD12	2.40	0.50
1:F:420:GLU:C	1:F:422:ILE:H	2.14	0.50
1:D:208:LEU:HD11	1:D:365:VAL:HG11	1.93	0.50
1:D:232:ILE:HG22	1:D:234:LEU:HD12	1.94	0.50
1:H:77:MET:O	1:H:80:GLU:HB2	2.12	0.50
1:B:25:ILE:HG23	1:B:104:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:MET:O	1:G:515:VAL:HA	2.12	0.50
1:B:269:LEU:N	1:B:269:LEU:HD22	2.27	0.50
1:H:269:LEU:O	1:H:273:VAL:HG23	2.12	0.50
1:A:268:MET:C	1:A:269:LEU:HD22	2.32	0.50
1:F:425:ARG:C	1:F:427:GLN:N	2.63	0.50
1:A:284:LEU:O	1:A:305:ALA:HA	2.11	0.50
1:C:118:THR:HA	1:C:121:VAL:HG12	1.93	0.50
1:G:135:LEU:HD21	1:G:411:LEU:HD22	1.94	0.50
1:D:109:GLU:O	1:D:113:GLN:HG3	2.12	0.50
1:C:82:ALA:HB2	1:C:97:VAL:CG2	2.42	0.50
3:A:545:ADP:O3B	4:A:546:SO4:S	2.70	0.50
3:B:545:ADP:O3B	4:B:546:SO4:O3	2.30	0.50
1:B:202:SER:OG	1:B:203:ILE:N	2.44	0.50
1:A:425:ARG:C	1:A:427:GLN:N	2.65	0.50
1:C:418:TYR:CE2	1:C:422:ILE:HD11	2.46	0.50
1:D:82:ALA:HB2	1:D:97:VAL:HG23	1.93	0.50
1:B:440:ILE:HB	1:B:441:PRO:HD3	1.93	0.50
1:G:202:SER:OG	1:G:370:ARG:HB2	2.12	0.50
1:B:201:ALA:HB2	1:C:497:GLN:CD	2.28	0.50
1:G:268:MET:C	1:G:269:LEU:HD22	2.31	0.50
1:H:208:LEU:HD11	1:H:365:VAL:HG11	1.91	0.50
1:B:49:VAL:HG12	1:B:50:ASP:N	2.26	0.50
1:E:59:ASN:O	1:E:59:ASN:OD1	2.30	0.49
1:D:57:VAL:CG2	1:E:512:ILE:HD11	2.42	0.49
1:C:269:LEU:HD22	1:C:269:LEU:N	2.27	0.49
1:A:450:LEU:HD21	1:A:478:GLY:HA2	1.94	0.49
1:G:450:LEU:HD21	1:G:478:GLY:HA2	1.94	0.49
1:E:419:ALA:O	1:E:427:GLN:HG3	2.13	0.49
1:E:425:ARG:C	1:E:427:GLN:N	2.64	0.49
1:G:425:ARG:C	1:G:427:GLN:H	2.15	0.49
1:C:420:GLU:C	1:C:422:ILE:H	2.14	0.49
1:H:25:ILE:O	1:H:29:ARG:HG3	2.12	0.49
1:D:46:LYS:HG3	1:D:64:ILE:CD1	2.35	0.49
1:G:169:LYS:O	1:G:173:ILE:HG13	2.12	0.49
1:C:51:ASP:HB2	1:D:519:GLU:CG	2.43	0.49
1:G:216:LYS:HG3	1:G:309:VAL:HG22	1.93	0.49
1:F:386:ASP:O	1:F:390:VAL:HG22	2.12	0.49
1:D:36:ARG:NH2	1:D:443:THR:HG22	2.27	0.49
1:F:197:LYS:HB3	1:F:377:ILE:CG2	2.41	0.49
1:C:468:ASN:C	1:C:470:CYS:H	2.15	0.49
1:B:77:MET:CE	1:B:509:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:THR:HG23	3:G:545:ADP:O2B	2.12	0.49
1:D:49:VAL:HG12	1:D:50:ASP:N	2.26	0.49
1:A:197:LYS:HB3	1:A:377:ILE:CG2	2.41	0.49
1:D:169:LYS:O	1:D:173:ILE:HG13	2.12	0.49
1:H:425:ARG:C	1:H:427:GLN:N	2.66	0.49
1:C:326:ILE:HD11	1:C:336:ASP:OD1	2.13	0.49
3:A:545:ADP:O1B	3:A:545:ADP:O2A	2.31	0.49
1:C:268:MET:C	1:C:269:LEU:HD22	2.32	0.49
1:F:189:ASP:HB3	1:F:192:LEU:CG	2.43	0.49
1:B:420:GLU:C	1:B:422:ILE:H	2.15	0.49
1:A:157:SER:HB2	1:A:390:VAL:HG21	1.94	0.49
1:E:146:ASP:OD1	1:E:149:ILE:HD12	2.13	0.49
1:G:39:LEU:HD21	1:G:444:LEU:HD21	1.91	0.49
1:D:372:THR:OG1	1:E:501:SER:HA	2.12	0.49
1:B:263:GLU:HA	1:B:269:LEU:CD2	2.38	0.49
1:D:269:LEU:HD22	1:D:269:LEU:N	2.28	0.49
1:H:273:VAL:HG21	1:H:297:TYR:HB2	1.95	0.49
1:D:450:LEU:HD21	1:D:478:GLY:HA2	1.95	0.49
1:A:468:ASN:C	1:A:470:CYS:H	2.15	0.49
1:F:419:ALA:O	1:F:427:GLN:HG3	2.13	0.49
1:H:284:LEU:O	1:H:305:ALA:HA	2.13	0.49
1:C:425:ARG:C	1:C:427:GLN:N	2.65	0.49
1:G:117:PRO:O	1:G:121:VAL:HG12	2.12	0.49
1:B:215:ASP:HA	1:B:353:MET:HG2	1.94	0.49
3:G:545:ADP:O3B	4:G:546:SO4:O3	2.31	0.49
1:C:202:SER:HB2	1:C:205:ASP:HB2	1.95	0.49
1:A:203:ILE:H	1:A:371:GLY:HA2	1.76	0.49
1:B:225:LYS:HB3	1:B:225:LYS:NZ	2.28	0.49
1:F:269:LEU:HD22	1:F:269:LEU:N	2.27	0.49
1:D:225:LYS:NZ	1:D:225:LYS:HB3	2.28	0.49
1:G:232:ILE:HG22	1:G:234:LEU:HD12	1.95	0.49
1:A:202:SER:HB2	1:A:205:ASP:HB2	1.94	0.49
1:G:273:VAL:HG21	1:G:297:TYR:HB2	1.95	0.49
1:D:50:ASP:OD1	1:D:51:ASP:N	2.45	0.49
1:F:232:ILE:HG22	1:F:234:LEU:HD12	1.95	0.49
1:B:386:ASP:O	1:B:390:VAL:HG22	2.12	0.49
1:G:464:ALA:O	1:G:466:ASN:OD1	2.30	0.49
1:E:438:GLU:C	1:E:441:PRO:HD2	2.33	0.49
1:E:440:ILE:HB	1:E:441:PRO:HD3	1.95	0.49
1:C:442:ARG:HD3	1:C:456:LEU:HD22	1.94	0.49
1:C:442:ARG:HG3	1:C:452:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:450:LEU:HD21	1:F:478:GLY:HA2	1.95	0.49
1:E:197:LYS:HB3	1:E:377:ILE:HG21	1.93	0.49
1:C:284:LEU:O	1:C:305:ALA:HA	2.12	0.49
1:D:425:ARG:C	1:D:427:GLN:N	2.65	0.49
1:H:442:ARG:CG	1:H:442:ARG:NH1	2.71	0.48
1:A:438:GLU:C	1:A:441:PRO:HD2	2.32	0.48
1:G:468:ASN:C	1:G:470:CYS:H	2.16	0.48
1:H:189:ASP:HB3	1:H:192:LEU:CG	2.42	0.48
1:C:232:ILE:HG22	1:C:234:LEU:HD12	1.95	0.48
1:E:117:PRO:O	1:E:121:VAL:HG12	2.13	0.48
1:F:490:GLU:OE1	1:F:495:LYS:HE3	2.12	0.48
1:E:442:ARG:CG	1:E:442:ARG:NH1	2.63	0.48
1:H:263:GLU:HA	1:H:269:LEU:CD2	2.38	0.48
1:H:415:LEU:HA	1:H:415:LEU:HD23	1.67	0.48
1:E:414:LYS:O	1:E:417:GLU:HG2	2.13	0.48
1:H:232:ILE:HG22	1:H:234:LEU:HD12	1.96	0.48
1:B:425:ARG:C	1:B:427:GLN:N	2.65	0.48
1:H:118:THR:HA	1:H:121:VAL:CG1	2.43	0.48
1:F:41:PRO:HG3	1:F:159:THR:HG22	1.95	0.48
1:D:49:VAL:CG2	1:E:73:PRO:HG3	2.41	0.48
1:C:225:LYS:HB3	1:C:225:LYS:NZ	2.28	0.48
1:B:11:ASN:HA	1:B:12:MET:HG3	1.95	0.48
1:E:197:LYS:HB3	1:E:377:ILE:CG2	2.43	0.48
1:G:154:ALA:HB2	1:G:391:VAL:HG23	1.95	0.48
1:C:169:LYS:O	1:C:173:ILE:HG13	2.13	0.48
1:D:419:ALA:O	1:D:427:GLN:HG3	2.12	0.48
1:B:82:ALA:HB2	1:B:97:VAL:HG23	1.95	0.48
1:A:138:ILE:HD12	1:A:410:GLU:HG2	1.93	0.48
1:B:454:GLU:O	1:B:457:VAL:N	2.46	0.48
1:A:39:LEU:HD21	1:A:444:LEU:HD21	1.94	0.48
1:A:414:LYS:O	1:A:417:GLU:HG2	2.13	0.48
1:C:419:ALA:O	1:C:427:GLN:HG3	2.14	0.48
1:D:118:THR:HA	1:D:121:VAL:HG12	1.96	0.48
1:D:453:ILE:O	1:D:457:VAL:HG23	2.13	0.48
1:E:133:GLU:O	1:E:137:THR:HG23	2.12	0.48
1:H:363:LYS:HD3	1:H:363:LYS:HA	1.57	0.48
1:C:438:GLU:C	1:C:441:PRO:HD2	2.34	0.48
1:C:46:LYS:HG3	1:C:64:ILE:CD1	2.38	0.48
1:B:442:ARG:HG3	1:B:452:ALA:HB1	1.96	0.48
1:G:263:GLU:HA	1:G:269:LEU:CD2	2.38	0.48
1:E:225:LYS:HB3	1:E:225:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:LEU:HD21	1:E:478:GLY:HA2	1.95	0.48
1:D:284:LEU:O	1:D:305:ALA:HA	2.13	0.48
1:A:216:LYS:HG3	1:A:309:VAL:HG22	1.95	0.48
1:H:453:ILE:O	1:H:457:VAL:HG23	2.13	0.48
1:C:117:PRO:O	1:C:121:VAL:HG12	2.14	0.48
1:F:236:ASN:HB2	1:F:325:VAL:CG1	2.43	0.48
1:A:269:LEU:N	1:A:269:LEU:HD22	2.29	0.48
1:F:225:LYS:NZ	1:F:225:LYS:HB3	2.28	0.48
1:A:236:ASN:HB2	1:A:325:VAL:CG1	2.43	0.48
1:A:512:ILE:HD13	1:H:47:MET:HB2	1.96	0.48
1:C:59:ASN:OD1	1:C:59:ASN:O	2.32	0.48
1:A:225:LYS:HB3	1:A:225:LYS:NZ	2.28	0.48
1:A:263:GLU:HA	1:A:269:LEU:CD2	2.37	0.48
1:H:450:LEU:HD21	1:H:478:GLY:HA2	1.95	0.48
1:E:157:SER:HB2	1:E:390:VAL:HG21	1.94	0.48
1:G:448:ALA:CB	1:G:450:LEU:HD12	2.43	0.48
1:A:232:ILE:HG22	1:A:234:LEU:HD12	1.95	0.48
1:E:232:ILE:HG22	1:E:234:LEU:HD12	1.95	0.48
1:D:386:ASP:O	1:D:390:VAL:HG22	2.14	0.48
1:F:363:LYS:HA	1:F:363:LYS:HD3	1.59	0.48
1:F:442:ARG:CG	1:F:442:ARG:NH1	2.70	0.48
1:C:372:THR:CB	1:D:501:SER:HB3	2.38	0.47
1:G:225:LYS:NZ	1:G:225:LYS:HB3	2.28	0.47
1:H:213:LEU:HD11	1:H:355:PHE:CE2	2.49	0.47
1:A:504:GLU:OE1	1:H:376:VAL:HG11	2.14	0.47
3:C:545:ADP:O3B	4:C:546:SO4:O3	2.32	0.47
1:C:39:LEU:HD11	1:C:95:THR:HG22	1.95	0.47
1:E:202:SER:HB2	1:E:205:ASP:HB2	1.96	0.47
1:D:372:THR:HG21	1:E:501:SER:N	2.29	0.47
1:G:442:ARG:HG3	1:G:452:ALA:HB1	1.96	0.47
1:F:189:ASP:HB3	1:F:192:LEU:CD1	2.44	0.47
1:F:388:VAL:O	1:F:388:VAL:HG12	2.14	0.47
1:E:234:LEU:HD21	1:E:317:LEU:CB	2.44	0.47
1:F:118:THR:HA	1:F:121:VAL:CG1	2.43	0.47
1:H:184:ASP:HA	1:H:185:GLU:HA	1.49	0.47
1:G:292:ASP:HB3	1:H:327:THR:HG21	1.95	0.47
1:C:80:GLU:O	1:C:84:THR:HG23	2.14	0.47
1:E:268:MET:C	1:E:269:LEU:HD22	2.34	0.47
1:H:225:LYS:NZ	1:H:225:LYS:HB3	2.28	0.47
1:H:80:GLU:O	1:H:84:THR:HG23	2.15	0.47
1:E:425:ARG:C	1:E:427:GLN:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:THR:HA	1:D:121:VAL:CG1	2.44	0.47
1:H:216:LYS:HG3	1:H:309:VAL:HG22	1.96	0.47
1:H:85:GLN:HG2	1:H:92:GLY:O	2.14	0.47
1:B:326:ILE:HD11	1:B:336:ASP:OD1	2.14	0.47
1:A:133:GLU:O	1:A:137:THR:HG23	2.14	0.47
1:A:46:LYS:HG3	1:A:64:ILE:CD1	2.38	0.47
1:G:102:GLU:HG2	1:G:439:VAL:HB	1.97	0.47
1:A:454:GLU:O	1:A:457:VAL:N	2.47	0.47
1:A:49:VAL:HG12	1:A:50:ASP:N	2.30	0.47
1:B:448:ALA:CB	1:B:450:LEU:HD12	2.42	0.47
1:C:102:GLU:HG2	1:C:439:VAL:HB	1.96	0.47
1:C:51:ASP:HB2	1:D:519:GLU:HG3	1.96	0.47
1:C:154:ALA:HB2	1:C:391:VAL:CG2	2.45	0.47
1:D:420:GLU:C	1:D:422:ILE:H	2.16	0.47
1:H:343:VAL:HG13	1:H:356:VAL:HG22	1.96	0.47
1:D:227:VAL:CG1	1:D:230:ALA:HB2	2.45	0.47
1:C:155:MET:HE3	1:C:171:ALA:HB2	1.96	0.47
1:F:82:ALA:HB2	1:F:97:VAL:CG2	2.45	0.47
1:B:203:ILE:H	1:B:371:GLY:HA2	1.78	0.47
1:G:269:LEU:N	1:G:269:LEU:HD22	2.29	0.47
1:D:213:LEU:HD11	1:D:355:PHE:CE2	2.49	0.47
1:D:202:SER:HB2	1:D:205:ASP:HB2	1.95	0.47
1:B:36:ARG:NH2	1:B:443:THR:HG22	2.30	0.47
1:C:425:ARG:C	1:C:427:GLN:H	2.17	0.47
1:H:153:ILE:HG13	1:H:489:VAL:HG23	1.96	0.47
1:B:227:VAL:HG12	1:B:230:ALA:HB2	1.97	0.47
1:G:326:ILE:HD11	1:G:336:ASP:OD1	2.15	0.47
1:B:310:LYS:O	1:B:314:MET:HG2	2.15	0.47
1:G:25:ILE:O	1:G:29:ARG:HG3	2.15	0.47
1:D:414:LYS:O	1:D:417:GLU:HG2	2.15	0.47
1:G:201:ALA:HB2	1:H:497:GLN:OE1	2.14	0.47
1:A:109:GLU:O	1:A:113:GLN:HG3	2.15	0.47
1:G:363:LYS:HD3	1:G:363:LYS:HA	1.59	0.47
1:G:236:ASN:HB2	1:G:325:VAL:CG1	2.45	0.47
1:F:454:GLU:O	1:F:457:VAL:N	2.47	0.47
1:H:326:ILE:HD11	1:H:336:ASP:OD1	2.15	0.47
1:B:384:VAL:O	1:B:388:VAL:HG23	2.15	0.47
1:F:216:LYS:HG3	1:F:309:VAL:HG22	1.96	0.47
1:B:236:ASN:HB2	1:B:325:VAL:CG1	2.44	0.47
1:B:155:MET:HE3	1:B:171:ALA:HB2	1.97	0.47
1:E:266:SER:HB3	1:E:268:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:448:ALA:CB	1:F:450:LEU:HD12	2.43	0.47
1:E:80:GLU:O	1:E:84:THR:HG23	2.15	0.47
1:H:342:LEU:CD2	1:H:344:GLU:HB2	2.45	0.47
1:G:343:VAL:HG13	1:G:356:VAL:HG22	1.95	0.47
1:G:284:LEU:O	1:G:305:ALA:HA	2.14	0.47
1:B:25:ILE:O	1:B:29:ARG:HG3	2.15	0.47
1:F:184:ASP:HA	1:F:185:GLU:HA	1.49	0.47
1:C:213:LEU:HD11	1:C:355:PHE:CE2	2.50	0.47
1:H:202:SER:OG	1:H:370:ARG:HB2	2.15	0.47
1:B:450:LEU:HD21	1:B:478:GLY:HA2	1.96	0.47
1:H:269:LEU:N	1:H:269:LEU:HD22	2.30	0.47
1:E:37:SER:OG	1:E:46:LYS:NZ	2.47	0.47
1:C:51:ASP:HB2	1:D:519:GLU:CB	2.45	0.47
1:D:233:ALA:HB2	1:D:337:LEU:HD22	1.97	0.47
1:D:189:ASP:HB3	1:D:192:LEU:CD1	2.44	0.47
1:A:25:ILE:O	1:A:29:ARG:HG3	2.14	0.47
1:H:218:ARG:NH1	1:H:225:LYS:HD3	2.30	0.46
1:F:269:LEU:O	1:F:273:VAL:HG23	2.14	0.46
1:E:468:ASN:C	1:E:470:CYS:H	2.18	0.46
1:F:425:ARG:C	1:F:427:GLN:H	2.17	0.46
1:D:459:VAL:O	1:D:463:HIS:HD2	1.98	0.46
1:C:202:SER:OG	1:C:370:ARG:HB2	2.15	0.46
1:B:202:SER:HB2	1:B:205:ASP:HB2	1.96	0.46
1:F:59:ASN:OD1	1:F:59:ASN:O	2.34	0.46
1:F:218:ARG:NH1	1:F:225:LYS:HD3	2.31	0.46
1:B:46:LYS:HG3	1:B:64:ILE:CD1	2.40	0.46
1:D:234:LEU:HD21	1:D:317:LEU:CB	2.45	0.46
1:B:425:ARG:C	1:B:427:GLN:H	2.19	0.46
1:D:146:ASP:OD1	1:D:149:ILE:HD12	2.16	0.46
1:G:39:LEU:HD12	1:G:94:THR:HG22	1.98	0.46
1:C:95:THR:HG23	3:C:545:ADP:O2B	2.16	0.46
1:E:202:SER:OG	1:E:203:ILE:N	2.46	0.46
1:H:297:TYR:O	1:H:301:GLU:HG2	2.15	0.46
1:E:218:ARG:NH1	1:E:225:LYS:HD3	2.31	0.46
1:A:11:ASN:HA	1:A:12:MET:HG3	1.93	0.46
1:B:80:GLU:O	1:B:84:THR:HG23	2.15	0.46
1:B:169:LYS:O	1:B:173:ILE:HG13	2.15	0.46
1:E:459:VAL:O	1:E:463:HIS:HD2	1.97	0.46
1:D:85:GLN:HG2	1:D:92:GLY:O	2.15	0.46
1:A:41:PRO:HG3	1:A:159:THR:HG22	1.97	0.46
1:C:297:TYR:O	1:C:301:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:ASN:HA	1:H:12:MET:HG3	1.96	0.46
1:D:373:THR:CG2	1:E:505:SER:HB3	2.41	0.46
1:G:415:LEU:HD23	1:G:415:LEU:HA	1.65	0.46
1:C:189:ASP:HB3	1:C:192:LEU:CG	2.45	0.46
1:D:363:LYS:HA	1:D:363:LYS:HD3	1.57	0.46
1:H:433:PHE:CD2	1:H:433:PHE:O	2.69	0.46
1:F:155:MET:HE3	1:F:171:ALA:HB2	1.96	0.46
1:H:34:THR:HG22	1:H:35:VAL:HG13	1.97	0.46
1:A:297:TYR:O	1:A:301:GLU:HG2	2.16	0.46
1:C:450:LEU:HD21	1:C:478:GLY:HA2	1.98	0.46
1:E:420:GLU:C	1:E:422:ILE:H	2.19	0.46
1:D:189:ASP:HB3	1:D:192:LEU:CG	2.45	0.46
1:H:233:ALA:HB2	1:H:337:LEU:HD22	1.98	0.46
1:H:342:LEU:HD23	1:H:343:VAL:N	2.31	0.46
1:E:232:ILE:O	1:E:337:LEU:HA	2.16	0.46
1:B:146:ASP:OD1	1:B:149:ILE:HD12	2.14	0.46
1:D:297:TYR:O	1:D:301:GLU:HG2	2.16	0.46
1:A:218:ARG:NH1	1:A:225:LYS:HD3	2.31	0.46
1:F:414:LYS:O	1:F:417:GLU:HG2	2.16	0.46
1:H:169:LYS:O	1:H:173:ILE:HG13	2.15	0.46
1:H:275:GLU:O	1:H:278:ALA:HB3	2.16	0.46
1:B:388:VAL:HG12	1:B:388:VAL:O	2.14	0.46
1:A:425:ARG:C	1:A:427:GLN:H	2.18	0.46
1:E:189:ASP:HB3	1:E:192:LEU:CG	2.45	0.46
1:H:146:ASP:OD1	1:H:149:ILE:HD12	2.16	0.46
1:G:109:GLU:O	1:G:113:GLN:HG3	2.15	0.46
1:H:438:GLU:C	1:H:441:PRO:HD2	2.36	0.46
1:E:208:LEU:HD11	1:E:365:VAL:HG11	1.96	0.46
1:H:178:VAL:HG13	1:H:188:VAL:HG11	1.97	0.46
1:C:343:VAL:HG13	1:C:356:VAL:HG22	1.96	0.46
1:A:118:THR:HA	1:A:121:VAL:CG1	2.46	0.46
1:E:49:VAL:HG12	1:E:50:ASP:N	2.30	0.46
1:E:109:GLU:O	1:E:113:GLN:HG3	2.16	0.46
1:D:275:GLU:O	1:D:278:ALA:HB3	2.16	0.46
1:A:234:LEU:HD21	1:A:317:LEU:HB2	1.98	0.46
1:C:82:ALA:HB2	1:C:97:VAL:HG23	1.98	0.46
1:H:213:LEU:HD11	1:H:355:PHE:CD2	2.51	0.46
1:B:109:GLU:O	1:B:113:GLN:HG3	2.15	0.46
1:E:194:LYS:HB2	1:E:316:LYS:NZ	2.31	0.46
1:E:202:SER:OG	1:E:370:ARG:HB2	2.16	0.46
1:E:297:TYR:O	1:E:301:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ARG:NH1	1:G:225:LYS:HD3	2.31	0.46
1:C:269:LEU:O	1:C:273:VAL:HG23	2.16	0.46
1:C:218:ARG:NH1	1:C:225:LYS:HD3	2.31	0.46
1:G:80:GLU:O	1:G:84:THR:HG23	2.16	0.46
1:A:234:LEU:HD21	1:A:317:LEU:CB	2.46	0.46
1:E:453:ILE:O	1:E:457:VAL:HG23	2.16	0.46
1:A:151:THR:OG1	1:A:175:VAL:HG21	2.16	0.46
1:C:236:ASN:HB2	1:C:325:VAL:CG1	2.46	0.46
1:B:369:ILE:O	1:B:370:ARG:HG2	2.16	0.46
1:E:415:LEU:HA	1:E:415:LEU:HD23	1.61	0.46
1:F:234:LEU:HD21	1:F:317:LEU:CB	2.45	0.46
1:G:189:ASP:HB3	1:G:192:LEU:CG	2.46	0.46
1:H:310:LYS:O	1:H:314:MET:HG2	2.16	0.46
1:A:184:ASP:HA	1:A:185:GLU:HA	1.48	0.46
1:G:128:ALA:O	1:G:132:GLN:HG2	2.16	0.46
1:H:46:LYS:HG3	1:H:64:ILE:CD1	2.39	0.45
1:G:45:ASP:O	1:H:512:ILE:HA	2.16	0.45
1:D:240:GLU:O	1:D:269:LEU:HG	2.16	0.45
1:D:218:ARG:NH1	1:D:225:LYS:HD3	2.31	0.45
1:E:34:THR:O	1:E:46:LYS:HE2	2.16	0.45
1:B:233:ALA:HB2	1:B:337:LEU:HD22	1.98	0.45
1:B:234:LEU:HD21	1:B:317:LEU:HB2	1.98	0.45
1:G:234:LEU:HD21	1:G:317:LEU:HB2	1.98	0.45
1:G:490:GLU:OE1	1:G:495:LYS:HE3	2.14	0.45
1:B:218:ARG:NH1	1:B:225:LYS:HD3	2.31	0.45
1:A:363:LYS:HA	1:A:363:LYS:HD3	1.54	0.45
1:C:516:ILE:HG22	1:C:516:ILE:O	2.16	0.45
1:A:227:VAL:CG1	1:A:230:ALA:HB2	2.46	0.45
1:G:269:LEU:O	1:G:273:VAL:HG23	2.16	0.45
1:C:266:SER:HB3	1:C:268:MET:CE	2.46	0.45
1:E:118:THR:HA	1:E:121:VAL:HG12	1.96	0.45
1:B:234:LEU:HD21	1:B:317:LEU:CB	2.46	0.45
1:G:342:LEU:CD2	1:G:344:GLU:HB2	2.45	0.45
1:E:234:LEU:HD21	1:E:317:LEU:HB2	1.98	0.45
1:G:454:GLU:O	1:G:457:VAL:N	2.47	0.45
1:B:213:LEU:HD11	1:B:355:PHE:CE2	2.51	0.45
1:F:403:GLY:O	1:F:406:SER:HB2	2.16	0.45
1:C:233:ALA:HB2	1:C:337:LEU:HD22	1.99	0.45
3:E:545:ADP:O3B	4:E:546:SO4:O3	2.35	0.45
1:D:442:ARG:HD3	1:D:456:LEU:HD22	1.99	0.45
1:D:47:MET:HG3	1:D:55:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:ARG:NH2	1:F:443:THR:HG22	2.31	0.45
1:D:266:SER:HB3	1:D:268:MET:CE	2.47	0.45
1:H:266:SER:HB3	1:H:268:MET:CE	2.46	0.45
1:E:269:LEU:HD22	1:E:269:LEU:N	2.32	0.45
1:F:233:ALA:HB2	1:F:337:LEU:HD22	1.99	0.45
1:D:234:LEU:HD21	1:D:317:LEU:HB2	1.99	0.45
1:C:219:VAL:CG2	1:C:307:ARG:HD3	2.47	0.45
1:D:425:ARG:C	1:D:427:GLN:H	2.19	0.45
1:B:41:PRO:HG3	1:B:159:THR:HG22	1.98	0.45
1:C:433:PHE:CD2	1:C:433:PHE:O	2.70	0.45
1:C:202:SER:OG	1:C:203:ILE:N	2.48	0.45
1:F:202:SER:OG	1:F:370:ARG:HB2	2.16	0.45
1:B:442:ARG:HD3	1:B:456:LEU:HD22	1.98	0.45
1:A:266:SER:HB3	1:A:268:MET:CE	2.46	0.45
1:B:415:LEU:HD23	1:B:415:LEU:HA	1.70	0.45
1:G:234:LEU:HD21	1:G:317:LEU:CB	2.46	0.45
1:A:178:VAL:HG13	1:A:188:VAL:HG11	1.98	0.45
1:D:25:ILE:O	1:D:29:ARG:HG3	2.17	0.45
1:C:85:GLN:HG2	1:C:92:GLY:O	2.16	0.45
1:F:476:PHE:O	1:F:477:THR:C	2.55	0.45
1:E:213:LEU:HD11	1:E:355:PHE:CE2	2.51	0.45
1:H:459:VAL:O	1:H:463:HIS:HD2	1.99	0.45
1:B:266:SER:HB3	1:B:268:MET:CE	2.46	0.45
1:E:36:ARG:NH2	1:E:443:THR:HG22	2.31	0.45
1:D:448:ALA:CB	1:D:450:LEU:HD12	2.43	0.45
1:B:154:ALA:HB2	1:B:391:VAL:CG2	2.47	0.45
1:D:153:ILE:HG13	1:D:489:VAL:HG23	1.98	0.45
1:F:117:PRO:O	1:F:121:VAL:HG12	2.16	0.45
1:H:49:VAL:HG12	1:H:50:ASP:N	2.31	0.45
1:A:403:GLY:O	1:A:406:SER:HB2	2.16	0.45
1:D:203:ILE:H	1:D:371:GLY:HA2	1.82	0.45
1:D:45:ASP:O	1:E:512:ILE:HA	2.16	0.45
1:A:417:GLU:C	1:A:419:ALA:N	2.70	0.45
1:A:189:ASP:HB3	1:A:192:LEU:CG	2.46	0.45
1:F:287:GLN:O	1:F:308:ARG:HA	2.17	0.45
1:G:516:ILE:O	1:G:516:ILE:HG22	2.16	0.45
1:A:202:SER:OG	1:A:203:ILE:N	2.49	0.45
1:H:425:ARG:C	1:H:427:GLN:H	2.20	0.45
1:A:233:ALA:HB2	1:A:337:LEU:HD22	1.97	0.45
1:A:519:GLU:HB2	1:H:51:ASP:HB2	1.99	0.45
1:G:442:ARG:HD3	1:G:456:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:THR:HG22	1:F:35:VAL:HG13	1.99	0.45
1:C:49:VAL:HG12	1:C:50:ASP:N	2.32	0.45
1:A:453:ILE:O	1:A:457:VAL:HG23	2.17	0.45
1:C:151:THR:OG1	1:C:175:VAL:HG21	2.17	0.45
1:F:202:SER:OG	1:F:203:ILE:N	2.48	0.44
1:D:34:THR:O	1:D:46:LYS:HE2	2.17	0.44
1:D:59:ASN:OD1	1:D:59:ASN:O	2.34	0.44
1:G:297:TYR:O	1:G:301:GLU:HG2	2.17	0.44
1:C:273:VAL:HG11	1:C:297:TYR:CB	2.47	0.44
1:H:189:ASP:HB3	1:H:192:LEU:CD1	2.47	0.44
1:B:153:ILE:HG13	1:B:489:VAL:HG23	1.99	0.44
1:C:41:PRO:HG3	1:C:159:THR:HG22	1.99	0.44
1:G:476:PHE:O	1:G:477:THR:C	2.55	0.44
1:C:184:ASP:HA	1:C:185:GLU:HA	1.47	0.44
1:D:184:ASP:HA	1:D:185:GLU:HA	1.47	0.44
1:F:297:TYR:O	1:F:301:GLU:HG2	2.16	0.44
1:D:468:ASN:C	1:D:470:CYS:H	2.20	0.44
1:B:372:THR:HG21	1:C:501:SER:CA	2.47	0.44
1:G:233:ALA:HB2	1:G:337:LEU:HD22	1.99	0.44
1:C:466:ASN:HB2	1:C:467:GLY:H	1.63	0.44
1:F:453:ILE:O	1:F:457:VAL:HG23	2.17	0.44
1:G:227:VAL:CG1	1:G:230:ALA:HB2	2.48	0.44
1:C:300:LYS:NZ	1:D:331:ASP:OD1	2.47	0.44
1:C:454:GLU:O	1:C:457:VAL:N	2.49	0.44
3:D:545:ADP:O3B	4:D:546:SO4:O3	2.36	0.44
1:G:202:SER:OG	1:G:203:ILE:N	2.50	0.44
1:D:376:VAL:HG11	1:E:504:GLU:OE1	2.17	0.44
1:D:57:VAL:CG1	1:E:512:ILE:HD11	2.48	0.44
1:D:273:VAL:HG11	1:D:297:TYR:CB	2.47	0.44
1:F:232:ILE:O	1:F:337:LEU:HA	2.18	0.44
1:C:49:VAL:HG22	1:D:73:PRO:HB3	1.99	0.44
1:D:388:VAL:O	1:D:388:VAL:HG12	2.18	0.44
1:D:216:LYS:HG3	1:D:309:VAL:HG22	1.98	0.44
1:C:85:GLN:HG2	1:C:93:THR:HA	1.99	0.44
1:G:213:LEU:HD11	1:G:355:PHE:CE2	2.53	0.44
1:G:41:PRO:HG3	1:G:159:THR:HG22	1.99	0.44
1:E:41:PRO:HG3	1:E:159:THR:HG22	2.00	0.44
1:A:459:VAL:O	1:A:463:HIS:HD2	1.99	0.44
1:G:403:GLY:O	1:G:406:SER:HB2	2.18	0.44
1:D:34:THR:HG22	1:D:35:VAL:HG13	2.00	0.44
1:G:450:LEU:HD22	1:G:455:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG22	1:B:388:VAL:HG13	1.99	0.44
1:D:232:ILE:O	1:D:337:LEU:HA	2.17	0.44
1:A:509:LEU:HA	1:A:509:LEU:HD23	1.69	0.44
1:C:403:GLY:O	1:C:406:SER:HB2	2.17	0.44
1:F:310:LYS:O	1:F:314:MET:HG2	2.18	0.44
1:B:240:GLU:O	1:B:269:LEU:HG	2.18	0.44
1:A:169:LYS:O	1:A:173:ILE:HG13	2.18	0.44
1:C:234:LEU:HD21	1:C:317:LEU:HB2	1.99	0.44
3:F:545:ADP:O3B	4:F:546:SO4:O3	2.35	0.44
1:E:442:ARG:HG3	1:E:452:ALA:HB1	1.99	0.44
1:F:102:GLU:HG2	1:F:439:VAL:HB	1.98	0.44
1:E:169:LYS:O	1:E:173:ILE:HG13	2.17	0.44
1:A:342:LEU:HD23	1:A:343:VAL:N	2.32	0.44
1:H:234:LEU:HD21	1:H:317:LEU:CB	2.48	0.44
1:E:342:LEU:CD2	1:E:344:GLU:HB2	2.47	0.44
1:B:342:LEU:CD2	1:B:344:GLU:HB2	2.48	0.44
1:C:194:LYS:HB2	1:C:316:LYS:NZ	2.32	0.44
1:H:348:ILE:CG2	1:H:348:ILE:O	2.65	0.44
1:A:118:THR:HA	1:A:121:VAL:HG12	1.98	0.44
1:F:47:MET:HG3	1:F:55:VAL:HG23	2.00	0.44
1:B:297:TYR:O	1:B:301:GLU:HG2	2.18	0.44
1:G:34:THR:HG22	1:G:35:VAL:HG13	2.00	0.44
1:C:240:GLU:O	1:C:269:LEU:HG	2.18	0.44
1:B:232:ILE:O	1:B:337:LEU:HA	2.18	0.44
1:C:213:LEU:HD11	1:C:355:PHE:CD2	2.52	0.44
1:G:413:MET:SD	1:G:463:HIS:O	2.76	0.44
1:A:85:GLN:HG2	1:A:92:GLY:O	2.17	0.44
1:A:213:LEU:HD11	1:A:355:PHE:CE2	2.52	0.44
1:G:47:MET:HG3	1:G:55:VAL:HG23	1.99	0.44
1:F:213:LEU:HD11	1:F:355:PHE:CE2	2.52	0.44
1:G:71:GLU:OE1	1:G:71:GLU:HA	2.18	0.44
1:G:240:GLU:O	1:G:269:LEU:HG	2.18	0.44
1:A:46:LYS:HD3	1:B:514:ASP:HB3	1.98	0.44
1:E:11:ASN:HA	1:E:12:MET:HG3	1.96	0.44
1:A:292:ASP:CB	1:B:327:THR:HG21	2.42	0.44
1:C:178:VAL:HG22	1:C:388:VAL:HG13	2.00	0.44
1:C:453:ILE:O	1:C:457:VAL:HG23	2.18	0.44
1:F:459:VAL:O	1:F:463:HIS:HD2	2.01	0.44
1:F:348:ILE:O	1:F:348:ILE:CG2	2.66	0.44
1:H:47:MET:HG3	1:H:55:VAL:HG23	1.98	0.43
1:C:234:LEU:HD21	1:C:317:LEU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:ASP:HB3	1:E:192:LEU:CD1	2.48	0.43
1:B:232:ILE:HG22	1:B:234:LEU:HD12	1.99	0.43
1:E:153:ILE:HG13	1:E:489:VAL:HG23	1.98	0.43
1:E:47:MET:HG3	1:E:55:VAL:HG23	2.00	0.43
1:B:202:SER:HG	1:B:203:ILE:N	2.16	0.43
1:A:372:THR:OG1	1:B:501:SER:HA	2.17	0.43
1:A:442:ARG:HG3	1:A:452:ALA:HB1	1.99	0.43
1:D:456:LEU:HA	1:D:456:LEU:HD12	1.90	0.43
1:A:59:ASN:OD1	1:A:59:ASN:O	2.36	0.43
1:H:240:GLU:O	1:H:269:LEU:HG	2.18	0.43
1:F:130:LYS:HG3	1:F:134:LEU:CD1	2.41	0.43
1:H:433:PHE:CD2	1:H:433:PHE:C	2.91	0.43
1:E:213:LEU:HD11	1:E:355:PHE:CD2	2.53	0.43
1:F:213:LEU:HD11	1:F:355:PHE:CD2	2.54	0.43
1:B:459:VAL:O	1:B:463:HIS:HD2	2.02	0.43
1:G:85:GLN:HG2	1:G:93:THR:HA	2.01	0.43
1:B:71:GLU:HA	1:B:71:GLU:OE1	2.18	0.43
1:H:202:SER:OG	1:H:203:ILE:N	2.48	0.43
1:H:34:THR:O	1:H:46:LYS:HE2	2.18	0.43
1:C:292:ASP:C	1:D:327:THR:HG21	2.38	0.43
1:E:275:GLU:O	1:E:278:ALA:HB3	2.18	0.43
1:H:234:LEU:HD21	1:H:317:LEU:HB2	2.00	0.43
1:B:414:LYS:O	1:B:417:GLU:HG2	2.18	0.43
1:G:142:VAL:HG11	1:G:149:ILE:HG21	2.00	0.43
1:E:184:ASP:HA	1:E:185:GLU:HA	1.47	0.43
1:D:292:ASP:O	1:E:327:THR:HG21	2.18	0.43
1:A:135:LEU:HD21	1:A:411:LEU:HD22	2.00	0.43
1:C:37:SER:OG	1:C:46:LYS:NZ	2.44	0.43
1:E:269:LEU:O	1:E:273:VAL:HG23	2.18	0.43
1:B:216:LYS:HG3	1:B:309:VAL:HG22	2.01	0.43
1:C:310:LYS:O	1:C:314:MET:HG2	2.19	0.43
1:E:490:GLU:OE1	1:E:495:LYS:HE3	2.17	0.43
1:B:184:ASP:HA	1:B:185:GLU:HA	1.48	0.43
1:C:34:THR:HG22	1:C:35:VAL:HG13	2.01	0.43
1:E:473:LEU:HD12	1:E:474:ASN:N	2.33	0.43
1:H:232:ILE:O	1:H:337:LEU:HA	2.18	0.43
1:F:342:LEU:CD2	1:F:344:GLU:HB2	2.48	0.43
1:G:459:VAL:O	1:G:463:HIS:HD2	2.02	0.43
1:A:201:ALA:HB2	1:B:497:GLN:CD	2.34	0.43
1:E:442:ARG:HD3	1:E:456:LEU:HD22	2.00	0.43
1:A:442:ARG:HD3	1:A:456:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:GLU:O	1:E:269:LEU:HG	2.18	0.43
1:F:154:ALA:HB2	1:F:391:VAL:HG23	2.00	0.43
1:G:189:ASP:HB3	1:G:192:LEU:CD1	2.48	0.43
1:E:342:LEU:HD23	1:E:343:VAL:N	2.33	0.43
1:A:153:ILE:HD13	1:A:394:THR:OG1	2.17	0.43
1:C:459:VAL:O	1:C:463:HIS:HD2	2.02	0.43
1:H:139:ALA:HB2	1:H:492:LEU:HD13	2.01	0.43
3:H:545:ADP:O3B	4:H:546:SO4:O3	2.37	0.43
1:D:269:LEU:O	1:D:273:VAL:HG23	2.18	0.43
1:F:240:GLU:O	1:F:269:LEU:HG	2.19	0.43
1:G:11:ASN:HA	1:G:12:MET:HG3	1.94	0.43
1:F:417:GLU:C	1:F:419:ALA:N	2.69	0.43
1:A:519:GLU:HB2	1:H:51:ASP:CB	2.49	0.43
1:E:454:GLU:O	1:E:457:VAL:N	2.51	0.43
1:B:213:LEU:HD11	1:B:355:PHE:CD2	2.54	0.43
1:G:414:LYS:O	1:G:417:GLU:HG2	2.19	0.43
1:A:128:ALA:O	1:A:132:GLN:HG2	2.18	0.43
1:E:433:PHE:C	1:E:433:PHE:CD2	2.92	0.43
1:H:442:ARG:HD3	1:H:456:LEU:HD22	2.01	0.43
1:D:438:GLU:C	1:D:441:PRO:HD2	2.39	0.43
1:C:39:LEU:HD12	1:C:94:THR:HG22	2.00	0.43
1:F:234:LEU:HD21	1:F:317:LEU:HB2	2.00	0.43
1:B:481:GLU:OE1	1:B:486:ASN:ND2	2.52	0.43
1:B:476:PHE:O	1:B:477:THR:C	2.57	0.43
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.91	0.43
1:B:167:LYS:HD2	1:B:167:LYS:HA	1.83	0.43
1:F:39:LEU:HD21	1:F:444:LEU:HD21	1.93	0.43
1:A:240:GLU:O	1:A:269:LEU:HG	2.18	0.43
1:D:217:GLU:O	1:D:218:ARG:C	2.57	0.43
1:G:77:MET:HE3	1:G:509:LEU:HD21	1.98	0.43
1:D:213:LEU:HD11	1:D:355:PHE:CD2	2.54	0.43
1:B:133:GLU:O	1:B:137:THR:HG23	2.19	0.43
1:A:155:MET:HE3	1:A:171:ALA:HB2	2.01	0.43
1:B:85:GLN:HG2	1:B:93:THR:HA	2.00	0.43
1:H:71:GLU:HA	1:H:71:GLU:OE1	2.17	0.43
1:G:438:GLU:C	1:G:441:PRO:HD2	2.38	0.43
1:C:39:LEU:HD21	1:C:444:LEU:HD21	1.94	0.43
3:C:545:ADP:PB	4:C:546:SO4:S	3.17	0.43
1:C:456:LEU:HA	1:C:456:LEU:HD12	1.86	0.43
1:D:46:LYS:HD3	1:E:514:ASP:CB	2.36	0.43
1:D:154:ALA:HB2	1:D:391:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:MET:HG3	1:C:55:VAL:HG23	2.00	0.43
1:C:342:LEU:CD2	1:C:344:GLU:HB2	2.48	0.43
1:E:343:VAL:HG13	1:E:356:VAL:HG22	2.00	0.43
1:A:15:TYR:O	1:A:20:ALA:HB2	2.19	0.43
1:C:57:VAL:CG1	1:D:512:ILE:HD11	2.49	0.43
1:F:202:SER:HB2	1:F:205:ASP:HB2	2.00	0.42
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.86	0.42
1:G:456:LEU:HA	1:G:456:LEU:HD12	1.85	0.42
1:E:102:GLU:HG2	1:E:439:VAL:HB	2.01	0.42
1:C:263:GLU:HA	1:C:269:LEU:CD2	2.39	0.42
1:H:509:LEU:HA	1:H:509:LEU:HD23	1.78	0.42
1:A:82:ALA:HB2	1:A:97:VAL:HG23	2.00	0.42
1:C:71:GLU:HA	1:C:71:GLU:OE1	2.19	0.42
1:E:217:GLU:O	1:E:218:ARG:C	2.58	0.42
1:G:34:THR:O	1:G:46:LYS:HE2	2.19	0.42
1:F:220:SER:HB3	1:F:223:MET:HG3	2.00	0.42
1:C:417:GLU:C	1:C:419:ALA:N	2.72	0.42
1:D:342:LEU:CD2	1:D:344:GLU:HB2	2.49	0.42
1:A:53:GLY:O	1:B:76:LYS:HE2	2.19	0.42
1:B:122:LYS:HD3	1:B:426:GLU:OE1	2.19	0.42
1:H:227:VAL:CG1	1:H:230:ALA:HB2	2.49	0.42
1:D:481:GLU:OE1	1:D:486:ASN:ND2	2.52	0.42
1:E:476:PHE:O	1:E:477:THR:C	2.57	0.42
1:E:481:GLU:OE1	1:E:486:ASN:ND2	2.52	0.42
1:C:227:VAL:CG1	1:C:230:ALA:HB2	2.49	0.42
1:A:34:THR:HG22	1:A:35:VAL:HG13	2.00	0.42
1:C:363:LYS:HD3	1:C:363:LYS:HA	1.56	0.42
1:G:202:SER:HB2	1:G:205:ASP:HB2	2.01	0.42
1:H:59:ASN:O	1:H:59:ASN:OD1	2.37	0.42
1:A:217:GLU:O	1:A:218:ARG:C	2.58	0.42
1:C:189:ASP:HB3	1:C:192:LEU:CD1	2.49	0.42
1:E:233:ALA:HB2	1:E:337:LEU:HD22	2.00	0.42
1:E:388:VAL:HG12	1:E:388:VAL:O	2.18	0.42
1:B:453:ILE:O	1:B:457:VAL:HG23	2.19	0.42
1:C:490:GLU:OE1	1:C:495:LYS:HE3	2.18	0.42
1:H:414:LYS:O	1:H:417:GLU:HG2	2.19	0.42
1:C:509:LEU:HD23	1:C:509:LEU:HA	1.76	0.42
1:E:273:VAL:HG11	1:E:297:TYR:CB	2.47	0.42
1:C:232:ILE:O	1:C:337:LEU:HA	2.19	0.42
1:A:490:GLU:OE1	1:A:495:LYS:HE3	2.19	0.42
1:A:37:SER:OG	1:A:46:LYS:NZ	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLU:O	1:B:218:ARG:C	2.57	0.42
1:G:178:VAL:HG13	1:G:188:VAL:HG11	2.00	0.42
1:G:342:LEU:HD23	1:G:343:VAL:N	2.35	0.42
1:F:343:VAL:HG13	1:F:356:VAL:HG22	2.02	0.42
1:A:118:THR:HG23	1:H:44:MET:HE1	2.02	0.42
1:H:50:ASP:OD1	1:H:51:ASP:N	2.53	0.42
1:D:85:GLN:HG2	1:D:93:THR:HA	2.01	0.42
1:G:227:VAL:HG12	1:G:230:ALA:HB2	2.02	0.42
1:B:52:LEU:C	1:B:54:ASP:H	2.23	0.42
1:A:189:ASP:HB3	1:A:192:LEU:CD1	2.49	0.42
1:E:417:GLU:C	1:E:419:ALA:N	2.69	0.42
1:D:342:LEU:HD23	1:D:343:VAL:N	2.34	0.42
1:F:219:VAL:CG2	1:F:307:ARG:HD3	2.49	0.42
1:D:227:VAL:HG12	1:D:230:ALA:HB2	2.00	0.42
1:B:194:LYS:HB2	1:B:316:LYS:NZ	2.34	0.42
1:B:142:VAL:HG12	1:B:143:GLY:N	2.34	0.42
1:H:442:ARG:CG	1:H:442:ARG:HH11	2.12	0.42
1:B:456:LEU:HA	1:B:456:LEU:HD12	1.82	0.42
1:B:267:GLU:C	1:B:269:LEU:N	2.72	0.42
1:C:269:LEU:HD12	1:C:272:MET:SD	2.60	0.42
1:E:46:LYS:HD3	1:F:514:ASP:CB	2.42	0.42
1:F:77:MET:O	1:F:80:GLU:HB2	2.20	0.42
1:G:466:ASN:HB2	1:G:467:GLY:H	1.60	0.42
1:E:128:ALA:O	1:E:132:GLN:HG2	2.20	0.42
1:E:310:LYS:O	1:E:314:MET:HG2	2.20	0.42
1:F:167:LYS:HD2	1:F:167:LYS:HA	1.83	0.42
1:H:357:GLU:H	1:H:357:GLU:HG2	1.70	0.42
1:G:220:SER:HB3	1:G:223:MET:HG3	2.01	0.42
1:B:37:SER:OG	1:B:46:LYS:NZ	2.45	0.42
1:D:415:LEU:HA	1:D:415:LEU:HD23	1.69	0.42
1:B:189:ASP:HB3	1:B:192:LEU:CG	2.49	0.42
1:H:394:THR:O	1:H:398:GLY:N	2.49	0.42
1:C:433:PHE:C	1:C:433:PHE:CD2	2.92	0.42
1:D:310:LYS:O	1:D:314:MET:HG2	2.19	0.42
1:H:476:PHE:O	1:H:477:THR:C	2.57	0.42
1:E:71:GLU:HA	1:E:71:GLU:OE1	2.18	0.42
1:D:348:ILE:CG2	1:D:348:ILE:O	2.67	0.42
1:H:468:ASN:C	1:H:470:CYS:H	2.22	0.42
1:G:232:ILE:O	1:G:337:LEU:HA	2.20	0.42
1:E:50:ASP:OD1	1:E:51:ASP:N	2.52	0.42
1:A:213:LEU:HD11	1:A:355:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:LYS:HB2	1:F:316:LYS:NZ	2.35	0.42
1:G:185:GLU:HA	1:G:186:GLY:HA2	1.81	0.42
1:D:158:ILE:O	1:D:161:LYS:HB2	2.20	0.42
1:A:368:LEU:HA	1:A:368:LEU:HD12	1.87	0.42
1:E:372:THR:HG21	1:F:501:SER:CA	2.50	0.42
1:A:154:ALA:HB2	1:A:391:VAL:CG2	2.50	0.42
1:G:146:ASP:OD1	1:G:149:ILE:HD12	2.20	0.42
1:A:296:HIS:CE1	1:B:331:ASP:OD2	2.73	0.42
1:E:158:ILE:O	1:E:161:LYS:HB2	2.20	0.42
1:F:433:PHE:O	1:F:433:PHE:CD2	2.72	0.42
1:G:194:LYS:HB2	1:G:316:LYS:NZ	2.34	0.42
1:F:85:GLN:HG2	1:F:93:THR:HA	2.02	0.42
1:A:269:LEU:O	1:A:273:VAL:HG23	2.19	0.41
1:B:220:SER:HB3	1:B:223:MET:HG3	2.02	0.41
1:A:342:LEU:CD2	1:A:344:GLU:HB2	2.49	0.41
1:G:49:VAL:CG2	1:H:73:PRO:HB3	2.50	0.41
1:D:133:GLU:O	1:D:137:THR:HG23	2.20	0.41
1:B:59:ASN:O	1:B:59:ASN:OD1	2.38	0.41
1:C:217:GLU:O	1:C:218:ARG:C	2.58	0.41
1:H:199:SER:HA	1:H:377:ILE:CD1	2.45	0.41
1:F:62:VAL:CG1	1:F:63:THR:N	2.81	0.41
1:B:178:VAL:HA	1:B:193:ILE:HD11	2.02	0.41
1:E:118:THR:HA	1:E:121:VAL:CG1	2.49	0.41
1:G:184:ASP:HA	1:G:185:GLU:HA	1.52	0.41
1:A:174:ILE:HD13	1:A:387:ALA:CB	2.50	0.41
1:E:403:GLY:O	1:E:406:SER:HB2	2.18	0.41
1:E:202:SER:HG	1:E:203:ILE:N	2.18	0.41
1:C:34:THR:O	1:C:46:LYS:HE2	2.20	0.41
1:H:269:LEU:HD12	1:H:272:MET:SD	2.61	0.41
1:G:273:VAL:HG11	1:G:297:TYR:CB	2.49	0.41
1:D:51:ASP:C	1:D:51:ASP:OD1	2.59	0.41
1:D:197:LYS:HD2	1:D:377:ILE:HG22	2.01	0.41
1:H:506:THR:O	1:H:510:LEU:HG	2.20	0.41
1:A:343:VAL:HG13	1:A:356:VAL:HG22	2.02	0.41
1:C:414:LYS:O	1:C:417:GLU:HG2	2.20	0.41
1:F:48:LEU:HG	1:G:516:ILE:HB	2.02	0.41
1:H:128:ALA:O	1:H:132:GLN:HG2	2.19	0.41
1:F:49:VAL:HG12	1:F:50:ASP:N	2.35	0.41
1:G:433:PHE:C	1:G:433:PHE:CD2	2.93	0.41
1:D:71:GLU:OE1	1:D:71:GLU:HA	2.19	0.41
1:C:52:LEU:C	1:C:54:ASP:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:SER:HA	1:D:377:ILE:CD1	2.43	0.41
1:D:373:THR:HB	1:E:80:GLU:HB3	2.03	0.41
1:C:506:THR:O	1:C:510:LEU:HG	2.21	0.41
1:B:417:GLU:C	1:B:419:ALA:N	2.71	0.41
1:F:185:GLU:HA	1:F:186:GLY:HA2	1.81	0.41
1:A:227:VAL:HG12	1:A:230:ALA:HB2	2.02	0.41
1:H:456:LEU:HA	1:H:456:LEU:HD12	1.95	0.41
1:B:269:LEU:O	1:B:273:VAL:HG23	2.20	0.41
1:B:273:VAL:HG11	1:B:297:TYR:CB	2.50	0.41
1:H:220:SER:HB3	1:H:223:MET:HG3	2.03	0.41
1:H:225:LYS:CG	1:H:345:GLU:HB3	2.51	0.41
1:B:197:LYS:HD2	1:B:377:ILE:HG22	2.03	0.41
1:F:178:VAL:HG22	1:F:388:VAL:HG13	2.01	0.41
1:A:25:ILE:HG23	1:A:104:LEU:HB3	2.02	0.41
1:D:357:GLU:HG2	1:D:357:GLU:H	1.71	0.41
1:E:267:GLU:C	1:E:269:LEU:N	2.74	0.41
1:F:273:VAL:HG11	1:F:297:TYR:CB	2.49	0.41
1:C:225:LYS:CG	1:C:345:GLU:HB3	2.51	0.41
1:C:413:MET:HG3	1:C:414:LYS:N	2.35	0.41
1:H:219:VAL:CG2	1:H:307:ARG:HD3	2.51	0.41
1:H:235:LEU:HD23	1:H:235:LEU:HA	1.91	0.41
1:H:273:VAL:HG11	1:H:297:TYR:CB	2.50	0.41
1:B:199:SER:HA	1:B:377:ILE:CD1	2.44	0.41
1:A:466:ASN:HB2	1:A:467:GLY:H	1.60	0.41
1:G:85:GLN:HG2	1:G:92:GLY:O	2.21	0.41
1:E:433:PHE:O	1:E:433:PHE:CD2	2.73	0.41
1:D:57:VAL:HG22	1:E:512:ILE:HD11	2.03	0.41
1:B:269:LEU:HD12	1:B:272:MET:SD	2.61	0.41
1:H:217:GLU:O	1:H:218:ARG:C	2.57	0.41
1:A:267:GLU:C	1:A:269:LEU:N	2.74	0.41
1:D:102:GLU:HG2	1:D:439:VAL:HB	2.02	0.41
1:D:225:LYS:CG	1:D:345:GLU:HB3	2.51	0.41
1:D:189:ASP:HB3	1:D:192:LEU:HD12	2.03	0.41
1:F:146:ASP:OD1	1:F:149:ILE:HD12	2.21	0.41
1:E:348:ILE:CG2	1:E:348:ILE:O	2.69	0.41
1:F:71:GLU:OE1	1:F:71:GLU:HA	2.19	0.41
1:H:441:PRO:HB2	1:H:456:LEU:CD1	2.51	0.41
1:F:369:ILE:O	1:F:370:ARG:HG2	2.20	0.41
1:E:225:LYS:CG	1:E:345:GLU:HB3	2.51	0.41
1:G:217:GLU:O	1:G:218:ARG:C	2.59	0.41
1:C:220:SER:HB3	1:C:223:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:506:THR:O	1:F:510:LEU:HG	2.20	0.41
1:A:413:MET:HG3	1:A:414:LYS:N	2.36	0.41
1:A:232:ILE:O	1:A:337:LEU:HA	2.21	0.41
1:F:342:LEU:HD23	1:F:343:VAL:N	2.35	0.41
1:C:219:VAL:HG23	1:C:307:ARG:HD3	2.03	0.41
1:E:219:VAL:CG2	1:E:307:ARG:HD3	2.51	0.41
1:G:49:VAL:HG12	1:G:50:ASP:N	2.36	0.41
1:G:135:LEU:CD2	1:G:411:LEU:HD22	2.51	0.41
1:E:196:GLU:HG2	1:E:213:LEU:HD23	2.03	0.41
1:F:413:MET:SD	1:F:463:HIS:O	2.79	0.41
1:F:433:PHE:CD2	1:F:433:PHE:C	2.94	0.41
1:C:142:VAL:HG12	1:C:143:GLY:N	2.34	0.41
1:G:235:LEU:HD23	1:G:235:LEU:HA	1.92	0.41
1:G:167:LYS:HD2	1:G:167:LYS:HA	1.85	0.41
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.95	0.41
1:F:174:ILE:HD13	1:F:387:ALA:CB	2.51	0.41
1:F:481:GLU:OE1	1:F:486:ASN:ND2	2.54	0.41
1:F:133:GLU:O	1:F:137:THR:HG23	2.20	0.41
1:C:95:THR:HG22	1:C:440:ILE:HD12	2.02	0.41
1:G:130:LYS:HG3	1:G:134:LEU:CD1	2.42	0.41
1:C:342:LEU:HD23	1:C:343:VAL:N	2.36	0.41
1:H:227:VAL:HG12	1:H:230:ALA:HB2	2.03	0.41
1:E:44:MET:HA	1:E:44:MET:CE	2.51	0.41
1:H:167:LYS:HD2	1:H:167:LYS:HA	1.82	0.41
1:B:433:PHE:CD2	1:B:433:PHE:C	2.95	0.41
1:C:174:ILE:HD13	1:C:387:ALA:CB	2.51	0.41
1:A:310:LYS:O	1:A:314:MET:HG2	2.21	0.41
1:A:202:SER:HG	1:A:370:ARG:HB2	1.87	0.40
1:C:130:LYS:HG3	1:C:134:LEU:CD1	2.41	0.40
1:G:77:MET:HA	1:G:80:GLU:CG	2.51	0.40
1:C:412:SER:HB2	1:C:434:ALA:O	2.20	0.40
1:B:189:ASP:HB3	1:B:192:LEU:CD1	2.51	0.40
1:H:44:MET:HA	1:H:44:MET:CE	2.51	0.40
1:B:342:LEU:HD23	1:B:343:VAL:N	2.36	0.40
1:G:348:ILE:CG2	1:G:348:ILE:O	2.69	0.40
1:C:369:ILE:O	1:C:370:ARG:HG2	2.21	0.40
1:D:202:SER:OG	1:D:370:ARG:HB2	2.20	0.40
1:G:267:GLU:C	1:G:269:LEU:N	2.73	0.40
1:G:266:SER:HB3	1:G:268:MET:CE	2.51	0.40
1:G:225:LYS:CG	1:G:345:GLU:HB3	2.51	0.40
1:G:225:LYS:HG3	1:G:345:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:VAL:HG11	1:A:297:TYR:CB	2.48	0.40
1:C:267:GLU:C	1:C:269:LEU:N	2.73	0.40
1:D:25:ILE:HG23	1:D:104:LEU:HB3	2.03	0.40
1:G:433:PHE:O	1:G:433:PHE:CD2	2.75	0.40
1:F:227:VAL:CG1	1:F:230:ALA:HB2	2.52	0.40
1:D:403:GLY:O	1:D:406:SER:HB2	2.22	0.40
1:E:56:VAL:O	1:E:56:VAL:HG13	2.21	0.40
1:B:348:ILE:O	1:B:348:ILE:CG2	2.70	0.40
1:D:155:MET:HE3	1:D:171:ALA:HB2	2.03	0.40
1:D:225:LYS:HG3	1:D:345:GLU:HB3	2.04	0.40
1:A:197:LYS:HD2	1:A:377:ILE:HG22	2.03	0.40
1:F:21:GLN:O	1:F:25:ILE:HG13	2.22	0.40
1:G:153:ILE:HG13	1:G:489:VAL:HG23	2.03	0.40
1:H:159:THR:HG22	1:H:160:GLY:N	2.36	0.40
1:G:453:ILE:O	1:G:457:VAL:HG23	2.21	0.40
1:D:476:PHE:O	1:D:477:THR:C	2.60	0.40
1:G:155:MET:HE3	1:G:171:ALA:HB2	2.03	0.40
1:G:158:ILE:O	1:G:161:LYS:HB2	2.21	0.40
1:E:79:ILE:O	1:E:83:LYS:HB2	2.21	0.40
1:B:174:ILE:HD13	1:B:387:ALA:CB	2.51	0.40
1:G:357:GLU:HG2	1:G:357:GLU:H	1.70	0.40
1:D:269:LEU:HD12	1:D:272:MET:SD	2.61	0.40
1:A:225:LYS:CG	1:A:345:GLU:HB3	2.51	0.40
1:H:197:LYS:HD2	1:H:377:ILE:HG22	2.03	0.40
1:H:178:VAL:HG22	1:H:388:VAL:HG13	2.02	0.40
1:D:516:ILE:O	1:D:516:ILE:HG22	2.21	0.40
1:F:82:ALA:HB2	1:F:97:VAL:HG23	2.01	0.40
1:C:474:ASN:HD22	1:C:486:ASN:HD22	1.70	0.40
1:D:48:LEU:HG	1:E:516:ILE:HB	2.04	0.40
1:A:476:PHE:O	1:A:477:THR:C	2.59	0.40
1:F:456:LEU:HA	1:F:456:LEU:HD12	1.87	0.40
1:G:202:SER:HG	1:G:203:ILE:N	2.19	0.40
1:F:34:THR:O	1:F:46:LYS:HE2	2.21	0.40
1:C:225:LYS:HG3	1:C:345:GLU:HB3	2.03	0.40
1:H:102:GLU:HG2	1:H:439:VAL:HB	2.02	0.40
1:E:174:ILE:HD13	1:E:387:ALA:CB	2.52	0.40
1:H:490:GLU:OE1	1:H:495:LYS:HE3	2.21	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:O	1:C:185:GLU:OE2[4_556]	1.91	0.29
1:E:148:GLU:OE1	1:G:130:LYS:NZ[4_445]	1.99	0.21
1:A:451:ASP:OD1	1:G:425:ARG:NH2[2_556]	2.03	0.17
1:E:465:SER:OG	1:F:176:GLU:OE2[4_445]	2.05	0.15
1:A:425:ARG:NH2	1:G:451:ASP:OD1[2_556]	2.05	0.15
1:B:169:LYS:NZ	1:H:228:THR:OG1[4_546]	2.07	0.13
1:A:145:GLN:CA	1:C:185:GLU:OE2[4_556]	2.12	0.08
1:E:468:ASN:O	1:F:169:LYS:NZ[4_445]	2.13	0.07
1:F:274:ALA:O	1:G:266:SER:OG[2_555]	2.16	0.04
1:A:145:GLN:N	1:C:185:GLU:CG[4_556]	2.16	0.04

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	485/521 (93%)	424 (87%)	53 (11%)	8 (2%)	12	55
1	B	485/521 (93%)	423 (87%)	55 (11%)	7 (1%)	14	58
1	C	485/521 (93%)	422 (87%)	56 (12%)	7 (1%)	14	58
1	D	485/521 (93%)	423 (87%)	54 (11%)	8 (2%)	12	55
1	E	485/521 (93%)	426 (88%)	52 (11%)	7 (1%)	14	58
1	F	485/521 (93%)	427 (88%)	50 (10%)	8 (2%)	12	55
1	G	485/521 (93%)	424 (87%)	54 (11%)	7 (1%)	14	58
1	H	485/521 (93%)	425 (88%)	52 (11%)	8 (2%)	12	55
All	All	3880/4168 (93%)	3394 (88%)	426 (11%)	60 (2%)	13	56

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	C	203	ILE
1	D	146	ASP

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Mol	Chain	Res	Type
1	D	199	SER
1	E	199	SER
1	F	199	SER
1	G	199	SER
1	H	199	SER
1	H	203	ILE
1	A	146	ASP
1	A	203	ILE
1	A	265	ALA
1	A	466	ASN
1	B	146	ASP
1	B	199	SER
1	B	203	ILE
1	B	265	ALA
1	B	466	ASN
1	C	146	ASP
1	C	199	SER
1	C	265	ALA
1	C	466	ASN
1	D	203	ILE
1	D	265	ALA
1	D	466	ASN
1	E	146	ASP
1	E	203	ILE
1	E	265	ALA
1	E	466	ASN
1	F	146	ASP
1	F	203	ILE
1	F	265	ALA
1	F	466	ASN
1	G	146	ASP
1	G	203	ILE
1	G	265	ALA
1	G	426	GLU
1	G	466	ASN
1	H	146	ASP
1	H	265	ALA
1	H	466	ASN
1	C	426	GLU
1	F	89	VAL
1	A	166	ALA
1	A	426	GLU

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Mol	Chain	Res	Type
1	B	426	GLU
1	D	426	GLU
1	E	89	VAL
1	E	166	ALA
1	H	426	GLU
1	A	89	VAL
1	D	89	VAL
1	D	166	ALA
1	F	166	ALA
1	G	89	VAL
1	H	166	ALA
1	B	89	VAL
1	F	426	GLU
1	C	89	VAL
1	H	89	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	388/413 (94%)	371 (96%)	17 (4%)	35	73
1	B	388/413 (94%)	369 (95%)	19 (5%)	31	70
1	C	388/413 (94%)	370 (95%)	18 (5%)	33	72
1	D	388/413 (94%)	370 (95%)	18 (5%)	33	72
1	E	388/413 (94%)	371 (96%)	17 (4%)	35	73
1	F	388/413 (94%)	370 (95%)	18 (5%)	33	72
1	G	388/413 (94%)	369 (95%)	19 (5%)	31	70
1	H	388/413 (94%)	372 (96%)	16 (4%)	37	74
All	All	3104/3304 (94%)	2962 (95%)	142 (5%)	33	72

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	34	THR
1	A	39	LEU
1	A	48	LEU
1	A	86	GLU
1	A	145	GLN
1	A	176	GLU
1	A	218	ARG
1	A	240	GLU
1	A	264	THR
1	A	286	CYS
1	A	304	VAL
1	A	307	ARG
1	A	373	THR
1	A	412	SER
1	A	466	ASN
1	A	519	GLU
1	B	34	THR
1	B	39	LEU
1	B	48	LEU
1	B	86	GLU
1	B	134	LEU
1	B	176	GLU
1	B	218	ARG
1	B	240	GLU
1	B	264	THR
1	B	286	CYS
1	B	304	VAL
1	B	307	ARG
1	B	373	THR
1	B	412	SER
1	B	442	ARG
1	B	466	ASN
1	B	480	VAL
1	B	501	SER
1	B	519	GLU
1	C	26	LEU
1	C	34	THR
1	C	39	LEU
1	C	48	LEU
1	C	176	GLU
1	C	185	GLU
1	C	218	ARG

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Mol	Chain	Res	Type
1	C	240	GLU
1	C	264	THR
1	C	286	CYS
1	C	304	VAL
1	C	307	ARG
1	C	373	THR
1	C	412	SER
1	C	442	ARG
1	C	466	ASN
1	C	501	SER
1	C	519	GLU
1	D	34	THR
1	D	39	LEU
1	D	48	LEU
1	D	86	GLU
1	D	176	GLU
1	D	218	ARG
1	D	240	GLU
1	D	264	THR
1	D	304	VAL
1	D	307	ARG
1	D	373	THR
1	D	412	SER
1	D	442	ARG
1	D	455	ILE
1	D	466	ASN
1	D	480	VAL
1	D	501	SER
1	D	519	GLU
1	E	34	THR
1	E	39	LEU
1	E	48	LEU
1	E	86	GLU
1	E	176	GLU
1	E	218	ARG
1	E	240	GLU
1	E	264	THR
1	E	304	VAL
1	E	307	ARG
1	E	373	THR
1	E	412	SER
1	E	442	ARG

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Mol	Chain	Res	Type
1	E	443	THR
1	E	466	ASN
1	E	480	VAL
1	E	519	GLU
1	F	26	LEU
1	F	34	THR
1	F	39	LEU
1	F	48	LEU
1	F	176	GLU
1	F	218	ARG
1	F	240	GLU
1	F	264	THR
1	F	286	CYS
1	F	304	VAL
1	F	307	ARG
1	F	373	THR
1	F	412	SER
1	F	442	ARG
1	F	443	THR
1	F	466	ASN
1	F	480	VAL
1	F	519	GLU
1	G	26	LEU
1	G	34	THR
1	G	39	LEU
1	G	48	LEU
1	G	86	GLU
1	G	176	GLU
1	G	218	ARG
1	G	240	GLU
1	G	264	THR
1	G	286	CYS
1	G	304	VAL
1	G	307	ARG
1	G	373	THR
1	G	412	SER
1	G	442	ARG
1	G	466	ASN
1	G	480	VAL
1	G	501	SER
1	G	519	GLU
1	H	26	LEU

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Mol	Chain	Res	Type
1	H	34	THR
1	H	39	LEU
1	H	48	LEU
1	H	86	GLU
1	H	176	GLU
1	H	218	ARG
1	H	240	GLU
1	H	264	THR
1	H	304	VAL
1	H	307	ARG
1	H	373	THR
1	H	412	SER
1	H	466	ASN
1	H	480	VAL
1	H	519	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	HIS
1	B	11	ASN
1	B	145	GLN
1	C	145	GLN
1	D	11	ASN
1	D	145	GLN
1	E	11	ASN
1	E	145	GLN
1	F	11	ASN
1	F	145	GLN
1	G	11	ASN
1	G	145	GLN
1	H	11	ASN
1	H	145	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADP	A	545	2	22,29,29	1.05	1 (4%)	27,45,45	2.30	6 (22%)
4	SO4	A	546	2	4,4,4	0.26	0	6,6,6	0.14	0
3	ADP	B	545	2	22,29,29	1.09	2 (9%)	27,45,45	2.10	6 (22%)
4	SO4	B	546	2	4,4,4	0.35	0	6,6,6	0.43	0
3	ADP	C	545	2	22,29,29	0.96	1 (4%)	27,45,45	2.25	7 (25%)
4	SO4	C	546	2	4,4,4	0.28	0	6,6,6	0.26	0
3	ADP	D	545	2	22,29,29	0.98	1 (4%)	27,45,45	2.31	6 (22%)
4	SO4	D	546	2	4,4,4	0.44	0	6,6,6	0.54	0
3	ADP	E	545	2	22,29,29	0.97	1 (4%)	27,45,45	2.35	7 (25%)
4	SO4	E	546	2	4,4,4	0.36	0	6,6,6	0.47	0
3	ADP	F	545	2	22,29,29	0.96	1 (4%)	27,45,45	2.23	5 (18%)
4	SO4	F	546	2	4,4,4	0.24	0	6,6,6	0.25	0
3	ADP	G	545	2	22,29,29	1.15	2 (9%)	27,45,45	2.32	7 (25%)
4	SO4	G	546	2	4,4,4	0.11	0	6,6,6	0.26	0
3	ADP	H	545	2	22,29,29	1.11	2 (9%)	27,45,45	2.27	8 (29%)
4	SO4	H	546	2	4,4,4	0.15	0	6,6,6	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	545	2	-	0/12/32/32	0/3/3/3
4	SO4	A	546	2	-	0/0/0/0	0/0/0/0
3	ADP	B	545	2	-	0/12/32/32	0/3/3/3
4	SO4	B	546	2	-	0/0/0/0	0/0/0/0
3	ADP	C	545	2	-	0/12/32/32	0/3/3/3
4	SO4	C	546	2	-	0/0/0/0	0/0/0/0
3	ADP	D	545	2	-	0/12/32/32	0/3/3/3
4	SO4	D	546	2	-	0/0/0/0	0/0/0/0
3	ADP	E	545	2	-	0/12/32/32	0/3/3/3
4	SO4	E	546	2	-	0/0/0/0	0/0/0/0
3	ADP	F	545	2	-	0/12/32/32	0/3/3/3
4	SO4	F	546	2	-	0/0/0/0	0/0/0/0
3	ADP	G	545	2	-	0/12/32/32	0/3/3/3
4	SO4	G	546	2	-	0/0/0/0	0/0/0/0
3	ADP	H	545	2	-	0/12/32/32	0/3/3/3
4	SO4	H	546	2	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	545	ADP	C5-C4	2.05	1.45	1.40
3	B	545	ADP	C2-N3	2.32	1.36	1.32
3	G	545	ADP	O4'-C1'	2.45	1.44	1.41
3	D	545	ADP	C5-C4	2.45	1.46	1.40
3	F	545	ADP	C5-C4	2.52	1.46	1.40
3	H	545	ADP	O4'-C1'	2.54	1.44	1.41
3	A	545	ADP	C5-C4	2.60	1.46	1.40
3	E	545	ADP	C5-C4	2.62	1.46	1.40
3	B	545	ADP	C5-C4	2.69	1.46	1.40
3	H	545	ADP	C5-C4	2.83	1.46	1.40
3	G	545	ADP	C5-C4	2.91	1.47	1.40

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	545	ADP	N3-C2-N1	-9.55	121.58	128.89
3	G	545	ADP	N3-C2-N1	-8.92	122.06	128.89
3	A	545	ADP	N3-C2-N1	-8.85	122.11	128.89
3	H	545	ADP	N3-C2-N1	-8.69	122.24	128.89
3	D	545	ADP	N3-C2-N1	-8.53	122.36	128.89
3	F	545	ADP	N3-C2-N1	-8.51	122.38	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	545	ADP	N3-C2-N1	-8.34	122.51	128.89
3	B	545	ADP	N3-C2-N1	-7.44	123.20	128.89
3	B	545	ADP	PA-O3A-PB	-4.00	119.26	132.67
3	G	545	ADP	PA-O3A-PB	-3.87	119.70	132.67
3	C	545	ADP	PA-O3A-PB	-3.84	119.80	132.67
3	D	545	ADP	PA-O3A-PB	-3.79	119.96	132.67
3	E	545	ADP	PA-O3A-PB	-3.67	120.38	132.67
3	H	545	ADP	PA-O3A-PB	-3.54	120.81	132.67
3	A	545	ADP	PA-O3A-PB	-3.47	121.03	132.67
3	F	545	ADP	PA-O3A-PB	-3.43	121.16	132.67
3	H	545	ADP	O3'-C3'-C2'	-3.43	100.67	111.83
3	D	545	ADP	O3'-C3'-C2'	-3.37	100.87	111.83
3	C	545	ADP	C4-C5-N7	-3.34	106.40	109.48
3	A	545	ADP	O2'-C2'-C3'	-3.32	101.02	111.83
3	A	545	ADP	O3'-C3'-C2'	-3.32	101.03	111.83
3	B	545	ADP	C4-C5-N7	-3.29	106.45	109.48
3	F	545	ADP	O3'-C3'-C2'	-3.01	102.03	111.83
3	G	545	ADP	O3'-C3'-C2'	-2.95	102.23	111.83
3	B	545	ADP	O3'-C3'-C2'	-2.91	102.35	111.83
3	B	545	ADP	O2'-C2'-C3'	-2.90	102.41	111.83
3	C	545	ADP	O2'-C2'-C3'	-2.84	102.59	111.83
3	C	545	ADP	O3'-C3'-C2'	-2.80	102.73	111.83
3	F	545	ADP	O2'-C2'-C3'	-2.76	102.86	111.83
3	D	545	ADP	C4-C5-N7	-2.63	107.06	109.48
3	D	545	ADP	O2'-C2'-C3'	-2.58	103.44	111.83
3	E	545	ADP	O2'-C2'-C3'	-2.53	103.58	111.83
3	E	545	ADP	O3'-C3'-C2'	-2.46	103.84	111.83
3	F	545	ADP	C4-C5-N7	-2.38	107.29	109.48
3	G	545	ADP	O2'-C2'-C3'	-2.33	104.24	111.83
3	H	545	ADP	O2'-C2'-C3'	-2.25	104.51	111.83
3	H	545	ADP	C4-C5-N7	-2.17	107.48	109.48
3	H	545	ADP	O2A-PA-O1A	2.00	123.38	112.53
3	E	545	ADP	O2B-PB-O1B	2.01	117.06	110.58
3	A	545	ADP	N6-C6-N1	2.02	123.53	119.20
3	G	545	ADP	O2A-PA-O1A	2.03	123.55	112.53
3	C	545	ADP	C2'-C3'-C4'	2.07	106.87	102.61
3	H	545	ADP	C2-N1-C6	2.07	122.47	118.77
3	B	545	ADP	O2B-PB-O1B	2.10	117.33	110.58
3	E	545	ADP	C2'-C3'-C4'	2.10	106.93	102.61
3	E	545	ADP	C2-N1-C6	2.19	122.68	118.77
3	C	545	ADP	O2B-PB-O1B	2.28	117.91	110.58
3	G	545	ADP	O2B-PB-O1B	2.36	118.17	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	545	ADP	C2'-C3'-C4'	2.42	107.59	102.61
3	A	545	ADP	C2'-C3'-C4'	2.44	107.62	102.61
3	H	545	ADP	C2'-C3'-C4'	2.46	107.66	102.61
3	D	545	ADP	C2'-C3'-C4'	2.46	107.67	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	545	ADP	5	0
4	A	546	SO4	3	0
3	B	545	ADP	6	0
4	B	546	SO4	4	0
3	C	545	ADP	7	0
4	C	546	SO4	5	0
3	D	545	ADP	6	0
4	D	546	SO4	4	0
3	E	545	ADP	6	0
4	E	546	SO4	4	0
3	F	545	ADP	6	0
4	F	546	SO4	4	0
3	G	545	ADP	6	0
4	G	546	SO4	4	0
3	H	545	ADP	6	0
4	H	546	SO4	4	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	487/521 (93%)	0.09	41 (8%)	14	12	26, 88, 243, 287	0
1	B	487/521 (93%)	-0.11	13 (2%)	58	47	38, 90, 196, 247	0
1	C	487/521 (93%)	0.25	44 (9%)	12	10	39, 88, 282, 341	0
1	D	487/521 (93%)	0.19	45 (9%)	11	10	42, 103, 243, 287	0
1	E	487/521 (93%)	0.23	55 (11%)	7	7	34, 94, 252, 294	0
1	F	487/521 (93%)	0.32	57 (11%)	6	6	41, 100, 258, 295	0
1	G	487/521 (93%)	0.35	44 (9%)	12	10	41, 122, 245, 291	0
1	H	487/521 (93%)	0.25	39 (8%)	15	12	64, 127, 229, 274	0
All	All	3896/4168 (93%)	0.20	338 (8%)	13	12	26, 102, 250, 341	0

All (338) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	327	THR	16.1
1	G	239	ILE	14.8
1	C	238	ALA	13.5
1	D	266	SER	11.9
1	G	238	ALA	11.1
1	C	239	ILE	10.2
1	F	281	ALA	9.9
1	E	281	ALA	9.9
1	C	289	GLY	9.6
1	E	303	ILE	9.2
1	D	281	ALA	8.9
1	F	268	MET	8.4
1	E	327	THR	8.3
1	C	281	ALA	8.1
1	E	298	LEU	8.1
1	C	264	THR	7.9

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Mol	Chain	Res	Type	RSRZ
1	F	266	SER	7.7
1	F	228	THR	7.6
1	D	267	GLU	7.4
1	A	239	ILE	7.3
1	F	335	GLN	7.1
1	G	279	SER	7.1
1	F	219	VAL	7.0
1	C	279	SER	6.8
1	F	275	GLU	6.8
1	C	303	ILE	6.8
1	F	290	ILE	6.8
1	F	282	ASN	6.7
1	C	267	GLU	6.6
1	G	240	GLU	6.6
1	H	294	ALA	6.5
1	A	327	THR	6.3
1	F	270	LYS	6.1
1	A	281	ALA	5.9
1	F	271	ASP	5.9
1	F	303	ILE	5.8
1	F	302	GLY	5.7
1	E	343	VAL	5.5
1	A	228	THR	5.5
1	E	266	SER	5.5
1	G	236	ASN	5.5
1	E	225	LYS	5.4
1	A	267	GLU	5.3
1	C	270	LYS	5.2
1	F	327	THR	5.2
1	E	230	ALA	5.2
1	G	303	ILE	5.2
1	C	335	GLN	5.1
1	E	267	GLU	5.1
1	A	303	ILE	5.1
1	A	279	SER	5.1
1	E	219	VAL	5.0
1	C	271	ASP	5.0
1	D	239	ILE	5.0
1	F	285	PHE	5.0
1	A	235	LEU	5.0
1	E	240	GLU	5.0
1	E	302	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	328	ASN	4.9
1	C	302	GLY	4.8
1	A	237	CYS	4.8
1	E	227	VAL	4.8
1	F	239	ILE	4.8
1	G	327	THR	4.8
1	G	237	CYS	4.7
1	E	294	ALA	4.7
1	F	265	ALA	4.7
1	C	263	GLU	4.7
1	A	236	ASN	4.7
1	C	290	ILE	4.7
1	D	303	ILE	4.6
1	G	266	SER	4.6
1	H	279	SER	4.6
1	E	276	ILE	4.6
1	G	235	LEU	4.6
1	E	264	THR	4.6
1	G	268	MET	4.6
1	H	230	ALA	4.5
1	G	330	LYS	4.5
1	A	276	ILE	4.5
1	C	343	VAL	4.4
1	F	238	ALA	4.4
1	C	268	MET	4.4
1	H	281	ALA	4.4
1	G	343	VAL	4.3
1	E	285	PHE	4.3
1	D	349	SER	4.3
1	D	236	ASN	4.3
1	H	178	VAL	4.3
1	C	230	ALA	4.3
1	A	240	GLU	4.3
1	F	291	ASP	4.3
1	D	294	ALA	4.3
1	C	282	ASN	4.2
1	C	273	VAL	4.2
1	C	276	ILE	4.2
1	H	266	SER	4.2
1	G	358	GLU	4.2
1	A	266	SER	4.2
1	G	234	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	291	ASP	4.1
1	F	320	ALA	4.1
1	A	234	LEU	4.1
1	D	298	LEU	4.1
1	F	330	LYS	4.1
1	D	219	VAL	4.1
1	G	290	ILE	4.1
1	E	297	TYR	4.0
1	C	326	ILE	4.0
1	F	236	ASN	4.0
1	E	349	SER	4.0
1	F	358	GLU	4.0
1	C	340	ALA	4.0
1	G	349	SER	4.0
1	C	237	CYS	4.0
1	A	238	ALA	3.9
1	E	223	MET	3.9
1	G	276	ILE	3.9
1	H	321	THR	3.9
1	F	294	ALA	3.8
1	D	285	PHE	3.8
1	C	227	VAL	3.8
1	E	265	ALA	3.8
1	A	326	ILE	3.8
1	E	271	ASP	3.8
1	F	274	ALA	3.8
1	E	220	SER	3.8
1	G	281	ALA	3.7
1	A	227	VAL	3.7
1	E	234	LEU	3.7
1	F	342	LEU	3.7
1	G	227	VAL	3.7
1	D	268	MET	3.7
1	A	265	ALA	3.7
1	E	232	ILE	3.6
1	A	268	MET	3.6
1	E	228	THR	3.6
1	D	350	GLY	3.6
1	B	267	GLU	3.6
1	C	240	GLU	3.6
1	D	282	ASN	3.6
1	F	267	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	53	GLY	3.5
1	F	227	VAL	3.5
1	C	220	SER	3.5
1	D	358	GLU	3.5
1	C	226	LYS	3.5
1	F	232	ILE	3.5
1	D	280	GLY	3.5
1	H	267	GLU	3.5
1	A	273	VAL	3.5
1	D	271	ASP	3.5
1	G	232	ILE	3.4
1	D	215	ASP	3.4
1	A	302	GLY	3.4
1	D	263	GLU	3.4
1	F	276	ILE	3.4
1	G	306	ALA	3.4
1	B	235	LEU	3.4
1	D	296	HIS	3.4
1	B	264	THR	3.4
1	B	327	THR	3.4
1	G	305	ALA	3.3
1	A	225	LYS	3.3
1	F	235	LEU	3.3
1	C	232	ILE	3.3
1	C	228	THR	3.2
1	C	336	ASP	3.2
1	B	266	SER	3.2
1	G	294	ALA	3.2
1	D	232	ILE	3.2
1	A	280	GLY	3.1
1	F	279	SER	3.1
1	E	331	ASP	3.1
1	A	294	ALA	3.1
1	G	334	ALA	3.1
1	D	351	ASP	3.1
1	G	285	PHE	3.1
1	E	293	LEU	3.1
1	F	298	LEU	3.1
1	H	317	LEU	3.1
1	F	341	GLY	3.1
1	H	268	MET	3.1
1	H	297	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	320	ALA	3.0
1	F	283	VAL	3.0
1	C	234	LEU	3.0
1	D	340	ALA	3.0
1	D	270	LYS	3.0
1	E	330	LYS	3.0
1	H	295	GLN	3.0
1	H	263	GLU	3.0
1	D	265	ALA	3.0
1	F	357	GLU	3.0
1	D	295	GLN	3.0
1	G	287	GLN	3.0
1	E	323	ALA	2.9
1	D	238	ALA	2.9
1	F	215	ASP	2.9
1	D	275	GLU	2.9
1	E	268	MET	2.9
1	F	234	LEU	2.9
1	E	289	GLY	2.9
1	F	305	ALA	2.9
1	F	237	CYS	2.8
1	C	215	ASP	2.8
1	D	144	ALA	2.8
1	D	53	GLY	2.8
1	D	342	LEU	2.8
1	E	233	ALA	2.8
1	F	334	ALA	2.8
1	G	342	LEU	2.8
1	D	327	THR	2.8
1	H	280	GLY	2.8
1	E	283	VAL	2.7
1	F	317	LEU	2.7
1	D	276	ILE	2.7
1	F	359	CYS	2.7
1	B	337	LEU	2.7
1	D	364	ALA	2.7
1	A	298	LEU	2.7
1	E	224	PRO	2.7
1	F	226	LYS	2.7
1	G	480	VAL	2.7
1	F	360	LYS	2.7
1	D	229	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	240	GLU	2.7
1	F	321	THR	2.7
1	H	351	ASP	2.7
1	A	330	LYS	2.7
1	A	328	ASN	2.7
1	A	290	ILE	2.6
1	F	337	LEU	2.6
1	C	280	GLY	2.6
1	E	280	GLY	2.6
1	H	210	LYS	2.6
1	E	337	LEU	2.6
1	H	219	VAL	2.6
1	C	292	ASP	2.6
1	C	266	SER	2.6
1	E	279	SER	2.6
1	F	351	ASP	2.6
1	D	287	GLN	2.6
1	B	239	ILE	2.6
1	B	290	ILE	2.6
1	H	303	ILE	2.6
1	C	355	PHE	2.6
1	D	359	CYS	2.6
1	G	320	ALA	2.6
1	H	239	ILE	2.6
1	G	331	ASP	2.6
1	E	215	ASP	2.6
1	A	329	ILE	2.6
1	H	264	THR	2.6
1	H	320	ALA	2.5
1	H	364	ALA	2.5
1	H	328	ASN	2.5
1	B	240	GLU	2.5
1	H	273	VAL	2.5
1	A	232	ILE	2.5
1	C	269	LEU	2.5
1	H	271	ASP	2.5
1	D	272	MET	2.5
1	D	264	THR	2.5
1	G	230	ALA	2.5
1	G	357	GLU	2.5
1	G	278	ALA	2.5
1	H	327	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	278	ALA	2.4
1	E	356	VAL	2.4
1	E	270	LYS	2.4
1	E	239	ILE	2.4
1	C	219	VAL	2.4
1	E	235	LEU	2.4
1	D	220	SER	2.4
1	C	328	ASN	2.4
1	B	295	GLN	2.4
1	F	229	ASP	2.4
1	H	232	ILE	2.4
1	G	222	GLN	2.4
1	E	238	ALA	2.4
1	F	280	GLY	2.3
1	G	356	VAL	2.3
1	G	226	LYS	2.3
1	B	298	LEU	2.3
1	G	291	ASP	2.3
1	A	519	GLU	2.3
1	F	53	GLY	2.3
1	H	341	GLY	2.3
1	E	321	THR	2.3
1	H	335	GLN	2.3
1	B	234	LEU	2.3
1	C	236	ASN	2.3
1	E	226	LYS	2.3
1	F	319	LYS	2.3
1	C	301	GLU	2.3
1	D	316	LYS	2.3
1	G	307	ARG	2.3
1	E	345	GLU	2.2
1	A	335	GLN	2.2
1	A	297	TYR	2.2
1	F	331	ASP	2.2
1	E	272	MET	2.2
1	H	177	ALA	2.2
1	H	215	ASP	2.2
1	A	299	ALA	2.2
1	F	264	THR	2.2
1	A	11	ASN	2.2
1	E	282	ASN	2.2
1	E	342	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	144	ALA	2.2
1	D	279	SER	2.2
1	G	144	ALA	2.2
1	A	337	LEU	2.1
1	F	304	VAL	2.1
1	B	518	ALA	2.1
1	G	283	VAL	2.1
1	E	291	ASP	2.1
1	G	335	GLN	2.1
1	H	184	ASP	2.1
1	F	336	ASP	2.1
1	H	240	GLU	2.1
1	G	143	GLY	2.1
1	E	301	GLU	2.1
1	G	319	LYS	2.1
1	D	321	THR	2.1
1	H	358	GLU	2.1
1	A	287	GLN	2.1
1	H	301	GLU	2.1
1	E	319	LYS	2.0
1	H	292	ASP	2.0
1	H	290	ILE	2.0
1	A	229	ASP	2.0
1	A	275	GLU	2.0
1	C	298	LEU	2.0
1	F	316	LYS	2.0
1	A	224	PRO	2.0
1	E	354	ILE	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
2	MG	F	544	1/1	0.97	0.32	7.03	83,83,83,83	0
2	MG	H	544	1/1	0.96	0.33	4.23	111,111,111,111	0
2	MG	B	544	1/1	0.97	0.24	2.92	58,58,58,58	0
2	MG	D	544	1/1	0.97	0.23	1.35	92,92,92,92	0
4	SO4	C	546	5/5	0.98	0.21	1.20	71,78,107,110	0
4	SO4	B	546	5/5	0.98	0.22	0.86	59,71,88,107	0
2	MG	G	544	1/1	0.96	0.25	0.83	111,111,111,111	0
2	MG	C	544	1/1	0.95	0.19	0.64	57,57,57,57	0
4	SO4	E	546	5/5	0.98	0.21	0.58	65,72,99,100	0
3	ADP	E	545	27/27	0.95	0.22	0.58	49,70,86,98	0
4	SO4	F	546	5/5	0.98	0.23	0.48	100,101,134,137	0
2	MG	E	544	1/1	0.97	0.21	0.37	55,55,55,55	0
2	MG	A	544	1/1	0.98	0.21	0.26	65,65,65,65	0
4	SO4	D	546	5/5	0.98	0.19	0.05	66,71,89,100	0
3	ADP	D	545	27/27	0.97	0.21	0.01	66,89,104,118	0
3	ADP	H	545	27/27	0.92	0.23	-0.06	72,100,114,124	0
4	SO4	A	546	5/5	0.98	0.20	-0.08	76,81,105,106	0
3	ADP	A	545	27/27	0.96	0.19	-0.15	38,59,78,83	0
3	ADP	F	545	27/27	0.96	0.21	-0.17	45,69,88,95	0
3	ADP	C	545	27/27	0.94	0.18	-0.19	46,68,88,95	0
4	SO4	G	546	5/5	0.97	0.18	-0.22	75,90,123,124	0
3	ADP	B	545	27/27	0.95	0.21	-0.31	47,65,83,90	0
3	ADP	G	545	27/27	0.95	0.20	-0.37	71,99,116,122	0
4	SO4	H	546	5/5	0.97	0.15	-0.81	96,104,122,137	0

6.5 Other polymers

There are no such residues in this entry.