



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

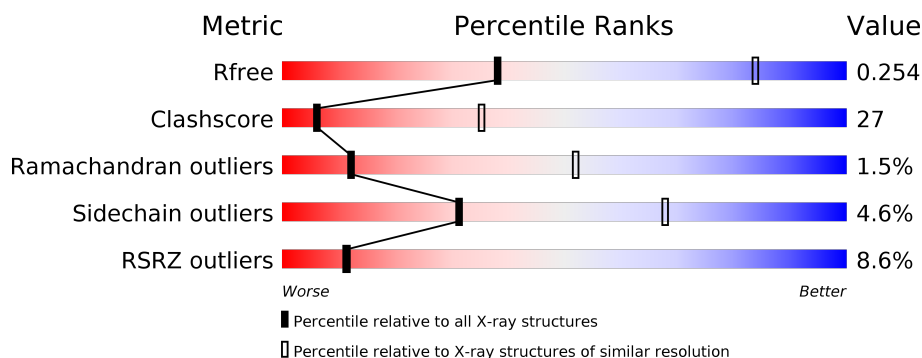
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	<div> <div>7%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>7%</div> </div> </div>
1	B	521	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>7%</div> </div> </div>
1	C	521	<div> <div>8%</div> <div> <div></div> <div>51%</div> <div>40%</div> <div>7%</div> </div> </div>
1	D	521	<div> <div>9%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>7%</div> </div> </div>
1	E	521	<div> <div>11%</div> <div> <div></div> <div>50%</div> <div>40%</div> <div>7%</div> </div> </div>
1	F	521	<div> <div>11%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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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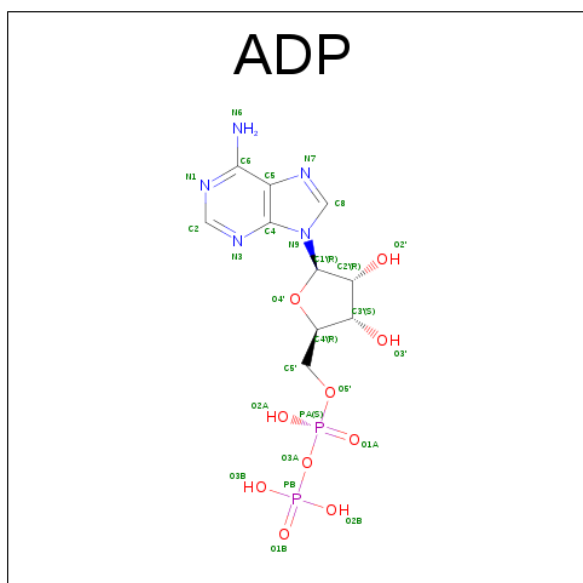
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Chain	Residue	Modelled	Actual	Comment	Reference
H	265	ALA	GLU	ENGINEERED	UNP Q877G8
H	266	SER	GLU	ENGINEERED	UNP Q877G8
H	267	GLU	LYS	ENGINEERED	UNP Q877G8

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

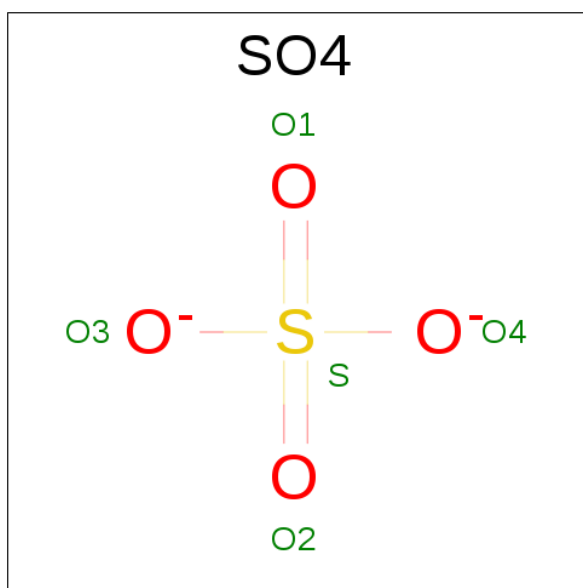
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- 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: O<sub>4</sub>S).



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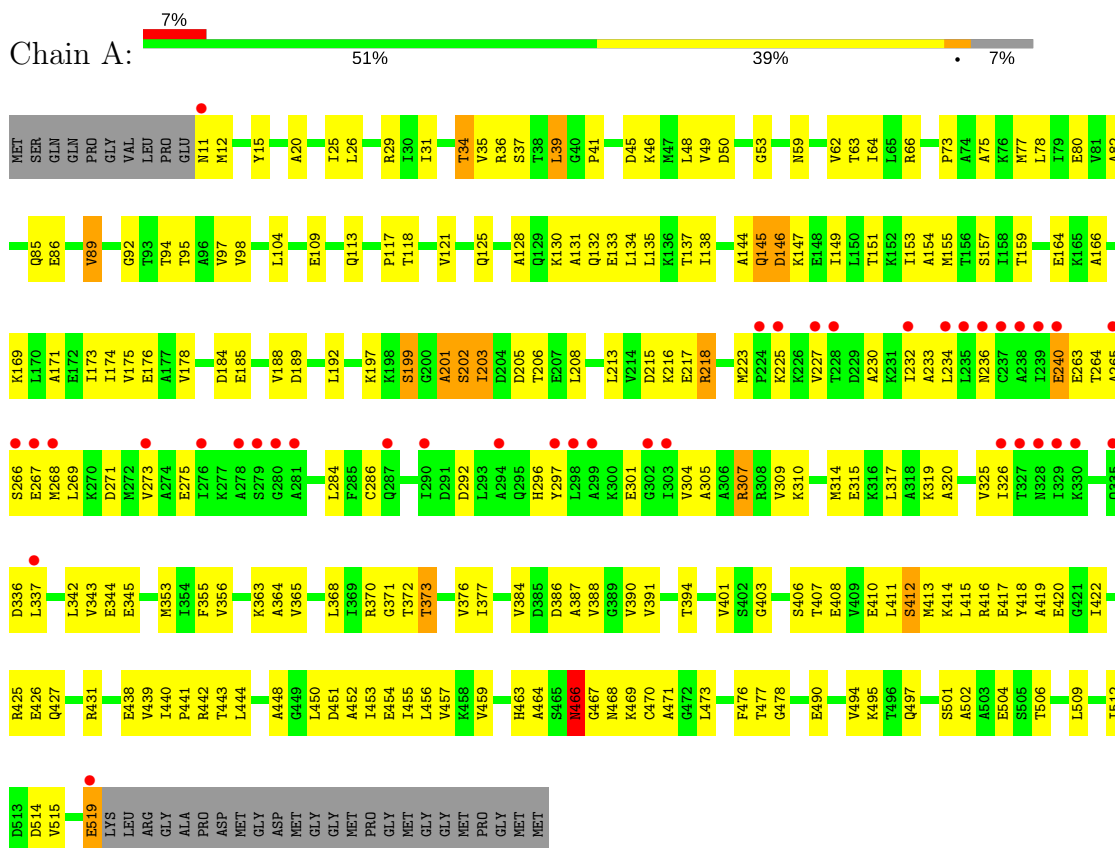
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

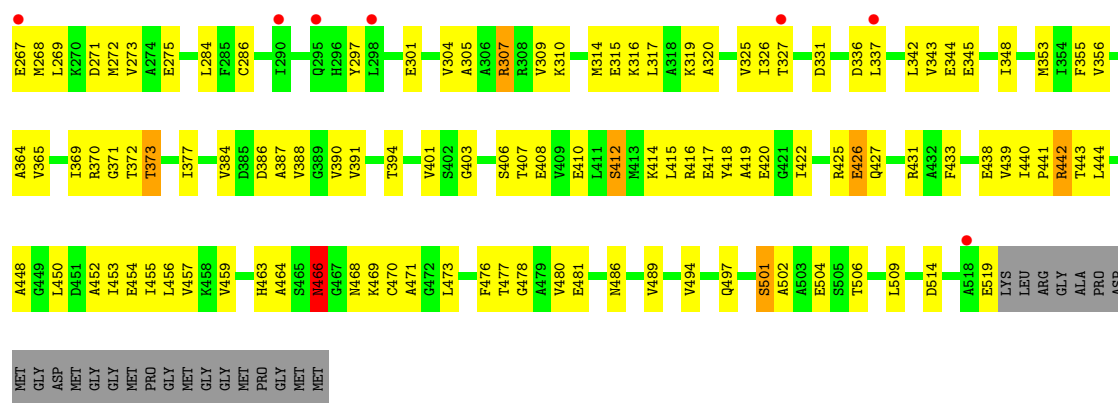
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Chaperonin

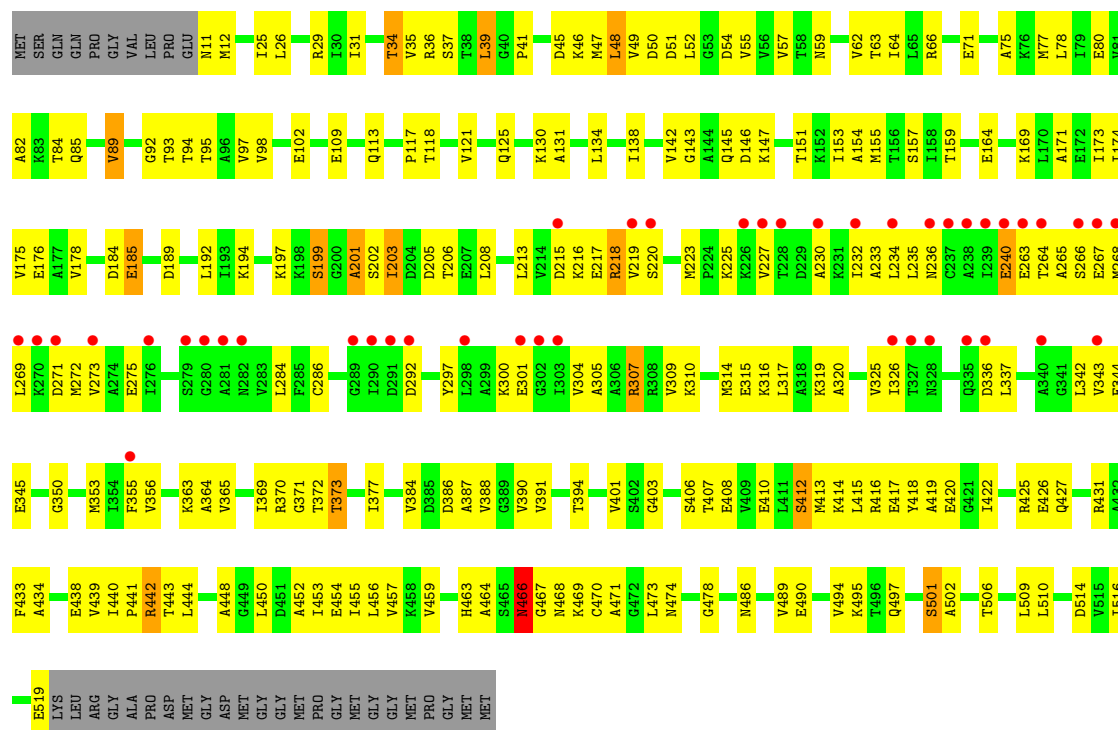


#### • Molecule 1: Chaperonin

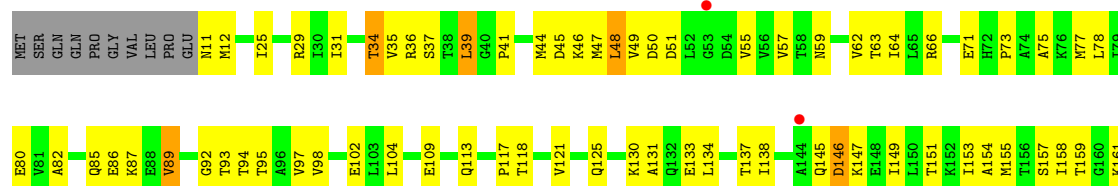


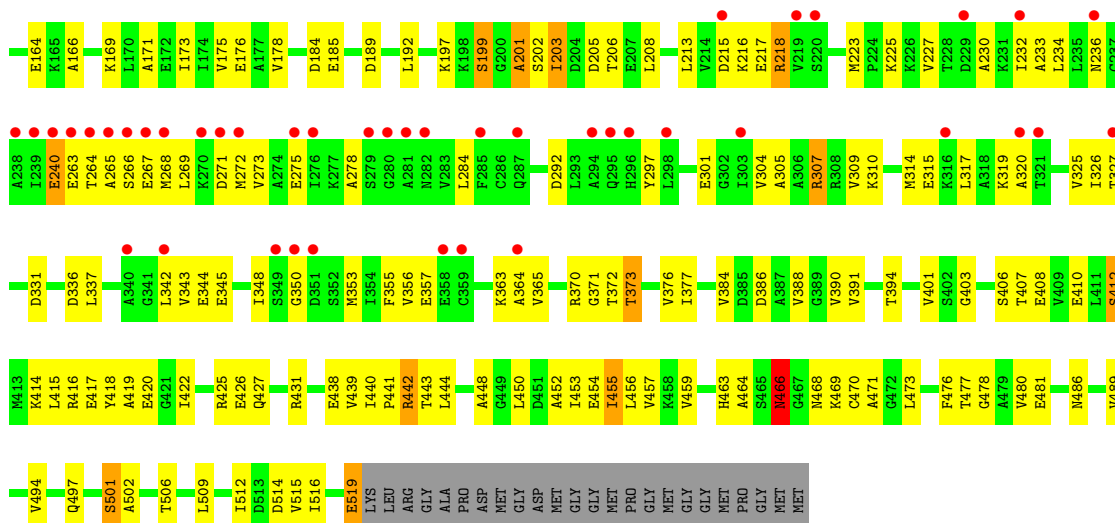


### • Molecule 1: Chaperonin

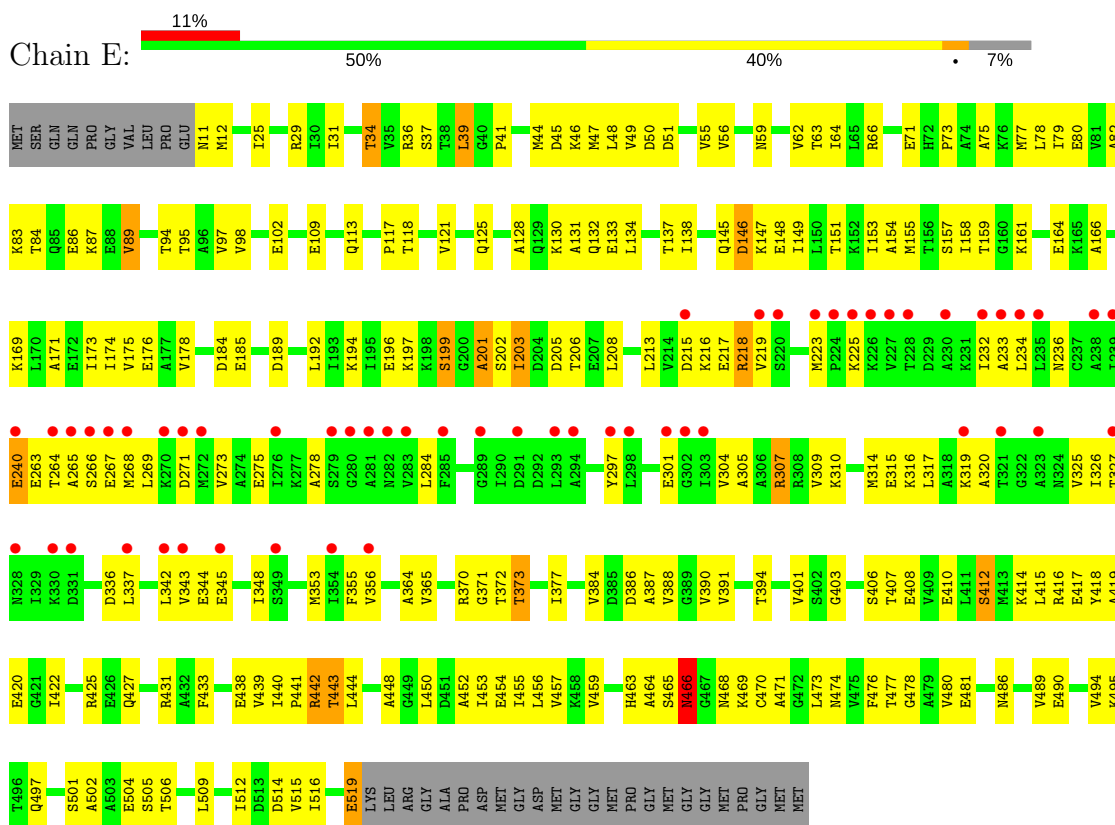


### • Molecule 1: Chaperonin

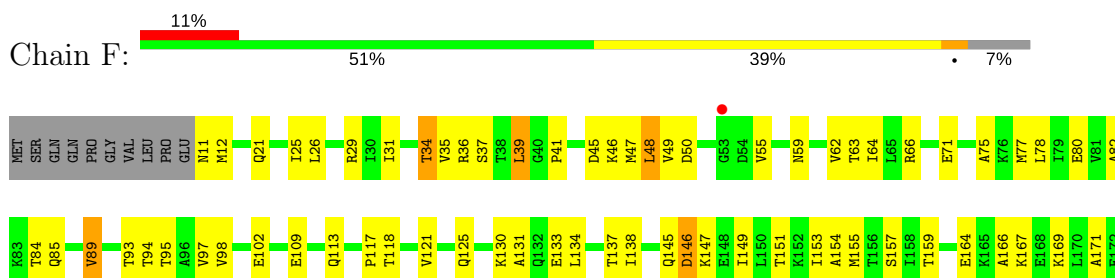


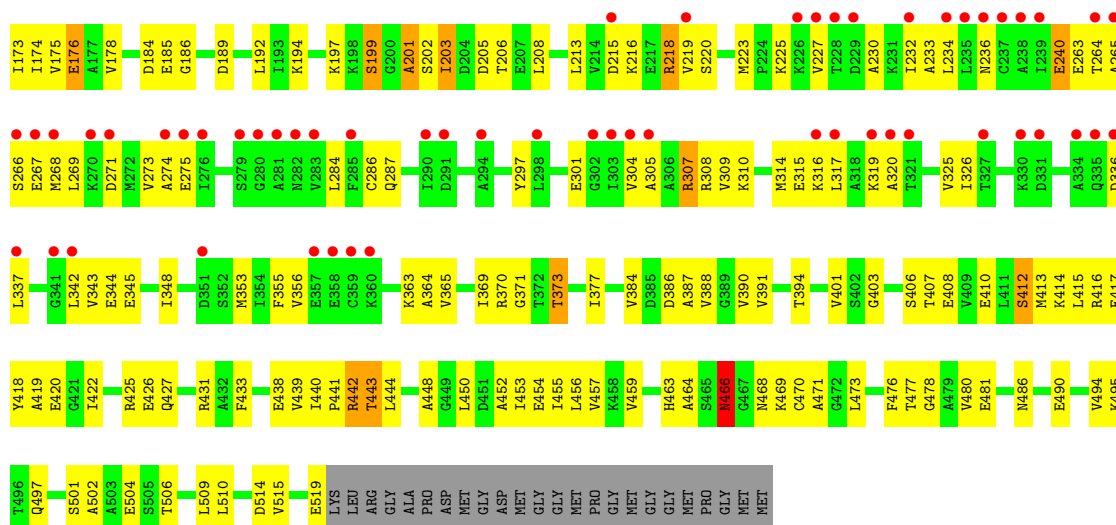


- Molecule 1: Chaperonin

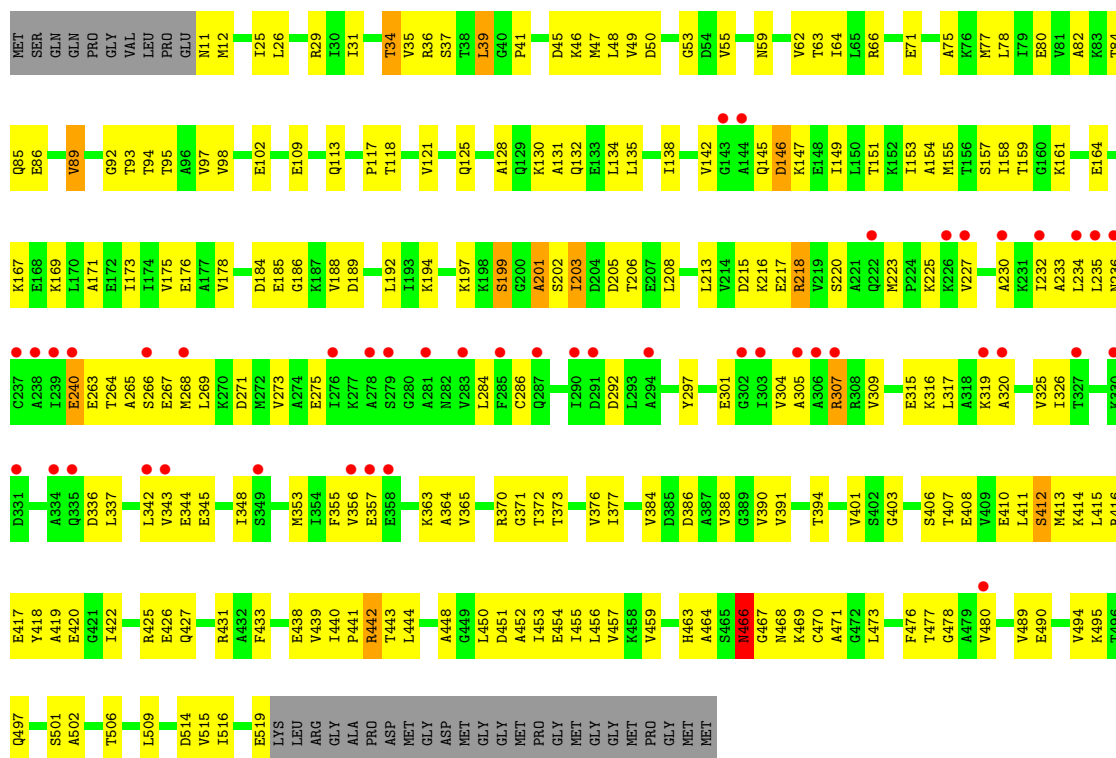


- Molecule 1: Chaperonin

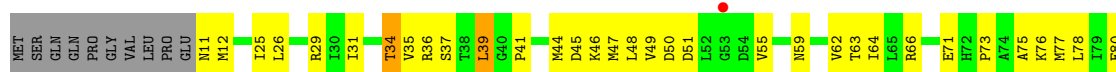




### • Molecule 1: Chaperonin



### • Molecule 1: Chaperonin



A502	A503	E504	S505	T506	L509	L510	R511	I512	D513	D514	E519	LYS	LEU	ARG	GLY	ALA	PRO	ASP	MET	GLY	ASP	MET	GLY	GLY	L456	L457	PRO	PRD	GLY	MET	GLY	H463	A464	S465	N466	Q467	N468	K469	C470	A471	G472	L473	F476	T477	G478	A479	V480	V489	E490	P491	L492	R493	V494	K495	T496	Q497	S501		
I422	R425	E426	Q427	R431	A432	F433	E438	V439	T440	P441	R442	T443	L444	A448	G449	L450	D451	A452	I453	E454	I455	L456	V457	V459	H463	A464	S465	N466	Q467	N468	K469	C470	A471	G472	L473	F476	T477	G478	A479	V480	V489	E490	P491	L492	R493	V494	K495	T496	Q497	S501									
G341	L342	V343	E344	E345	T348	D351	S352	M353	I354	F355	V356	E357	E358	K363	A364	V365	R370	G371	T372	T373	V376	I377	V384	D385	D386	A387	V388	G389	V390	V391	T394	G398	V401	T407	E408	V409	E410	L411	S412	M413	K414	L415	R416	E417	Y418	A419	E420	G421											
N236	I239	E240	T264	A265	S266	E267	M268	L269	K270	D271	M272	V273	E275	A278	S279	G280	A281	L284	I290	A294	Q295	H296	Y297	E301	G302	I303	V304	A305	A306	R307	R308	V309	K310	M314	E315	K316	L317	K318	P319	A320	T321	V325	I326	D329	T327	N328	Q335	D336	L337										
K165	A166	K167	E168	K169	L170	A171	E172	I173	I174	V175	E176	A177	V178	D184	E185	V188	D189	L192	K197	K198	S199	G200	A201	S202	I203	D204	D205	T206	A131	Q132	E133	L134	L213	V214	D215	K216	E217	R218	V219	S220	M223	P224	K225	K226	V227	T228	T151	K152	T153	A154	M155	T156	S157	K281	I232	A233	L234	L235	E164
V81	A82	K83	T84	Q85	E86	V89	G92	T93	T94	T95	A96	V97	V98	E102	E109	Q113	P117	T118	V121	Q125	A128	Q129	K130	A131	Q132	E133	L134	T138	A139	Q144	A145	D146	K147	E148	I149	L150	T151	K152	T153	A154	M155	T156	S157	T158	T159	G160	E164												



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.232 , 0.269 0.224 , 0.254	Depositor DCC
$R_{free}$ test set	2796 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 77.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.053 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	29296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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:A:201:ALA:HB2	1:B:497:GLN:OE1	1.54	1.08
1:C:39:LEU:HD23	1:C:444:LEU:HD23	1.36	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:E:39:LEU:HD23	1:E:444:LEU:HD23	1.34	1.06
1:G:39:LEU:HD23	1:G:444:LEU:HD23	1.32	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:A:206:THR:HG22	1:A:370:ARG:H	1.15	1.03
1:F:39:LEU:HD23	1:F:444:LEU:HD23	1.34	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:C:442:ARG:HH11	1:C:442:ARG:HG2	1.28	0.94
1:D:372:THR:HB	1:E:501:SER:HB3	1.48	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:D:442:ARG:HH11	1:D:442:ARG:HG2	1.34	0.92
1:G:206:THR:HG22	1:G:370:ARG:N	1.85	0.92
1:B:130:LYS:HG3	1:B:134:LEU:HD12	1.51	0.91
1:B:39:LEU:CD2	1:B:444:LEU:CD2	2.49	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:G:39:LEU:CD2	1:G:444:LEU:CD2	2.48	0.90
1:H:39:LEU:HD23	1:H:444:LEU:HD21	1.50	0.90
1:E:45:ASP:OD1	1:E:59:ASN:HB2	1.70	0.90
1:C:201:ALA:HB2	1:D:497:GLN:OE1	1.72	0.90
1:F:39:LEU:CD2	1:F:444:LEU:CD2	2.49	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:B:45:ASP:OD1	1:B:59:ASN:HB2	1.74	0.88
1:F:45:ASP:OD1	1:F:59:ASN:HB2	1.73	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: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:G:39:LEU:CD2	1:G:444:LEU:HD21	2.07	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:G:268:MET:O	1:G:269:LEU:HD13	1.76	0.84
1:H:39:LEU:CD2	1:H:444:LEU:HD21	2.04	0.84
1:A:218:ARG:HG3	1:A:345:GLU:OE1	1.78	0.84
1:A:125:GLN:OE1	1:H:164:GLU:HB2	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: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:130:LYS:HG3	1:G:134:LEU:HD12	1.59	0.83
1:G:46:LYS:HG3	1:G:64:ILE:HD13	1.58	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:A:268:MET:O	1:A:269:LEU:HD13	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:LYS:HG3	1:F:134:LEU:HD12	1.60	0.82
1:G:218:ARG:HG3	1:G:345:GLU:OE1	1.79	0.82
1:H:218:ARG:NH2	1:H:223:MET:O	2.12	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:B:31:ILE:HD13	1:B:75:ALA:HB1	1.62	0.82
1:D:31:ILE:HD13	1:D:75:ALA:HB1	1.60	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: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:E:39:LEU:CD2	1:E:444:LEU:HD21	2.10	0.81
1:H:218:ARG:HG3	1:H:345:GLU:OE1	1.81	0.81
1:B:439:VAL:O	1:B:443:THR:HG23	1.81	0.81
1:F:46:LYS:HG3	1:F:64:ILE:HD13	1.60	0.81
1:C:268:MET:O	1:C:269:LEU:HD13	1.80	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:46:LYS:HG3	1:C:64:ILE:HD13	1.60	0.81
1:F:268:MET:O	1:F:269:LEU:HD13	1.81	0.80
1:F:206:THR:CG2	1:F:370:ARG:H	1.92	0.80
1:D:218:ARG:NH2	1:D:223:MET:O	2.13	0.80
1:D:439:VAL:O	1:D:443:THR:HG23	1.79	0.80
1:C:218:ARG:HG3	1:C:345:GLU:OE1	1.82	0.80
1:E:31:ILE:HD13	1:E:75:ALA:HB1	1.62	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:A:130:LYS:HG3	1:A:134:LEU:HD12	1.63	0.80
1:E:218:ARG:CG	1:E:345:GLU:OE1	2.29	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:B:11:ASN:HA	1:B:12:MET:CG	2.12	0.80
1:C:218:ARG:NH2	1:C:223:MET:O	2.13	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: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:E:46:LYS:HD3	1:F:514:ASP:HB3	1.63	0.79
1:H:263:GLU:HA	1:H:269:LEU:HD21	1.64	0.79
1:F:201:ALA:HB2	1:G:497:GLN:OE1	1.82	0.79
1:B:468:ASN:HB2	1:B:471:ALA:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:GLU:HA	1:C:269:LEU:HD21	1.64	0.79
1:D:11:ASN:HA	1:D:12:MET:CG	2.13	0.79
1:D:199:SER:HA	1:D:377:ILE:HD11	1.65	0.79
1:A:455:ILE:HG21	1:A:473:LEU:HD22	1.64	0.79
1:F:11:ASN:HA	1:F:12:MET:CG	2.12	0.79
1:E:201:ALA:HB2	1:F:497:GLN:OE1	1.83	0.79
1:C:468:ASN:HB2	1:C:471:ALA:HB2	1.65	0.79
1:G:218:ARG:CG	1:G:345:GLU:OE1	2.31	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:F:218:ARG:CG	1:F:345:GLU:OE1	2.32	0.78
1:G:263:GLU:HA	1:G:269:LEU:HD21	1.63	0.78
1:C:31:ILE:HD13	1:C:75:ALA:HB1	1.64	0.78
1:D:468:ASN:HB2	1:D:471:ALA:HB2	1.64	0.78
1:A:11:ASN:HA	1:A:12:MET:CG	2.12	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:H:11:ASN:HA	1:H:12:MET:CG	2.14	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:B:11:ASN:HA	1:B:12:MET:HG2	1.65	0.77
1:H:218:ARG:CG	1:H:345:GLU:OE1	2.32	0.77
1:E:455:ILE:HG21	1:E:473:LEU:HD22	1.67	0.77
1:G:218:ARG:NH2	1:G:223:MET:O	2.14	0.77
1:E:11:ASN:HA	1:E:12:MET:CG	2.15	0.77
1:H:199:SER:HA	1:H:377:ILE:HD11	1.66	0.77
1:B:46:LYS:HG3	1:B:64:ILE:HD13	1.64	0.77
1:D:130:LYS:HG3	1:D:134:LEU:HD12	1.67	0.77
1:H:320:ALA:HB2	1:H:364:ALA:HB3	1.66	0.77
1:B:199:SER:HA	1:B:377:ILE:HD11	1.65	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:D:320:ALA:HB2	1:D:364:ALA:HB3	1.66	0.77
1:A:501:SER:HB3	1:H:372:THR:HB	1.65	0.77
1:C:206:THR:CG2	1:C:370:ARG:H	1.94	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:E:320:ALA:HB2	1:E:364:ALA:HB3	1.67	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
1:B:372:THR:HB	1:C:501:SER:HB3	1.65	0.76
3:C:545:ADP:O1B	4:C:546:SO4:O2	2.03	0.76
1:A:439:VAL:O	1:A:443:THR:HG23	1.84	0.76
1:E:372:THR:HB	1:F:501:SER:HB3	1.66	0.76
1:C:218:ARG:CG	1:C:345:GLU:OE1	2.33	0.76
1:C:455:ILE:HG21	1:C:473:LEU:HD22	1.66	0.76
1:G:199:SER:HA	1:G:377:ILE:HD11	1.65	0.76
1:G:468:ASN:HB2	1:G:471:ALA:HB2	1.67	0.76
1:D:373:THR:HG21	1:E:505:SER:HB3	1.68	0.76
1:C:11:ASN:HA	1:C:12:MET:HG2	1.68	0.75
1:D:218:ARG:CG	1:D:345:GLU:OE1	2.34	0.75
1:A:320:ALA:HB2	1:A:364:ALA:HB3	1.69	0.75
1:B:164:GLU:HB2	1:C:125:GLN:OE1	1.85	0.75
1:F:320:ALA:HB2	1:F:364:ALA:HB3	1.66	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:11:ASN:HA	1:F:12:MET:HG2	1.69	0.74
1:F:218:ARG:NH2	1:F:223:MET:O	2.14	0.74
1:H:63:THR:HG22	1:H:66:ARG:NH2	2.03	0.74
1:C:320:ALA:HB2	1:C:364:ALA:HB3	1.69	0.73
1:H:468:ASN:HB2	1:H:471:ALA:HB2	1.70	0.73
1:C:442:ARG:HG2	1:C:442:ARG:NH1	2.03	0.73
1:F:468:ASN:HB2	1:F:471:ALA:HB2	1.70	0.73
1:G:11:ASN:HA	1:G:12:MET:HG2	1.70	0.73
1:E:199:SER:HA	1:E:377:ILE:HD11	1.70	0.73
1:G:46:LYS:HD3	1:H:514:ASP:HB3	1.71	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: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:F:46:LYS:HD3	1:G:514:ASP:HB3	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:F:416:ARG:O	1:F:419:ALA:HB3	1.92	0.70
1:H:206:THR:CG2	1:H:370:ARG:H	1.95	0.70
1:G:320:ALA:HB2	1:G:364:ALA:HB3	1.72	0.70
1:G:206:THR:CG2	1:G:370:ARG:H	1.96	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
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
3:G:545:ADP:O1B	4:G:546:SO4:O2	2.11	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:178:VAL:HG11	1:D:391:VAL:HG12	1.73	0.69
1:D:49:VAL:HG21	1:E:73:PRO:HG3	1.75	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:D:63:THR:HG22	1:D:66:ARG:HH22	1.59	0.68
1:E:63:THR:HG22	1:E:66:ARG:NH2	2.09	0.68
1:G:39:LEU:CD2	1:G:444:LEU:HD23	2.18	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:F:208:LEU:HD11	1:F:365:VAL:CG1	2.24	0.67
1:G:502:ALA:O	1:G:506:THR:HG23	1.93	0.67
1:E:401:VAL:HB	1:E:407:THR:HG21	1.77	0.67
1:H:202:SER:OG	1:H:205:ASP:HB2	1.94	0.67
1:H:131:ALA:HB2	1:H:415:LEU:HD11	1.75	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:F:39:LEU:HD11	1:F:95:THR:HG22	1.76	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: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:G:440:ILE:O	1:G:444:LEU:HG	1.96	0.66
1:H:39:LEU:CD2	1:H:444:LEU:HD23	2.17	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:F:373:THR:HB	1:G:80:GLU:HB3	1.77	0.66
1:H:271:ASP:O	1:H:275:GLU:HG3	1.95	0.66
1:G:448:ALA:HB3	1:G:450:LEU:HD12	1.77	0.66
1:C:51:ASP:CB	1:D:519:GLU:HB2	2.26	0.66
1:E:178:VAL:HG11	1:E:391:VAL:HG12	1.78	0.66
1:E:173:ILE:HG23	1:E:208:LEU:HB2	1.78	0.65
1:F:440:ILE:O	1:F:444:LEU:HG	1.95	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
1:B:39:LEU:CD2	1:B:444:LEU:HD23	2.19	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:545:ADP:PB	4:C:546:SO4:O2	2.55	0.65
1:D:131:ALA:HB2	1:D:415:LEU:HD11	1.79	0.65
1:G:376:VAL:HG11	1:H:504:GLU:OE1	1.96	0.65
1:H:173:ILE:HG23	1:H:208:LEU:HB2	1.77	0.65
1:A:356:VAL:HG12	1:A:356:VAL:O	1.97	0.65
1:B:440:ILE:O	1:B:444:LEU:HG	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
1:H:39:LEU:HD11	1:H:95:THR:HG22	1.79	0.65
1:B:178:VAL:HG11	1:B:391:VAL:HG12	1.78	0.65
3:F:545:ADP:O1B	4:F:546:SO4:O2	2.15	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:B:401:VAL:HB	1:B:407:THR:HG21	1.77	0.64
1:F:468:ASN:O	1:F:469:LYS:HG2	1.98	0.64
1:H:440:ILE:O	1:H:444:LEU:HG	1.96	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:G:31:ILE:HD13	1:G:75:ALA:CB	2.27	0.64
1:C:202:SER:OG	1:C:205:ASP:HB2	1.98	0.64
1:B:46:LYS:HD3	1:C:514:ASP:HB3	1.79	0.64
1:E:440:ILE:O	1:E:444:LEU:HG	1.98	0.64
1:G:468:ASN:O	1:G:469:LYS:HG2	1.97	0.64
1:A:401:VAL:HB	1:A:407:THR:HG21	1.80	0.64
1:E:164:GLU:HB2	1:F:125:GLN:OE1	1.97	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:A:173:ILE:HG23	1:A:208:LEU:HB2	1.80	0.64
1:A:502:ALA:O	1:A:506:THR:HG23	1.98	0.64
1:F:178:VAL:HG11	1:F:391:VAL:HG12	1.80	0.64
1:G:202:SER:OG	1:G:205:ASP:HB2	1.98	0.64
1:A:189:ASP:HB3	1:A:192:LEU:HG	1.80	0.63
1:C:233:ALA:O	1:C:284:LEU:HD12	1.98	0.63
1:C:502:ALA:O	1:C:506:THR:HG23	1.97	0.63
1:C:189:ASP:HB3	1:C:192:LEU:HG	1.80	0.63
1:C:440:ILE:O	1:C:444:LEU:HG	1.98	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:D:233:ALA:O	1:D:284:LEU:HD12	1.99	0.63
1:E:373:THR:HB	1:F:80:GLU:HB3	1.80	0.63
1:E:94:THR:O	1:E:98:VAL:HG23	1.99	0.63
1:F:271:ASP:O	1:F:275:GLU:HG3	1.99	0.63
1:D:89:VAL:HG11	1:D:494:VAL:HG22	1.81	0.63
1:E:95:THR:HG23	3:E:545:ADP:O2B	1.99	0.63
1:B:271:ASP:O	1:B:275:GLU:HG3	1.98	0.62
1:F:420:GLU:HG2	1:F:431:ARG:HH22	1.63	0.62
1:F:62:VAL:HG13	1:F:63:THR:N	2.14	0.62
1:G:189:ASP:HB3	1:G:192:LEU:HG	1.81	0.62
1:H:77:MET:HA	1:H:80:GLU:HG2	1.81	0.62
1:D:271:ASP:O	1:D:275:GLU:HG3	1.99	0.62
1:D:44:MET:HE1	1:E:118:THR:HG23	1.80	0.62
1:E:189:ASP:HB3	1:E:192:LEU:HG	1.80	0.62
1:H:203:ILE:HA	1:H:370:ARG:O	2.00	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
1:B:131:ALA:HB2	1:B:415:LEU:HD11	1.81	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
3:G:545:ADP:PB	4:G:546:SO4:O2	2.58	0.62
1:H:401:VAL:HB	1:H:407:THR:HG21	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:C:408:GLU:O	1:C:412:SER:HB3	2.00	0.62
1:E:468:ASN:O	1:E:469:LYS:HG2	2.00	0.62
1:F:202:SER:OG	1:F:205:ASP:HB2	1.99	0.62
1:H:408:GLU:O	1:H:412:SER:HB3	1.99	0.62
1:C:271:ASP:O	1:C:275:GLU:HG3	2.00	0.62
1:E:416:ARG:O	1:E:419:ALA:HB3	1.99	0.62
1:B:39:LEU:HD11	1:B:95:THR:HG22	1.82	0.61
1:D:189:ASP:HB3	1:D:192:LEU:HG	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: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:B:31:ILE:HD11	1:B:78:LEU:HB2	1.81	0.61
1:C:468:ASN:O	1:C:469:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:SER:OG	1:E:205:ASP:HB2	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: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:E:203:ILE:HA	1:E:370:ARG:O	2.01	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: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: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:B:189:ASP:HB3	1:B:192:LEU:HG	1.83	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:315:GLU:O	1:B:319:LYS:HG3	2.01	0.61
1:B:468:ASN:O	1:B:469:LYS:HG2	2.01	0.61
1:D:372:THR:HB	1:E:501:SER:CB	2.27	0.61
1:E:386:ASP:O	1:E:390:VAL:HG22	2.01	0.61
1:H:233:ALA:O	1:H:284:LEU:HD12	2.01	0.61
1:A:408:GLU:O	1:A:412:SER:HB3	2.01	0.60
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: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:C:31:ILE:HD11	1:C:78:LEU:HB2	1.83	0.60
1:D:420:GLU:HG2	1:D:431:ARG:HH22	1.66	0.60
1:G:173:ILE:HG23	1:G:208:LEU:HB2	1.82	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: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
1:G:37:SER:OG	1:G:46:LYS:NZ	2.33	0.60
1:B:408:GLU:O	1:B:412:SER:HB3	2.01	0.60
1:D:401:VAL:HB	1:D:407:THR:HG21	1.82	0.60
1:D:201:ALA:HB2	1:E:497:GLN:OE1	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:C:273:VAL:HG11	1:C:297:TYR:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:545:ADP:O1B	4:E:546:SO4:O2	2.18	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:D:31:ILE:HD11	1:D:78:LEU:HB2	1.84	0.60
1:F:203:ILE:HA	1:F:370:ARG:O	2.02	0.60
1:G:342:LEU:HD21	1:G:344:GLU:HB2	1.84	0.60
1:A:31:ILE:HD13	1:A:75:ALA:CB	2.31	0.60
3:D:545:ADP:O1B	3:D:545:ADP:O2A	2.19	0.60
1:E:77:MET:CE	1:E:509:LEU:HD21	2.31	0.60
1:F:89:VAL:HG11	1:F:494:VAL:HG22	1.84	0.60
1:G:233:ALA:O	1:G:284:LEU:HD12	2.01	0.60
1:C:416:ARG:O	1:C:419:ALA:HB3	2.01	0.60
1:C:31:ILE:HD13	1:C:75:ALA:CB	2.32	0.60
1:C:164:GLU:HB2	1:D:125:GLN:OE1	2.02	0.60
1:E:273:VAL:HG11	1:E:297:TYR:HB3	1.84	0.60
1:F:315:GLU:O	1:F:319:LYS:HG3	2.01	0.60
1:G:31:ILE:HD11	1:G:78:LEU:HB2	1.83	0.60
1:G:384:VAL:O	1:G:388:VAL:HG23	2.02	0.60
1:H:94:THR:O	1:H:98:VAL:HG23	2.02	0.60
1:A:233:ALA:O	1:A:284:LEU:HD12	2.02	0.59
1:A:208:LEU:HD11	1:A:365:VAL:CG1	2.31	0.59
1:D:356:VAL:O	1:D:356:VAL:HG12	2.02	0.59
1:D:77:MET:CE	1:D:509:LEU:HD21	2.32	0.59
1:H:420:GLU:HG2	1:H:431:ARG:HH22	1.66	0.59
1:H:31:ILE:HD13	1:H:75:ALA:CB	2.30	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:H:77:MET:CE	1:H:509:LEU:HD21	2.32	0.59
1:H:31:ILE:HD11	1:H:78:LEU:HB2	1.84	0.59
1:B:273:VAL:HG11	1:B:297:TYR:HB3	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: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:E:233:ALA:O	1:E:284:LEU:HD12	2.02	0.59
1:E:315:GLU:O	1:E:319:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:VAL:HG11	1:G:297:TYR:HB3	1.84	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:315:GLU:O	1:D:319:LYS:HG3	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:C:203:ILE:HA	1:C:370:ARG:O	2.03	0.59
1:B:418:TYR:CE2	1:B:422:ILE:HD11	2.37	0.58
1:F:173:ILE:HG23	1:F:208:LEU:HB2	1.83	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:A:273:VAL:HG11	1:A:297:TYR:HB3	1.85	0.58
1:F:95:THR:HG23	3:F:545:ADP:O2B	2.02	0.58
1:A:178:VAL:HG11	1:A:391:VAL:HG12	1.86	0.58
3:D:545:ADP:O1B	4:D:546:SO4:O2	2.21	0.58
1:E:408:GLU:O	1:E:412:SER:HB3	2.02	0.58
1:H:273:VAL:HG11	1:H:297:TYR:HB3	1.86	0.58
1:C:89:VAL:HG11	1:C:494:VAL:HG22	1.85	0.58
1:D:62:VAL:HG13	1:D:63:THR:N	2.18	0.58
1:E:89:VAL:HG11	1:E:494:VAL:HG22	1.85	0.58
1:H:145:GLN:O	1:H:147:LYS:N	2.36	0.58
1:D:94:THR:O	1:D:98:VAL:HG23	2.04	0.58
1:F:425:ARG:O	1:F:427:GLN:N	2.37	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
3:G:545:ADP:O2A	3:G:545:ADP:O1B	2.22	0.58
1:H:418:TYR:CE2	1:H:422:ILE:HD11	2.38	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:G:203:ILE:HA	1:G:370:ARG:O	2.03	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:F:31:ILE:HD13	1:F:75:ALA:CB	2.34	0.58
1:E:138:ILE:HD12	1:E:410:GLU:HG2	1.86	0.58
1:G:218:ARG:HG2	1:G:345:GLU:OE1	2.03	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:A:89:VAL:HG11	1:A:494:VAL:HG22	1.85	0.57
1:B:145:GLN:O	1:B:147:LYS:N	2.37	0.57
1:H:138:ILE:HD12	1:H:410:GLU:HG2	1.86	0.57
1:H:425:ARG:O	1:H:427:GLN:N	2.37	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:153:ILE:HD13	1:D:394:THR:OG1	2.03	0.57
1:D:384:VAL:O	1:D:388:VAL:HG23	2.04	0.57
1:A:216:LYS:HE2	1:A:307:ARG:O	2.05	0.57
1:A:94:THR:O	1:A:98:VAL:HG23	2.05	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:E:425:ARG:O	1:E:427:GLN:N	2.37	0.57
1:E:39:LEU:CD2	1:E:444:LEU:HD23	2.21	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:A:376:VAL:HG11	1:B:504:GLU:OE1	2.05	0.57
1:D:202:SER:CB	1:D:205:ASP:HB2	2.35	0.57
1:D:342:LEU:HD21	1:D:344:GLU:HB2	1.87	0.57
1:E:47:MET:O	1:F:515:VAL:HA	2.04	0.57
1:E:31:ILE:HD11	1:E:78:LEU:HB2	1.86	0.57
3:H:545:ADP:O1B	4:H:546:SO4:O2	2.23	0.57
1:A:425:ARG:O	1:A:427:GLN:N	2.37	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:E:464:ALA:O	1:E:466:ASN:OD1	2.23	0.57
1:H:356:VAL:HG12	1:H:356:VAL:O	2.05	0.57
1:A:31:ILE:HD11	1:A:78:LEU:HB2	1.86	0.57
1:B:202:SER:OG	1:B:205:ASP:HB2	2.04	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:D:95:THR:HG23	3:D:545:ADP:O2B	2.05	0.57
1:F:267:GLU:C	1:F:269:LEU:H	2.09	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:E:145:GLN:O	1:E:147:LYS:N	2.38	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:B:153:ILE:HD13	1:B:394:THR:OG1	2.06	0.56
1:C:216:LYS:HE2	1:C:307:ARG:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:LYS:HE2	1:E:307:ARG:O	2.06	0.56
1:D:372:THR:OG1	1:E:504:GLU:HB2	2.04	0.56
1:F:145:GLN:O	1:F:147:LYS:N	2.38	0.56
1:A:267:GLU:C	1:A:269:LEU:H	2.08	0.56
1:B:77:MET:HA	1:B:80:GLU:HG2	1.87	0.56
1:F:326:ILE:HD11	1:F:336:ASP:OD1	2.06	0.56
1:G:36:ARG:NH2	1:G:443:THR:HG22	2.19	0.56
1:A:117:PRO:O	1:A:121:VAL:HG12	2.06	0.56
1:A:202:SER:CB	1:A:205:ASP:HB2	2.36	0.56
1:A:342:LEU:HD21	1:A:344:GLU:HB2	1.87	0.56
1:B:267:GLU:C	1:B:269:LEU:H	2.07	0.56
1:B:425:ARG:O	1:B:427:GLN:N	2.38	0.56
1:B:94:THR:O	1:B:98:VAL:HG23	2.05	0.56
1:C:342:LEU:HD21	1:C:344:GLU:HB2	1.87	0.56
1:A:36:ARG:NH2	1:A:443:THR:HG22	2.20	0.56
1:B:203:ILE:HA	1:B:370:ARG:O	2.04	0.56
1:E:151:THR:OG1	1:E:175:VAL:HG21	2.06	0.56
1:A:418:TYR:CE2	1:A:422:ILE:HD11	2.41	0.56
1:G:154:ALA:HB2	1:G:391:VAL:CG2	2.35	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:D:151:THR:OG1	1:D:175:VAL:HG21	2.05	0.56
1:H:95:THR:HG23	3:H:545:ADP:O2B	2.06	0.56
1:B:372:THR:CB	1:C:501:SER:HB3	2.35	0.56
3:B:545:ADP:O3B	4:B:546:SO4:S	2.64	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:F:25:ILE:O	1:F:29:ARG:HG3	2.05	0.56
1:F:77:MET:HA	1:F:80:GLU:HG2	1.87	0.56
1:G:138:ILE:HD12	1:G:410:GLU:HG2	1.87	0.56
1:H:267:GLU:C	1:H:269:LEU:H	2.09	0.56
1:H:386:ASP:O	1:H:390:VAL:HG22	2.05	0.56
1:B:218:ARG:HG2	1:B:345:GLU:OE1	2.05	0.56
1:G:94:THR:O	1:G:98:VAL:HG23	2.05	0.56
1:A:77:MET:HA	1:A:80:GLU:HG2	1.88	0.55
1:D:138:ILE:HD12	1:D:410:GLU:HG2	1.88	0.55
1:G:153:ILE:HD13	1:G:394:THR:OG1	2.05	0.55
1:D:51:ASP:HB2	1:E:519:GLU:CB	2.36	0.55
1:E:267:GLU:C	1:E:269:LEU:H	2.09	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:D:425:ARG:O	1:D:427:GLN:N	2.40	0.55
1:F:94:THR:O	1:F:98:VAL:HG23	2.06	0.55
1:H:218:ARG:HG2	1:H:345:GLU:OE1	2.04	0.55
1:D:117:PRO:O	1:D:121:VAL:HG12	2.06	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:A:39:LEU:HD11	1:A:95:THR:HG22	1.89	0.55
3:E:545:ADP:O3B	4:E:546:SO4:S	2.65	0.55
1:G:157:SER:HB2	1:G:390:VAL:HG21	1.88	0.55
1:G:268:MET:C	1:G:269:LEU:HD13	2.27	0.55
3:H:545:ADP:O1B	3:H:545:ADP:O2A	2.24	0.55
1:H:197:LYS:HB3	1:H:377:ILE:CG2	2.37	0.55
1:H:39:LEU:HD21	1:H:444:LEU:HD21	1.87	0.55
1:H:82:ALA:HB2	1:H:97:VAL:HG23	1.89	0.55
1:A:384:VAL:O	1:A:388:VAL:HG23	2.06	0.55
1:D:268:MET:C	1:D:269:LEU:HD13	2.27	0.55
3:H:545:ADP:PB	4:H:546:SO4:O2	2.65	0.55
1:B:157:SER:HB2	1:B:390:VAL:HG21	1.89	0.55
1:H:153:ILE:HD13	1:H:394:THR:OG1	2.07	0.55
1:B:62:VAL:HG13	1:B:63:THR:N	2.21	0.54
1:D:39:LEU:HD11	1:D:95:THR:HG22	1.88	0.54
1:C:77:MET:HA	1:C:80:GLU:HG2	1.90	0.54
1:D:39:LEU:HD21	1:D:444:LEU:HD21	1.90	0.54
1:F:266:SER:HB3	1:F:268:MET:CE	2.37	0.54
1:G:356:VAL:O	1:G:356:VAL:HG12	2.06	0.54
1:A:442:ARG:CG	1:A:442:ARG:NH1	2.67	0.54
1:A:95:THR:HG23	3:A:545:ADP:O2B	2.08	0.54
1:B:268:MET:C	1:B:269:LEU:HD13	2.27	0.54
1:B:450:LEU:HD22	1:B:455:ILE:HD11	1.89	0.54
1:H:203:ILE:H	1:H:371:GLY:HA2	1.71	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
3:F:545:ADP:PB	4:F:546:SO4:O2	2.65	0.54
1:A:215:ASP:HA	1:A:353:MET:HG2	1.89	0.54
1:B:118:THR:HA	1:B:121:VAL:CG1	2.38	0.54
1:C:145:GLN:O	1:C:147:LYS:N	2.40	0.54
1:D:197:LYS:HB3	1:D:377:ILE:HG21	1.90	0.54
1:F:151:THR:OG1	1:F:175:VAL:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:ARG:CG	1:F:442:ARG:HH11	2.12	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:A:464:ALA:O	1:A:466:ASN:OD1	2.25	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:D:215:ASP:HA	1:D:353:MET:HG2	1.90	0.54
1:A:315:GLU:O	1:A:319:LYS:HG3	2.06	0.54
1:E:46:LYS:HG3	1:E:64:ILE:CD1	2.36	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: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:39:LEU:HD11	1:G:95:THR:HG22	1.88	0.54
1:E:202:SER:CB	1:E:205:ASP:HB2	2.38	0.54
3:F:545:ADP:O3B	4:F:546:SO4:S	2.66	0.54
1:G:440:ILE:HB	1:G:441:PRO:HD3	1.90	0.54
1:H:450:LEU:HD22	1:H:455:ILE:HD11	1.89	0.54
1:B:216:LYS:HE2	1:B:307:ARG:O	2.08	0.53
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
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:F:154:ALA:HB2	1:F:391:VAL:CG2	2.38	0.53
3:F:545:ADP:O2A	3:F:545:ADP:O1B	2.26	0.53
1:G:145:GLN:O	1:G:147:LYS:N	2.41	0.53
1:G:62:VAL:HG13	1:G:63:THR:N	2.23	0.53
1:H:36:ARG:NH2	1:H:443:THR:HG22	2.23	0.53
1:A:268:MET:C	1:A:269:LEU:HD13	2.28	0.53
1:B:117:PRO:O	1:B:121:VAL:HG12	2.08	0.53
1:C:440:ILE:HB	1:C:441:PRO:HD3	1.89	0.53
1:C:77:MET:CE	1:C:509:LEU:HD21	2.38	0.53
1:F:11:ASN:HA	1:F:12:MET:HG3	1.90	0.53
1:F:440:ILE:HB	1:F:441:PRO:HD3	1.90	0.53
1:F:450:LEU:HD22	1:F:455:ILE:HD11	1.90	0.53
1:H:202:SER:HB2	1:H:205:ASP:HB2	1.90	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
1:B:284:LEU:O	1:B:305:ALA:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ASN:HA	1:C:12:MET:HG3	1.91	0.53
3:E:545:ADP:O1B	3:E:545:ADP:O2A	2.25	0.53
1:H:448:ALA:CB	1:H:450:LEU:HD12	2.39	0.53
1:D:154:ALA:HB2	1:D:391:VAL:CG2	2.39	0.53
1:E:203:ILE:H	1:E:371:GLY:HA2	1.74	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: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:A:146:ASP:OD1	1:A:149:ILE:HD12	2.08	0.53
1:B:442:ARG:CG	1:B:442:ARG:NH1	2.69	0.53
1:B:464:ALA:O	1:B:466:ASN:OD1	2.26	0.53
1:D:202:SER:OG	1:D:203:ILE:N	2.42	0.53
1:G:418:TYR:CE2	1:G:422:ILE:HD11	2.44	0.53
1:G:59:ASN:OD1	1:G:59:ASN:O	2.27	0.53
1:B:151:THR:OG1	1:B:175:VAL:HG21	2.09	0.53
1:C:442:ARG:CG	1:C:442:ARG:NH1	2.68	0.53
1:F:138:ILE:HD12	1:F:410:GLU:HG2	1.90	0.53
1:G:442:ARG:CG	1:G:442:ARG:NH1	2.70	0.53
1:H:41:PRO:HG3	1:H:159:THR:HG22	1.91	0.53
1:B:202:SER:CB	1:B:205:ASP:HB2	2.39	0.53
1:B:342:LEU:HD21	1:B:344:GLU:HB2	1.89	0.53
1:C:138:ILE:HD12	1:C:410:GLU:HG2	1.89	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
1:G:49:VAL:HG22	1:H:73:PRO:HB3	1.90	0.53
1:B:268:MET:C	1:B:269:LEU:HD22	2.29	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
3:D:545:ADP:PB	4:D:546:SO4:O2	2.67	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:G:203:ILE:H	1:G:371:GLY:HA2	1.73	0.53
1:C:450:LEU:HD22	1:C:455:ILE:HD11	1.91	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:E:77:MET:HA	1:E:80:GLU: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:F:215:ASP:HA	1:F:353:MET:HG2	1.91	0.52
1:G:386:ASP:O	1:G:390:VAL:HG22	2.09	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:B:138:ILE:HD12	1:B:410:GLU:HG2	1.92	0.52
1:F:77:MET:CE	1:F:509:LEU:HD21	2.38	0.52
1:A:197:LYS:HB3	1:A:377:ILE:HG21	1.90	0.52
1:A:386:ASP:O	1:A:390:VAL:HG22	2.10	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:F:157:SER:HB2	1:F:390:VAL:HG21	1.90	0.52
1:C:25:ILE:O	1:C:29:ARG:HG3	2.09	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:448:ALA:CB	1:C:450:LEU:HD12	2.39	0.52
1:E:263:GLU:HA	1:E:269:LEU:CD2	2.34	0.52
1:F:118:THR:HA	1:F:121:VAL:HG12	1.91	0.52
1:F:202:SER:CB	1:F:205:ASP:HB2	2.40	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:G:208:LEU:HD11	1:G:365:VAL:HG11	1.90	0.52
1:B:118:THR:HA	1:B:121:VAL:HG12	1.91	0.52
1:D:37:SER:OG	1:D:46:LYS:NZ	2.39	0.52
3:D:545:ADP:O3B	4:D:546:SO4:S	2.68	0.52
1:E:326:ILE:HD11	1:E:336:ASP:OD1	2.08	0.52
1:F:169:LYS:O	1:F:173:ILE:HG13	2.10	0.52
1:F:268:MET:C	1:F:269:LEU:HD13	2.29	0.52
1:G:202:SER:CB	1:G:205:ASP:HB2	2.40	0.52
1:A:419:ALA:O	1:A:427:GLN:HG3	2.10	0.52
1:A:440:ILE:HB	1:A:441:PRO:HD3	1.92	0.52
1:C:350:GLY:HA3	1:D:87:LYS:HE2	1.92	0.52
1:E:62:VAL:HG13	1:E:63:THR:N	2.25	0.52
1:F:273:VAL:HG21	1:F:297:TYR:HB2	1.92	0.52
1:G:118:THR:HA	1:G:121:VAL:HG12	1.90	0.52
1:D:216:LYS:HE2	1:D:307:ARG:O	2.09	0.52
1:E:372:THR:OG1	1:F:504:GLU:HB2	2.10	0.52
1:A:273:VAL:HG21	1:A:297:TYR:HB2	1.93	0.51
1:A:208:LEU:HD11	1:A:365:VAL:HG11	1.92	0.51
1:C:268:MET:C	1:C:269:LEU:HD13	2.31	0.51
1:F:109:GLU:O	1:F:113:GLN:HG3	2.10	0.51
1:H:155:MET:HE3	1:H:171:ALA:HB2	1.92	0.51
1:H:419:ALA:O	1:H:427:GLN:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ALA:CB	1:A:450:LEU:HD12	2.40	0.51
1:A:73:PRO:HG3	1:H:49:VAL:HG21	1.91	0.51
1:C:384:VAL:O	1:C:388:VAL:HG23	2.10	0.51
1:D:41:PRO:HG3	1:D:159:THR:HG22	1.93	0.51
1:F:263:GLU:HA	1:F:269:LEU:CD2	2.37	0.51
1:H:154:ALA:HB2	1:H:391:VAL:CG2	2.40	0.51
1:B:130:LYS:HG3	1:B:134:LEU:CD1	2.34	0.51
1:C:157:SER:HB2	1:C:390:VAL:HG21	1.91	0.51
3:E:545:ADP:PB	4:E:546:SO4:O2	2.68	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:B:419:ALA:O	1:B:427:GLN:HG3	2.10	0.51
1:D:273:VAL:HG21	1:D:297:TYR:HB2	1.92	0.51
1:D:442:ARG:CG	1:D:442:ARG:NH1	2.68	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: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:F:80:GLU:O	1:F:84:THR:HG23	2.10	0.51
1:G:215:ASP:HA	1:G:353:MET:HG2	1.92	0.51
1:H:216:LYS:HE2	1:H:307:ARG:O	2.10	0.51
1:B:39:LEU:HD21	1:B:444:LEU:HD21	1.90	0.51
1:C:386:ASP:O	1:C:390:VAL:HG22	2.11	0.51
1:D:454:GLU:O	1:D:457:VAL:N	2.44	0.51
1:E:273:VAL:HG21	1:E:297:TYR:HB2	1.92	0.51
1:E:39:LEU:HD21	1:E:444:LEU:HD21	1.92	0.51
1:F:464:ALA:O	1:F:466:ASN:OD1	2.28	0.51
1:F:46:LYS:HG3	1:F:64:ILE:CD1	2.34	0.51
1:G:46:LYS:HG3	1:G:64:ILE:CD1	2.34	0.51
1:F:268:MET:C	1:F:269:LEU:HD22	2.31	0.51
1:A:82:ALA:HB2	1:A:97:VAL:CG2	2.40	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:F:442:ARG:HG3	1:F:452:ALA:HB1	1.93	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:B:273:VAL:HG21	1:B:297:TYR:HB2	1.91	0.51
1:B:468:ASN:C	1:B:470:CYS:H	2.13	0.51
1:C:208:LEU:HD11	1:C:365:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:NH2	1:C:443:THR:HG22	2.25	0.51
1:E:155:MET:HE3	1:E:171:ALA:HB2	1.93	0.51
1:F:438:GLU:C	1:F:441:PRO:HD2	2.31	0.51
1:F:468:ASN:C	1:F:470:CYS:H	2.14	0.51
1:G:419:ALA:O	1:G:427:GLN:HG3	2.11	0.51
1:A:326:ILE:HD11	1:A:336:ASP:OD1	2.10	0.51
1:C:49:VAL:CG2	1:D:73:PRO:HG3	2.41	0.51
1:E:154:ALA:HB2	1:E:391:VAL:CG2	2.41	0.51
3:H:545:ADP:O3B	4:H:546:SO4:S	2.68	0.51
1:B:227:VAL:CG1	1:B:230:ALA:HB2	2.41	0.50
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:C:215:ASP:HA	1:C:353:MET:HG2	1.93	0.50
1:B:403:GLY:O	1:B:406:SER:HB2	2.11	0.50
1:D:268:MET:C	1:D:269:LEU:HD22	2.31	0.50
1:D:442:ARG:HG3	1:D:452:ALA:HB1	1.93	0.50
1:H:236:ASN:HB2	1:H:325:VAL:CG1	2.40	0.50
1:A:420:GLU:C	1:A:422:ILE:H	2.15	0.50
1:C:109:GLU:O	1:C:113:GLN:HG3	2.11	0.50
1:H:215:ASP:HA	1:H:353:MET:HG2	1.93	0.50
1:H:420:GLU:C	1:H:422:ILE:H	2.15	0.50
1:A:512:ILE:HA	1:H:45:ASP:O	2.11	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:C:216:LYS:HG3	1:C:309:VAL:HG22	1.92	0.50
1:C:94:THR:O	1:C:98:VAL:HG23	2.12	0.50
1:D:236:ASN:HB2	1:D:325:VAL:CG1	2.42	0.50
1:G:151:THR:OG1	1:G:175:VAL:HG21	2.11	0.50
1:G:425:ARG:C	1:G:427:GLN:N	2.64	0.50
1:H:268:MET:C	1:H:269:LEU:HD22	2.31	0.50
1:C:273:VAL:HG21	1:C:297:TYR:HB2	1.92	0.50
1:C:39:LEU:CD2	1:C:444:LEU:HD23	2.21	0.50
1:D:11:ASN:HA	1:D:12:MET:HG3	1.94	0.50
1:D:440:ILE:HB	1:D:441:PRO:HD3	1.94	0.50
1:E:448:ALA:CB	1:E:450:LEU:HD12	2.40	0.50
1:F:197:LYS:HB3	1:F:377:ILE:HG21	1.92	0.50
1:F:420:GLU:C	1:F:422:ILE:H	2.14	0.50
1:B:25:ILE:HG23	1:B:104:LEU:HB3	1.94	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:F:47:MET:O	1:G:515:VAL:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:MET:O	1:H:80:GLU:HB2	2.12	0.50
1:A:268:MET:C	1:A:269:LEU:HD22	2.32	0.50
1:A:284:LEU:O	1:A:305:ALA:HA	2.11	0.50
1:B:269:LEU:HD22	1:B:269:LEU:N	2.27	0.50
1:C:118:THR:HA	1:C:121:VAL:HG12	1.93	0.50
1:C:82:ALA:HB2	1:C:97:VAL:CG2	2.42	0.50
1:D:109:GLU:O	1:D:113:GLN:HG3	2.12	0.50
1:F:425:ARG:C	1:F:427:GLN:N	2.63	0.50
1:G:135:LEU:HD21	1:G:411:LEU:HD22	1.94	0.50
1:H:269:LEU:O	1:H:273:VAL:HG23	2.12	0.50
1:A:425:ARG:C	1:A:427:GLN:N	2.65	0.50
3:A:545:ADP:O3B	4:A:546:SO4:S	2.70	0.50
1:B:202:SER:OG	1:B:203:ILE:N	2.44	0.50
3:B:545:ADP:O3B	4:B:546:SO4:O3	2.30	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:201:ALA:HB2	1:C:497:GLN:CD	2.28	0.50
1:B:440:ILE:HB	1:B:441:PRO:HD3	1.93	0.50
1:B:49:VAL:HG12	1:B:50:ASP:N	2.26	0.50
1:G:202:SER:OG	1:G:370:ARG:HB2	2.12	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:A:450:LEU:HD21	1:A:478:GLY:HA2	1.94	0.49
1:C:269:LEU:N	1:C:269:LEU:HD22	2.27	0.49
1:C:420:GLU:C	1:C:422:ILE:H	2.14	0.49
1:D:57:VAL:CG2	1:E:512:ILE:HD11	2.42	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:E:59:ASN:O	1:E:59:ASN:OD1	2.30	0.49
1:G:425:ARG:C	1:G:427:GLN:H	2.15	0.49
1:G:450:LEU:HD21	1:G:478:GLY:HA2	1.94	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:C:51:ASP:HB2	1:D:519:GLU:CG	2.43	0.49
1:F:386:ASP:O	1:F:390:VAL:HG22	2.12	0.49
1:G:169:LYS:O	1:G:173:ILE:HG13	2.12	0.49
1:G:216:LYS:HG3	1:G:309:VAL:HG22	1.93	0.49
1:B:77:MET:CE	1:B:509:LEU:HD21	2.42	0.49
1:C:468:ASN:C	1:C:470:CYS:H	2.15	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:LYS:HB3	1:E:377:ILE:HG21	1.93	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:F:450:LEU:HD21	1:F:478:GLY:HA2	1.95	0.49
1:A:438:GLU:C	1:A:441:PRO:HD2	2.32	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: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:H:442:ARG:CG	1:H:442:ARG:NH1	2.71	0.48
1:B:425:ARG:C	1:B:427:GLN:N	2.65	0.48
1:E:414:LYS:O	1:E:417:GLU:HG2	2.13	0.48
1:E:442:ARG:CG	1:E:442:ARG:NH1	2.63	0.48
1:F:41:PRO:HG3	1:F:159:THR:HG22	1.95	0.48
1:H:118:THR:HA	1:H:121:VAL:CG1	2.43	0.48
1:H:232:ILE:HG22	1:H:234:LEU:HD12	1.96	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:A:138:ILE:HD12	1:A:410:GLU:HG2	1.93	0.48
1:B:11:ASN:HA	1:B:12:MET:HG3	1.95	0.48
1:B:454:GLU:O	1:B:457:VAL:N	2.46	0.48
1:B:82:ALA:HB2	1:B:97:VAL:HG23	1.95	0.48
1:C:169:LYS:O	1:C:173:ILE:HG13	2.13	0.48
1:C:225:LYS:HB3	1:C:225:LYS:NZ	2.28	0.48
1:D:419:ALA:O	1:D:427:GLN:HG3	2.12	0.48
1:D:49:VAL:CG2	1:E:73:PRO:HG3	2.41	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:A:414:LYS:O	1:A:417:GLU:HG2	2.13	0.48
1:A:39:LEU:HD21	1:A:444:LEU:HD21	1.94	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:A:216:LYS:HG3	1:A:309:VAL:HG22	1.95	0.48
1:B:442:ARG:HG3	1:B:452:ALA:HB1	1.96	0.48
1:C:117:PRO:O	1:C:121:VAL:HG12	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:O	1:D:305:ALA:HA	2.13	0.48
1:E:225:LYS:NZ	1:E:225:LYS:HB3	2.28	0.48
1:E:450:LEU:HD21	1:E:478:GLY:HA2	1.95	0.48
1:F:236:ASN:HB2	1:F:325:VAL:CG1	2.43	0.48
1:G:263:GLU:HA	1:G:269:LEU:CD2	2.38	0.48
1:H:453:ILE:O	1:H:457:VAL:HG23	2.13	0.48
1:A:269:LEU:N	1:A:269:LEU:HD22	2.29	0.48
1:A:236:ASN:HB2	1:A:325:VAL:CG1	2.43	0.48
1:F:225:LYS:NZ	1:F:225:LYS:HB3	2.28	0.48
1:A:225:LYS:NZ	1:A:225:LYS:HB3	2.28	0.48
1:A:263:GLU:HA	1:A:269:LEU:CD2	2.37	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:E:157:SER:HB2	1:E:390:VAL:HG21	1.94	0.48
1:H:450:LEU:HD21	1:H:478:GLY:HA2	1.95	0.48
1:A:232:ILE:HG22	1:A:234:LEU:HD12	1.95	0.48
1:D:386:ASP:O	1:D:390:VAL:HG22	2.14	0.48
1:E:232:ILE:HG22	1:E:234:LEU:HD12	1.95	0.48
1:F:363:LYS:HA	1:F:363:LYS:HD3	1.59	0.48
1:G:448:ALA:CB	1:G:450:LEU:HD12	2.43	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:D:372:THR:HG21	1:E:501:SER:N	2.29	0.47
1:E:202:SER:HB2	1:E:205:ASP:HB2	1.96	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: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:G:442:ARG:HG3	1:G:452:ALA:HB1	1.96	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:A:133:GLU:O	1:A:137:THR:HG23	2.14	0.47
1:B:326:ILE:HD11	1:B:336:ASP:OD1	2.14	0.47
1:C:80:GLU:O	1:C:84:THR:HG23	2.14	0.47
1:D:118:THR:HA	1:D:121:VAL:CG1	2.44	0.47
1:E:268:MET:C	1:E:269:LEU:HD22	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:ARG:C	1:E:427:GLN:H	2.18	0.47
1:H:216:LYS:HG3	1:H:309:VAL:HG22	1.96	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:H:85:GLN:HG2	1:H:92:GLY:O	2.14	0.47
1:A:454:GLU:O	1:A:457:VAL:N	2.47	0.47
1:A:46:LYS:HG3	1:A:64:ILE:CD1	2.38	0.47
1:A:49:VAL:HG12	1:A:50:ASP:N	2.30	0.47
1:G:102:GLU:HG2	1:G:439:VAL:HB	1.97	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:155:MET:HE3	1:C:171:ALA:HB2	1.96	0.47
1:C:154:ALA:HB2	1:C:391:VAL:CG2	2.45	0.47
1:C:51:ASP:HB2	1:D:519:GLU:HG3	1.96	0.47
1:D:227:VAL:CG1	1:D:230:ALA:HB2	2.45	0.47
1:D:420:GLU:C	1:D:422:ILE:H	2.16	0.47
1:F:82:ALA:HB2	1:F:97:VAL:CG2	2.45	0.47
1:H:343:VAL:HG13	1:H:356:VAL:HG22	1.96	0.47
1:B:203:ILE:H	1:B:371:GLY:HA2	1.78	0.47
1:D:213:LEU:HD11	1:D:355:PHE:CE2	2.49	0.47
1:G:269:LEU:N	1:G:269:LEU:HD22	2.29	0.47
1:A:109:GLU:O	1:A:113:GLN:HG3	2.15	0.47
1:B:227:VAL:HG12	1:B:230:ALA:HB2	1.97	0.47
1:B:310:LYS:O	1:B:314:MET:HG2	2.15	0.47
1:D:202:SER:HB2	1:D:205:ASP:HB2	1.95	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:G:25:ILE:O	1:G:29:ARG:HG3	2.15	0.47
1:G:326:ILE:HD11	1:G:336:ASP:OD1	2.15	0.47
1:G:363:LYS:HD3	1:G:363:LYS:HA	1.59	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:F:454:GLU:O	1:F:457:VAL:N	2.47	0.47
1:G:236:ASN:HB2	1:G:325:VAL:CG1	2.45	0.47
1:H:326:ILE:HD11	1:H:336:ASP:OD1	2.15	0.47
1:H:153:ILE:HG13	1:H:489:VAL:HG23	1.96	0.47
1:B:155:MET:HE3	1:B:171:ALA:HB2	1.97	0.47
1:B:236:ASN:HB2	1:B:325:VAL:CG1	2.44	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:25:ILE:O	1:B:29:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:HD11	1:C:355:PHE:CE2	2.50	0.47
1:E:266:SER:HB3	1:E:268:MET:CE	2.45	0.47
1:E:80:GLU:O	1:E:84:THR:HG23	2.15	0.47
1:F:184:ASP:HA	1:F:185:GLU:HA	1.49	0.47
1:F:448:ALA:CB	1:F:450:LEU:HD12	2.43	0.47
1:G:284:LEU:O	1:G:305:ALA:HA	2.14	0.47
1:G:343:VAL:HG13	1:G:356:VAL:HG22	1.95	0.47
1:H:342:LEU:CD2	1:H:344:GLU:HB2	2.45	0.47
1:A:25:ILE:O	1:A:29:ARG:HG3	2.14	0.47
1:B:450:LEU:HD21	1:B:478:GLY:HA2	1.96	0.47
1:D:189:ASP:HB3	1:D:192:LEU:CD1	2.44	0.47
1:D:233:ALA:HB2	1:D:337:LEU:HD22	1.97	0.47
1:C:51:ASP:HB2	1:D:519:GLU:CB	2.45	0.47
1:E:37:SER:OG	1:E:46:LYS:NZ	2.47	0.47
1:H:202:SER:OG	1:H:370:ARG:HB2	2.15	0.47
1:H:269:LEU:N	1:H:269:LEU:HD22	2.30	0.47
1:D:459:VAL:O	1:D:463:HIS:HD2	1.98	0.46
1:E:468:ASN:C	1:E:470:CYS:H	2.18	0.46
1:F:269:LEU:O	1:F:273:VAL:HG23	2.14	0.46
1:F:425:ARG:C	1:F:427:GLN:H	2.17	0.46
1:H:218:ARG:NH1	1:H:225:LYS:HD3	2.30	0.46
1:B:202:SER:HB2	1:B:205:ASP:HB2	1.96	0.46
1:B:425:ARG:C	1:B:427:GLN:H	2.19	0.46
1:B:46:LYS:HG3	1:B:64:ILE:CD1	2.40	0.46
1:C:202:SER:OG	1:C:370:ARG:HB2	2.15	0.46
1:D:146:ASP:OD1	1:D:149:ILE:HD12	2.16	0.46
1:D:234:LEU:HD21	1:D:317:LEU:CB	2.45	0.46
1:F:218:ARG:NH1	1:F:225:LYS:HD3	2.31	0.46
1:F:59:ASN:OD1	1:F:59:ASN:O	2.34	0.46
1:A:11:ASN:HA	1:A:12:MET:HG3	1.93	0.46
1:A:41:PRO:HG3	1:A:159:THR:HG22	1.97	0.46
1:B:169:LYS:O	1:B:173:ILE:HG13	2.15	0.46
1:B:80:GLU:O	1:B:84:THR:HG23	2.15	0.46
1:C:95:THR:HG23	3:C:545:ADP:O2B	2.16	0.46
1:D:85:GLN:HG2	1:D:92:GLY:O	2.15	0.46
1:E:202:SER:OG	1:E:203:ILE:N	2.46	0.46
1:E:218:ARG:NH1	1:E:225:LYS:HD3	2.31	0.46
1:E:459:VAL:O	1:E:463:HIS:HD2	1.97	0.46
1:G:39:LEU:HD12	1:G:94:THR:HG22	1.98	0.46
1:H:297:TYR:O	1:H:301:GLU:HG2	2.15	0.46
1:C:189:ASP:HB3	1:C:192:LEU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TYR:O	1:C:301:GLU:HG2	2.16	0.46
1:D:363:LYS:HA	1:D:363:LYS:HD3	1.57	0.46
1:D:373:THR:CG2	1:E:505:SER:HB3	2.41	0.46
1:F:155:MET:HE3	1:F:171:ALA:HB2	1.96	0.46
1:G:415:LEU:HD23	1:G:415:LEU:HA	1.65	0.46
1:H:11:ASN:HA	1:H:12:MET:HG3	1.96	0.46
1:H:433:PHE:CD2	1:H:433:PHE:O	2.69	0.46
1:A:297:TYR:O	1:A:301:GLU:HG2	2.16	0.46
1:B:146:ASP:OD1	1:B:149:ILE:HD12	2.14	0.46
1:C:450:LEU:HD21	1:C:478:GLY:HA2	1.98	0.46
1:D:189:ASP:HB3	1:D:192:LEU:CG	2.45	0.46
1:E:232:ILE:O	1:E:337:LEU:HA	2.16	0.46
1:E:420:GLU:C	1:E:422:ILE:H	2.19	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:H:34:THR:HG22	1:H:35:VAL:HG13	1.97	0.46
1:A:218:ARG:NH1	1:A:225:LYS:HD3	2.31	0.46
1:A:425:ARG:C	1:A:427:GLN:H	2.18	0.46
1:B:388:VAL:HG12	1:B:388:VAL:O	2.14	0.46
1:D:297:TYR:O	1:D:301:GLU:HG2	2.16	0.46
1:E:189:ASP:HB3	1:E:192:LEU:CG	2.45	0.46
1:F:414:LYS:O	1:F:417:GLU:HG2	2.16	0.46
1:G:109:GLU:O	1:G:113:GLN:HG3	2.15	0.46
1:H:146:ASP:OD1	1:H:149:ILE:HD12	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:A:118:THR:HA	1:A:121:VAL:CG1	2.46	0.46
1:C:343:VAL:HG13	1:C:356:VAL:HG22	1.96	0.46
1:E:109:GLU:O	1:E:113:GLN:HG3	2.16	0.46
1:E:208:LEU:HD11	1:E:365:VAL:HG11	1.96	0.46
1:E:49:VAL:HG12	1:E:50:ASP:N	2.30	0.46
1:H:178:VAL:HG13	1:H:188:VAL:HG11	1.97	0.46
1:H:438:GLU:C	1:H:441:PRO:HD2	2.36	0.46
1:A:234:LEU:HD21	1:A:317:LEU:HB2	1.98	0.46
1:B:109:GLU:O	1:B:113:GLN:HG3	2.15	0.46
1:C:82:ALA:HB2	1:C:97:VAL:HG23	1.98	0.46
1:D:275:GLU:O	1:D:278:ALA:HB3	2.16	0.46
1:E:194:LYS:HB2	1:E:316:LYS:NZ	2.31	0.46
1:H:213:LEU:HD11	1:H:355:PHE:CD2	2.51	0.46
1:A:151:THR:OG1	1:A:175:VAL:HG21	2.16	0.46
1:A:234:LEU:HD21	1:A:317:LEU:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ARG:NH1	1:C:225:LYS:HD3	2.31	0.46
1:C:236:ASN:HB2	1:C:325:VAL:CG1	2.46	0.46
1:C:269:LEU:O	1:C:273:VAL:HG23	2.16	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
1:E:453:ILE:O	1:E:457:VAL:HG23	2.16	0.46
1:G:218:ARG:NH1	1:G:225:LYS:HD3	2.31	0.46
1:G:80:GLU:O	1:G:84:THR:HG23	2.16	0.46
1:A:184:ASP:HA	1:A:185:GLU:HA	1.48	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:128:ALA:O	1:G:132:GLN:HG2	2.16	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: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:D:218:ARG:NH1	1:D:225:LYS:HD3	2.31	0.45
1:D:240:GLU:O	1:D:269:LEU:HG	2.16	0.45
1:E:34:THR:O	1:E:46:LYS:HE2	2.16	0.45
1:G:234:LEU:HD21	1:G:317:LEU:HB2	1.98	0.45
1:G:45:ASP:O	1:H:512:ILE:HA	2.16	0.45
1:G:490:GLU:OE1	1:G:495:LYS:HE3	2.14	0.45
1:H:46:LYS:HG3	1:H:64:ILE:CD1	2.39	0.45
1:A:227:VAL:CG1	1:A:230:ALA:HB2	2.46	0.45
1:A:363:LYS:HD3	1:A:363:LYS:HA	1.54	0.45
1:B:218:ARG:NH1	1:B:225:LYS:HD3	2.31	0.45
1:C:516:ILE:O	1:C:516:ILE:HG22	2.16	0.45
1:B:234:LEU:HD21	1:B:317:LEU:CB	2.46	0.45
1:B:213:LEU:HD11	1:B:355:PHE:CE2	2.51	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:E:234:LEU:HD21	1:E:317:LEU:HB2	1.98	0.45
1:F:403:GLY:O	1:F:406:SER:HB2	2.16	0.45
1:G:269:LEU:O	1:G:273:VAL:HG23	2.16	0.45
1:G:342:LEU:CD2	1:G:344:GLU:HB2	2.45	0.45
1:G:454:GLU:O	1:G:457:VAL:N	2.47	0.45
1:C:233:ALA:HB2	1:C:337:LEU:HD22	1.99	0.45
1:B:41:PRO:HG3	1:B:159:THR:HG22	1.98	0.45
1:C:219:VAL:CG2	1:C:307:ARG:HD3	2.47	0.45
1:C:433:PHE:CD2	1:C:433:PHE:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LEU:HD21	1:D:317:LEU:HB2	1.99	0.45
1:D:266:SER:HB3	1:D:268:MET:CE	2.47	0.45
1:D:425:ARG:C	1:D:427:GLN:H	2.19	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
1:E:269:LEU:N	1:E:269:LEU:HD22	2.32	0.45
3:E:545:ADP:O3B	4:E:546:SO4:O3	2.35	0.45
1:F:233:ALA:HB2	1:F:337:LEU:HD22	1.99	0.45
1:F:36:ARG:NH2	1:F:443:THR:HG22	2.31	0.45
1:H:266:SER:HB3	1:H:268:MET:CE	2.46	0.45
1:A:178:VAL:HG13	1:A:188:VAL:HG11	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:B:442:ARG:HD3	1:B:456:LEU:HD22	1.98	0.45
1:C:202:SER:OG	1:C:203:ILE:N	2.48	0.45
1:C:85:GLN:HG2	1:C:92:GLY:O	2.16	0.45
1:D:25:ILE:O	1:D:29:ARG:HG3	2.17	0.45
1:E:213:LEU:HD11	1:E:355:PHE:CE2	2.51	0.45
1:F:202:SER:OG	1:F:370:ARG:HB2	2.16	0.45
1:F:476:PHE:O	1:F:477:THR:C	2.55	0.45
1:G:234:LEU:HD21	1:G:317:LEU:CB	2.46	0.45
1:H:459:VAL:O	1:H:463:HIS:HD2	1.99	0.45
1:A:403:GLY:O	1:A:406:SER:HB2	2.16	0.45
1:B:154:ALA:HB2	1:B:391:VAL:CG2	2.47	0.45
1:B:266:SER:HB3	1:B:268:MET:CE	2.46	0.45
1:D:448:ALA:CB	1:D:450:LEU:HD12	2.43	0.45
1:D:153:ILE:HG13	1:D:489:VAL:HG23	1.98	0.45
1:E:36:ARG:NH2	1:E:443:THR:HG22	2.31	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:189:ASP:HB3	1:A:192:LEU:CG	2.46	0.45
1:A:417:GLU:C	1:A:419:ALA:N	2.70	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: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:A:233:ALA:HB2	1:A:337:LEU:HD22	1.97	0.45
1:H:425:ARG:C	1:H:427:GLN:H	2.20	0.45
1:A:519:GLU:HB2	1:H:51:ASP:HB2	1.99	0.45
1:A:453:ILE:O	1:A:457:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:THR:OG1	1:C:175:VAL:HG21	2.17	0.45
1:C:49:VAL:HG12	1:C:50:ASP:N	2.32	0.45
1:F:34:THR:HG22	1:F:35:VAL:HG13	1.99	0.45
1:G:442:ARG:HD3	1:G:456:LEU:HD22	1.99	0.45
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:C:184:ASP:HA	1:C:185:GLU:HA	1.47	0.44
1:C:273:VAL:HG11	1:C:297:TYR:CB	2.47	0.44
1:D:184:ASP:HA	1:D:185:GLU:HA	1.47	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:F:202:SER:OG	1:F:203:ILE:N	2.48	0.44
1:G:297:TYR:O	1:G:301:GLU:HG2	2.17	0.44
1:G:476:PHE:O	1:G:477:THR:C	2.55	0.44
1:H:189:ASP:HB3	1:H:192:LEU:CD1	2.47	0.44
1:C:454:GLU:O	1:C:457:VAL:N	2.49	0.44
1:C:466:ASN:HB2	1:C:467:GLY:H	1.63	0.44
1:B:372:THR:HG21	1:C:501:SER:CA	2.47	0.44
1:C:300:LYS:NZ	1:D:331:ASP:OD1	2.47	0.44
1:D:468:ASN:C	1:D:470:CYS:H	2.20	0.44
1:F:297:TYR:O	1:F:301:GLU:HG2	2.16	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:G:233:ALA:HB2	1:G:337:LEU:HD22	1.99	0.44
1:A:459:VAL:O	1:A:463:HIS:HD2	1.99	0.44
1:C:85:GLN:HG2	1:C:93:THR:HA	1.99	0.44
1:D:273:VAL:HG11	1:D:297:TYR:CB	2.47	0.44
1:D:216:LYS:HG3	1:D:309:VAL:HG22	1.98	0.44
1:D:388:VAL:O	1:D:388:VAL:HG12	2.18	0.44
3:D:545:ADP:O3B	4:D:546:SO4:O3	2.36	0.44
1:D:57:VAL:CG1	1:E:512:ILE:HD11	2.48	0.44
1:C:49:VAL:HG22	1:D:73:PRO:HB3	1.99	0.44
1:E:41:PRO:HG3	1:E:159:THR:HG22	2.00	0.44
1:D:376:VAL:HG11	1:E:504:GLU:OE1	2.17	0.44
1:F:232:ILE:O	1:F:337:LEU:HA	2.18	0.44
1:G:202:SER:OG	1:G:203:ILE:N	2.50	0.44
1:G:213:LEU:HD11	1:G:355:PHE:CE2	2.53	0.44
1:G:403:GLY:O	1:G:406:SER:HB2	2.18	0.44
1:G:41:PRO:HG3	1:G:159:THR:HG22	1.99	0.44
1:A:509:LEU:HA	1:A:509:LEU:HD23	1.69	0.44
1:B:178:VAL:HG22	1:B:388:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:GLY:O	1:C:406:SER:HB2	2.17	0.44
1:D:232:ILE:O	1:D:337:LEU:HA	2.17	0.44
1:D:34:THR:HG22	1:D:35:VAL:HG13	2.00	0.44
1:F:310:LYS:O	1:F:314:MET:HG2	2.18	0.44
1:G:450:LEU:HD22	1:G:455:ILE:HD11	1.98	0.44
1:A:169:LYS:O	1:A:173:ILE:HG13	2.18	0.44
1:B:240:GLU:O	1:B:269:LEU:HG	2.18	0.44
1:C:234:LEU:HD21	1:C:317:LEU:HB2	1.99	0.44
1:A:342:LEU:HD23	1:A:343:VAL:N	2.32	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:E:169:LYS:O	1:E:173:ILE:HG13	2.17	0.44
1:E:342:LEU:CD2	1:E:344:GLU:HB2	2.47	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
3:F:545:ADP:O3B	4:F:546:SO4:O3	2.35	0.44
1:H:234:LEU:HD21	1:H:317:LEU:CB	2.48	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:A:213:LEU:HD11	1:A:355:PHE:CE2	2.52	0.44
1:A:85:GLN:HG2	1:A:92:GLY:O	2.17	0.44
1:B:297:TYR:O	1:B:301:GLU:HG2	2.18	0.44
1:B:232:ILE:O	1:B:337:LEU:HA	2.18	0.44
1:C:240:GLU:O	1:C:269:LEU:HG	2.18	0.44
1:C:213:LEU:HD11	1:C:355:PHE:CD2	2.52	0.44
1:F:213:LEU:HD11	1:F:355:PHE:CE2	2.52	0.44
1:G:34:THR:HG22	1:G:35:VAL:HG13	2.00	0.44
1:G:413:MET:SD	1:G:463:HIS:O	2.76	0.44
1:G:47:MET:HG3	1:G:55:VAL:HG23	1.99	0.44
1:G:71:GLU:OE1	1:G:71:GLU:HA	2.18	0.44
1:A:292:ASP:CB	1:B:327:THR:HG21	2.42	0.44
1:A:46:LYS:HD3	1:B:514:ASP:HB3	1.98	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:E:11:ASN:HA	1:E:12:MET:HG3	1.96	0.44
1:F:348:ILE:O	1:F:348:ILE:CG2	2.66	0.44
1:F:459:VAL:O	1:F:463:HIS:HD2	2.01	0.44
1:G:240:GLU:O	1:G:269:LEU:HG	2.18	0.44
1:B:232:ILE:HG22	1:B:234:LEU:HD12	1.99	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:E:47:MET:HG3	1:E:55:VAL:HG23	2.00	0.43
1:E:153:ILE:HG13	1:E:489:VAL:HG23	1.98	0.43
1:H:47:MET:HG3	1:H:55:VAL:HG23	1.98	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:A:59:ASN:OD1	1:A:59:ASN:O	2.36	0.43
1:B:202:SER:HG	1:B:203:ILE:N	2.16	0.43
1:B:459:VAL:O	1:B:463:HIS:HD2	2.02	0.43
1:B:71:GLU:HA	1:B:71:GLU:OE1	2.18	0.43
1:D:456:LEU:HA	1:D:456:LEU:HD12	1.90	0.43
1:E:213:LEU:HD11	1:E:355:PHE:CD2	2.53	0.43
1:F:130:LYS:HG3	1:F:134:LEU:CD1	2.41	0.43
1:F:213:LEU:HD11	1:F:355:PHE:CD2	2.54	0.43
1:G:85:GLN:HG2	1:G:93:THR:HA	2.01	0.43
1:H:240:GLU:O	1:H:269:LEU:HG	2.18	0.43
1:H:433:PHE:CD2	1:H:433:PHE:C	2.91	0.43
1:A:135:LEU:HD21	1:A:411:LEU:HD22	2.00	0.43
1:B:414:LYS:O	1:B:417:GLU:HG2	2.18	0.43
1:D:292:ASP:O	1:E:327:THR:HG21	2.18	0.43
1:C:292:ASP:C	1:D:327:THR:HG21	2.38	0.43
1:E:184:ASP:HA	1:E:185:GLU:HA	1.47	0.43
1:E:275:GLU:O	1:E:278:ALA:HB3	2.18	0.43
1:G:142:VAL:HG11	1:G:149:ILE:HG21	2.00	0.43
1:H:202:SER:OG	1:H:203:ILE:N	2.48	0.43
1:H:234:LEU:HD21	1:H:317:LEU:HB2	2.00	0.43
1:H:34:THR:O	1:H:46:LYS:HE2	2.18	0.43
1:B:184:ASP:HA	1:B:185:GLU:HA	1.48	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: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:E:490:GLU:OE1	1:E:495:LYS:HE3	2.17	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: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:H:232:ILE:O	1:H:337:LEU:HA	2.18	0.43
1:A:153:ILE:HD13	1:A:394:THR:OG1	2.17	0.43
1:A:201:ALA:HB2	1:B:497:GLN:CD	2.34	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:C:459:VAL:O	1:C:463:HIS:HD2	2.02	0.43
1:E:240:GLU:O	1:E:269:LEU:HG	2.18	0.43
1:E:342:LEU:HD23	1:E:343:VAL:N	2.33	0.43
1:E:442:ARG:HD3	1:E:456:LEU:HD22	2.00	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:H:139:ALA:HB2	1:H:492:LEU:HD13	2.01	0.43
1:A:128:ALA:O	1:A:132:GLN:HG2	2.18	0.43
1:B:213:LEU:HD11	1:B:355:PHE:CD2	2.54	0.43
1:D:269:LEU:O	1:D:273:VAL:HG23	2.18	0.43
1:E:433:PHE:C	1:E:433:PHE:CD2	2.92	0.43
1:E:454:GLU:O	1:E:457:VAL:N	2.51	0.43
1:F:240:GLU:O	1:F:269:LEU:HG	2.19	0.43
1:F:417:GLU:C	1:F:419:ALA:N	2.69	0.43
1:G:11:ASN:HA	1:G:12:MET:HG3	1.94	0.43
1:G:414:LYS:O	1:G:417:GLU:HG2	2.19	0.43
1:A:519:GLU:HB2	1:H:51:ASP:CB	2.49	0.43
3:H:545:ADP:O3B	4:H:546:SO4:O3	2.37	0.43
1:B:167:LYS:HD2	1:B:167:LYS:HA	1.83	0.43
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.91	0.43
1:B:476:PHE:O	1:B:477:THR:C	2.57	0.43
1:B:481:GLU:OE1	1:B:486:ASN:ND2	2.52	0.43
1:C:39:LEU:HD12	1:C:94:THR:HG22	2.00	0.43
1:D:438:GLU:C	1:D:441:PRO:HD2	2.39	0.43
1:F:234:LEU:HD21	1:F:317:LEU:HB2	2.00	0.43
1:H:442:ARG:HD3	1:H:456:LEU:HD22	2.01	0.43
1:A:155:MET:HE3	1:A:171:ALA:HB2	2.01	0.43
1:A:240:GLU:O	1:A:269:LEU:HG	2.18	0.43
1:B:133:GLU:O	1:B:137:THR:HG23	2.19	0.43
1:B:85:GLN:HG2	1:B:93:THR:HA	2.00	0.43
1:D:217:GLU:O	1:D:218:ARG:C	2.57	0.43
1:D:213:LEU:HD11	1:D:355:PHE:CD2	2.54	0.43
1:F:39:LEU:HD21	1:F:444:LEU:HD21	1.93	0.43
1:G:77:MET:HE3	1:G:509:LEU:HD21	1.98	0.43
1:H:71:GLU:HA	1:H:71:GLU:OE1	2.17	0.43
1:A:15:TYR:O	1:A:20:ALA:HB2	2.19	0.43
1:C:342:LEU:CD2	1:C:344:GLU:HB2	2.48	0.43
1:C:39:LEU:HD21	1:C:444:LEU:HD21	1.94	0.43
1:C:456:LEU:HA	1:C:456:LEU:HD12	1.86	0.43
3:C:545:ADP:PB	4:C:546:SO4:S	3.17	0.43
1:C:47:MET:HG3	1:C:55:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:CG1	1:D:512:ILE:HD11	2.49	0.43
1:D:154:ALA:HB2	1:D:391:VAL:HG23	2.00	0.43
1:D:46:LYS:HD3	1:E:514:ASP:CB	2.36	0.43
1:E:343:VAL:HG13	1:E:356:VAL:HG22	2.00	0.43
1:G:438:GLU:C	1:G:441:PRO:HD2	2.38	0.43
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.86	0.42
1:A:82:ALA:HB2	1:A:97:VAL:HG23	2.00	0.42
1:C:263:GLU:HA	1:C:269:LEU:CD2	2.39	0.42
1:C:71:GLU:HA	1:C:71:GLU:OE1	2.19	0.42
1:E:102:GLU:HG2	1:E:439:VAL:HB	2.01	0.42
1:F:202:SER:HB2	1:F:205:ASP:HB2	2.00	0.42
1:G:456:LEU:HD12	1:G:456:LEU:HA	1.85	0.42
1:H:509:LEU:HA	1:H:509:LEU:HD23	1.78	0.42
1:A:34:THR:HG22	1:A:35:VAL:HG13	2.00	0.42
1:B:122:LYS:HD3	1:B:426:GLU:OE1	2.19	0.42
1:A:53:GLY:O	1:B:76:LYS:HE2	2.19	0.42
1:C:227:VAL:CG1	1:C:230:ALA:HB2	2.49	0.42
1:C:363:LYS:HD3	1:C:363:LYS:HA	1.56	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:D:481:GLU:OE1	1:D:486:ASN:ND2	2.52	0.42
1:E:217:GLU:O	1:E:218:ARG:C	2.58	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:F:220:SER:HB3	1:F:223:MET:HG3	2.00	0.42
1:G:34:THR:O	1:G:46:LYS:HE2	2.19	0.42
1:H:227:VAL:CG1	1:H:230:ALA:HB2	2.49	0.42
1:A:217:GLU:O	1:A:218:ARG:C	2.58	0.42
1:B:453:ILE:O	1:B:457:VAL:HG23	2.19	0.42
1:C:189:ASP:HB3	1:C:192:LEU:CD1	2.49	0.42
1:C:490:GLU:OE1	1:C:495:LYS:HE3	2.18	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:G:202:SER:HB2	1:G:205:ASP:HB2	2.01	0.42
1:H:414:LYS:O	1:H:417:GLU:HG2	2.19	0.42
1:H:59:ASN:O	1:H:59:ASN:OD1	2.37	0.42
1:A:490:GLU:OE1	1:A:495:LYS:HE3	2.19	0.42
1:C:232:ILE:O	1:C:337:LEU:HA	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: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:B:52:LEU:C	1:B:54:ASP:H	2.23	0.42
1:D:85:GLN:HG2	1:D:93:THR:HA	2.01	0.42
1:F:343:VAL:HG13	1:F:356:VAL:HG22	2.02	0.42
1:G:178:VAL:HG13	1:G:188:VAL:HG11	2.00	0.42
1:G:227:VAL:HG12	1:G:230:ALA:HB2	2.02	0.42
1:G:342:LEU:HD23	1:G:343:VAL:N	2.35	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:A:189:ASP:HB3	1:A:192:LEU:CD1	2.49	0.42
1:B:142:VAL:HG12	1:B:143:GLY:N	2.34	0.42
1:B:194:LYS:HB2	1:B:316:LYS:NZ	2.34	0.42
1:D:227:VAL:HG12	1:D:230:ALA:HB2	2.00	0.42
1:D:342:LEU:HD23	1:D:343:VAL:N	2.34	0.42
1:E:417:GLU:C	1:E:419:ALA:N	2.69	0.42
1:F:219:VAL:CG2	1:F:307:ARG:HD3	2.49	0.42
1:B:267:GLU:C	1:B:269:LEU:N	2.72	0.42
1:B:456:LEU:HA	1:B:456:LEU:HD12	1.82	0.42
1:C:269:LEU:HD12	1:C:272:MET:SD	2.60	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:E:46:LYS:HD3	1:F:514:ASP:CB	2.42	0.42
1:F:167:LYS:HD2	1:F:167:LYS:HA	1.83	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:H:357:GLU:H	1:H:357:GLU:HG2	1.70	0.42
1:H:442:ARG:CG	1:H:442:ARG:HH11	2.12	0.42
1:B:189:ASP:HB3	1:B:192:LEU:CG	2.49	0.42
1:B:37:SER:OG	1:B:46:LYS:NZ	2.45	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:D:348:ILE:CG2	1:D:348:ILE:O	2.67	0.42
1:D:415:LEU:HA	1:D:415:LEU:HD23	1.69	0.42
1:E:71:GLU:HA	1:E:71:GLU:OE1	2.18	0.42
1:G:220:SER:HB3	1:G:223:MET:HG3	2.01	0.42
1:H:394:THR:O	1:H:398:GLY:N	2.49	0.42
1:H:476:PHE:O	1:H:477:THR:C	2.57	0.42
1:A:213:LEU:HD11	1:A:355:PHE:CD2	2.55	0.42
1:A:368:LEU:HA	1:A:368:LEU:HD12	1.87	0.42
1:D:158:ILE:O	1:D:161:LYS:HB2	2.20	0.42
1:E:50:ASP:OD1	1:E:51:ASP:N	2.52	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:G:232:ILE:O	1:G:337:LEU:HA	2.20	0.42
1:H:468:ASN:C	1:H:470:CYS:H	2.22	0.42
1:A:154:ALA:HB2	1:A:391:VAL:CG2	2.50	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:E:372:THR:HG21	1:F:501:SER:CA	2.50	0.42
1:F:85:GLN:HG2	1:F:93:THR:HA	2.02	0.42
1:G:146:ASP:OD1	1:G:149:ILE:HD12	2.20	0.42
1:G:194:LYS:HB2	1:G:316:LYS:NZ	2.34	0.42
1:A:269:LEU:O	1:A:273:VAL:HG23	2.19	0.41
1:A:342:LEU:CD2	1:A:344:GLU:HB2	2.49	0.41
1:B:220:SER:HB3	1:B:223:MET:HG3	2.02	0.41
1:D:133:GLU:O	1:D:137:THR:HG23	2.20	0.41
1:G:49:VAL:CG2	1:H:73:PRO:HB3	2.50	0.41
1:A:174:ILE:HD13	1:A:387:ALA:CB	2.50	0.41
1:B:178:VAL:HA	1:B:193:ILE:HD11	2.02	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:E:118:THR:HA	1:E:121:VAL:CG1	2.49	0.41
1:E:403:GLY:O	1:E:406:SER:HB2	2.18	0.41
1:F:62:VAL:CG1	1:F:63:THR:N	2.81	0.41
1:G:184:ASP:HA	1:G:185:GLU:HA	1.52	0.41
1:H:199:SER:HA	1:H:377:ILE:CD1	2.45	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:C:34:THR:O	1:C:46:LYS:HE2	2.20	0.41
1:C:52:LEU:C	1:C:54:ASP:H	2.22	0.41
1:D:197:LYS:HD2	1:D:377:ILE:HG22	2.01	0.41
1:D:51:ASP:C	1:D:51:ASP:OD1	2.59	0.41
1:D:71:GLU:OE1	1:D:71:GLU:HA	2.19	0.41
1:E:202:SER:HG	1:E:203:ILE:N	2.18	0.41
1:F:48:LEU:HG	1:G:516:ILE:HB	2.02	0.41
1:F:49:VAL:HG12	1:F:50:ASP:N	2.35	0.41
1:G:273:VAL:HG11	1:G:297:TYR:CB	2.49	0.41
1:G:433:PHE:C	1:G:433:PHE:CD2	2.93	0.41
1:H:128:ALA:O	1:H:132:GLN:HG2	2.19	0.41
1:H:269:LEU:HD12	1:H:272:MET:SD	2.61	0.41
1:H:506:THR:O	1:H:510:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG12	1:A:230:ALA:HB2	2.02	0.41
1:B:417:GLU:C	1:B:419:ALA:N	2.71	0.41
1:C:506:THR:O	1:C:510:LEU:HG	2.21	0.41
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:F:185:GLU:HA	1:F:186:GLY:HA2	1.81	0.41
1:A:25:ILE:HG23	1:A:104:LEU:HB3	2.02	0.41
1:B:197:LYS:HD2	1:B:377:ILE:HG22	2.03	0.41
1:B:273:VAL:HG11	1:B:297:TYR:CB	2.50	0.41
1:B:269:LEU:O	1:B:273:VAL:HG23	2.20	0.41
1:D:357:GLU:HG2	1:D:357:GLU:H	1.71	0.41
1:F:178:VAL:HG22	1:F:388:VAL:HG13	2.01	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:H:456:LEU:HA	1:H:456:LEU:HD12	1.95	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: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:H:235:LEU:HD23	1:H:235:LEU:HA	1.91	0.41
1:H:219:VAL:CG2	1:H:307:ARG:HD3	2.51	0.41
1:A:466:ASN:HB2	1:A:467:GLY:H	1.60	0.41
1:B:199:SER:HA	1:B:377:ILE:CD1	2.44	0.41
1:E:433:PHE:O	1:E:433:PHE:CD2	2.73	0.41
1:G:85:GLN:HG2	1:G:92:GLY:O	2.21	0.41
1:H:273:VAL:HG11	1:H:297:TYR:CB	2.50	0.41
1:A:267:GLU:C	1:A:269:LEU:N	2.74	0.41
1:B:269:LEU:HD12	1:B:272:MET:SD	2.61	0.41
1:D:102:GLU:HG2	1:D:439:VAL:HB	2.02	0.41
1:D:189:ASP:HB3	1:D:192:LEU:HD12	2.03	0.41
1:D:225:LYS:CG	1:D:345:GLU:HB3	2.51	0.41
1:E:348:ILE:CG2	1:E:348:ILE:O	2.69	0.41
1:D:57:VAL:HG22	1:E:512:ILE:HD11	2.03	0.41
1:F:146:ASP:OD1	1:F:149:ILE:HD12	2.21	0.41
1:F:71:GLU:OE1	1:F:71:GLU:HA	2.19	0.41
1:H:217:GLU:O	1:H:218:ARG:C	2.57	0.41
1:A:413:MET:HG3	1:A:414:LYS:N	2.36	0.41
1:C:142:VAL:HG12	1:C:143:GLY:N	2.34	0.41
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.95	0.41
1:E:225:LYS:CG	1:E:345:GLU:HB3	2.51	0.41
1:F:369:ILE:O	1:F:370:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:PHE:CD2	1:F:433:PHE:C	2.94	0.41
1:F:506:THR:O	1:F:510:LEU:HG	2.20	0.41
1:G:167:LYS:HD2	1:G:167:LYS:HA	1.85	0.41
1:G:235:LEU:HD23	1:G:235:LEU:HA	1.92	0.41
1:A:232:ILE:O	1:A:337:LEU:HA	2.21	0.41
1:C:219:VAL:HG23	1:C:307:ARG:HD3	2.03	0.41
1:C:220:SER:HB3	1:C:223:MET:HG3	2.02	0.41
1:E:196:GLU:HG2	1:E:213:LEU:HD23	2.03	0.41
1:E:219:VAL:CG2	1:E:307:ARG:HD3	2.51	0.41
1:F:133:GLU:O	1:F:137:THR:HG23	2.20	0.41
1:F:342:LEU:HD23	1:F:343:VAL:N	2.35	0.41
1:F:174:ILE:HD13	1:F:387:ALA:CB	2.51	0.41
1:F:413:MET:SD	1:F:463:HIS:O	2.79	0.41
1:F:481:GLU:OE1	1:F:486:ASN:ND2	2.54	0.41
1:G:217:GLU:O	1:G:218:ARG:C	2.59	0.41
1:G:135:LEU:CD2	1:G:411:LEU:HD22	2.51	0.41
1:G:49:VAL:HG12	1:G:50:ASP:N	2.36	0.41
1:H:441:PRO:HB2	1:H:456:LEU:CD1	2.51	0.41
1:A:310:LYS:O	1:A:314:MET:HG2	2.21	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:C:342:LEU:HD23	1:C:343:VAL:N	2.36	0.41
1:C:95:THR:HG22	1:C:440:ILE:HD12	2.02	0.41
1:E:44:MET:HA	1:E:44:MET:CE	2.51	0.41
1:G:130:LYS:HG3	1:G:134:LEU:CD1	2.42	0.41
1:H:167:LYS:HD2	1:H:167:LYS:HA	1.82	0.41
1:H:227:VAL:HG12	1:H:230:ALA:HB2	2.03	0.41
1:A:202:SER:HG	1:A:370:ARG:HB2	1.87	0.40
1:B:189:ASP:HB3	1:B:192:LEU:CD1	2.51	0.40
1:B:342:LEU:HD23	1:B:343:VAL:N	2.36	0.40
1:C:130:LYS:HG3	1:C:134:LEU:CD1	2.41	0.40
1:C:412:SER:HB2	1:C:434:ALA:O	2.20	0.40
1:G:348:ILE:CG2	1:G:348:ILE:O	2.69	0.40
1:G:77:MET:HA	1:G:80:GLU:CG	2.51	0.40
1:H:44:MET:HA	1:H:44:MET:CE	2.51	0.40
1:A:273:VAL:HG11	1:A:297:TYR:CB	2.48	0.40
1:B:348:ILE:O	1:B:348:ILE:CG2	2.70	0.40
1:C:267:GLU:C	1:C:269:LEU:N	2.73	0.40
1:C:369:ILE:O	1:C:370:ARG:HG2	2.21	0.40
1:D:155:MET:HE3	1:D:171:ALA:HB2	2.03	0.40
1:D:25:ILE:HG23	1:D:104:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:SER:OG	1:D:370:ARG:HB2	2.20	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:F:227:VAL:CG1	1:F:230:ALA:HB2	2.52	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
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:433:PHE:O	1:G:433:PHE:CD2	2.75	0.40
1:A:197:LYS:HD2	1:A:377:ILE:HG22	2.03	0.40
1:B:174:ILE:HD13	1:B:387:ALA:CB	2.51	0.40
1:D:225:LYS:HG3	1:D:345:GLU:HB3	2.04	0.40
1:D:476:PHE:O	1:D:477:THR:C	2.60	0.40
1:E:79:ILE:O	1:E:83:LYS:HB2	2.21	0.40
1:F:21:GLN:O	1:F:25:ILE:HG13	2.22	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:G:357:GLU:HG2	1:G:357:GLU:H	1.70	0.40
1:G:453:ILE:O	1:G:457:VAL:HG23	2.21	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:A:225:LYS:CG	1:A:345:GLU:HB3	2.51	0.40
1:A:476:PHE:O	1:A:477:THR:C	2.59	0.40
1:C:474:ASN:HD22	1:C:486:ASN:HD22	1.70	0.40
1:D:269:LEU:HD12	1:D:272:MET:SD	2.61	0.40
1:D:48:LEU:HG	1:E:516:ILE:HB	2.04	0.40
1:D:516:ILE:O	1:D:516:ILE:HG22	2.21	0.40
1:F:456:LEU:HA	1:F:456:LEU:HD12	1.87	0.40
1:F:82:ALA:HB2	1:F:97:VAL:HG23	2.01	0.40
1:H:178:VAL:HG22	1:H:388:VAL:HG13	2.02	0.40
1:H:197:LYS:HD2	1:H:377:ILE:HG22	2.03	0.40
1:C:225:LYS:HG3	1:C:345:GLU:HB3	2.03	0.40
1:E:174:ILE:HD13	1:E:387:ALA:CB	2.52	0.40
1:F:34:THR:O	1:F:46:LYS:HE2	2.21	0.40
1:G:202:SER:HG	1:G:203:ILE:N	2.19	0.40
1:H:102:GLU:HG2	1:H:439:VAL:HB	2.02	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%)	11	50
1	B	485/521 (93%)	423 (87%)	55 (11%)	7 (1%)	13	53
1	C	485/521 (93%)	422 (87%)	56 (12%)	7 (1%)	13	53
1	D	485/521 (93%)	423 (87%)	54 (11%)	8 (2%)	11	50
1	E	485/521 (93%)	426 (88%)	52 (11%)	7 (1%)	13	53
1	F	485/521 (93%)	427 (88%)	50 (10%)	8 (2%)	11	50
1	G	485/521 (93%)	424 (87%)	54 (11%)	7 (1%)	13	53
1	H	485/521 (93%)	425 (88%)	52 (11%)	8 (2%)	11	50
All	All	3880/4168 (93%)	3394 (88%)	426 (11%)	60 (2%)	12	52

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%)	33	69
1	B	388/413 (94%)	369 (95%)	19 (5%)	29	66
1	C	388/413 (94%)	370 (95%)	18 (5%)	31	68
1	D	388/413 (94%)	370 (95%)	18 (5%)	31	68
1	E	388/413 (94%)	371 (96%)	17 (4%)	33	69
1	F	388/413 (94%)	370 (95%)	18 (5%)	31	68
1	G	388/413 (94%)	369 (95%)	19 (5%)	29	66
1	H	388/413 (94%)	372 (96%)	16 (4%)	35	71
All	All	3104/3304 (94%)	2962 (95%)	142 (5%)	31	68

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	25,29,29	1.08	2 (8%)	24,45,45	2.18	6 (25%)
4	SO4	A	546	2	4,4,4	0.20	0	6,6,6	0.20	0
3	ADP	B	545	2	25,29,29	1.05	2 (8%)	24,45,45	1.93	4 (16%)
4	SO4	B	546	2	4,4,4	0.14	0	6,6,6	0.28	0
3	ADP	C	545	2	25,29,29	0.95	1 (4%)	24,45,45	2.09	5 (20%)
4	SO4	C	546	2	4,4,4	0.17	0	6,6,6	0.23	0
3	ADP	D	545	2	25,29,29	1.03	1 (4%)	24,45,45	2.16	5 (20%)
4	SO4	D	546	2	4,4,4	0.21	0	6,6,6	0.31	0
3	ADP	E	545	2	25,29,29	0.95	1 (4%)	24,45,45	2.18	5 (20%)
4	SO4	E	546	2	4,4,4	0.25	0	6,6,6	0.30	0
3	ADP	F	545	2	25,29,29	1.01	1 (4%)	24,45,45	2.09	5 (20%)
4	SO4	F	546	2	4,4,4	0.13	0	6,6,6	0.24	0
3	ADP	G	545	2	25,29,29	1.14	3 (12%)	24,45,45	2.14	5 (20%)
4	SO4	G	546	2	4,4,4	0.19	0	6,6,6	0.30	0
3	ADP	H	545	2	25,29,29	1.17	3 (12%)	24,45,45	2.13	6 (25%)
4	SO4	H	546	2	4,4,4	0.25	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	545	ADP	PB-O3A	2.04	1.63	1.60
3	C	545	ADP	C5-C4	2.05	1.45	1.40
3	G	545	ADP	C2-N3	2.11	1.35	1.32
3	G	545	ADP	O4'-C1'	2.20	1.44	1.41
3	H	545	ADP	O4'-C1'	2.28	1.44	1.41
3	D	545	ADP	C5-C4	2.45	1.46	1.40
3	B	545	ADP	C2-N3	2.46	1.36	1.32
3	F	545	ADP	C5-C4	2.52	1.46	1.40
3	H	545	ADP	PB-O3A	2.52	1.64	1.60
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 (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	545	ADP	N3-C2-N1	-8.35	121.58	128.86
3	G	545	ADP	N3-C2-N1	-7.80	122.06	128.86
3	A	545	ADP	N3-C2-N1	-7.74	122.11	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	545	ADP	N3-C2-N1	-7.60	122.24	128.86
3	D	545	ADP	N3-C2-N1	-7.46	122.36	128.86
3	F	545	ADP	N3-C2-N1	-7.44	122.38	128.86
3	C	545	ADP	N3-C2-N1	-7.29	122.51	128.86
3	B	545	ADP	N3-C2-N1	-6.50	123.20	128.86
3	H	545	ADP	O3'-C3'-C2'	-3.48	100.67	111.83
3	D	545	ADP	O3'-C3'-C2'	-3.42	100.87	111.83
3	A	545	ADP	O2'-C2'-C3'	-3.38	101.02	111.83
3	A	545	ADP	O3'-C3'-C2'	-3.37	101.03	111.83
3	C	545	ADP	C4-C5-N7	-3.11	106.40	109.41
3	B	545	ADP	C4-C5-N7	-3.06	106.45	109.41
3	F	545	ADP	O3'-C3'-C2'	-3.06	102.03	111.83
3	G	545	ADP	O3'-C3'-C2'	-3.00	102.23	111.83
3	B	545	ADP	O3'-C3'-C2'	-2.96	102.35	111.83
3	B	545	ADP	O2'-C2'-C3'	-2.94	102.41	111.83
3	C	545	ADP	O2'-C2'-C3'	-2.88	102.59	111.83
3	C	545	ADP	O3'-C3'-C2'	-2.84	102.73	111.83
3	F	545	ADP	O2'-C2'-C3'	-2.80	102.86	111.83
3	D	545	ADP	O2'-C2'-C3'	-2.62	103.44	111.83
3	E	545	ADP	O2'-C2'-C3'	-2.57	103.58	111.83
3	E	545	ADP	O3'-C3'-C2'	-2.50	103.84	111.83
3	D	545	ADP	C4-C5-N7	-2.43	107.06	109.41
3	G	545	ADP	O2'-C2'-C3'	-2.37	104.24	111.83
3	H	545	ADP	O2'-C2'-C3'	-2.29	104.51	111.83
3	F	545	ADP	C4-C5-N7	-2.19	107.29	109.41
3	A	545	ADP	C2-N1-C6	2.04	122.34	118.77
3	F	545	ADP	C2'-C3'-C4'	2.09	106.69	102.62
3	H	545	ADP	C2-N1-C6	2.11	122.47	118.77
3	H	545	ADP	O2A-PA-O1A	2.14	123.38	112.28
3	G	545	ADP	O2A-PA-O1A	2.18	123.55	112.28
3	C	545	ADP	C2'-C3'-C4'	2.18	106.87	102.62
3	E	545	ADP	C2'-C3'-C4'	2.21	106.93	102.62
3	E	545	ADP	C2-N1-C6	2.24	122.68	118.77
3	A	545	ADP	N6-C6-N1	2.40	123.53	118.77
3	G	545	ADP	C2'-C3'-C4'	2.55	107.59	102.62
3	A	545	ADP	C2'-C3'-C4'	2.57	107.62	102.62
3	H	545	ADP	C2'-C3'-C4'	2.59	107.66	102.62
3	D	545	ADP	C2'-C3'-C4'	2.60	107.67	102.62

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	487/521 (93%)	0.06	39 (8%)	13	12	26, 88, 243, 287	0
1	B	487/521 (93%)	-0.14	13 (2%)	55	46	38, 90, 196, 247	0
1	C	487/521 (93%)	0.22	44 (9%)	10	10	39, 88, 282, 341	0
1	D	487/521 (93%)	0.16	45 (9%)	10	10	42, 103, 243, 287	0
1	E	487/521 (93%)	0.21	55 (11%)	6	7	34, 94, 252, 294	0
1	F	487/521 (93%)	0.29	57 (11%)	5	6	41, 100, 258, 295	0
1	G	487/521 (93%)	0.33	45 (9%)	10	10	41, 122, 245, 291	0
1	H	487/521 (93%)	0.22	37 (7%)	15	13	64, 127, 229, 274	0
All	All	3896/4168 (93%)	0.17	335 (8%)	11	11	26, 102, 250, 341	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	327	THR	16.1
1	G	239	ILE	15.0
1	C	238	ALA	13.4
1	D	266	SER	11.7
1	G	238	ALA	11.0
1	C	239	ILE	10.4
1	F	281	ALA	9.9
1	E	281	ALA	9.9
1	C	289	GLY	9.7
1	E	303	ILE	9.3
1	D	281	ALA	8.9
1	F	268	MET	8.5
1	E	327	THR	8.3
1	E	298	LEU	8.1
1	C	281	ALA	8.1
1	C	264	THR	7.9

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Mol	Chain	Res	Type	RSRZ
1	F	266	SER	7.6
1	F	228	THR	7.6
1	A	239	ILE	7.4
1	D	267	GLU	7.3
1	F	219	VAL	7.1
1	F	335	GLN	7.1
1	G	279	SER	6.9
1	C	303	ILE	6.9
1	F	290	ILE	6.9
1	F	275	GLU	6.7
1	C	279	SER	6.7
1	F	282	ASN	6.6
1	C	267	GLU	6.4
1	H	294	ALA	6.4
1	G	240	GLU	6.4
1	A	327	THR	6.3
1	F	270	LYS	6.2
1	F	303	ILE	5.9
1	A	281	ALA	5.9
1	F	271	ASP	5.8
1	F	302	GLY	5.7
1	E	343	VAL	5.5
1	E	225	LYS	5.5
1	A	228	THR	5.5
1	G	236	ASN	5.4
1	C	270	LYS	5.4
1	E	266	SER	5.4
1	G	303	ILE	5.3
1	F	327	THR	5.2
1	A	303	ILE	5.2
1	A	267	GLU	5.2
1	E	230	ALA	5.2
1	C	335	GLN	5.1
1	D	239	ILE	5.1
1	E	219	VAL	5.1
1	E	267	GLU	5.0
1	F	285	PHE	5.0
1	A	235	LEU	5.0
1	E	302	GLY	5.0
1	A	279	SER	5.0
1	C	271	ASP	5.0
1	C	302	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	239	ILE	4.9
1	E	240	GLU	4.9
1	E	227	VAL	4.9
1	E	328	ASN	4.8
1	G	327	THR	4.8
1	C	290	ILE	4.7
1	E	294	ALA	4.7
1	D	303	ILE	4.7
1	F	265	ALA	4.7
1	E	276	ILE	4.7
1	G	235	LEU	4.6
1	A	236	ASN	4.6
1	C	263	GLU	4.6
1	G	268	MET	4.6
1	G	330	LYS	4.6
1	E	264	THR	4.6
1	A	276	ILE	4.6
1	A	237	CYS	4.5
1	G	266	SER	4.5
1	H	279	SER	4.5
1	H	230	ALA	4.5
1	C	343	VAL	4.5
1	G	237	CYS	4.4
1	C	268	MET	4.4
1	F	238	ALA	4.4
1	G	343	VAL	4.4
1	H	281	ALA	4.4
1	E	285	PHE	4.3
1	H	178	VAL	4.3
1	C	276	ILE	4.3
1	C	230	ALA	4.3
1	C	273	VAL	4.2
1	D	294	ALA	4.2
1	D	236	ASN	4.2
1	D	349	SER	4.2
1	A	240	GLU	4.2
1	F	330	LYS	4.2
1	G	234	LEU	4.2
1	F	291	ASP	4.2
1	A	234	LEU	4.1
1	C	282	ASN	4.1
1	D	298	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	290	ILE	4.1
1	H	266	SER	4.1
1	F	320	ALA	4.1
1	C	326	ILE	4.1
1	G	358	GLU	4.1
1	D	219	VAL	4.1
1	A	266	SER	4.1
1	C	291	ASP	4.1
1	E	297	TYR	4.0
1	F	236	ASN	4.0
1	C	340	ALA	4.0
1	G	276	ILE	4.0
1	E	349	SER	3.9
1	E	223	MET	3.9
1	F	358	GLU	3.9
1	A	238	ALA	3.9
1	G	349	SER	3.9
1	H	321	THR	3.9
1	C	227	VAL	3.8
1	A	326	ILE	3.8
1	D	285	PHE	3.8
1	F	294	ALA	3.8
1	E	265	ALA	3.8
1	A	227	VAL	3.8
1	F	274	ALA	3.7
1	E	234	LEU	3.7
1	F	342	LEU	3.7
1	G	281	ALA	3.7
1	C	237	CYS	3.7
1	E	271	ASP	3.7
1	G	227	VAL	3.7
1	D	268	MET	3.7
1	E	232	ILE	3.7
1	E	220	SER	3.7
1	A	265	ALA	3.6
1	D	350	GLY	3.6
1	A	268	MET	3.6
1	E	228	THR	3.6
1	H	53	GLY	3.6
1	C	226	LYS	3.6
1	F	227	VAL	3.5
1	F	232	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	267	GLU	3.5
1	D	282	ASN	3.5
1	C	240	GLU	3.5
1	D	280	GLY	3.5
1	G	232	ILE	3.5
1	D	296	HIS	3.5
1	A	273	VAL	3.5
1	A	302	GLY	3.5
1	F	267	GLU	3.5
1	F	276	ILE	3.4
1	C	220	SER	3.4
1	D	358	GLU	3.4
1	B	235	LEU	3.4
1	D	271	ASP	3.4
1	H	267	GLU	3.4
1	G	306	ALA	3.4
1	A	225	LYS	3.4
1	D	215	ASP	3.4
1	B	264	THR	3.3
1	B	327	THR	3.3
1	D	263	GLU	3.3
1	C	232	ILE	3.3
1	F	235	LEU	3.3
1	G	305	ALA	3.3
1	C	228	THR	3.2
1	D	232	ILE	3.2
1	A	280	GLY	3.2
1	G	294	ALA	3.1
1	C	336	ASP	3.1
1	A	294	ALA	3.1
1	G	334	ALA	3.1
1	F	341	GLY	3.1
1	B	266	SER	3.1
1	D	270	LYS	3.1
1	E	293	LEU	3.1
1	F	298	LEU	3.1
1	H	317	LEU	3.1
1	E	330	LYS	3.1
1	E	331	ASP	3.1
1	F	279	SER	3.1
1	H	268	MET	3.1
1	G	285	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	283	VAL	3.1
1	C	234	LEU	3.0
1	D	351	ASP	3.0
1	H	297	TYR	3.0
1	D	320	ALA	3.0
1	D	340	ALA	3.0
1	H	295	GLN	3.0
1	D	265	ALA	3.0
1	D	295	GLN	2.9
1	G	287	GLN	2.9
1	H	263	GLU	2.9
1	E	289	GLY	2.9
1	D	238	ALA	2.9
1	E	323	ALA	2.9
1	F	234	LEU	2.9
1	E	268	MET	2.9
1	F	357	GLU	2.9
1	D	53	GLY	2.9
1	F	215	ASP	2.8
1	F	305	ALA	2.8
1	D	342	LEU	2.8
1	D	275	GLU	2.8
1	D	144	ALA	2.8
1	E	233	ALA	2.8
1	F	334	ALA	2.8
1	G	342	LEU	2.8
1	H	280	GLY	2.8
1	C	215	ASP	2.8
1	D	327	THR	2.8
1	D	276	ILE	2.7
1	E	283	VAL	2.7
1	F	226	LYS	2.7
1	F	317	LEU	2.7
1	F	360	LYS	2.7
1	B	337	LEU	2.7
1	A	330	LYS	2.7
1	A	298	LEU	2.7
1	E	224	PRO	2.7
1	H	210	LYS	2.7
1	D	364	ALA	2.7
1	G	480	VAL	2.7
1	A	290	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	280	GLY	2.7
1	F	321	THR	2.7
1	E	280	GLY	2.7
1	F	337	LEU	2.7
1	F	237	CYS	2.7
1	E	337	LEU	2.6
1	H	219	VAL	2.6
1	B	239	ILE	2.6
1	B	290	ILE	2.6
1	H	303	ILE	2.6
1	D	229	ASP	2.6
1	H	239	ILE	2.6
1	A	328	ASN	2.6
1	D	240	GLU	2.6
1	H	351	ASP	2.6
1	A	329	ILE	2.6
1	C	355	PHE	2.6
1	D	287	GLN	2.6
1	C	292	ASP	2.6
1	G	320	ALA	2.6
1	C	266	SER	2.6
1	F	351	ASP	2.5
1	E	279	SER	2.5
1	H	264	THR	2.5
1	A	232	ILE	2.5
1	F	359	CYS	2.5
1	H	320	ALA	2.5
1	C	269	LEU	2.5
1	G	331	ASP	2.5
1	H	273	VAL	2.5
1	E	215	ASP	2.5
1	H	364	ALA	2.5
1	D	272	MET	2.5
1	H	328	ASN	2.5
1	E	270	LYS	2.5
1	D	264	THR	2.5
1	G	230	ALA	2.5
1	B	240	GLU	2.4
1	E	356	VAL	2.4
1	G	278	ALA	2.4
1	H	271	ASP	2.4
1	H	327	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	359	CYS	2.4
1	E	239	ILE	2.4
1	A	278	ALA	2.4
1	G	357	GLU	2.4
1	C	219	VAL	2.4
1	E	235	LEU	2.4
1	H	232	ILE	2.4
1	F	280	GLY	2.4
1	G	226	LYS	2.4
1	B	295	GLN	2.3
1	F	53	GLY	2.3
1	G	356	VAL	2.3
1	H	341	GLY	2.3
1	C	328	ASN	2.3
1	B	298	LEU	2.3
1	E	238	ALA	2.3
1	G	222	GLN	2.3
1	D	220	SER	2.3
1	E	226	LYS	2.3
1	F	229	ASP	2.3
1	G	307	ARG	2.3
1	F	319	LYS	2.3
1	B	234	LEU	2.3
1	D	316	LYS	2.3
1	E	321	THR	2.3
1	H	335	GLN	2.3
1	G	291	ASP	2.3
1	A	519	GLU	2.2
1	C	236	ASN	2.2
1	E	272	MET	2.2
1	A	297	TYR	2.2
1	A	335	GLN	2.2
1	C	301	GLU	2.2
1	E	342	LEU	2.2
1	H	177	ALA	2.2
1	F	331	ASP	2.2
1	A	299	ALA	2.2
1	F	264	THR	2.2
1	E	345	GLU	2.2
1	A	337	LEU	2.2
1	H	144	ALA	2.1
1	F	304	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	283	VAL	2.1
1	A	11	ASN	2.1
1	E	282	ASN	2.1
1	G	144	ALA	2.1
1	H	215	ASP	2.1
1	B	518	ALA	2.1
1	G	319	LYS	2.1
1	D	279	SER	2.1
1	G	335	GLN	2.1
1	G	143	GLY	2.1
1	E	319	LYS	2.1
1	E	291	ASP	2.1
1	H	184	ASP	2.1
1	H	290	ILE	2.1
1	F	316	LYS	2.0
1	D	321	THR	2.0
1	A	287	GLN	2.0
1	F	336	ASP	2.0
1	E	354	ILE	2.0
1	H	240	GLU	2.0
1	A	224	PRO	2.0
1	C	298	LEU	2.0
1	E	301	GLU	2.0
1	G	302	GLY	2.0
1	H	358	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	F	544	1/1	0.97	0.32	6.98	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	1.36	92,92,92,92	0
4	SO4	C	546	5/5	0.98	0.21	1.21	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	0.84	111,111,111,111	0
2	MG	C	544	1/1	0.95	0.19	0.65	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	-0.19	75,90,123,124	0
3	ADP	B	545	27/27	0.95	0.21	-0.30	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.