



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:04 PM UTC

PDB ID : 3KFE / pdb_00003kfe
Title : Crystal structures of a group II chaperonin from *Methanococcus maripaludis*
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.; Meyer, D.; Knee, K.M.; Goulet, D.R.; King, J.A.; Frydman, J.; Adams, P.D.
Deposited on : 2009-10-27
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

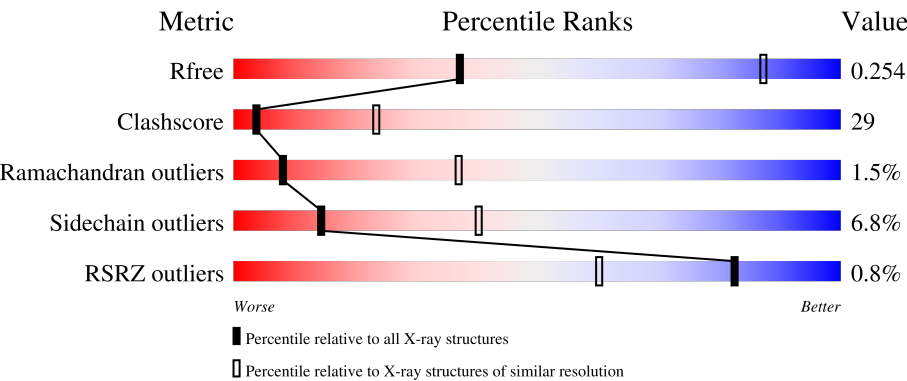
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	49%39%7%
1	B	521	50%39%7%
1	C	521	% 49%40%5%7%
1	D	521	% 49%38%6%7%
1	E	521	% 48%40%5%7%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 mutation	UNP Q877G8
A	265	ALA	GLU	engineered mutation	UNP Q877G8
A	266	SER	GLU	engineered mutation	UNP Q877G8
A	267	GLU	LYS	engineered mutation	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 mutation	UNP Q877G8
B	265	ALA	GLU	engineered mutation	UNP Q877G8
B	266	SER	GLU	engineered mutation	UNP Q877G8
B	267	GLU	LYS	engineered mutation	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 mutation	UNP Q877G8
C	265	ALA	GLU	engineered mutation	UNP Q877G8
C	266	SER	GLU	engineered mutation	UNP Q877G8
C	267	GLU	LYS	engineered mutation	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 mutation	UNP Q877G8
D	265	ALA	GLU	engineered mutation	UNP Q877G8
D	266	SER	GLU	engineered mutation	UNP Q877G8
D	267	GLU	LYS	engineered mutation	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 mutation	UNP Q877G8
E	265	ALA	GLU	engineered mutation	UNP Q877G8
E	266	SER	GLU	engineered mutation	UNP Q877G8
E	267	GLU	LYS	engineered mutation	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 mutation	UNP Q877G8
F	265	ALA	GLU	engineered mutation	UNP Q877G8
F	266	SER	GLU	engineered mutation	UNP Q877G8
F	267	GLU	LYS	engineered mutation	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 mutation	UNP Q877G8
G	265	ALA	GLU	engineered mutation	UNP Q877G8
G	266	SER	GLU	engineered mutation	UNP Q877G8
G	267	GLU	LYS	engineered mutation	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 mutation	UNP Q877G8

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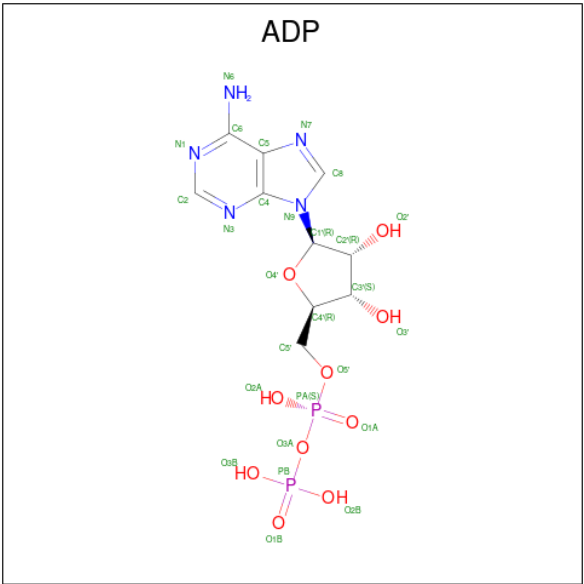
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Chain	Residue	Modelled	Actual	Comment	Reference
H	265	ALA	GLU	engineered mutation	UNP Q877G8
H	266	SER	GLU	engineered mutation	UNP Q877G8
H	267	GLU	LYS	engineered mutation	UNP Q877G8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

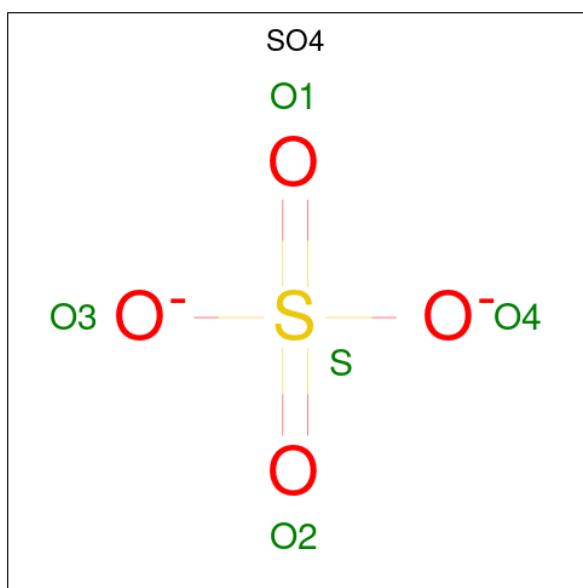
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 (CCD ID: SO4) (formula: O₄S).



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

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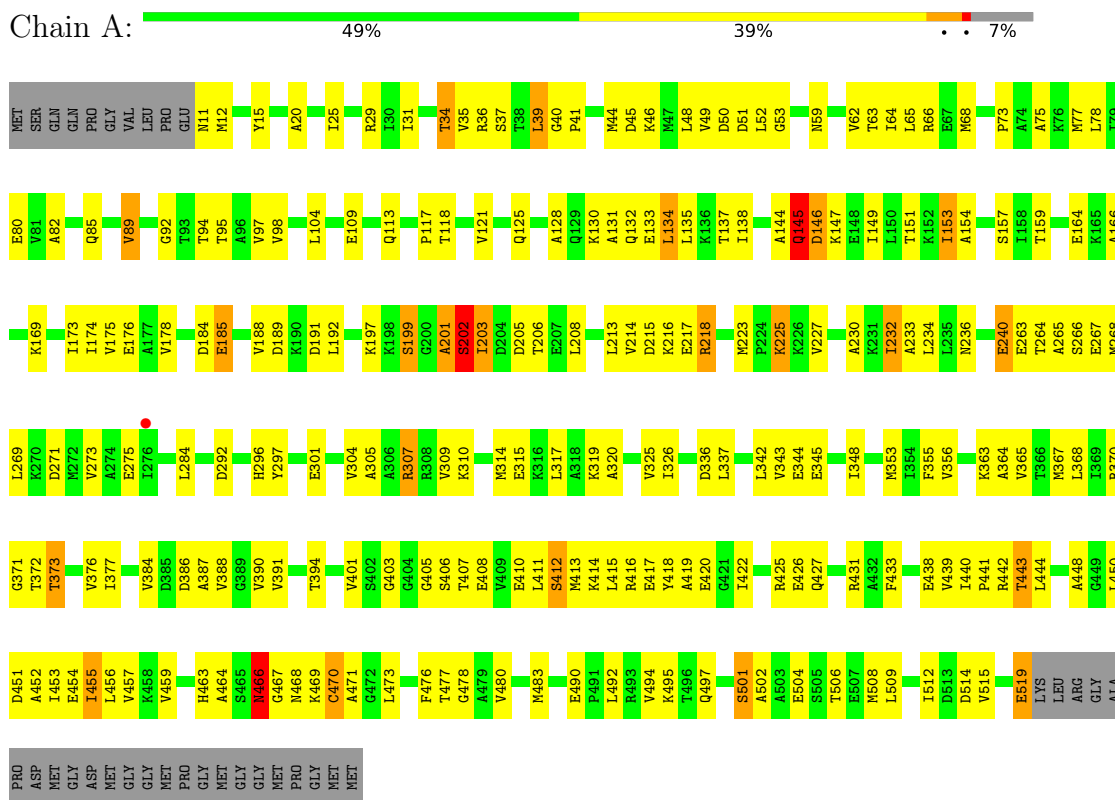
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

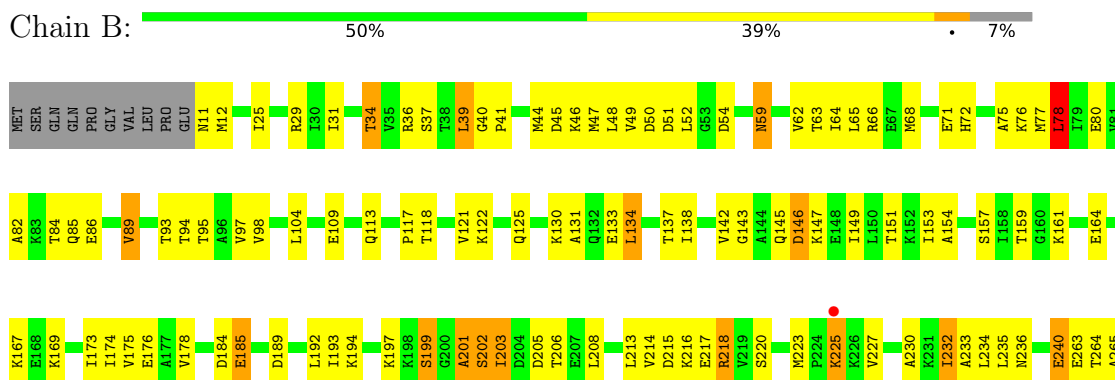
3 Residue-property plots [i](#)

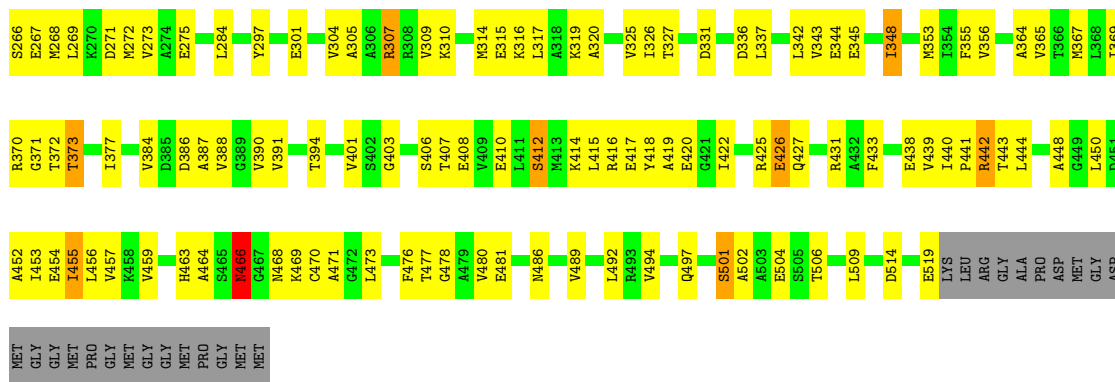
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

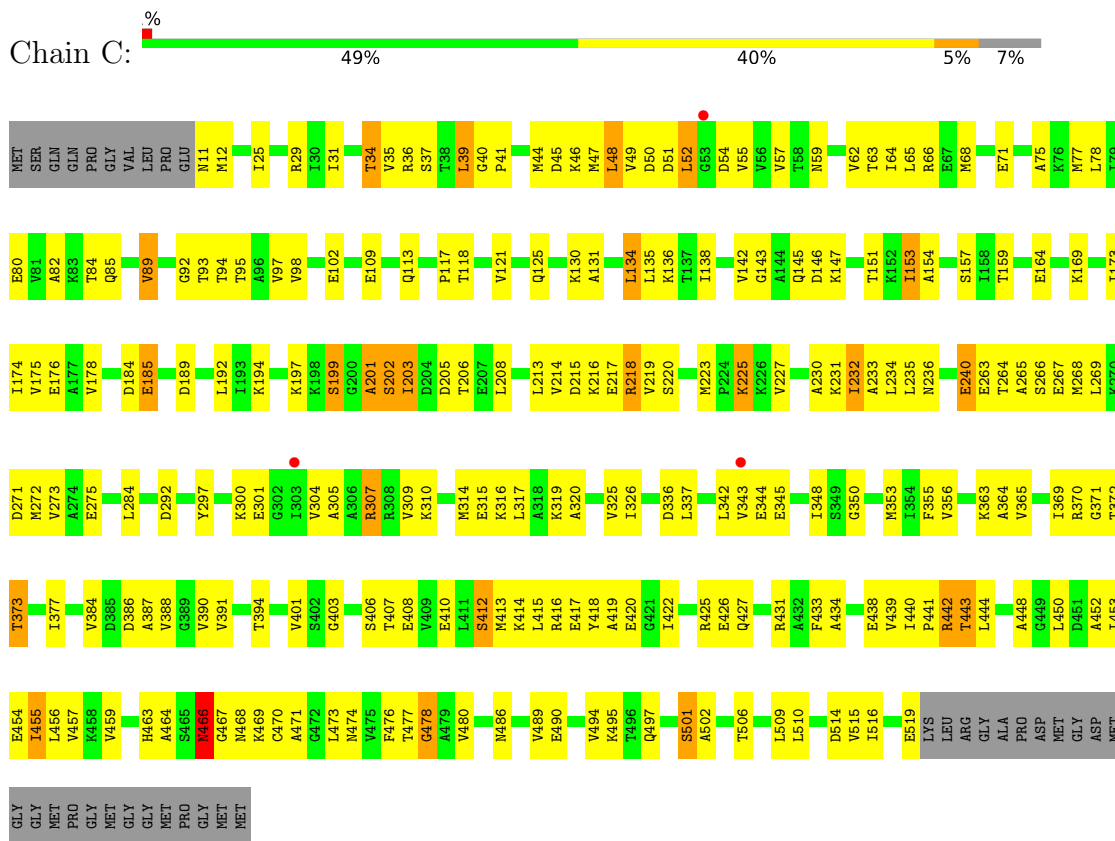


• Molecule 1: Chaperonin

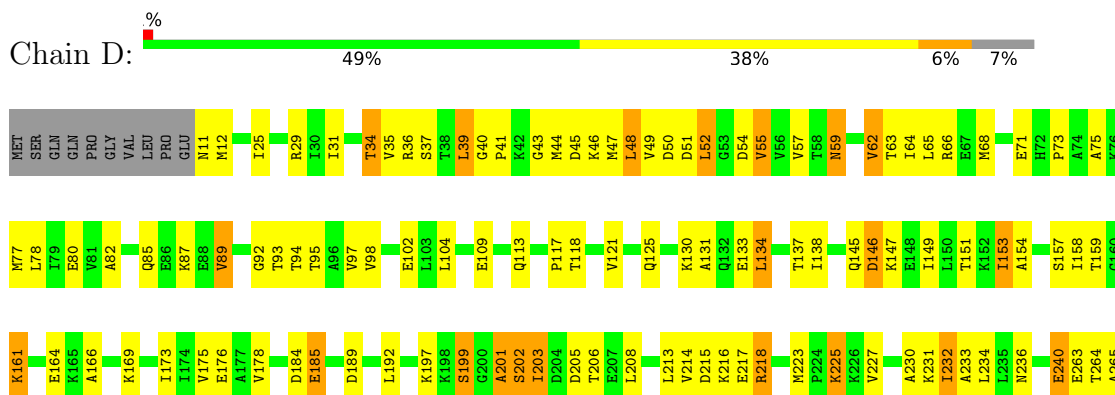




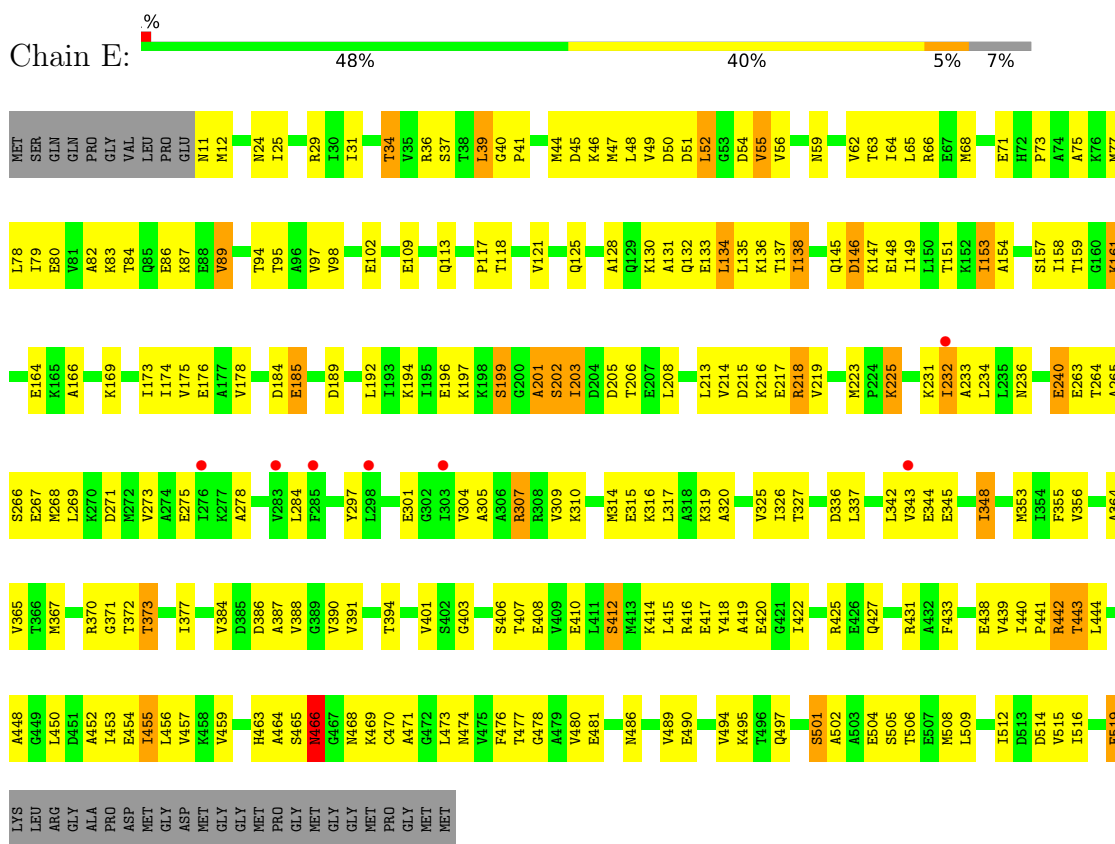
- Molecule 1: Chaperonin



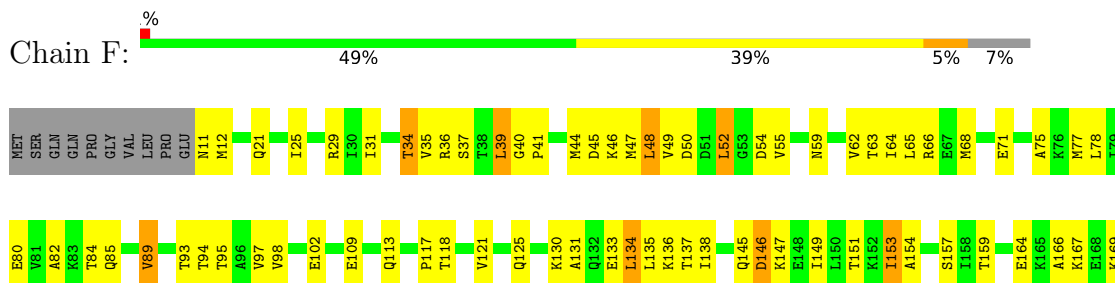
- Molecule 1: Chaperonin

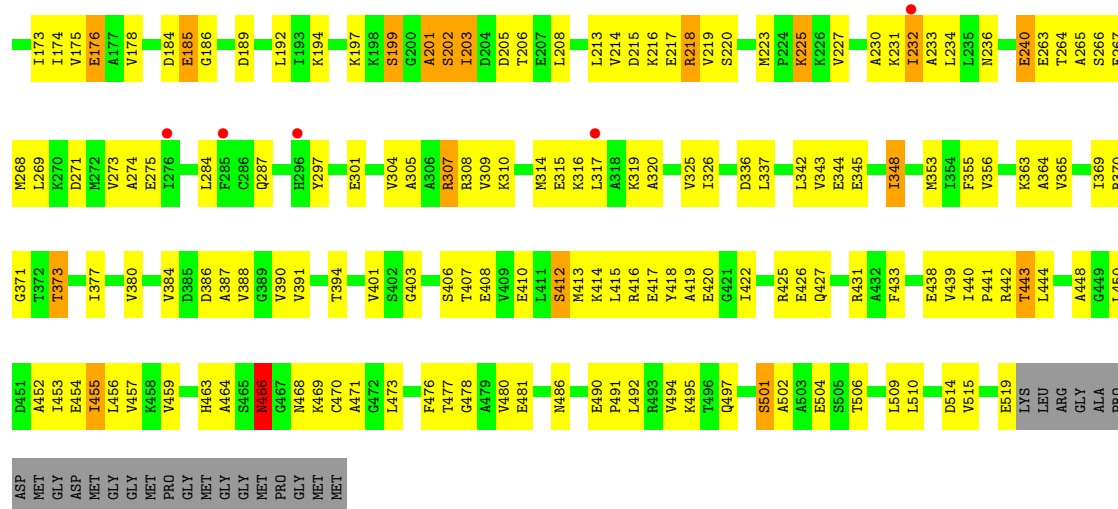


- Molecule 1: Chaperonin

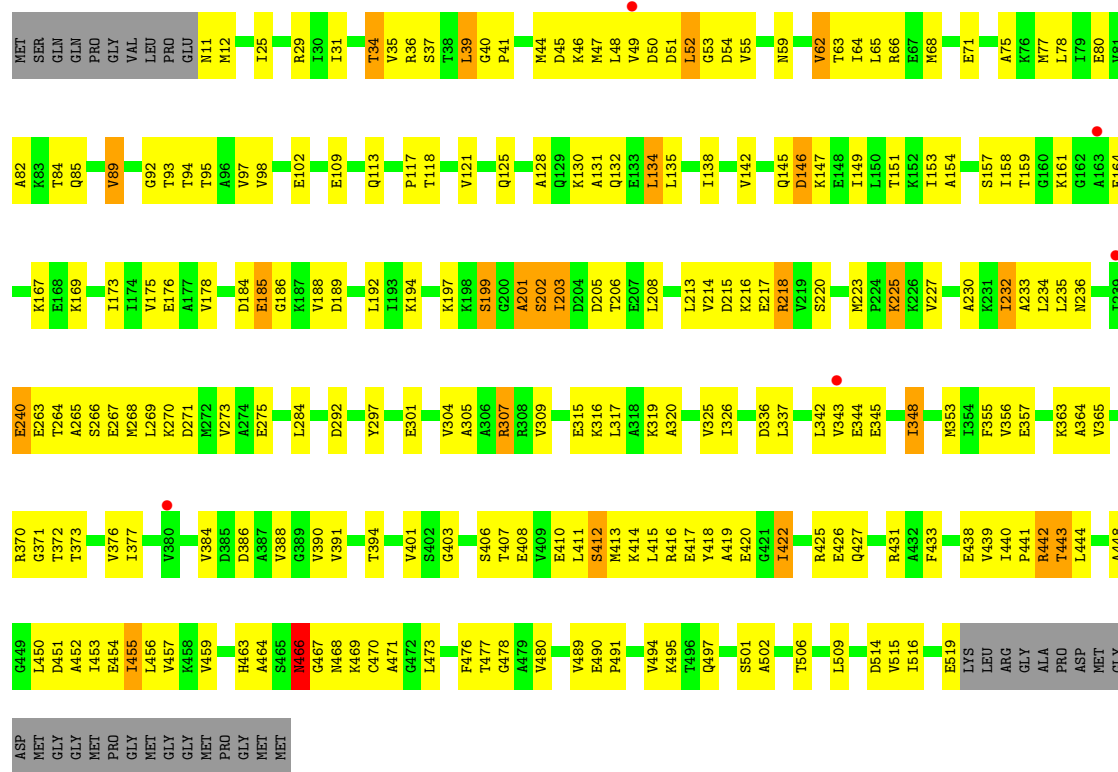


- Molecule 1: Chaperonin

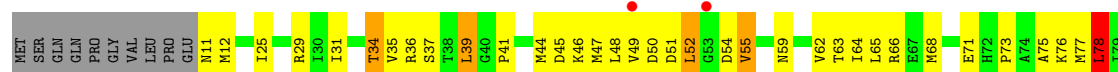




• Molecule 1: Chaperonin



• Molecule 1: Chaperonin



PRO	A80	E81	A82	F83	T84	Q85		V89	G92	T93	T94	T95	A96	V97	V98		E102		E109		Q113		P117	T118		V121	Q125		A128	Q129	K130	A131	Q132	E133	L134		I138	A139		Q145	D146	K147	E148	I149	L150	T151	K152	I153	A154	M155	T156	S157	I158	T159	G160		E164	K165																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
	A166	K167	E168	K169		I173	I174	V175	E176	A177	V178		D184	E185		V188	D189		L192		K197	K198	S199	A201	S202	T203	D204	D205	T206	E207	L208		L213	V214	D215	K216	E217	R218	V219	S220		W223	P224	K225	K226	V227	T228	D229	A230	K231	I232	A233	L234	L235	W236		E240	E263	T264																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
	A265	S266	E267	M268	L269	K270	D271	M272	V273	A274	E275		A278		L284		Y297		E301		V304	A305	A306	R307	R308	V309	K310	M314	E315	K316	L317	A318	K319	A320		V325	T326	T327		D336	L337		L342	V343	E344	E345		K348		K353	T354	F355	V356	E357		K363	A364	V365	T366																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
	K367		R370	G371	T372	T373	V376	I377		V384	D385	D386	A387	V388		V390	V391		T394		G398		V401	T407	E408	V409	E410	L411	S412	M413	K414	L415	R416	E417	Y418	A419	E420	G421	L422		R425	E426	Q427		R431	A432	F433		E438	V439	I440	P441	V442	T443	L444		A448	G449																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
	L450	D451	A452	I453	E454	I455	L456	V457	K458	V459		H463	A464	S465	N466	G467	N468	K469	C470	A471	G472	L473		F476	T477	G478	A479	V480		V489	E490	P491	L492	R493	V494	K495	T496	Q497		S501	A502	A503	E504	S505	T506	E507	M508	L509	L510	R511	I512	D513	D514		E519	LYS	LEU	ARG	GLY	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
	ASP	A508	E509	F510	T511	Q512		V515	G516	T517	T518	T519	T520	A521	V522		E525		E529		Q533		P537	T538		V541	Q542		A545	Q546	K547	L548	A549	Q550	E551	L552		I555	A556		Q559	D560	K561	E562	I563	A564	M565	T566	S567	I568	T569	G570		E574	K575																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
	MET	A576	S577	E578	M579	L580	K581	D582	M583	V584	A585	E586		A589		L592		Y593		E597		V600	A601	A602	R603	R604	V605	K606	M607	E608	L609	P610	L611	R612	A613	A614	E615		D618	L619		L622	V623		L626	V627		L630	V631	I632	A633	L634	L635	W636		E640	E663	T664																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
	ASP	K637		R638	G639	T640	T641	V642	I643		V646	D647	D648	A649	V650		V652		T656		G659		V662		V665	T666	E667	E668	L669	S670	M671	K672	L673	A674	A675	R676	A677	E678		D681	L682		L685	V686		L689	V690		L693	V694		L697	V698		L700	V701		L704	V705		L708	V709		L712	V713		L716	V717		L720	V721		L724	V725		L728	V729		L732	V733		L736	V737		L740	V741		L744	V745		L748	V749		L752	V753		L756	V757		L760	V761		L764	V765		L768	V769		L772	V773		L776	V777		L780	V781		L784	V785		L788	V789		L792	V793		L796	V797		L800	V801		L804	V805		L808	V809		L812	V813		L816	V817		L820	V821		L824	V825		L828	V829		L832	V833		L836	V837		L840	V841		L844	V845		L848	V849		L852	V853		L856	V857		L860	V861		L864	V865		L868	V869		L872	V873		L876	V877		L880	V881		L884	V885		L888	V889		L892	V893		L896	V897		L900	V901		L904	V905		L908	V909		L912	V913		L916	V917		L920	V921		L924	V925		L928	V929		L932	V933		L936	V937		L940	V941		L944	V945		L948	V949		L952	V953		L956	V957		L960	V961		L964	V965		L968	V969		L972	V973		L976	V977		L980	V981		L984	V985		L988	V989		L992	V993		L996	V997		L1000	V1001		L1004	V1005		L1008	V1009		L1012	V1013		L1016	V1017		L1020	V1021		L1024	V1025		L1028	V1029		L1032	V1033		L1036	V1037		L1040	V1041		L1044	V1045		L1048	V1049		L1052	V1053		L1056	V1057		L1060	V1061		L1064	V1065		L1068	V1069		L1072	V1073		L1076	V1077		L1080	V1081		L1084	V1085		L1088	V1089		L1092	V1093		L1096	V1097		L1100	V1101		L1104	V1105		L1108	V1109		L1112	V1113		L1116	V1117		L1120	V1121		L1124	V1125		L1128	V1129		L1132	V1133		L1136	V1137		L1140	V1141		L1144	V1145		L1148	V1149		L1152	V1153		L1156	V1157		L1160	V1161		L1164	V1165		L1168	V1169		L1172	V1173		L1176	V1177		L1180	V1181		L1184	V1185		L1188	V1189		L1192	V1193		L1196	V1197		L1200	V1201		L1204	V1205		L1208	V1209		L1212	V1213		L1216	V1217		L1220	V1221		L1224	V1225		L1228	V1229		L1232	V1233		L1236	V1237		L1240	V1241		L1244	V1245		L1248	V1249		L1252	V1253		L1256	V1257		L1260	V1261		L1264	V1265		L1268	V1269		L1272	V1273		L1276	V1277		L1280	V1281		L1284	V1285		L1288	V1289		L1292	V1293		L1296	V1297		L1300	V1301		L1304	V1305		L1308	V1309		L1312	V1313		L1316	V1317		L1320	V1321		L1324	V1325		L1328	V1329		L1332	V1333		L1336	V1337		L1340	V1341		L1344	V1345		L1348	V1349		L1352	V1353		L1356	V1357		L1360	V1361		L1364	V1365		L1368	V1369		L1372	V1373		L1376	V1377		L1380	V1381		L1384	V1385		L1388	V1389		L1392	V1393		L1396	V1397		L1400	V1401		L1404	V1405		L1408	V1409		L1412	V1413		L1416	V1417		L1420	V1421		L1424	V1425		L1428	V1429		L1432	V1433		L1436	V1437		L1440	V1441		L1444	V1445		L1448	V1449		L1452	V1453		L1456	V1457		L1460	V1461		L1464	V1465		L1468	V1469		L1472	V1473		L1476	V1477		L1480	V1481		L1484	V1485		L1488	V1489		L1492	V1493		L1496	V1497		L1500	V1501		L1504	V1505		L1508	V1509		L1512	V1513		L1516	V1517		L1520	V1521		L1524	V1525		L1528	V1529		L1532	V1533		L1536	V1537		L1540	V1541		L1544	V1545		L1548	V1549		L1552	V1553		L1556	V1557		L1560	V1561		L1564	V1565		L1568	V1569		L1572	V1573		L1576	V1577		L1580	V1581		L1584	V1585		L1588	V1589		L1592	V1593		L1596	V1597		L1600	V1601		L1604	V1605		L1608	V1609		L1612	V1613		L1616	V1617		L1620	V1621		L1624	V1625		L1628	V1629		L1632	V1633		L1636	V1637		L1640	V1641		L1644	V1645		L1648	V1649		L1652	V1653		L1656	V1657		L1660	V1661		L1664	V1665		L1668	V1669		L1672	V1673		L1676	V1677		L1680	V1681		L1684	V1685		L1688	V1689		L1692	V1693		L1696	V1697		L1700	V1701		L1704	V1705		L1708	V1709		L1712	V1713		L1716	V1717		L1720	V1721		L1724	V1725		L1728	V1729		L1732	V1733		L1736	V1737		L1740	V1741		L1744	V1745		L1748	V1749		L1752	V1753		L1756	V1757		L1760	V1761		L1764	V1765		L1768	V1769		L1772	V1773		L1776	V1777		L1780	V1781		L1784	V1785		L1788	V1789		L1792	V1793		L1796	V1797		L1800	V1801		L1804	V1805		L1808	V1809		L1812	V1813		L1816	V1817		L1820	V1821		L1824	V1825		L1828	V1829		L1832	V1833		L1836	V1837		L1840	V1841		L1844	V1845		L1848	V1849		L1852	V1853		L1856	V1857		L1860	V1861		L1864	V1865		L1868	V1869		L1872	V1873		L1876	V1877		L1880	V1881		L1884	V1885		L1888	V1889		L1892	V1893		L1896	V1897		L1900	V1901		L1904	V1905		L1908	V1909		L1912	V1913		L1916	V1917		L1920	V1921		L1924	V1925		L1928	V1929		L1932	V1933		L1936	V1937		L1940	V1941		L1944	V1945		L1948	V1949		L1952	V1953		L1956	V1957		L1960	V1961		L1964	V1965		L1968	V1969		L1972	V1973		L1976	V1977		L1980	V1981		L1984	V1985		L1988	V1989		L1992	V1993		L1996	V1997		L2000	V2001		L2004	V2005		L2008	V2009		L2012	V2013		L2016	V2017		L2020	V2021		L2024	V2025		L2028	V2029		L2032	V2033		L2036	V2037		L2040	V2041		L2044	V2045		L2048	V2049		L2052	V2053		L2056	V2057		L2060	V2061		L2064	V2065		L2068	V2069		L2072	V2073		L2076	V2077		L2080	V2081		L2084	V2085		L2088	V2089		L2092	V2093		L2096	V2097		L2100	V2101		L2104	V2105		L2108	V2109		L2112	V2113		L2116	V2117		L2120	V2121		L2124	V2125		L2128	V2129		L2132	V2133		L2136	V2137		L2140	V2141		L2144	V2145		L2148	V2149		L2152	V2153		L2156	V2157		L2160	V2161		L2164	V2165		L2168	V2169		L2172	V2173		L2176	V2177		L2180	V2181		L2184	V2185		L2188	V2189		L2192	V2193		L2196	V2197		L2200	V2201		L2204	V2205		L2208	V2209		L2212	V2213		L2216	V2217		L2220	V2221		L2224	V2225		L2228	V2229		L2232	V2233		L2236	V2237		L2240	V2241		L2244	V2245		L2248	V2249		L2252	V2253		L2256	V2257		L2260	V2261		L2264	V2265		L2268	V2269		L2272	V2273		L2276	V2277		L2280	V2281		L2284	V2285		L2288	V2289		L2292	V2293		L2296	V2297		L2300	V2301		L2304	V2305		L2308	V2309		L2312	V2313		L2316	V2317		L2320	V2321		L2324	V2325		L2328	V2329		L2332	V2333		L2336	V2337		L2340	V2341		L2344	V2345		L2348	V2349		L2352	V2353		L2356	V

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.45Å 161.92Å 147.37Å 90.00° 124.12° 90.00°	Depositor
Resolution (Å)	54.49 – 3.50 54.49 – 3.50	Depositor EDS
% Data completeness (in resolution range)	77.1 (54.49-3.50) 86.4 (54.49-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.232 , 0.269 0.226 , 0.254	Depositor DCC
R_{free} test set	2797 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 98.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	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 ²)	124.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

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	0.68	1/3649 (0.0%)	0.97	7/4911 (0.1%)
1	B	0.69	3/3649 (0.1%)	0.97	9/4911 (0.2%)
1	C	0.68	0/3649	0.97	5/4911 (0.1%)
1	D	0.64	0/3649	0.97	9/4911 (0.2%)
1	E	0.68	0/3649	0.96	5/4911 (0.1%)
1	F	0.65	0/3649	0.96	6/4911 (0.1%)
1	G	0.62	1/3649 (0.0%)	0.96	5/4911 (0.1%)
1	H	0.60	0/3649	0.94	4/4911 (0.1%)
All	All	0.66	5/29192 (0.0%)	0.96	50/39288 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	HIS	CG-CD2	11.31	1.48	1.35
1	A	145	GLN	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	HIS	CB-CG	-6.08	1.41	1.50
1	B	72	HIS	ND1-CE1	-5.87	1.26	1.32
1	G	202	SER	CA-C	5.45	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	SER	N-CA-C	9.35	122.89	108.30
1	C	202	SER	N-CA-C	8.90	122.19	108.30
1	G	202	SER	N-CA-C	8.89	122.17	108.30
1	F	202	SER	N-CA-C	8.53	121.61	108.30
1	B	202	SER	N-CA-C	8.39	121.39	108.30
1	A	202	SER	N-CA-C	8.39	121.39	108.30
1	B	40	GLY	CA-C-N	6.63	126.08	118.85
1	B	40	GLY	C-N-CA	6.63	126.08	118.85
1	A	40	GLY	CA-C-N	6.29	125.71	118.85
1	A	40	GLY	C-N-CA	6.29	125.71	118.85
1	F	40	GLY	CA-C-N	6.20	125.61	118.85
1	F	40	GLY	C-N-CA	6.20	125.61	118.85
1	B	72	HIS	ND1-CG-CD2	-5.97	100.13	106.10
1	A	232	ILE	N-CA-C	5.91	116.62	107.99
1	D	62	VAL	N-CA-C	5.79	115.98	110.42
1	C	40	GLY	CA-C-N	5.66	125.02	118.85
1	C	40	GLY	C-N-CA	5.66	125.02	118.85
1	F	232	ILE	N-CA-C	5.65	116.24	107.99
1	B	232	ILE	N-CA-C	5.64	116.23	107.99
1	G	62	VAL	N-CA-C	5.60	115.79	110.42
1	H	232	ILE	N-CA-C	5.58	116.14	107.99
1	H	202	SER	N-CA-C	5.54	122.59	110.80
1	F	202	SER	O-C-N	5.53	124.92	120.83
1	D	232	ILE	N-CA-C	5.41	115.89	107.99
1	E	202	SER	N-CA-C	5.37	122.24	110.80
1	C	232	ILE	N-CA-C	5.37	115.83	107.99
1	A	470	CYS	N-CA-C	-5.37	105.02	113.02
1	G	40	GLY	CA-C-N	5.37	124.70	118.85
1	G	40	GLY	C-N-CA	5.37	124.70	118.85
1	G	232	ILE	N-CA-C	5.36	115.82	107.99
1	H	478	GLY	N-CA-C	-5.27	108.42	114.69
1	D	478	GLY	N-CA-C	-5.26	108.43	114.69
1	F	492	LEU	N-CA-C	-5.26	105.72	111.82
1	E	40	GLY	CA-C-N	5.25	124.57	118.85
1	E	40	GLY	C-N-CA	5.25	124.57	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASN	N-CA-C	-5.23	106.84	114.12
1	D	161	LYS	N-CA-C	-5.20	106.69	112.57
1	H	78	LEU	N-CA-C	-5.20	106.45	112.89
1	A	492	LEU	N-CA-C	-5.17	105.82	111.82
1	E	161	LYS	N-CA-C	-5.16	107.50	112.97
1	D	40	GLY	CA-C-N	5.14	124.46	118.85
1	D	40	GLY	C-N-CA	5.14	124.46	118.85
1	A	405	GLY	N-CA-C	-5.11	108.22	115.43
1	B	78	LEU	N-CA-C	-5.10	106.56	112.89
1	D	470	CYS	N-CA-C	-5.10	105.42	113.02
1	E	232	ILE	N-CA-C	5.09	115.65	108.36
1	D	59	ASN	N-CA-C	-5.05	106.54	113.30
1	B	161	LYS	N-CA-C	-5.04	106.88	112.57
1	C	478	GLY	N-CA-C	-5.03	108.70	114.69
1	B	492	LEU	N-CA-C	-5.02	106.00	111.82

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	208	5
1	B	3629	0	3762	215	1
1	C	3629	0	3762	227	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3629	0	3762	246	0
1	E	3629	0	3762	235	3
1	F	3629	0	3762	214	3
1	G	3629	0	3762	221	4
1	H	3629	0	3762	224	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
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	1710	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 29.

All (1710) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:206:THR:HG22	1:F:370:ARG:H	1.07	1.10
1:H:39:LEU:HD23	1:H:444:LEU:HD23	1.30	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
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:HG2	1:C:442:ARG:HH11	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:HG2	1:D:442:ARG:HH11	1.34	0.92
1:G:206:THR:HG22	1:G:370:ARG:N	1.85	0.92
1:B:39:LEU:CD2	1:B:444:LEU:CD2	2.49	0.91
1:B:130:LYS:HG3	1:B:134:LEU:HD12	1.51	0.91
1:D:39:LEU:CD2	1:D:444:LEU:CD2	2.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:ARG:HG2	1:F:442:ARG:HH11	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:HG2	1:G:442:ARG:HH11	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
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:HH11	1:H:442:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:ILE:HD13	1:A:75:ALA:HB1	1.60	0.84
1:A:125:GLN:OE1	1:H:164:GLU:HB2	1.78	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:46:LYS:HG3	1:G:64:ILE:HD13	1.58	0.83
1:G:130:LYS:HG3	1:G:134:LEU:HD12	1.59	0.83
1:A:46:LYS:HG3	1:A:64:ILE:HD13	1.61	0.83
1:E:439:VAL:O	1:E:443:THR:HG23	1.77	0.83
1:D:39:LEU:CD2	1:D:444:LEU:HD21	2.08	0.83
1:H:130:LYS:HG3	1:H:134:LEU:HD12	1.60	0.83
1:C:39:LEU:CD2	1:C:444:LEU:HD21	2.07	0.83
1:C:130:LYS:HG3	1:C:134:LEU:HD12	1.59	0.82
1:A:268:MET:O	1:A:269:LEU:HD13	1.80	0.82
1:F:130:LYS:HG3	1:F:134:LEU:HD12	1.60	0.82
1: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:206:THR:CG2	1:F:370:ARG:H	1.92	0.80
1:F:268:MET:O	1:F:269:LEU:HD13	1.81	0.80
1:D: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:44:MET:HE2	1:E:44:MET:HA	1.67	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:H:44:MET:HE2	1:H:44:MET:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:MET:HE2	1:D:44:MET:HA	1.69	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:B:34:THR:HG21	1:B:68:MET:HE1	1.69	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:F:44:MET:HA	1:F:44:MET:HE2	1.71	0.72
1:G:34:THR:HG21	1:G:68:MET:HE1	1.71	0.72
1:A:34:THR:HG21	1:A:68:MET:HE1	1.71	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
1:A:292:ASP:HB3	1:B:327:THR:HG21	1.70	0.72
1:G:44:MET:HE2	1:G:44:MET:HA	1.72	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:HG2	1:A:442:ARG:NH1	2.02	0.72
1:B:320:ALA:HB2	1:B:364:ALA:HB3	1.72	0.72
1:C:44:MET:HA	1:C:44:MET:HE2	1.72	0.71
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:C:34:THR:HG21	1:C:68:MET:HE1	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:34:THR:HG21	1:E:68:MET:HE1	1.74	0.70
1:G:206:THR:CG2	1:G:370:ARG:H	1.96	0.70
1:G:320:ALA:HB2	1:G:364:ALA:HB3	1.72	0.70
1:H:208:LEU:HD11	1:H:365:VAL:CG1	2.21	0.70
1:E:448:ALA:HB3	1:E:450:LEU:HD12	1.73	0.69
1:A:448:ALA:HB3	1:A:450:LEU:HD12	1.73	0.69
1:B:44:MET:HE2	1:B:44:MET:HA	1.74	0.69
1:D:34:THR:HG21	1:D:68:MET:HE1	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:HG2	1:F:442:ARG:NH1	2.08	0.69
1:H:448:ALA:HB3	1:H:450:LEU:HD12	1.74	0.69
1:D:49:VAL:HG21	1:E:73:PRO:HG3	1.75	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:A:63:THR:HG22	1:A:66:ARG:HH22	1.58	0.68
1:H:34:THR:HG21	1:H:68:MET:HE1	1.75	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:F:34:THR:HG21	1:F:68:MET:HE1	1.74	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
1:F:448:ALA:HB3	1:F:450:LEU:HD12	1.76	0.67
1:G:442:ARG:HG2	1:G:442:ARG:NH1	2.08	0.67
1:H:189:ASP:HB3	1:H:192:LEU:HG	1.76	0.67
1:E:442:ARG:HH11	1:E:442:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:GLY:HA3	1:E:87:LYS:HE2	1.77	0.67
1:F:39:LEU:HD11	1:F:95:THR:HG22	1.76	0.67
1:F:401:VAL:HB	1:F:407:THR:HG21	1.77	0.67
1:H:89:VAL:HG11	1:H:494:VAL:HG22	1.76	0.67
1:B:448:ALA:HB3	1:B:450:LEU:HD12	1.75	0.67
1:C:63:THR:HG22	1:C:66:ARG:HH22	1.59	0.67
1:G:178:VAL:HG11	1:G:391:VAL:HG12	1.77	0.67
1:B:206:THR:CG2	1:B:370:ARG:H	2.04	0.66
1:H:442:ARG:HG2	1:H:442:ARG:NH1	2.10	0.66
1:H:502:ALA:O	1:H:506:THR:HG23	1.94	0.66
1:B:502:ALA:O	1:B:506:THR:HG23	1.94	0.66
1:E:39:LEU:HD11	1:E:95:THR:HG22	1.78	0.66
1:F:164:GLU:HB2	1:G:125:GLN:OE1	1.95	0.66
1:D:63:THR:HG22	1:D:66:ARG:NH2	2.10	0.66
1: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:F:373:THR:HB	1:G:80:GLU:HB3	1.77	0.66
1:G:420:GLU:HG2	1:G:431:ARG:HH22	1.61	0.66
1:H:271:ASP:O	1:H:275:GLU:HG3	1.95	0.66
1: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:A:44:MET:HE2	1:A:44:MET:HA	1.76	0.65
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
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:O	1:A:356:VAL:HG12	1.97	0.65
1:B:63:THR:HG22	1:B:66:ARG:HH22	1.61	0.65
1:B:440:ILE:O	1:B:444:LEU:HG	1.97	0.65
1:D:208:LEU:HD11	1:D:365:VAL:CG1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:131:ALA:HB2	1:A:415:LEU:HD11	1.80	0.62
1:A:206:THR:CG2	1:A:370:ARG:H	2.00	0.62
1:B:233:ALA:O	1:B:284:LEU:HD12	2.00	0.62
1:B:63:THR:HG22	1:B:66:ARG:NH2	2.14	0.62
1:B:131:ALA:HB2	1:B:415:LEU:HD11	1.81	0.62
1:D:173:ILE:HG23	1:D:208:LEU:HB2	1.80	0.62
1:F:62:VAL:HG13	1:F:63:THR:N	2.14	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:G:267:GLU:C	1:G:269:LEU:H	2.07	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:31:ILE:HD13	1:D:75:ALA:CB	2.30	0.61
1:D:189:ASP:HB3	1:D:192:LEU:HG	1.82	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
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:267:GLU:C	1:D:269:LEU:H	2.09	0.61
1:D:440:ILE:O	1:D:444:LEU:HG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:SER:CB	1:H:205:ASP:HB2	2.31	0.61
1:A:267:GLU:C	1:A:269:LEU:H	2.08	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:153:ILE:HD13	1:E:394:THR:OG1	2.01	0.61
1:E:208:LEU:HD11	1:E:365:VAL:CG1	2.29	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:B:267:GLU:C	1:B:269:LEU:H	2.07	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:31:ILE:HD11	1:C:78:LEU:HB2	1.83	0.60
1:C:420:GLU:HG2	1:C:431:ARG:HH22	1.65	0.60
1:D:420:GLU:HG2	1:D:431:ARG:HH22	1.66	0.60
1: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:C:267:GLU:C	1:C:269:LEU:H	2.08	0.60
1:G:37:SER:OG	1:G:46:LYS:NZ	2.33	0.60
1:G:408:GLU:O	1:G:412:SER:HB3	2.01	0.60
1:H:267:GLU:C	1:H:269:LEU:H	2.09	0.60
1:B:408:GLU:O	1:B:412:SER:HB3	2.01	0.60
1:D:201:ALA:HB2	1:E:497:GLN:OE1	2.01	0.60
1:D:401:VAL:HB	1:D:407:THR:HG21	1.82	0.60
1:E:267:GLU:C	1:E:269:LEU:H	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:47:MET:HE1	1:E:24:ASN:OD1	2.02	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:H:268:MET:C	1:H:269:LEU:HD13	2.26	0.60
1:A:31:ILE:HD13	1:A:75:ALA:CB	2.31	0.60
3:D:545:ADP:O2A	3:D:545:ADP:O1B	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: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:C:416:ARG:O	1:C:419:ALA:HB3	2.01	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:208:LEU:HD11	1:A:365:VAL:CG1	2.31	0.59
1:A:233:ALA:O	1:A:284:LEU:HD12	2.02	0.59
1:D:77:MET:CE	1:D:509:LEU:HD21	2.32	0.59
1:D:356:VAL:O	1:D:356:VAL:HG12	2.02	0.59
1:G:268:MET:C	1:G:269:LEU:HD13	2.27	0.59
1:H:31:ILE:HD13	1:H:75:ALA:CB	2.30	0.59
1:H:420:GLU:HG2	1:H:431:ARG:HH22	1.66	0.59
1:B:201:ALA:HB2	1:C:497:GLN:CD	2.28	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:F:267:GLU:C	1:F:269:LEU:H	2.09	0.59
1:G:82:ALA:HB2	1:G:97:VAL:CG2	2.33	0.59
1:H:31:ILE:HD11	1:H:78:LEU:HB2	1.84	0.59
1:H:77:MET:CE	1:H:509:LEU:HD21	2.32	0.59
1: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:268:MET:C	1:D:269:LEU:HD13	2.27	0.59
1:D:408:GLU:O	1:D:412:SER:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:268:MET:C	1:B:269:LEU:HD13	2.27	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:G:420:GLU:C	1:G:422:ILE:H	2.10	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:A:268:MET:C	1:A:269:LEU:HD13	2.28	0.58
1:F:418:TYR:CE2	1:F:422:ILE:HD11	2.39	0.58
3:G:545:ADP:O1B	3:G:545:ADP:O2A	2.22	0.58
1:H:418:TYR:CE2	1:H:422:ILE:HD11	2.38	0.58
1:A:77:MET:CE	1:A:509:LEU:HD21	2.34	0.58
1:A:145:GLN:O	1:A:147:LYS:N	2.36	0.58
1:G:203:ILE:HA	1:G:370:ARG:O	2.03	0.58
1:C:356:VAL:O	1:C:356:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:356:VAL:O	1:F:356:VAL:HG12	2.03	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
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:268:MET:C	1:B:269:LEU:HD22	2.29	0.57
1:B:442:ARG:HH11	1:B:442:ARG:CG	2.10	0.57
1:D:44:MET:CE	1:E:118:THR:HG23	2.34	0.57
1:E:268:MET:C	1:E:269:LEU:HD13	2.29	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:94:THR:O	1:A:98:VAL:HG23	2.05	0.57
1:A:216:LYS:HE2	1:A:307:ARG:O	2.05	0.57
3:B:545:ADP:O1B	3:B:545:ADP:O2A	2.21	0.57
1:D:47:MET:HB2	1:E:512:ILE:CD1	2.34	0.57
1:D:372:THR:CB	1:E:501:SER:HA	2.35	0.57
1:E:39:LEU:CD2	1:E:444:LEU:HD23	2.21	0.57
1:E:425:ARG:O	1:E:427:GLN:N	2.37	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:31:ILE:HD11	1:E:78:LEU:HB2	1.86	0.57
1:E:47:MET:O	1:F:515:VAL:HA	2.04	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:MET:HE3	1:C:515:VAL:HG13	1.87	0.56
1:C:62:VAL:HG13	1:C:63:THR:N	2.21	0.56
1:E:145:GLN:O	1:E:147:LYS:N	2.38	0.56
1:F:268:MET:C	1:F:269:LEU:HD13	2.29	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:77:MET:HA	1:B:80:GLU:HG2	1.87	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
1:D:372:THR:OG1	1:E:504:GLU:HB2	2.04	0.56
1:E:216:LYS:HE2	1:E:307:ARG:O	2.06	0.56
1:F:145:GLN:O	1:F:147:LYS:N	2.38	0.56
1:F:326:ILE:HD11	1:F:336:ASP:OD1	2.06	0.56
1: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:94:THR:O	1:B:98:VAL:HG23	2.05	0.56
1:B:425:ARG:O	1:B:427:GLN:N	2.38	0.56
1:C:268:MET:C	1:C:269:LEU:HD13	2.31	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:82:ALA:HB2	1:G:97:VAL:HG23	1.87	0.56
1:G:154:ALA:HB2	1:G:391:VAL:CG2	2.35	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:44:MET:HE3	1:E:118:THR:HG23	1.88	0.56
1:F:425:ARG:C	1:F:427:GLN:N	2.63	0.56
1:D:151:THR:OG1	1:D:175:VAL:HG21	2.05	0.56
1:E:47:MET:HE3	1:F:515:VAL:HG13	1.88	0.56
1:F:468:ASN:C	1:F:470:CYS:H	2.14	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: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:F:268:MET:C	1:F:269:LEU:HD22	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:ILE:HD12	1:G:410:GLU:HG2	1.87	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:F:438:GLU:C	1:F:441:PRO:HD2	2.31	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:B:438:GLU:C	1:B:441:PRO:HD2	2.32	0.55
1:B:468:ASN:C	1:B:470:CYS:H	2.13	0.55
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:A:420:GLU:C	1:A:422:ILE:H	2.15	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:H:420:GLU:C	1:H:422:ILE:H	2.15	0.55
1:A:39:LEU:HD11	1:A:95:THR:HG22	1.89	0.55
1:C:268:MET:C	1:C:269:LEU:HD22	2.32	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:H:268:MET:C	1:H:269:LEU:HD22	2.31	0.55
3:H:545:ADP:O1B	3:H:545:ADP:O2A	2.24	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:H:197:LYS:HB3	1:H:377:ILE:CG2	2.37	0.55
1:A:384:VAL:O	1:A:388:VAL:HG23	2.06	0.55
1:F:47:MET:HE3	1:G:515:VAL:HG13	1.89	0.55
1:F:420:GLU:C	1:F:422:ILE:H	2.14	0.55
3:H:545:ADP:PB	4:H:546:SO4:O2	2.65	0.55
1:A:268:MET:C	1:A:269:LEU:HD22	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:THR:HG23	3:A:545:ADP:O2B	2.08	0.54
1:A:442:ARG:NH1	1:A:442:ARG:CG	2.67	0.54
1:B:450:LEU:HD22	1:B:455:ILE:HD11	1.89	0.54
1:C:420:GLU:C	1:C:422:ILE:H	2.14	0.54
1:C:425:ARG:C	1:C:427:GLN:N	2.65	0.54
1:D:268:MET:C	1:D:269:LEU:HD22	2.31	0.54
1:G:268:MET:C	1:G:269:LEU:HD22	2.31	0.54
1:G:425:ARG:C	1:G:427:GLN:H	2.15	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
1:E:425:ARG:C	1:E:427:GLN:N	2.64	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
1:F:442:ARG:HH11	1:F:442:ARG:CG	2.12	0.54
1:H:65:LEU:HD23	1:H:68:MET:HE2	1.90	0.54
1:A:62:VAL:HG13	1:A:63:THR:N	2.23	0.54
1:C:468:ASN:C	1:C:470:CYS:H	2.15	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:G:425:ARG:C	1:G:427:GLN:N	2.64	0.54
1:A:315:GLU:O	1:A:319:LYS:HG3	2.06	0.54
1:B:420:GLU:C	1:B:422:ILE:H	2.15	0.54
1:E:46:LYS:HG3	1:E:64:ILE:CD1	2.36	0.54
1:F:37:SER:OG	1:F:46:LYS:NZ	2.40	0.54
1:F:203:ILE:H	1:F:371:GLY:HA2	1.72	0.54
1:B:89:VAL:HG11	1:B:494:VAL:HG22	1.90	0.54
1:B:197:LYS:HB3	1:B:377:ILE:HG21	1.90	0.54
1:E:47:MET:HE3	1:F:515:VAL:CG1	2.37	0.54
1:G:39:LEU:HD11	1:G:95:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLU:C	1:A:441:PRO:HD2	2.32	0.54
1:A:468:ASN:C	1:A:470:CYS:H	2.15	0.54
1:B:425:ARG:C	1:B:427:GLN:N	2.65	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:A:425:ARG:C	1:A:427:GLN:N	2.65	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:O1B	3:F:545:ADP:O2A	2.26	0.53
1:G:62:VAL:HG13	1:G:63:THR:N	2.23	0.53
1:G:145:GLN:O	1:G:147:LYS:N	2.41	0.53
1:H:36:ARG:NH2	1:H:443:THR:HG22	2.23	0.53
1:B:117:PRO:O	1:B:121:VAL:HG12	2.08	0.53
1:C:77:MET:CE	1:C:509:LEU:HD21	2.38	0.53
1:C:440:ILE:HB	1:C:441:PRO:HD3	1.89	0.53
1:E:438:GLU:C	1:E:441:PRO:HD2	2.33	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
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:A:515:VAL:HA	1:H:47:MET:O	2.09	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:HG12	1:E:356:VAL:O	2.07	0.53
1:H:62:VAL:HG13	1:H:63:THR:N	2.24	0.53
1:H:109:GLU:O	1:H:113:GLN:HG3	2.09	0.53
1:A:146:ASP:OD1	1:A:149:ILE:HD12	2.08	0.53
1:B:442:ARG:NH1	1:B:442:ARG:CG	2.69	0.53
1:B:464:ALA:O	1:B:466:ASN:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:GLU:C	1:C:441:PRO:HD2	2.34	0.53
1:G:59:ASN:OD1	1:G:59:ASN:O	2.27	0.53
1:G:418:TYR:CE2	1:G:422:ILE:HD11	2.44	0.53
1:G:468:ASN:C	1:G:470:CYS:H	2.16	0.53
1:B:151:THR:OG1	1:B:175:VAL:HG21	2.09	0.53
1:C:442:ARG:NH1	1:C:442:ARG:CG	2.68	0.53
1:F:138:ILE:HD12	1:F:410:GLU:HG2	1.90	0.53
1:G:442:ARG:NH1	1:G:442:ARG:CG	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: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: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:D:425:ARG:C	1:D:427:GLN:N	2.65	0.52
1:E:77:MET:HA	1:E:80:GLU:HG2	1.90	0.52
1:E:215:ASP:HA	1:E:353:MET:HG2	1.90	0.52
1:G:118:THR:HA	1:G:121:VAL:CG1	2.40	0.52
1:C:203:ILE:H	1:C:371:GLY:HA2	1.73	0.52
1: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:LYS:HG3	1:E:309:VAL:HG22	1.92	0.52
1:E:268:MET:C	1:E:269:LEU:HD22	2.34	0.52
1:E:425:ARG:C	1:E:427:GLN:H	2.18	0.52
1:C:448:ALA:CB	1:C:450:LEU:HD12	2.39	0.52
1:D:420:GLU:C	1:D:422:ILE:H	2.16	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:E:468:ASN:C	1:E:470:CYS:H	2.18	0.52
1:F:169:LYS:O	1:F:173:ILE:HG13	2.10	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:C:425:ARG:C	1:C:427:GLN:H	2.17	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:208:LEU:HD11	1:A:365:VAL:HG11	1.92	0.51
1:A:273:VAL:HG21	1:A:297:TYR:HB2	1.93	0.51
1:F:109:GLU:O	1:F:113:GLN:HG3	2.10	0.51
1:H:419:ALA:O	1:H:427:GLN:HG3	2.09	0.51
1:H:425:ARG:C	1:H:427:GLN:N	2.66	0.51
1:A:65:LEU:HD23	1:A:68:MET:HE2	1.92	0.51
1:A:73:PRO:HG3	1:H:49:VAL:HG21	1.91	0.51
1:A:448:ALA:CB	1:A:450:LEU:HD12	2.40	0.51
1:C:384:VAL:O	1:C:388:VAL:HG23	2.10	0.51
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:545:ADP:PB	4:E:546:SO4:O2	2.68	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:NH1	1:D:442:ARG:CG	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:B:425:ARG:C	1:B:427:GLN:H	2.19	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:39:LEU:HD21	1:E:444:LEU:HD21	1.92	0.51
1:E:273:VAL:HG21	1:E:297:TYR:HB2	1.92	0.51
1:F:46:LYS:HG3	1:F:64:ILE:CD1	2.34	0.51
1:F:425:ARG:C	1:F:427:GLN:H	2.17	0.51
1:F:464:ALA:O	1:F:466:ASN:OD1	2.28	0.51
1:G:46:LYS:HG3	1:G:64:ILE:CD1	2.34	0.51
1:A:82:ALA:HB2	1:A:97:VAL:CG2	2.40	0.51
1:E:82:ALA:HB2	1:E:97:VAL:HG23	1.92	0.51
1:E:450:LEU:HD22	1:E:455:ILE:HD11	1.91	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:A:425:ARG:C	1:A:427:GLN:H	2.18	0.51
1:B:273:VAL:HG21	1:B:297:TYR:HB2	1.91	0.51
1:C:36:ARG:NH2	1:C:443:THR:HG22	2.25	0.51
1:C:208:LEU:HD11	1:C:365:VAL:HG11	1.92	0.51
1:E:420:GLU:C	1:E:422:ILE:H	2.19	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
1:H:438:GLU:C	1:H:441:PRO:HD2	2.36	0.51
3:H:545:ADP:O3B	4:H:546:SO4:S	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:CG1	1:B:230:ALA:HB2	2.41	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:442:ARG:HG3	1:D:452:ALA:HB1	1.93	0.50
1:F:266:SER:HB3	1:F:268:MET:HE2	1.93	0.50
1:H:236:ASN:HB2	1:H:325:VAL:CG1	2.40	0.50
1:A:512:ILE:HA	1:H:45:ASP:O	2.11	0.50
1: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:A:450:LEU:HD22	1:A:455:ILE:HD11	1.93	0.50
1:C:94:THR:O	1:C:98:VAL:HG23	2.12	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: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:B:65:LEU:HD23	1:B:68:MET:HE2	1.93	0.50
1:C:39:LEU:CD2	1:C:444:LEU:HD23	2.21	0.50
1:C:273:VAL:HG21	1:C:297:TYR:HB2	1.92	0.50
1: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: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
1:H:77:MET:O	1:H:80:GLU:HB2	2.12	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:65:LEU:HD23	1:C:68:MET:HE2	1.92	0.50
1:C:82:ALA:HB2	1:C:97:VAL:CG2	2.42	0.50
1:C:118:THR:HA	1:C:121:VAL:HG12	1.93	0.50
1:D:109:GLU:O	1:D:113:GLN:HG3	2.12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:MET:HE3	1:C:515:VAL:CG1	2.41	0.50
1:B:49:VAL:HG12	1:B:50:ASP:N	2.26	0.50
1:B:440:ILE:HB	1:B:441:PRO:HD3	1.93	0.50
1:D:425:ARG:C	1:D:427:GLN:H	2.19	0.50
1:F:476:PHE:O	1:F:477:THR:C	2.55	0.50
1:G:202:SER:OG	1:G:370:ARG:HB2	2.12	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:HD22	1:C:269:LEU:N	2.27	0.49
1:D:57:VAL:CG2	1:E:512:ILE:HD11	2.42	0.49
1:E:59:ASN:OD1	1:E:59:ASN:O	2.30	0.49
1:E:419:ALA:O	1:E:427:GLN:HG3	2.13	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:C:51:ASP:HB2	1:D:519:GLU:CG	2.43	0.49
1:D:46:LYS:HG3	1:D:64:ILE:CD1	2.35	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:202:SER:HG	1:G:370:ARG:HB2	1.77	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:D:36:ARG:NH2	1:D:443:THR:HG22	2.27	0.49
1:F:197:LYS:HB3	1:F:377:ILE:CG2	2.41	0.49
1:A:197:LYS:HB3	1:A:377:ILE:CG2	2.41	0.49
1:D:49:VAL:HG12	1:D:50:ASP:N	2.26	0.49
1:D:169:LYS:O	1:D:173:ILE:HG13	2.12	0.49
1:G:95:THR:HG23	3:G:545:ADP:O2B	2.12	0.49
1:C:326:ILE:HD11	1:C:336:ASP:OD1	2.13	0.49
1:F:65:LEU:HD23	1:F:68:MET:HE2	1.94	0.49
1:G:476:PHE:O	1:G:477:THR:C	2.55	0.49
1:H:425:ARG:C	1:H:427:GLN:H	2.20	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: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:B:215:ASP:HA	1:B:353:MET:HG2	1.94	0.49
1:B:263:GLU:HA	1:B:269:LEU:CD2	2.38	0.49
1:D:269:LEU:HD22	1:D:269:LEU:N	2.28	0.49
1: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:D:468:ASN:C	1:D:470:CYS:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:ALA:O	1:F:427:GLN:HG3	2.13	0.49
1:G:39:LEU:HD21	1:G:444:LEU:HD21	1.91	0.49
1:G:117:PRO:O	1:G:121:VAL:HG12	2.12	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:NZ	1:B:225:LYS:HB3	2.28	0.49
1:B:367:MET:HE3	1:B:367:MET:HB3	1.74	0.49
1:C:202:SER:HB2	1:C:205:ASP:HB2	1.95	0.49
1:D:225:LYS:HB3	1:D:225:LYS:NZ	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:HD3	1:C:456:LEU:HD22	1.94	0.49
1:C:442:ARG:HG3	1:C:452:ALA:HB1	1.95	0.49
1:E:197:LYS:HB3	1:E:377:ILE:HG21	1.93	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: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:H:189:ASP:HB3	1:H:192:LEU:CG	2.42	0.48
1:H:442:ARG:NH1	1:H:442:ARG:CG	2.71	0.48
1:E:414:LYS:O	1:E:417:GLU:HG2	2.13	0.48
1:E:442:ARG:NH1	1:E:442:ARG:CG	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:HD23	1:H:415:LEU:HA	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:82:ALA:HB2	1:B:97:VAL:HG23	1.95	0.48
1:B:454:GLU:O	1:B:457:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:SER:OG	1:C:46:LYS:NZ	2.44	0.48
1:C:169:LYS:O	1:C:173:ILE:HG13	2.13	0.48
1:C:225:LYS:NZ	1:C:225:LYS:HB3	2.28	0.48
1:D:49:VAL:CG2	1:E:73:PRO:HG3	2.41	0.48
1:D:419:ALA:O	1:D:427:GLN:HG3	2.12	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:39:LEU:HD21	1:A:444:LEU:HD21	1.94	0.48
1:A:414:LYS:O	1:A:417:GLU:HG2	2.13	0.48
1:A:417:GLU:C	1:A:419:ALA:N	2.70	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:H:433:PHE:C	1:H:433:PHE:CD2	2.91	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:46:LYS:HG3	1:C:64:ILE:CD1	2.38	0.48
1:C:117:PRO:O	1:C:121:VAL:HG12	2.14	0.48
1:D:65:LEU:HD23	1:D:68:MET:HE2	1.96	0.48
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:236:ASN:HB2	1:A:325:VAL:CG1	2.43	0.48
1:A:269:LEU:HD22	1:A:269:LEU:N	2.29	0.48
1:C:292:ASP:C	1:D:327:THR:HG21	2.38	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:O	1:C:59:ASN:OD1	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:HD3	1:F:363:LYS:HA	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:448:ALA:CB	1:G:450:LEU:HD12	2.43	0.48
1:A:201:ALA:HB2	1:B:497:GLN:CD	2.34	0.48
1:E:202:SER:HG	1:E:203:ILE:N	2.12	0.48
1:F:442:ARG:NH1	1:F:442:ARG:CG	2.70	0.48
1:B:476:PHE:O	1:B:477:THR:C	2.57	0.48
1:D:438:GLU:C	1:D:441:PRO:HD2	2.39	0.48
1:E:433:PHE:C	1:E:433:PHE:CD2	2.92	0.48
1:A:504:GLU:OE1	1:H:376:VAL:HG11	2.14	0.47
1:B:417:GLU:C	1:B:419:ALA:N	2.71	0.47
1:C:372:THR:CB	1:D:501:SER:HB3	2.38	0.47
1:G:225:LYS:HB3	1:G:225:LYS:NZ	2.28	0.47
1:H:213:LEU:HD11	1:H:355:PHE:CE2	2.49	0.47
1:C:39:LEU:HD11	1:C:95:THR:HG22	1.95	0.47
3:C:545:ADP:O3B	4:C:546:SO4:O3	2.32	0.47
1:D:217:GLU:O	1:D:218:ARG:C	2.57	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:F:417:GLU:C	1:F:419:ALA:N	2.69	0.47
1:G:292:ASP:HB3	1:H:327:THR:HG21	1.95	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: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:G:438:GLU:C	1:G:441:PRO:HD2	2.38	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: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: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:A:454:GLU:O	1:A:457:VAL:N	2.47	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:51:ASP:HB2	1:D:519:GLU:HG3	1.96	0.47
1:C:102:GLU:HG2	1:C:439:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ALA:HB2	1:C:391:VAL:CG2	2.45	0.47
1:D:227:VAL:CG1	1:D:230:ALA:HB2	2.45	0.47
1:E:217:GLU:O	1:E:218:ARG:C	2.58	0.47
1:E:476:PHE:O	1:E:477:THR:C	2.57	0.47
1:F:82:ALA:HB2	1:F:97:VAL:CG2	2.45	0.47
1:G:267:GLU:C	1:G:269:LEU:N	2.73	0.47
1:H:343:VAL:HG13	1:H:356:VAL:HG22	1.96	0.47
1:A:217:GLU:O	1:A:218:ARG:C	2.58	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:HD22	1:G:269:LEU:N	2.29	0.47
1:A:109:GLU:O	1:A:113:GLN:HG3	2.15	0.47
1:B:36:ARG:NH2	1:B:443:THR:HG22	2.30	0.47
1:B:52:LEU:C	1:B:54:ASP:H	2.23	0.47
1:B:217:GLU:O	1:B:218:ARG:C	2.57	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:F:454:GLU:O	1:F:457:VAL:N	2.47	0.47
1:G:25:ILE:O	1:G:29:ARG:HG3	2.15	0.47
1:G:201:ALA:HB2	1:H:497:GLN:OE1	2.14	0.47
1:G:236:ASN:HB2	1:G:325:VAL:CG1	2.45	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:H:153:ILE:HG13	1:H:489:VAL:HG23	1.96	0.47
1:H:326:ILE:HD11	1:H:336:ASP:OD1	2.15	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
1:C:213:LEU:HD11	1:C:355:PHE:CE2	2.50	0.47
1:C:433:PHE:C	1:C:433:PHE:CD2	2.92	0.47
1:D:202:SER:HG	1:D:203:ILE:N	2.13	0.47
1:E:80:GLU:O	1:E:84:THR:HG23	2.15	0.47
1:E:266:SER:HB3	1:E:268:MET:CE	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:51:ASP:HB2	1:D:519:GLU:CB	2.45	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:E:37:SER:OG	1:E:46:LYS:NZ	2.47	0.47
1:E:417:GLU:C	1:E:419:ALA:N	2.69	0.47
1:H:202:SER:OG	1:H:370:ARG:HB2	2.15	0.47
1:H:269:LEU:HD22	1:H:269:LEU:N	2.30	0.47
1:H:476:PHE:O	1:H:477:THR:C	2.57	0.47
1:D:459:VAL:O	1:D:463:HIS:HD2	1.98	0.46
1:E:65:LEU:HD23	1:E:68:MET:HE2	1.95	0.46
1:F:269:LEU:O	1:F:273:VAL:HG23	2.14	0.46
1:H:218:ARG:NH1	1:H:225:LYS:HD3	2.30	0.46
1:A:267:GLU:C	1:A:269:LEU:N	2.74	0.46
1:B:46:LYS:HG3	1:B:64:ILE:CD1	2.40	0.46
1:B:202:SER:HB2	1:B:205:ASP:HB2	1.96	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:59:ASN:O	1:F:59:ASN:OD1	2.34	0.46
1:F:218:ARG:NH1	1:F:225:LYS:HD3	2.31	0.46
1:H:468:ASN:C	1:H:470:CYS:H	2.22	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:80:GLU:O	1:B:84:THR:HG23	2.15	0.46
1:B:169:LYS:O	1:B:173:ILE:HG13	2.15	0.46
1: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
1:C:217:GLU:O	1:C:218:ARG:C	2.58	0.46
1:C:297:TYR:O	1:C:301:GLU:HG2	2.16	0.46
1:D:363:LYS:HD3	1:D:363:LYS:HA	1.57	0.46
1:D:373:THR:CG2	1:E:505:SER:HB3	2.41	0.46
1:G:415:LEU:HD23	1:G:415:LEU:HA	1.65	0.46
1:H:11:ASN:HA	1:H:12:MET:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:266:SER:HB3	1:G:268:MET:HE2	1.98	0.46
1:G:433:PHE:C	1:G:433:PHE:CD2	2.93	0.46
1:H:34:THR:HG22	1:H:35:VAL:HG13	1.97	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:A:218:ARG:NH1	1:A:225:LYS:HD3	2.31	0.46
1:B:388:VAL:HG12	1:B:388:VAL:O	2.14	0.46
1:D:267:GLU:C	1:D:269:LEU:N	2.74	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:267:GLU:C	1:F:269:LEU:N	2.74	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:A:118:THR:HG23	1:H:44:MET:HE3	1.98	0.46
1:C:52:LEU:C	1:C:54:ASP:H	2.22	0.46
1:C:343:VAL:HG13	1:C:356:VAL:HG22	1.96	0.46
1:E:49:VAL:HG12	1:E:50:ASP:N	2.30	0.46
1:E:109:GLU:O	1:E:113:GLN:HG3	2.16	0.46
1:E:208:LEU:HD11	1:E:365:VAL:HG11	1.96	0.46
1:F:47:MET:HE3	1:G:515:VAL:CG1	2.44	0.46
1:H:178:VAL:HG13	1:H:188:VAL:HG11	1.97	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:H:367:MET:HE3	1:H:367:MET:HB3	1.70	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
1:C:218:ARG:NH1	1:C:225:LYS:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:GLU:O	1:G:84:THR:HG23	2.16	0.46
1:G:218:ARG:NH1	1:G:225:LYS:HD3	2.31	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:HD23	1:E:415:LEU:HA	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:217:GLU:O	1:H:218:ARG:C	2.57	0.46
1:H:310:LYS:O	1:H:314:MET:HG2	2.16	0.46
1:A:266:SER:HB3	1:A:268:MET:HE2	1.98	0.45
1:B:233:ALA:HB2	1:B:337:LEU:HD22	1.98	0.45
1:B:234:LEU:HD21	1:B:317:LEU:HB2	1.98	0.45
1: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:F:433:PHE:C	1:F:433:PHE:CD2	2.94	0.45
1:G:45:ASP:O	1:H:512:ILE:HA	2.16	0.45
1:G:65:LEU:HD23	1:G:68:MET:HE2	1.97	0.45
1:G:234:LEU:HD21	1:G:317:LEU:HB2	1.98	0.45
1:G:490:GLU:OE1	1:G:495:LYS:HE3	2.14	0.45
1:H:46:LYS:HG3	1:H:64:ILE:CD1	2.39	0.45
1:H:202:SER:HG	1:H:203:ILE:N	2.14	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:HG22	1:C:516:ILE:O	2.16	0.45
1:G:217:GLU:O	1:G:218:ARG:C	2.59	0.45
1:B:213:LEU:HD11	1:B:355:PHE:CE2	2.51	0.45
1:B:234:LEU:HD21	1:B:317:LEU:CB	2.46	0.45
1:C:266:SER:HB3	1:C:268:MET:CE	2.46	0.45
1:D:417:GLU:C	1:D:419:ALA:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:433:PHE:C	1:B:433:PHE:CD2	2.95	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
1:D:47:MET:HG3	1:D:55:VAL:HG23	1.99	0.45
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:442:ARG:HD3	1:D:456:LEU:HD22	1.99	0.45
1:D:476:PHE:O	1:D:477:THR:C	2.60	0.45
1:E:269:LEU:HD22	1:E:269:LEU:N	2.32	0.45
3:E:545:ADP:O3B	4:E:546:SO4:O3	2.35	0.45
1:F:36:ARG:NH2	1:F:443:THR:HG22	2.31	0.45
1:F:233:ALA:HB2	1:F:337:LEU:HD22	1.99	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:85:GLN:HG2	1:C:92:GLY:O	2.16	0.45
1:C:202:SER:OG	1:C:203:ILE:N	2.48	0.45
1:C:267:GLU:C	1:C:269:LEU:N	2.73	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:E:267:GLU:C	1:E:269:LEU:N	2.74	0.45
1:F:202:SER:OG	1:F:370:ARG:HB2	2.16	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:A:476:PHE:O	1:A:477:THR:C	2.59	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:153:ILE:HG13	1:D:489:VAL:HG23	1.98	0.45
1:D:448:ALA:CB	1:D:450:LEU:HD12	2.43	0.45
1:E:36:ARG:NH2	1:E:443:THR:HG22	2.31	0.45
1:E:266:SER:HB3	1:E:268:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ASP:O	1:E:512:ILE:HA	2.16	0.45
1:D:203:ILE:H	1:D:371:GLY:HA2	1.82	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:H:267:GLU:C	1:H:269:LEU:N	2.75	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:A:433:PHE:C	1:A:433:PHE:CD2	2.94	0.45
1:A:519:GLU:HB2	1:H:51:ASP:HB2	1.99	0.45
1:B:267:GLU:C	1:B:269:LEU:N	2.72	0.45
1:G:63:THR:O	1:G:64:ILE:C	2.59	0.45
1:A:453:ILE:O	1:A:457:VAL:HG23	2.17	0.45
1:C:49:VAL:HG12	1:C:50:ASP:N	2.32	0.45
1:C:151:THR:OG1	1:C:175:VAL:HG21	2.17	0.45
1:C:417:GLU:C	1:C:419:ALA:N	2.72	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: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:D:184:ASP:HA	1:D:185:GLU:HA	1.47	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:H:189:ASP:HB3	1:H:192:LEU:CD1	2.47	0.44
1:B:225:LYS:HB3	1:B:225:LYS:HZ3	1.82	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: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:D:266:SER:HB3	1:D:268:MET:HE2	1.99	0.44
1:F:52:LEU:C	1:F:54:ASP:H	2.25	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:H:51:ASP:C	1:H:51:ASP:OD1	2.59	0.44
1:A:459:VAL:O	1:A:463:HIS:HD2	1.99	0.44
1:C:49:VAL:HG22	1:D:73:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLN:HG2	1:C:93:THR:HA	1.99	0.44
1:C:476:PHE:O	1:C:477:THR:C	2.59	0.44
1:D:51:ASP:C	1:D:51:ASP:OD1	2.59	0.44
1:D:57:VAL:CG1	1:E:512:ILE:HD11	2.48	0.44
1:D:216:LYS:HG3	1:D:309:VAL:HG22	1.98	0.44
1:D:273:VAL:HG11	1:D:297:TYR:CB	2.47	0.44
1:D:376:VAL:HG11	1:E:504:GLU:OE1	2.17	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:E:41:PRO:HG3	1:E:159:THR:HG22	2.00	0.44
1:F:232:ILE:O	1:F:337:LEU:HA	2.18	0.44
1:G:41:PRO:HG3	1:G:159:THR:HG22	1.99	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:H:417:GLU:C	1:H:419:ALA:N	2.75	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
1:C:403:GLY:O	1:C:406:SER:HB2	2.17	0.44
1:D:34:THR:HG22	1:D:35:VAL:HG13	2.00	0.44
1:D:232:ILE:O	1:D:337:LEU:HA	2.17	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:H:266:SER:HB3	1:H:268:MET:HE2	1.99	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:G:52:LEU:C	1:G:54:ASP:H	2.26	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:417:GLU:C	1:E:419:ALA:H	2.26	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:O	1:H:348:ILE:CG2	2.65	0.44
1:A:118:THR:HA	1:A:121:VAL:HG12	1.98	0.44
1:D:433:PHE:C	1:D:433:PHE:CD2	2.95	0.44
1:F:47:MET:HG3	1:F:55:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:HG2	1:A:92:GLY:O	2.17	0.44
1:A:213:LEU:HD11	1:A:355:PHE:CE2	2.52	0.44
1:B:232:ILE:O	1:B:337:LEU:HA	2.18	0.44
1:B:297:TYR:O	1:B:301:GLU:HG2	2.18	0.44
1:C:213:LEU:HD11	1:C:355:PHE:CD2	2.52	0.44
1:C:240:GLU:O	1:C:269:LEU:HG	2.18	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:47:MET:HG3	1:G:55:VAL:HG23	1.99	0.44
1:G:75:ALA:C	1:G:77:MET:N	2.76	0.44
1:G:413:MET:SD	1:G:463:HIS:O	2.76	0.44
1:A:46:LYS:HD3	1:B:514:ASP:HB3	1.98	0.44
1:A:292:ASP:CB	1:B:327:THR:HG21	2.42	0.44
1:B:75:ALA:C	1:B:77:MET:N	2.75	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:217:GLU:O	1:F:218:ARG:C	2.59	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:B:266:SER:HB3	1:B:268:MET:HE2	1.99	0.43
1:C:135:LEU:O	1:C:136:LYS:C	2.61	0.43
1:C:234:LEU:HD21	1:C:317:LEU:CB	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:E:189:ASP:HB3	1:E:192:LEU:CD1	2.48	0.43
1:H:47:MET:HG3	1:H:55:VAL:HG23	1.98	0.43
1:A:59:ASN:OD1	1:A:59:ASN:O	2.36	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:B:71:GLU:OE1	1:B:71:GLU:HA	2.18	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:D:456:LEU:HD12	1:D:456:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:34:THR:O	1:H:46:LYS:HE2	2.18	0.43
1:H:234:LEU:HD21	1:H:317:LEU:HB2	2.00	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: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:D:75:ALA:C	1:D:77:MET:N	2.76	0.43
1:D:367:MET:HE3	1:D:367:MET:HB3	1.71	0.43
1:E:473:LEU:HD12	1:E:474:ASN:N	2.33	0.43
1:F:135:LEU:O	1:F:136:LYS:C	2.61	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:442:ARG:HD3	1:A:456:LEU:HD22	2.00	0.43
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:F:417:GLU:C	1:F:419:ALA:H	2.26	0.43
1:G:51:ASP:OD1	1:G:51:ASP:C	2.62	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:A:519:GLU:HB2	1:H:51:ASP:CB	2.49	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: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: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:G:490:GLU:O	1:G:491:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:545:ADP:O3B	4:H:546:SO4:O3	2.37	0.43
1:B:167:LYS:HA	1:B:167:LYS:HD2	1.83	0.43
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.91	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: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:240:GLU:O	1:A:269:LEU:HG	2.18	0.43
1:B:85:GLN:HG2	1:B:93:THR:HA	2.00	0.43
1:B:133:GLU:O	1:B:137:THR:HG23	2.19	0.43
1:D:202:SER:OG	1:D:203:ILE:N	2.42	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:420:GLU:C	1:G:422:ILE:N	2.76	0.43
1:H:71:GLU:OE1	1:H:71:GLU:HA	2.17	0.43
1:A:15:TYR:O	1:A:20:ALA:HB2	2.19	0.43
1:A:417:GLU:C	1:A:419:ALA:H	2.27	0.43
1:C:39:LEU:HD21	1:C:444:LEU:HD21	1.94	0.43
1:C:47:MET:HG3	1:C:55:VAL:HG23	2.00	0.43
1:C:57:VAL:CG1	1:D:512:ILE:HD11	2.49	0.43
1:C:342:LEU:CD2	1:C:344:GLU:HB2	2.48	0.43
1:C:456:LEU:HD12	1:C:456:LEU:HA	1.86	0.43
3:C:545:ADP:PB	4:C:546:SO4:S	3.17	0.43
1:D:46:LYS:HD3	1:E:514:ASP:CB	2.36	0.43
1:D:154:ALA:HB2	1:D:391:VAL:HG23	2.00	0.43
1:E:343:VAL:HG13	1:E:356:VAL:HG22	2.00	0.43
1:A:82:ALA:HB2	1:A:97:VAL:HG23	2.00	0.42
1:A:456:LEU:HA	1:A:456:LEU:HD12	1.86	0.42
1:C:71:GLU:OE1	1:C:71:GLU:HA	2.19	0.42
1:C:263:GLU:HA	1:C:269:LEU:CD2	2.39	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:HD23	1:H:509:LEU:HA	1.78	0.42
1:A:34:THR:HG22	1:A:35:VAL:HG13	2.00	0.42
1:A:53:GLY:O	1:B:76:LYS:HE2	2.19	0.42
1:A:367:MET:HE3	1:A:367:MET:HB3	1.69	0.42
1:B:122:LYS:HD3	1:B:426:GLU:OE1	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:D:342:LEU:CD2	1:D:344:GLU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:GLU:OE1	1:D:486:ASN:ND2	2.52	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:G:417:GLU:C	1:G:419:ALA:N	2.74	0.42
1:H:227:VAL:CG1	1:H:230:ALA:HB2	2.49	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:63:THR:O	1:E:64:ILE:C	2.61	0.42
1:E:201:ALA:HB2	1:F:497:GLN:CD	2.42	0.42
1:E:233:ALA:HB2	1:E:337:LEU:HD22	2.00	0.42
1:E:388:VAL:O	1:E:388:VAL:HG12	2.18	0.42
1:G:202:SER:HB2	1:G:205:ASP:HB2	2.01	0.42
1:H:59:ASN:O	1:H:59:ASN:OD1	2.37	0.42
1:H:414:LYS:O	1:H:417:GLU:HG2	2.19	0.42
1:A:483:MET:HE2	1:A:483:MET:HA	2.01	0.42
1:A:490:GLU:OE1	1:A:495:LYS:HE3	2.19	0.42
1:B:51:ASP:C	1:B:51:ASP:OD1	2.63	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
1:A:51:ASP:C	1:A:51:ASP:OD1	2.61	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:267:GLU:CD	1:G:270:LYS:HD3	2.44	0.42
1:G:342:LEU:HD23	1:G:343:VAL:N	2.35	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:C:266:SER:HB3	1:C:268:MET:HE2	1.99	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:F:219:VAL:CG2	1:F:307:ARG:HD3	2.49	0.42
1:B:456:LEU:HD12	1:B:456:LEU:HA	1.82	0.42
1:C:269:LEU:HD12	1:C:272:MET:SD	2.60	0.42
1:E:46:LYS:HD3	1:F:514:ASP:CB	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:ALA:O	1:E:132:GLN:HG2	2.20	0.42
1:E:310:LYS:O	1:E:314:MET:HG2	2.20	0.42
1:F:77:MET:O	1:F:80:GLU:HB2	2.20	0.42
1:F:167:LYS:HD2	1:F:167:LYS:HA	1.83	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:HH11	1:H:442:ARG:CG	2.12	0.42
1:B:37:SER:OG	1:B:46:LYS:NZ	2.45	0.42
1:B:189:ASP:HB3	1:B:192:LEU:CG	2.49	0.42
1:D:310:LYS:O	1:D:314:MET:HG2	2.19	0.42
1:D:348:ILE:O	1:D:348:ILE:CG2	2.67	0.42
1:D:415:LEU:HD23	1:D:415:LEU:HA	1.69	0.42
1:E:71:GLU:OE1	1:E:71:GLU:HA	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:A:213:LEU:HD11	1:A:355:PHE:CD2	2.55	0.42
1:A:368:LEU:HD12	1:A:368:LEU:HA	1.87	0.42
1:B:417:GLU:C	1:B:419:ALA:H	2.27	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
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: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: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:F:433:PHE:CD2	1:F:433:PHE:O	2.72	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:F:490:GLU:O	1:F:491:PRO:C	2.62	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:59:ASN:OD1	1:B:59:ASN:O	2.38	0.41
1:B:178:VAL:HA	1:B:193:ILE:HD11	2.02	0.41
1:E:118:THR:HA	1:E:121:VAL:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:THR:O	1:C:46:LYS:HE2	2.20	0.41
1:C:52:LEU:C	1:C:54:ASP:N	2.78	0.41
1:C:414:LYS:O	1:C:417:GLU:HG2	2.20	0.41
1:D:197:LYS:HD2	1:D:377:ILE:HG22	2.01	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:77:MET:HE3	1:G:509:LEU:HD21	2.01	0.41
1:G:273:VAL:HG11	1:G:297:TYR:CB	2.49	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
1:A:227:VAL:HG12	1:A:230:ALA:HB2	2.02	0.41
1:C:417:GLU:C	1:C:419:ALA:H	2.28	0.41
1:C:506:THR:O	1:C:510:LEU:HG	2.21	0.41
1:D:71:GLU:OE1	1:D:71:GLU:HA	2.19	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:D:375:HIS:O	1:E:508:MET:HE1	2.21	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:269:LEU:O	1:B:273:VAL:HG23	2.20	0.41
1:B:273:VAL:HG11	1:B:297:TYR:CB	2.50	0.41
1:D:357:GLU:H	1:D:357:GLU:HG2	1.71	0.41
1:F:178:VAL:HG22	1:F:388:VAL:HG13	2.01	0.41
1:F:353:MET:HE3	1:F:353:MET:HB2	1.97	0.41
1:G:202:SER:OG	1:G:203:ILE:N	2.50	0.41
1:H:52:LEU:C	1:H:54:ASP:H	2.28	0.41
1:H:63:THR:O	1:H:64:ILE:C	2.63	0.41
1:H:202:SER:OG	1:H:203:ILE:N	2.48	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:HD12	1:H:456:LEU:HA	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:D:52:LEU:C	1:D:54:ASP:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:LEU:O	1:E:136:LYS:C	2.63	0.41
1:F:273:VAL:HG11	1:F:297:TYR:CB	2.49	0.41
1:H:219:VAL:CG2	1:H:307:ARG:HD3	2.51	0.41
1:H:235:LEU:HD23	1:H:235:LEU:HA	1.91	0.41
1: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:CD2	1:E:433:PHE:O	2.73	0.41
1:G:71:GLU:OE1	1:G:71:GLU:HA	2.18	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:468:ASN:C	1:A:470:CYS:N	2.78	0.41
1:B:269:LEU:HD12	1:B:272:MET:SD	2.61	0.41
1:D:57:VAL:HG22	1:E:512:ILE:HD11	2.03	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:O	1:E:348:ILE:CG2	2.69	0.41
1:E:367:MET:HE3	1:E:367:MET:HB3	1.68	0.41
1:F:71:GLU:OE1	1:F:71:GLU:HA	2.19	0.41
1:F:146:ASP:OD1	1:F:149:ILE:HD12	2.21	0.41
1:A:232:ILE:O	1:A:337:LEU:HA	2.21	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: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:C:235:LEU:HD23	1:C:235:LEU:HA	1.95	0.41
1:D:63:THR:O	1:D:64:ILE:C	2.64	0.41
1:E:51:ASP:OD1	1:E:51:ASP:C	2.63	0.41
1:E:52:LEU:C	1:E:54:ASP:H	2.29	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:E:225:LYS:CG	1:E:345:GLU:HB3	2.51	0.41
1:F:133:GLU:O	1:F:137:THR:HG23	2.20	0.41
1:F:174:ILE:HD13	1:F:387:ALA:CB	2.51	0.41
1:F:342:LEU:HD23	1:F:343:VAL:N	2.35	0.41
1:F:369:ILE:O	1:F:370:ARG:HG2	2.20	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:F:506:THR:O	1:F:510:LEU:HG	2.20	0.41
1:G:49:VAL:HG12	1:G:50:ASP:N	2.36	0.41
1:G:135:LEU:CD2	1:G:411:LEU:HD22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:418:TYR:CD2	1:G:418:TYR:C	2.99	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:C:95:THR:HG22	1:C:440:ILE:HD12	2.02	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: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: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:51:ASP:C	1:C:51:ASP:OD1	2.64	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:77:MET:HA	1:G:80:GLU:CG	2.51	0.40
1:G:348:ILE:O	1:G:348:ILE:CG2	2.69	0.40
1:G:515:VAL:C	1:G:516:ILE:HG13	2.46	0.40
1:H:353:MET:HE3	1:H:353:MET:HB2	1.94	0.40
1:A:273:VAL:HG11	1:A:297:TYR:CB	2.48	0.40
1:B:65:LEU:O	1:B:66:ARG:C	2.64	0.40
1:B:348:ILE:O	1:B:348:ILE:CG2	2.70	0.40
1:B:468:ASN:C	1:B:470:CYS:N	2.78	0.40
1:C:369:ILE:O	1:C:370:ARG:HG2	2.21	0.40
1:D:25:ILE:HG23	1:D:104:LEU:HB3	2.03	0.40
1:D:41:PRO:C	1:D:43:GLY:H	2.30	0.40
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:F:266:SER:HB3	1:F:268:MET:HE3	2.04	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:266:SER:HB3	1:G:268:MET:CE	2.51	0.40
1:G:433:PHE:CD2	1:G:433:PHE:O	2.75	0.40
1:H:508:MET:HE3	1:H:508:MET:HB2	1.88	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:E:79:ILE:O	1:E:83:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:GLN:O	1:F:25:ILE:HG13	2.22	0.40
1:G:153:ILE:HG13	1:G:489:VAL:HG23	2.03	0.40
1:G:158:ILE:O	1:G:161:LYS:HB2	2.21	0.40
1:G:357:GLU:H	1:G:357:GLU:HG2	1.70	0.40
1:G:453:ILE:O	1:G:457:VAL:HG23	2.21	0.40
1:H:159:THR:HG22	1:H:160:GLY:N	2.36	0.40
1:A:189:ASP:C	1:A:191:ASP:H	2.30	0.40
1:A:225:LYS:CG	1:A:345:GLU:HB3	2.51	0.40
1:B:353:MET:HE3	1:B:353:MET:HB2	1.96	0.40
1:C:474:ASN:HD22	1:C:486:ASN:HD22	1.70	0.40
1:D:48:LEU:HG	1:E:516:ILE:HB	2.04	0.40
1:D:269:LEU:HD12	1:D:272:MET:SD	2.61	0.40
1:D:516:ILE:O	1:D:516:ILE:HG22	2.21	0.40
1:F:82:ALA:HB2	1:F:97:VAL:HG23	2.01	0.40
1:F:456:LEU:HD12	1:F:456:LEU:HA	1.87	0.40
1:H:75:ALA:C	1:H:77:MET:N	2.80	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:A:75:ALA:C	1:A:77:MET:N	2.78	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:E:353:MET:HE3	1:E:353:MET:HB2	1.96	0.40
1:F:34:THR:O	1:F:46:LYS:HE2	2.21	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:A:425:ARG:NH2	1:G:451:ASP:OD1[2_556]	2.05	0.15
1:E:465:SER:OG	1:F:176:GLU:OE2[4_445]	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:A:145:GLN:N	1:C:185:GLU:CG[4_556]	2.16	0.04
1:F:274:ALA:O	1:G:266:SER:OG[2_555]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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%)	7	36
1	B	485/521 (93%)	423 (87%)	55 (11%)	7 (1%)	9	38
1	C	485/521 (93%)	422 (87%)	56 (12%)	7 (1%)	9	38
1	D	485/521 (93%)	423 (87%)	54 (11%)	8 (2%)	7	36
1	E	485/521 (93%)	426 (88%)	52 (11%)	7 (1%)	9	38
1	F	485/521 (93%)	427 (88%)	50 (10%)	8 (2%)	7	36
1	G	485/521 (93%)	424 (87%)	54 (11%)	7 (1%)	9	38
1	H	485/521 (93%)	425 (88%)	52 (11%)	8 (2%)	7	36
All	All	3880/4168 (93%)	3394 (88%)	426 (11%)	60 (2%)	8	37

All (60) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	362 (93%)	26 (7%)	15	41
1	B	388/413 (94%)	364 (94%)	24 (6%)	16	43
1	C	388/413 (94%)	362 (93%)	26 (7%)	15	41
1	D	388/413 (94%)	359 (92%)	29 (8%)	12	37
1	E	388/413 (94%)	359 (92%)	29 (8%)	12	37
1	F	388/413 (94%)	362 (93%)	26 (7%)	15	41
1	G	388/413 (94%)	363 (94%)	25 (6%)	16	42
1	H	388/413 (94%)	363 (94%)	25 (6%)	16	42
All	All	3104/3304 (94%)	2894 (93%)	210 (7%)	14	40

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	39	LEU
1	A	48	LEU
1	A	52	LEU
1	A	134	LEU
1	A	145	GLN
1	A	153	ILE
1	A	176	GLU
1	A	185	GLU
1	A	214	VAL
1	A	218	ARG
1	A	225	LYS
1	A	240	GLU
1	A	264	THR

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Mol	Chain	Res	Type
1	A	304	VAL
1	A	307	ARG
1	A	348	ILE
1	A	373	THR
1	A	412	SER
1	A	443	THR
1	A	455	ILE
1	A	466	ASN
1	A	480	VAL
1	A	501	SER
1	A	508	MET
1	A	519	GLU
1	B	34	THR
1	B	39	LEU
1	B	48	LEU
1	B	78	LEU
1	B	86	GLU
1	B	134	LEU
1	B	176	GLU
1	B	185	GLU
1	B	214	VAL
1	B	218	ARG
1	B	225	LYS
1	B	240	GLU
1	B	264	THR
1	B	304	VAL
1	B	307	ARG
1	B	348	ILE
1	B	373	THR
1	B	412	SER
1	B	442	ARG
1	B	455	ILE
1	B	466	ASN
1	B	480	VAL
1	B	501	SER
1	B	519	GLU
1	C	34	THR
1	C	39	LEU
1	C	48	LEU
1	C	52	LEU
1	C	134	LEU
1	C	153	ILE

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Mol	Chain	Res	Type
1	C	176	GLU
1	C	185	GLU
1	C	214	VAL
1	C	218	ARG
1	C	225	LYS
1	C	231	LYS
1	C	240	GLU
1	C	264	THR
1	C	304	VAL
1	C	307	ARG
1	C	348	ILE
1	C	373	THR
1	C	412	SER
1	C	442	ARG
1	C	443	THR
1	C	455	ILE
1	C	466	ASN
1	C	480	VAL
1	C	501	SER
1	C	519	GLU
1	D	34	THR
1	D	39	LEU
1	D	48	LEU
1	D	52	LEU
1	D	55	VAL
1	D	134	LEU
1	D	153	ILE
1	D	176	GLU
1	D	185	GLU
1	D	214	VAL
1	D	218	ARG
1	D	225	LYS
1	D	231	LYS
1	D	240	GLU
1	D	264	THR
1	D	304	VAL
1	D	307	ARG
1	D	348	ILE
1	D	373	THR
1	D	380	VAL
1	D	412	SER
1	D	442	ARG

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Mol	Chain	Res	Type
1	D	443	THR
1	D	455	ILE
1	D	466	ASN
1	D	480	VAL
1	D	501	SER
1	D	508	MET
1	D	519	GLU
1	E	34	THR
1	E	39	LEU
1	E	48	LEU
1	E	52	LEU
1	E	55	VAL
1	E	86	GLU
1	E	134	LEU
1	E	138	ILE
1	E	153	ILE
1	E	176	GLU
1	E	185	GLU
1	E	214	VAL
1	E	218	ARG
1	E	225	LYS
1	E	231	LYS
1	E	240	GLU
1	E	264	THR
1	E	304	VAL
1	E	307	ARG
1	E	348	ILE
1	E	373	THR
1	E	412	SER
1	E	442	ARG
1	E	443	THR
1	E	455	ILE
1	E	466	ASN
1	E	480	VAL
1	E	501	SER
1	E	519	GLU
1	F	34	THR
1	F	39	LEU
1	F	48	LEU
1	F	52	LEU
1	F	134	LEU
1	F	153	ILE

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Mol	Chain	Res	Type
1	F	176	GLU
1	F	185	GLU
1	F	214	VAL
1	F	218	ARG
1	F	225	LYS
1	F	231	LYS
1	F	240	GLU
1	F	264	THR
1	F	304	VAL
1	F	307	ARG
1	F	348	ILE
1	F	373	THR
1	F	380	VAL
1	F	412	SER
1	F	443	THR
1	F	455	ILE
1	F	466	ASN
1	F	480	VAL
1	F	501	SER
1	F	519	GLU
1	G	34	THR
1	G	39	LEU
1	G	48	LEU
1	G	52	LEU
1	G	134	LEU
1	G	176	GLU
1	G	185	GLU
1	G	214	VAL
1	G	218	ARG
1	G	225	LYS
1	G	240	GLU
1	G	264	THR
1	G	304	VAL
1	G	307	ARG
1	G	348	ILE
1	G	373	THR
1	G	412	SER
1	G	422	ILE
1	G	442	ARG
1	G	443	THR
1	G	455	ILE
1	G	466	ASN

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Mol	Chain	Res	Type
1	G	480	VAL
1	G	501	SER
1	G	519	GLU
1	H	34	THR
1	H	39	LEU
1	H	48	LEU
1	H	52	LEU
1	H	55	VAL
1	H	78	LEU
1	H	134	LEU
1	H	155	MET
1	H	176	GLU
1	H	185	GLU
1	H	214	VAL
1	H	218	ARG
1	H	225	LYS
1	H	240	GLU
1	H	264	THR
1	H	304	VAL
1	H	307	ARG
1	H	348	ILE
1	H	373	THR
1	H	412	SER
1	H	443	THR
1	H	455	ILE
1	H	466	ASN
1	H	480	VAL
1	H	519	GLU

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

Mol	Chain	Res	Type
1	A	296	HIS
1	A	361	HIS
1	A	500	GLN
1	B	145	GLN
1	B	361	HIS
1	B	500	GLN
1	C	145	GLN
1	C	361	HIS
1	C	474	ASN
1	C	500	GLN

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Mol	Chain	Res	Type
1	D	145	GLN
1	D	361	HIS
1	D	500	GLN
1	E	145	GLN
1	E	361	HIS
1	F	145	GLN
1	F	361	HIS
1	G	145	GLN
1	G	361	HIS
1	H	145	GLN
1	H	361	HIS
1	H	500	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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	D	545	2	28,29,29	1.44	6 (21%)	43,45,45	2.18	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	G	545	2	28,29,29	1.49	5 (17%)	43,45,45	2.02	13 (30%)
4	SO4	A	546	2	4,4,4	0.29	0	6,6,6	0.22	0
4	SO4	C	546	2	4,4,4	0.26	0	6,6,6	0.23	0
4	SO4	D	546	2	4,4,4	0.31	0	6,6,6	0.36	0
4	SO4	F	546	2	4,4,4	0.22	0	6,6,6	0.27	0
3	ADP	A	545	2	28,29,29	1.51	5 (17%)	43,45,45	2.00	13 (30%)
4	SO4	H	546	2	4,4,4	0.32	0	6,6,6	0.25	0
4	SO4	G	546	2	4,4,4	0.26	0	6,6,6	0.25	0
3	ADP	F	545	2	28,29,29	1.43	6 (21%)	43,45,45	2.07	13 (30%)
3	ADP	C	545	2	28,29,29	1.40	6 (21%)	43,45,45	2.19	12 (27%)
4	SO4	E	546	2	4,4,4	0.34	0	6,6,6	0.35	0
4	SO4	B	546	2	4,4,4	0.24	0	6,6,6	0.33	0
3	ADP	E	545	2	28,29,29	1.38	6 (21%)	43,45,45	2.02	12 (27%)
3	ADP	B	545	2	28,29,29	1.49	6 (21%)	43,45,45	2.11	10 (23%)
3	ADP	H	545	2	28,29,29	1.55	5 (17%)	43,45,45	2.06	13 (30%)

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	D	545	2	-	5/16/32/32	0/3/3/3
3	ADP	G	545	2	-	5/16/32/32	0/3/3/3
3	ADP	A	545	2	-	5/16/32/32	0/3/3/3
3	ADP	F	545	2	-	5/16/32/32	0/3/3/3
3	ADP	C	545	2	-	5/16/32/32	0/3/3/3
3	ADP	E	545	2	-	5/16/32/32	0/3/3/3
3	ADP	B	545	2	-	5/16/32/32	0/3/3/3
3	ADP	H	545	2	-	5/16/32/32	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	545	ADP	C5-C4	4.47	1.47	1.39
3	H	545	ADP	C5-C4	4.37	1.46	1.39
3	B	545	ADP	C5-C4	4.19	1.46	1.39
3	E	545	ADP	C5-C4	4.11	1.46	1.39
3	A	545	ADP	C5-C4	4.08	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	545	ADP	C5-C4	3.97	1.46	1.39
3	D	545	ADP	C5-C4	3.89	1.46	1.39
3	H	545	ADP	PA-O3A	3.75	1.63	1.59
3	A	545	ADP	PA-O3A	3.40	1.63	1.59
3	C	545	ADP	C5-C4	3.39	1.45	1.39
3	C	545	ADP	C5-N7	-3.07	1.33	1.39
3	A	545	ADP	C5-N7	-3.03	1.33	1.39
3	F	545	ADP	C5-N7	-2.96	1.33	1.39
3	G	545	ADP	C5-N7	-2.88	1.33	1.39
3	B	545	ADP	C5-C6	2.79	1.48	1.41
3	F	545	ADP	PA-O3A	2.78	1.62	1.59
3	B	545	ADP	C5-N7	-2.76	1.34	1.39
3	E	545	ADP	C5-N7	-2.75	1.34	1.39
3	B	545	ADP	C4-N9	-2.72	1.32	1.37
3	D	545	ADP	C5-C6	2.61	1.48	1.41
3	D	545	ADP	C4-N9	-2.61	1.32	1.37
3	D	545	ADP	C5-N7	-2.59	1.34	1.39
3	A	545	ADP	C4-N9	-2.58	1.32	1.37
3	C	545	ADP	C4-N9	-2.57	1.32	1.37
3	H	545	ADP	C5-N7	-2.53	1.34	1.39
3	C	545	ADP	C5-C6	2.52	1.48	1.41
3	H	545	ADP	C5-C6	2.50	1.47	1.41
3	G	545	ADP	PA-O3A	2.42	1.62	1.59
3	D	545	ADP	PA-O3A	2.41	1.62	1.59
3	A	545	ADP	C8-N7	2.38	1.36	1.31
3	F	545	ADP	C4-N9	-2.35	1.32	1.37
3	G	545	ADP	C5-C6	2.35	1.47	1.41
3	G	545	ADP	C8-N7	2.29	1.36	1.31
3	C	545	ADP	C8-N9	-2.29	1.33	1.37
3	F	545	ADP	C8-N7	2.29	1.36	1.31
3	H	545	ADP	C8-N7	2.27	1.36	1.31
3	E	545	ADP	C8-N7	2.26	1.36	1.31
3	E	545	ADP	C5-C6	2.24	1.47	1.41
3	B	545	ADP	C8-N7	2.20	1.35	1.31
3	E	545	ADP	C4-N9	-2.16	1.33	1.37
3	B	545	ADP	PA-O3A	2.14	1.61	1.59
3	D	545	ADP	C8-N7	2.12	1.35	1.31
3	F	545	ADP	C5-C6	2.11	1.46	1.41
3	C	545	ADP	C8-N7	2.06	1.35	1.31
3	E	545	ADP	PA-O3A	2.00	1.61	1.59

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	545	ADP	C5-C4-N3	-6.67	117.53	126.72
3	B	545	ADP	C5-C4-N3	-6.09	118.33	126.72
3	D	545	ADP	C5-C4-N3	-6.02	118.43	126.72
3	F	545	ADP	C5-C4-N3	-5.55	119.08	126.72
3	E	545	ADP	C5-C4-N3	-5.43	119.24	126.72
3	H	545	ADP	C5-C4-N3	-5.35	119.36	126.72
3	A	545	ADP	C5-C4-N3	-5.29	119.43	126.72
3	C	545	ADP	N3-C4-N9	5.27	136.12	127.17
3	G	545	ADP	C5-C4-N3	-5.24	119.50	126.72
3	D	545	ADP	N3-C4-N9	5.22	136.04	127.17
3	B	545	ADP	N3-C4-N9	5.04	135.75	127.17
3	E	545	ADP	N3-C4-N9	4.89	135.48	127.17
3	F	545	ADP	N3-C4-N9	4.86	135.43	127.17
3	H	545	ADP	N3-C4-N9	4.84	135.40	127.17
3	G	545	ADP	N3-C4-N9	4.83	135.39	127.17
3	E	545	ADP	N3-C2-N1	-4.62	121.58	128.58
3	A	545	ADP	N3-C4-N9	4.57	134.95	127.17
3	C	545	ADP	C2-N3-C4	4.55	122.95	111.83
3	D	545	ADP	C2-N3-C4	4.32	122.39	111.83
3	G	545	ADP	N3-C2-N1	-4.31	122.06	128.58
3	A	545	ADP	N3-C2-N1	-4.27	122.11	128.58
3	H	545	ADP	N3-C2-N1	-4.19	122.24	128.58
3	E	545	ADP	C2-N3-C4	4.16	122.00	111.83
3	D	545	ADP	C4-N9-C8	4.16	110.11	105.74
3	D	545	ADP	N3-C2-N1	-4.11	122.36	128.58
3	F	545	ADP	N3-C2-N1	-4.10	122.38	128.58
3	B	545	ADP	C4-N9-C8	4.05	109.99	105.74
3	B	545	ADP	C2-N3-C4	4.05	121.72	111.83
3	C	545	ADP	N3-C2-N1	-4.01	122.51	128.58
3	A	545	ADP	C2-N3-C4	3.98	121.55	111.83
3	F	545	ADP	C2-N3-C4	3.94	121.47	111.83
3	H	545	ADP	C2-N3-C4	3.91	121.37	111.83
3	G	545	ADP	C2-N3-C4	3.87	121.28	111.83
3	F	545	ADP	C4-N9-C8	3.86	109.79	105.74
3	H	545	ADP	C4-N9-C8	3.81	109.73	105.74
3	C	545	ADP	C4-C5-N7	-3.65	106.40	110.58
3	B	545	ADP	C4-C5-N7	-3.61	106.45	110.58
3	B	545	ADP	N3-C2-N1	-3.56	123.20	128.58
3	E	545	ADP	C4-N9-C8	3.53	109.45	105.74
3	C	545	ADP	C4-N9-C8	3.49	109.40	105.74
3	H	545	ADP	O3'-C3'-C2'	-3.48	100.67	111.82
3	G	545	ADP	C4-N9-C8	3.47	109.38	105.74
3	D	545	ADP	O3'-C3'-C2'	-3.42	100.87	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	545	ADP	O2'-C2'-C3'	-3.37	101.02	111.82
3	A	545	ADP	O3'-C3'-C2'	-3.36	101.03	111.82
3	A	545	ADP	C4-N9-C8	3.23	109.13	105.74
3	B	545	ADP	N9-C8-N7	-3.23	109.36	113.94
3	D	545	ADP	C4-C5-N7	-3.08	107.06	110.58
3	B	545	ADP	C5-N7-C8	3.07	108.28	103.45
3	D	545	ADP	N9-C8-N7	-3.06	109.59	113.94
3	F	545	ADP	O3'-C3'-C2'	-3.05	102.03	111.82
3	C	545	ADP	N9-C8-N7	-3.03	109.64	113.94
3	C	545	ADP	C5-N7-C8	3.02	108.20	103.45
3	F	545	ADP	N9-C8-N7	-3.02	109.65	113.94
3	G	545	ADP	O3'-C3'-C2'	-2.99	102.23	111.82
3	H	545	ADP	N9-C8-N7	-2.96	109.73	113.94
3	B	545	ADP	O3'-C3'-C2'	-2.95	102.35	111.82
3	B	545	ADP	O2'-C2'-C3'	-2.93	102.41	111.82
3	C	545	ADP	O2'-C2'-C3'	-2.88	102.59	111.82
3	F	545	ADP	C4-C5-N7	-2.88	107.29	110.58
3	C	545	ADP	O3'-C3'-C2'	-2.84	102.73	111.82
3	F	545	ADP	O2'-C2'-C3'	-2.79	102.86	111.82
3	H	545	ADP	C5-N7-C8	2.77	107.80	103.45
3	F	545	ADP	C5-N7-C8	2.75	107.78	103.45
3	D	545	ADP	C5-N7-C8	2.71	107.71	103.45
3	H	545	ADP	C4-C5-N7	-2.71	107.48	110.58
3	E	545	ADP	N9-C8-N7	-2.69	110.12	113.94
3	G	545	ADP	N9-C8-N7	-2.65	110.17	113.94
3	D	545	ADP	C2'-C3'-C4'	2.62	107.67	102.61
3	H	545	ADP	C2'-C3'-C4'	2.62	107.66	102.61
3	D	545	ADP	O2'-C2'-C3'	-2.61	103.44	111.82
3	A	545	ADP	C2'-C3'-C4'	2.59	107.62	102.61
3	G	545	ADP	C2'-C3'-C4'	2.58	107.59	102.61
3	E	545	ADP	O2'-C2'-C3'	-2.57	103.58	111.82
3	G	545	ADP	C5-N7-C8	2.53	107.43	103.45
3	E	545	ADP	O3'-C3'-C2'	-2.49	103.84	111.82
3	A	545	ADP	N9-C8-N7	-2.48	110.41	113.94
3	E	545	ADP	C2-N1-C6	2.41	122.68	118.73
3	G	545	ADP	O2A-PA-O1A	2.39	123.55	112.44
3	E	545	ADP	C5-N7-C8	2.38	107.19	103.45
3	G	545	ADP	O2'-C2'-C3'	-2.36	104.24	111.82
3	H	545	ADP	O2A-PA-O1A	2.35	123.38	112.44
3	G	545	ADP	C4-C5-N7	-2.34	107.91	110.58
3	A	545	ADP	N6-C6-N1	2.31	123.53	118.38
3	E	545	ADP	C4-C5-N7	-2.29	107.97	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	545	ADP	O2'-C2'-C3'	-2.28	104.51	111.82
3	H	545	ADP	C2-N1-C6	2.28	122.47	118.73
3	E	545	ADP	C2'-C3'-C4'	2.24	106.93	102.61
3	A	545	ADP	C4-C5-N7	-2.23	108.03	110.58
3	C	545	ADP	C2'-C3'-C4'	2.21	106.87	102.61
3	A	545	ADP	C2-N1-C6	2.20	122.34	118.73
3	A	545	ADP	C5-N7-C8	2.13	106.80	103.45
3	F	545	ADP	C2'-C3'-C4'	2.11	106.69	102.61
3	G	545	ADP	C2-N1-C6	2.10	122.18	118.73
3	C	545	ADP	O2A-PA-O1A	2.09	122.15	112.44
3	F	545	ADP	O2A-PA-O1A	2.07	122.10	112.44
3	F	545	ADP	C2-N1-C6	2.04	122.08	118.73
3	D	545	ADP	O2A-PA-O1A	2.01	121.79	112.44

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	545	ADP	C5'-O5'-PA-O1A
3	A	545	ADP	C5'-O5'-PA-O2A
3	A	545	ADP	C5'-O5'-PA-O3A
3	B	545	ADP	C5'-O5'-PA-O1A
3	B	545	ADP	C5'-O5'-PA-O2A
3	B	545	ADP	C5'-O5'-PA-O3A
3	C	545	ADP	C5'-O5'-PA-O1A
3	C	545	ADP	C5'-O5'-PA-O2A
3	C	545	ADP	C5'-O5'-PA-O3A
3	D	545	ADP	C5'-O5'-PA-O1A
3	D	545	ADP	C5'-O5'-PA-O2A
3	D	545	ADP	C5'-O5'-PA-O3A
3	E	545	ADP	C5'-O5'-PA-O1A
3	E	545	ADP	C5'-O5'-PA-O2A
3	E	545	ADP	C5'-O5'-PA-O3A
3	F	545	ADP	C5'-O5'-PA-O1A
3	F	545	ADP	C5'-O5'-PA-O2A
3	F	545	ADP	C5'-O5'-PA-O3A
3	G	545	ADP	C5'-O5'-PA-O1A
3	G	545	ADP	C5'-O5'-PA-O2A
3	G	545	ADP	C5'-O5'-PA-O3A
3	H	545	ADP	C5'-O5'-PA-O1A
3	H	545	ADP	C5'-O5'-PA-O2A
3	H	545	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	A	545	ADP	C3'-C4'-C5'-O5'
3	B	545	ADP	C3'-C4'-C5'-O5'
3	C	545	ADP	C3'-C4'-C5'-O5'
3	D	545	ADP	C3'-C4'-C5'-O5'
3	E	545	ADP	C3'-C4'-C5'-O5'
3	F	545	ADP	C3'-C4'-C5'-O5'
3	G	545	ADP	C3'-C4'-C5'-O5'
3	H	545	ADP	C3'-C4'-C5'-O5'
3	C	545	ADP	O4'-C4'-C5'-O5'
3	E	545	ADP	O4'-C4'-C5'-O5'
3	A	545	ADP	O4'-C4'-C5'-O5'
3	B	545	ADP	O4'-C4'-C5'-O5'
3	D	545	ADP	O4'-C4'-C5'-O5'
3	F	545	ADP	O4'-C4'-C5'-O5'
3	G	545	ADP	O4'-C4'-C5'-O5'
3	H	545	ADP	O4'-C4'-C5'-O5'

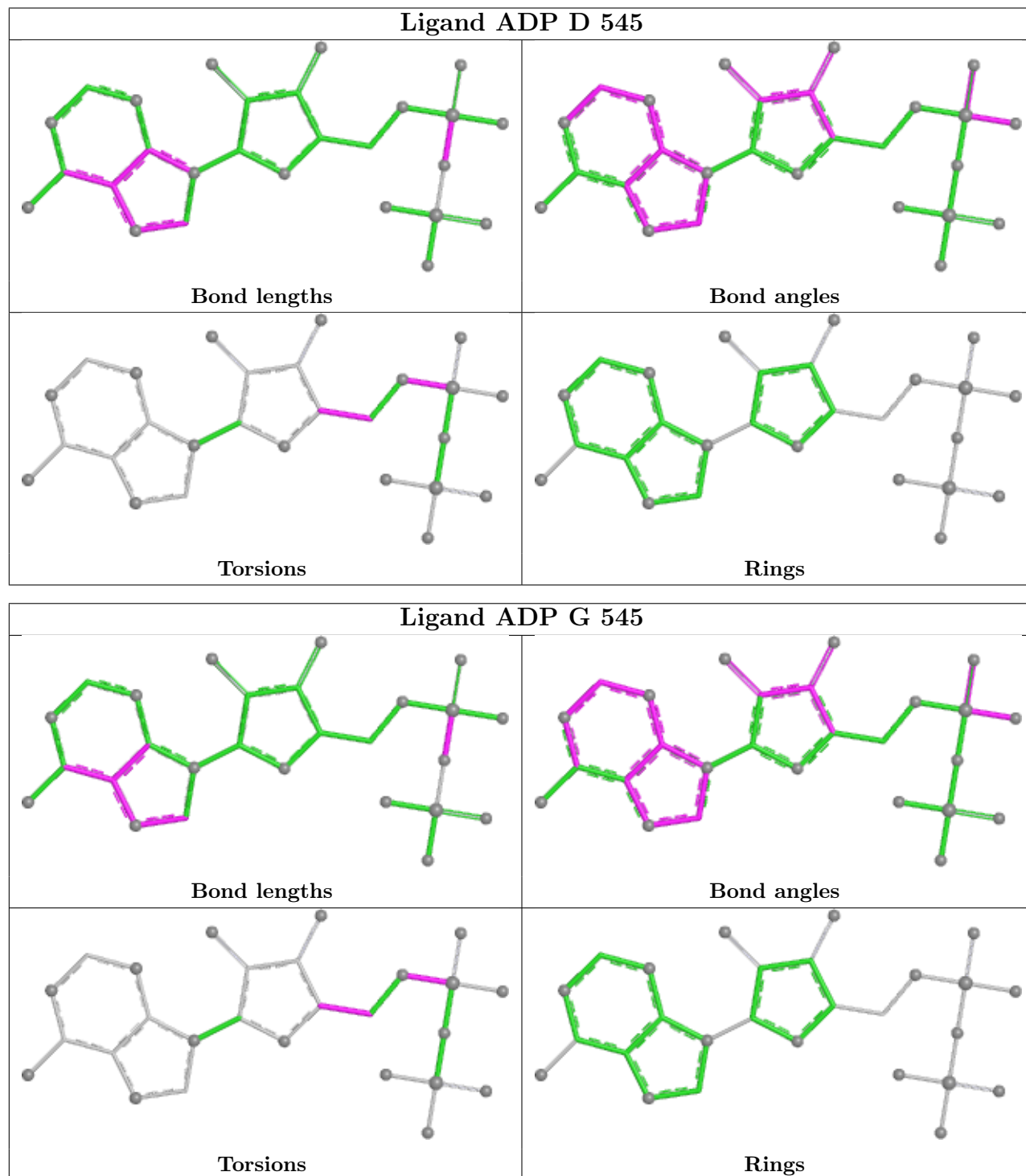
There are no ring outliers.

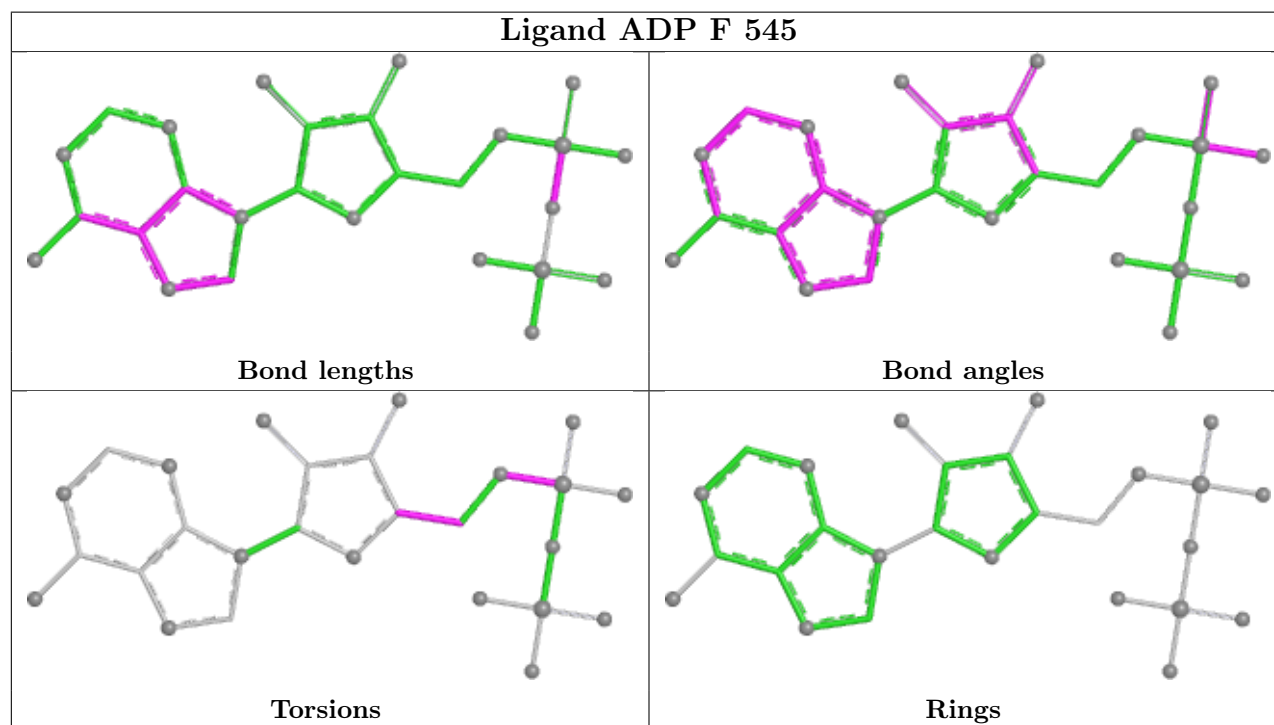
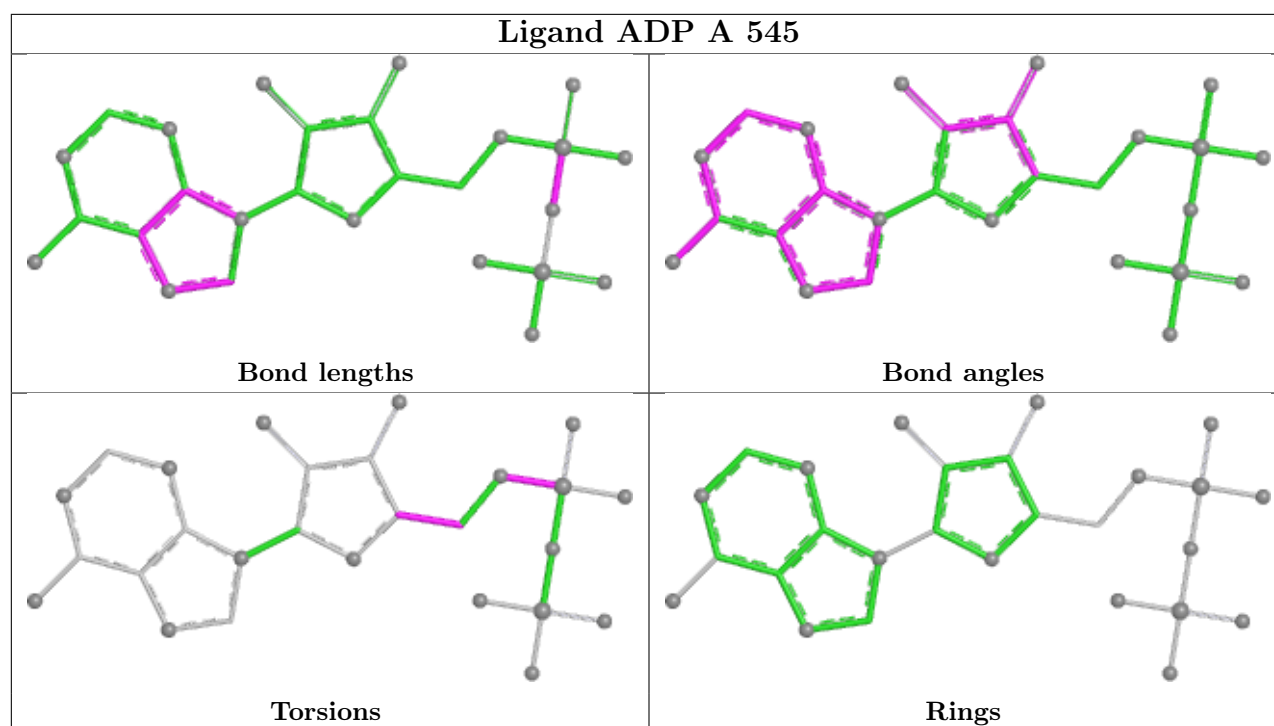
16 monomers are involved in 48 short contacts:

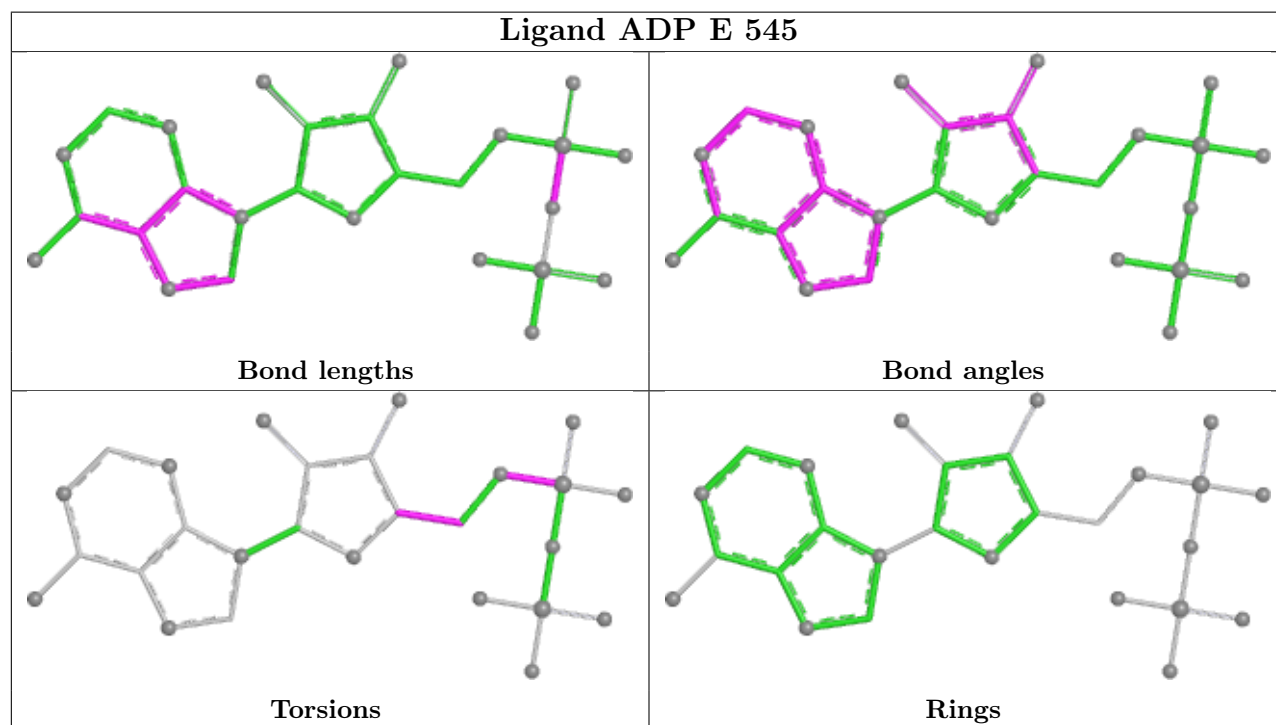
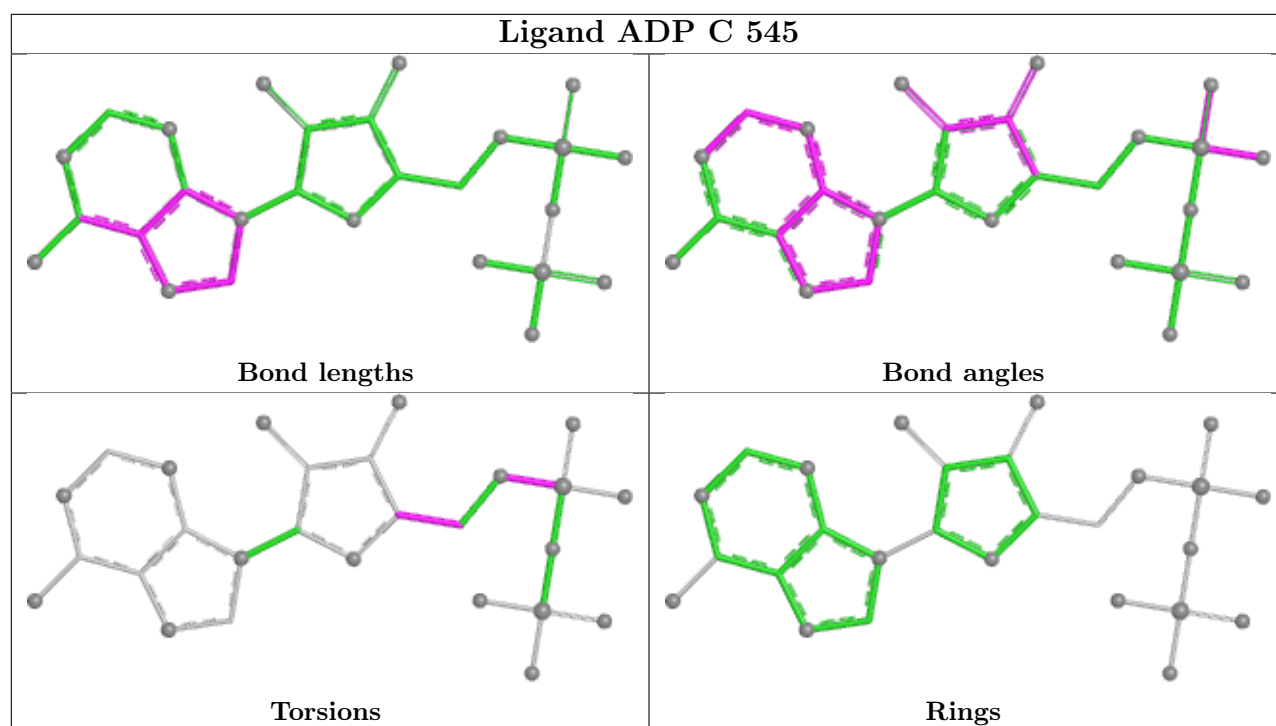
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	545	ADP	6	0
3	G	545	ADP	6	0
4	A	546	SO4	3	0
4	C	546	SO4	5	0
4	D	546	SO4	4	0
4	F	546	SO4	4	0
3	A	545	ADP	5	0
4	H	546	SO4	4	0
4	G	546	SO4	4	0
3	F	545	ADP	6	0
3	C	545	ADP	7	0
4	E	546	SO4	4	0
4	B	546	SO4	4	0
3	E	545	ADP	6	0
3	B	545	ADP	6	0
3	H	545	ADP	6	0

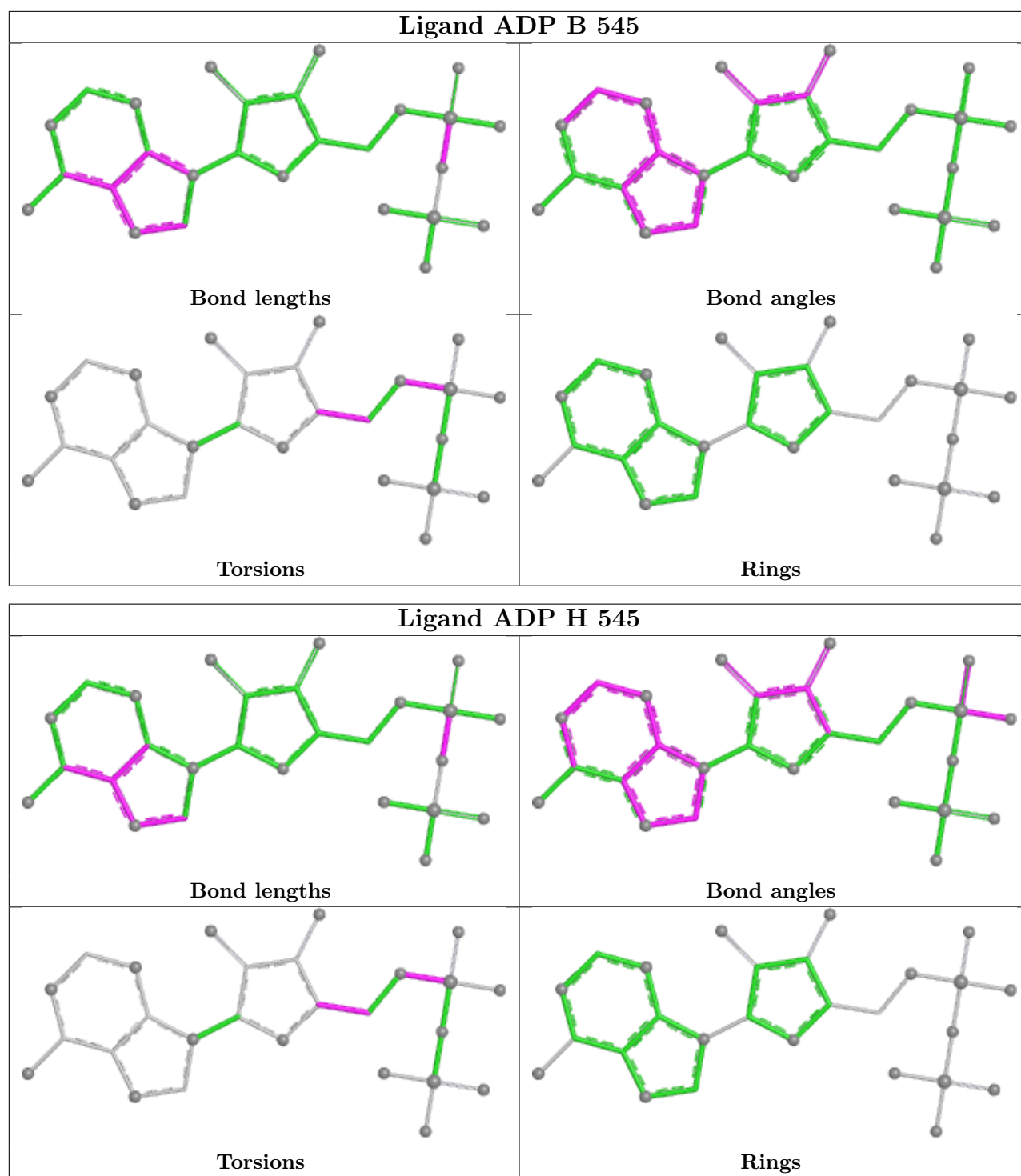
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	487/521 (93%)	-0.09	1 (0%) 91 82	26, 88, 242, 287	0
1	B	487/521 (93%)	-0.15	1 (0%) 91 82	38, 90, 196, 247	0
1	C	487/521 (93%)	-0.10	3 (0%) 85 65	39, 88, 282, 341	0
1	D	487/521 (93%)	-0.08	3 (0%) 85 65	42, 103, 243, 287	0
1	E	487/521 (93%)	0.02	7 (1%) 73 48	34, 94, 252, 294	0
1	F	487/521 (93%)	0.01	5 (1%) 79 56	41, 100, 258, 295	0
1	G	487/521 (93%)	0.02	5 (1%) 79 56	41, 122, 245, 291	0
1	H	487/521 (93%)	0.07	5 (1%) 79 56	64, 127, 229, 274	0
All	All	3896/4168 (93%)	-0.04	30 (0%) 82 60	26, 102, 250, 341	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	343	VAL	5.0
1	H	53	GLY	4.2
1	G	239	ILE	4.1
1	E	232	ILE	4.1
1	E	298	LEU	3.8
1	H	178	VAL	3.7
1	E	303	ILE	3.6
1	C	343	VAL	3.5
1	E	276	ILE	3.5
1	F	285	PHE	3.2
1	H	348	ILE	3.1
1	H	118	THR	3.0
1	C	53	GLY	2.9
1	G	49	VAL	2.9
1	G	380	VAL	2.6
1	G	343	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	285	PHE	2.4
1	H	49	VAL	2.4
1	D	329	ILE	2.3
1	D	348	ILE	2.3
1	G	163	ALA	2.3
1	E	283	VAL	2.3
1	F	296	HIS	2.2
1	F	232	ILE	2.2
1	F	317	LEU	2.1
1	C	303	ILE	2.1
1	A	276	ILE	2.1
1	B	225	LYS	2.1
1	F	276	ILE	2.0
1	D	267	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	G	544	1/1	0.89	0.12	111,111,111,111	0
2	MG	B	544	1/1	0.93	0.18	58,58,58,58	0
3	ADP	H	545	27/27	0.93	0.10	72,100,114,124	0
2	MG	C	544	1/1	0.94	0.10	57,57,57,57	0
3	ADP	E	545	27/27	0.95	0.09	49,70,86,98	0
3	ADP	G	545	27/27	0.95	0.08	71,99,116,122	0
2	MG	H	544	1/1	0.95	0.10	111,111,111,111	0
4	SO4	B	546	5/5	0.95	0.08	59,71,88,107	0
4	SO4	E	546	5/5	0.95	0.07	65,72,99,100	0

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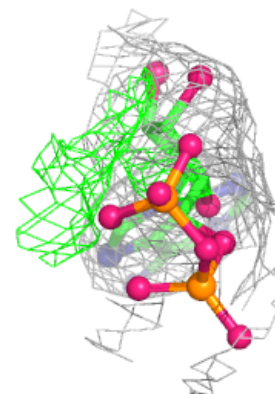
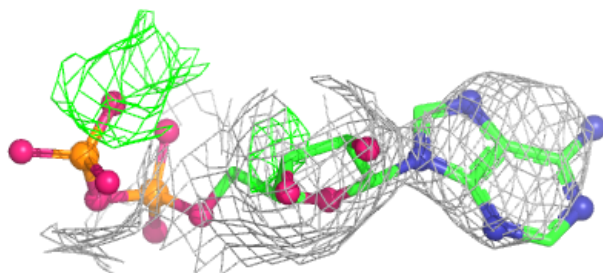
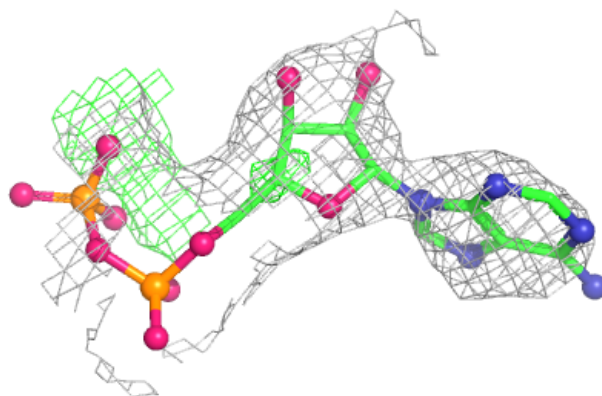
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	H	546	5/5	0.95	0.05	96,104,122,137	0
2	MG	E	544	1/1	0.96	0.06	55,55,55,55	0
3	ADP	A	545	27/27	0.96	0.08	38,59,78,83	0
4	SO4	A	546	5/5	0.96	0.06	76,81,105,106	0
3	ADP	B	545	27/27	0.96	0.09	47,65,83,90	0
4	SO4	C	546	5/5	0.96	0.08	71,78,107,110	0
4	SO4	D	546	5/5	0.96	0.06	66,71,89,100	0
3	ADP	C	545	27/27	0.96	0.07	46,68,88,95	0
2	MG	D	544	1/1	0.96	0.10	92,92,92,92	0
2	MG	A	544	1/1	0.97	0.05	65,65,65,65	0
3	ADP	D	545	27/27	0.97	0.08	66,89,104,118	0
2	MG	F	544	1/1	0.97	0.08	83,83,83,83	0
4	SO4	F	546	5/5	0.97	0.08	100,101,134,137	0
4	SO4	G	546	5/5	0.97	0.06	75,90,123,124	0
3	ADP	F	545	27/27	0.97	0.07	45,69,88,95	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

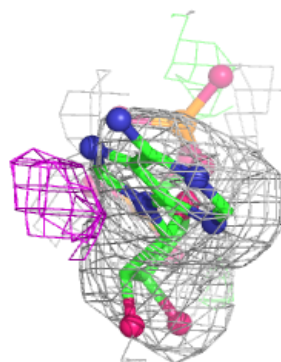
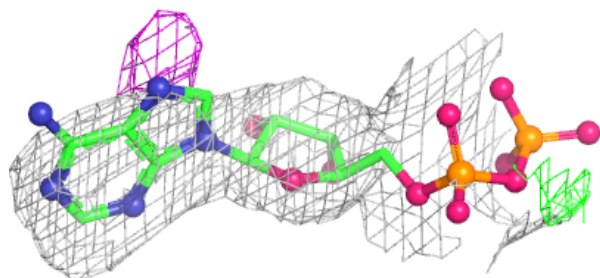
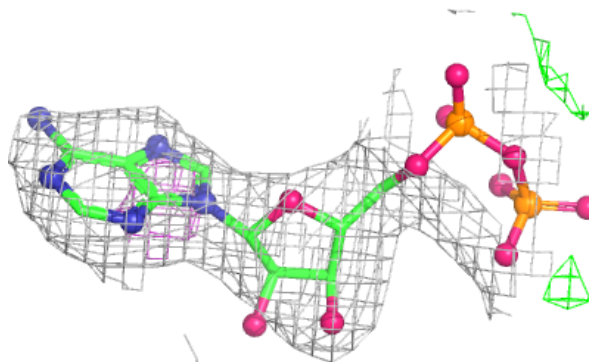
Electron density around ADP H 545:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

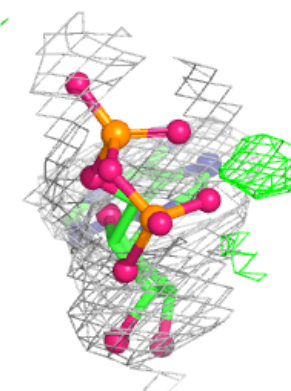
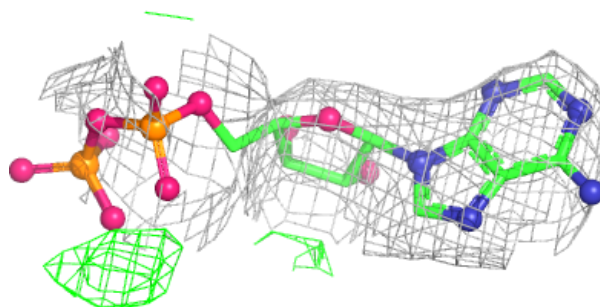
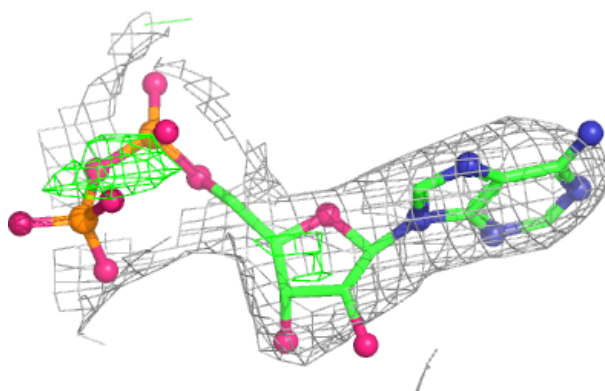


Electron density around ADP E 545:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

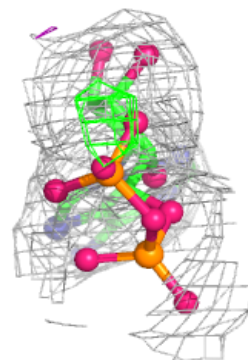
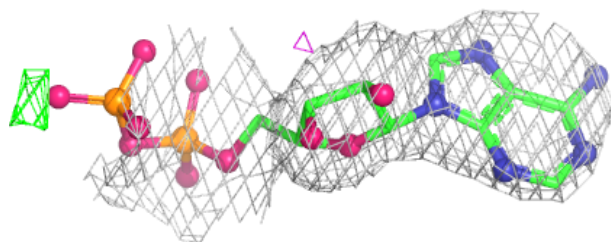
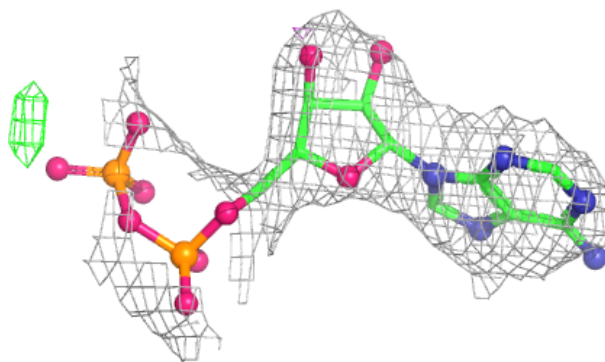
**Electron density around ADP G 545:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

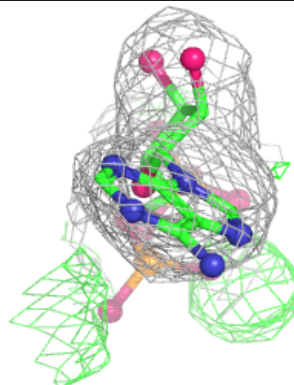
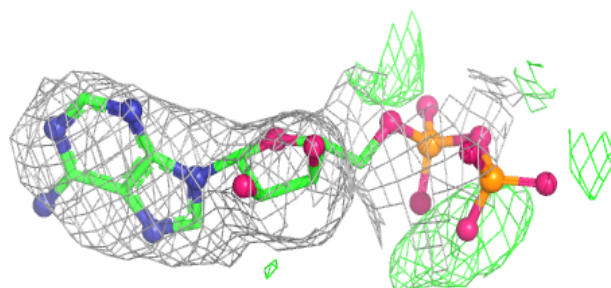
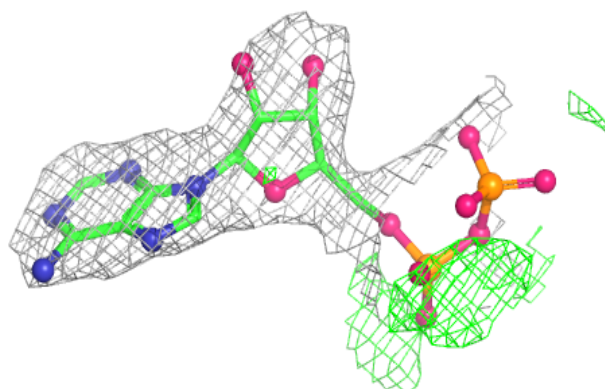


Electron density around ADP A 545:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

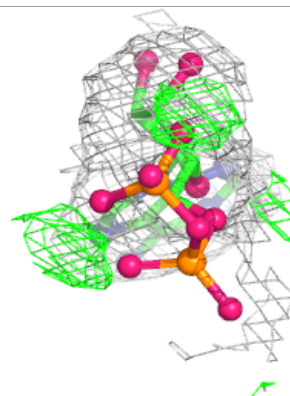
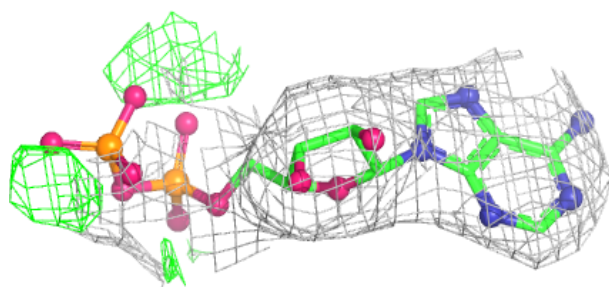
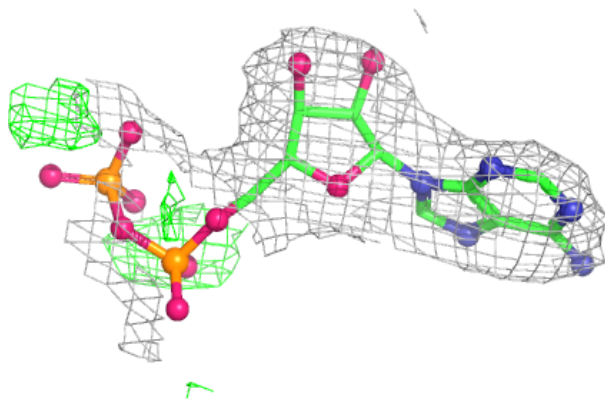
**Electron density around ADP B 545:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

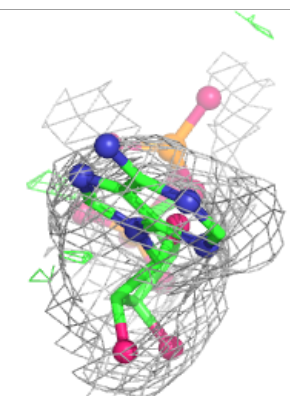
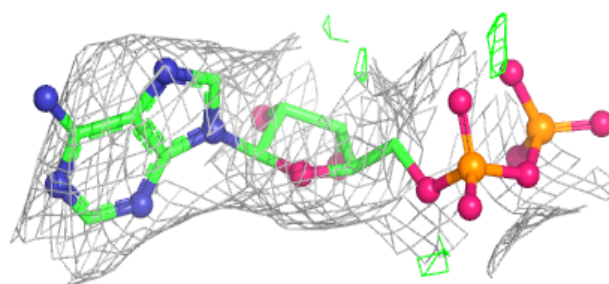
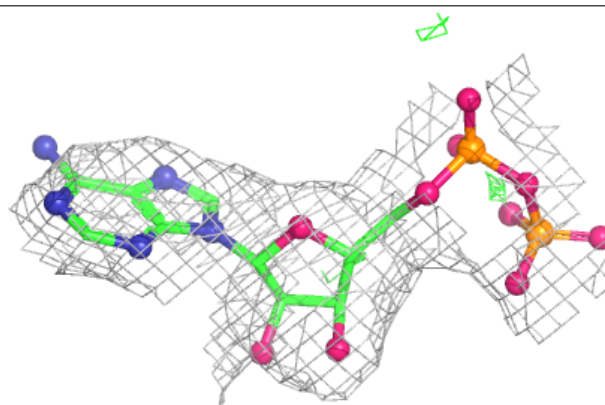


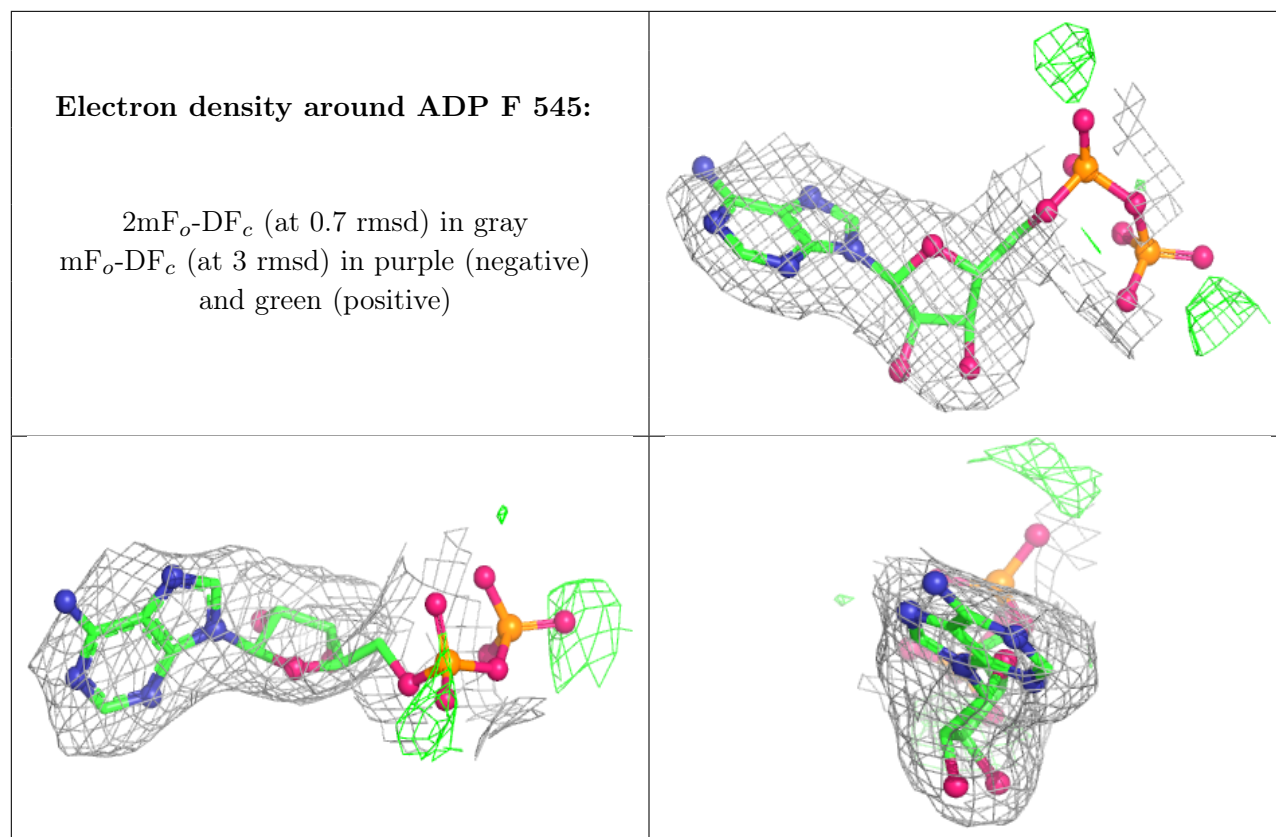
Electron density around ADP C 545:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP D 545:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.