Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 11:16 PM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

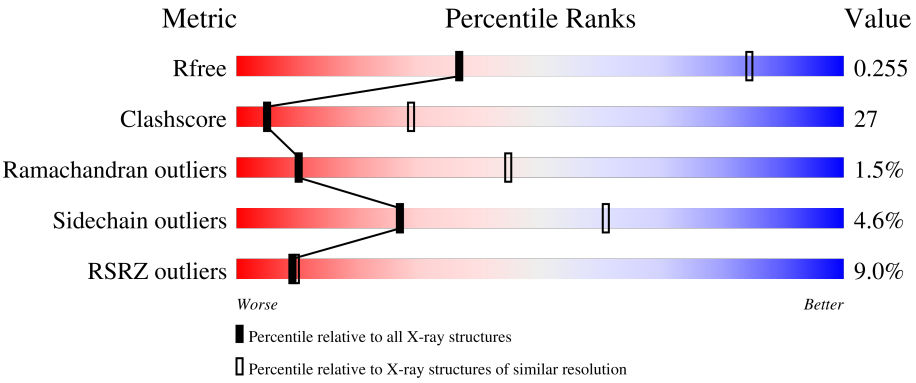
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	8% 51% 39% • 7%
1	B	521	3% 51% 39% • 7%
1	C	521	8% 51% 40% • 7%
1	D	521	10% 51% 39% • 7%
1	E	521	11% 50% 40% • 7%

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Mol	Chain	Length	Quality of chain
1	F	521	11% 51% 39% 7%
1	G	521	9% 50% 40% 7%
1	H	521	7% 50% 40% 7%

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 (i)

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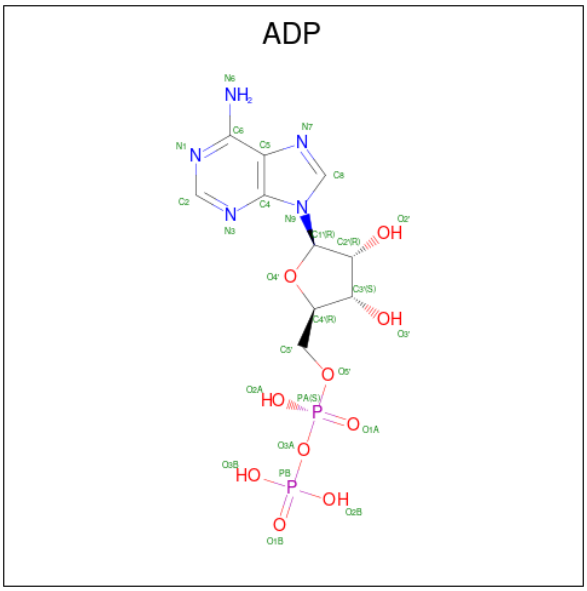
Chain	Residue	Modelled	Actual	Comment	Reference
H	265	ALA	GLU	engineered mutation	UNP Q877G8
H	266	SER	GLU	engineered mutation	UNP Q877G8
H	267	GLU	LYS	engineered mutation	UNP Q877G8

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

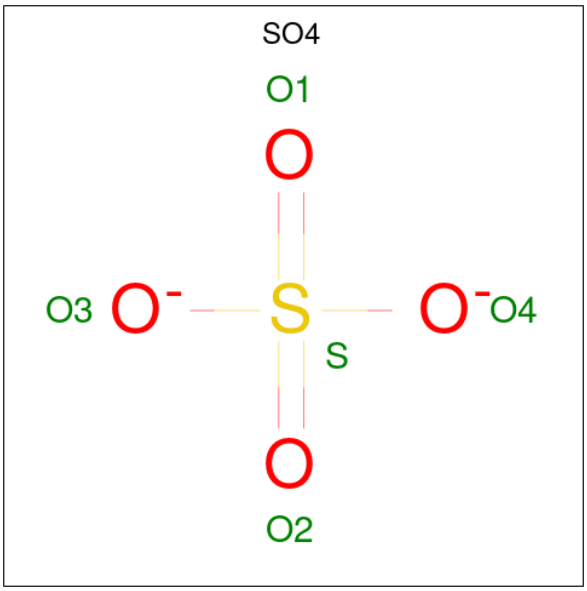
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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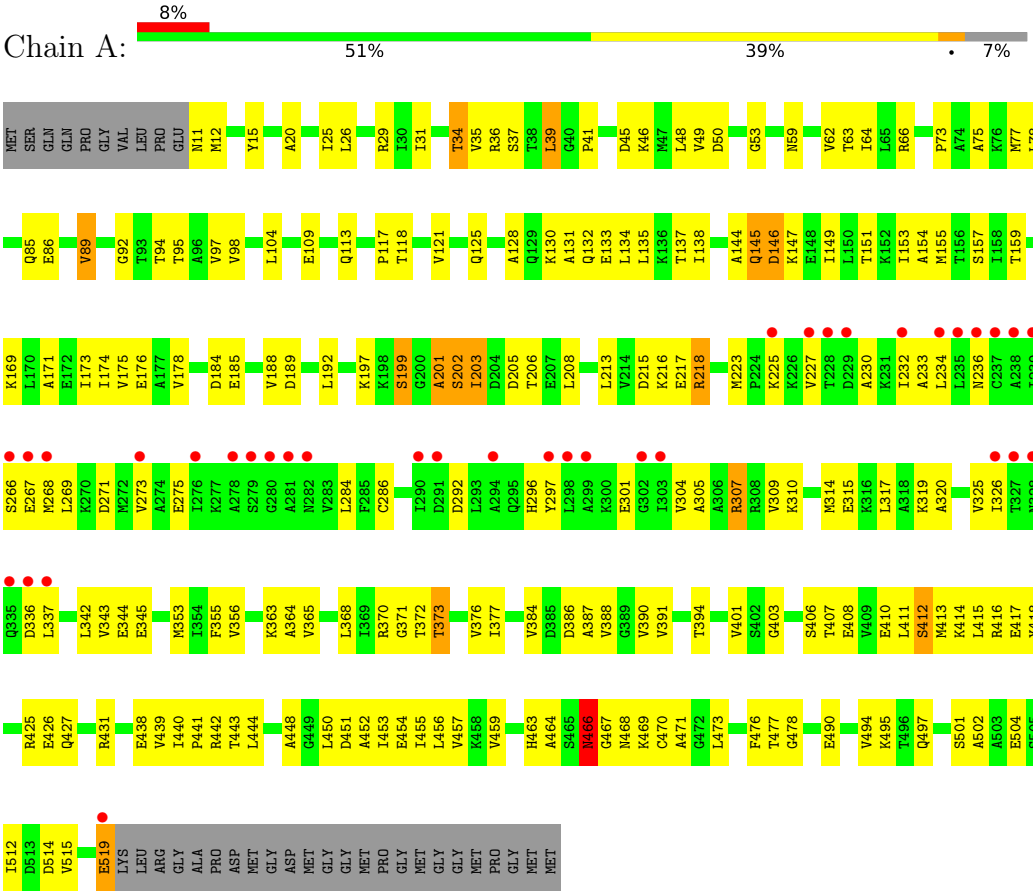
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

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.

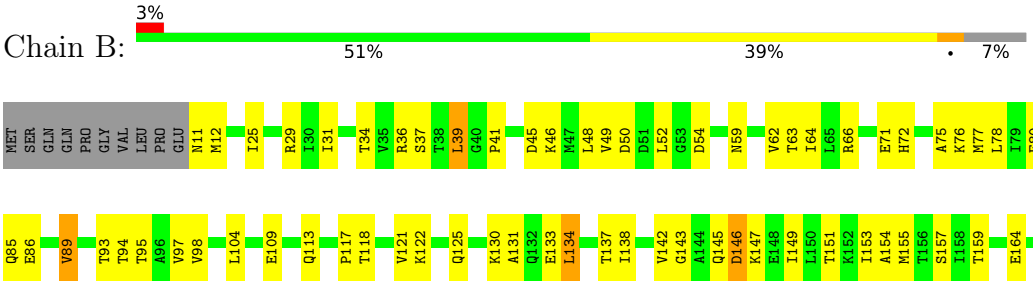
• Molecule 1: Chaperonin

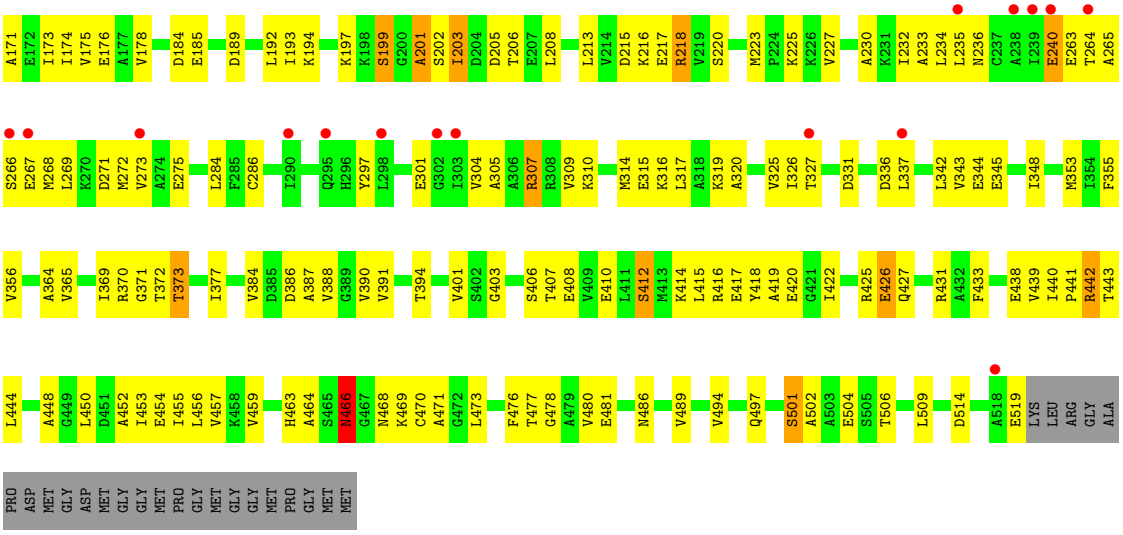
Chain A:



• Molecule 1: Chaperonin

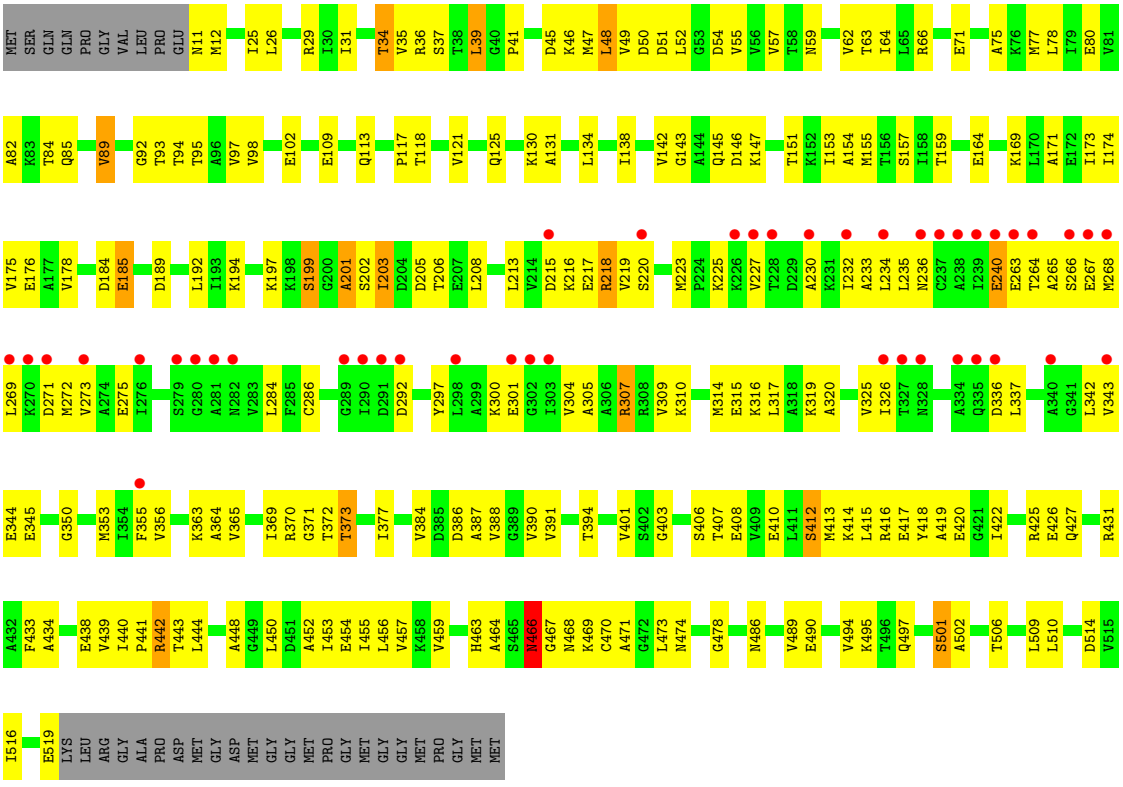
Chain B:





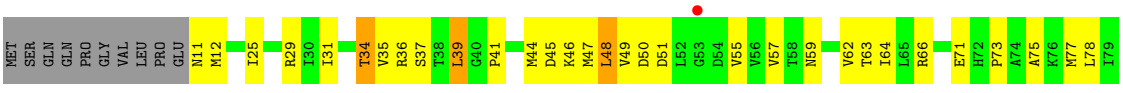
• Molecule 1: Chaperonin

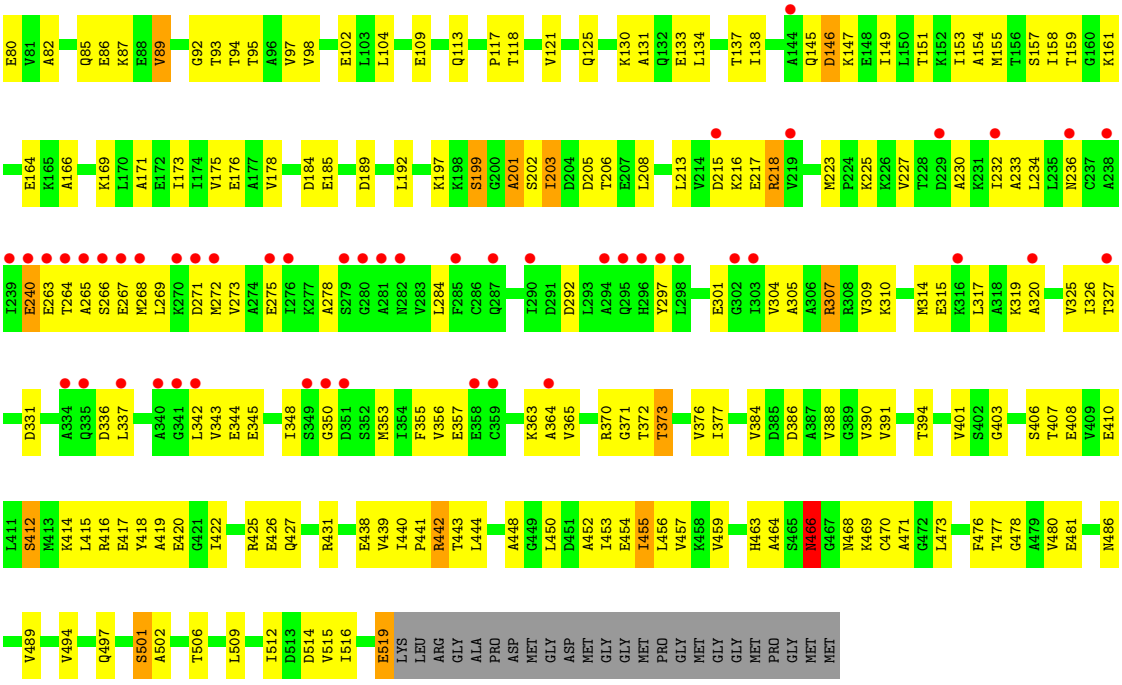
Chain C:



• Molecule 1: Chaperonin

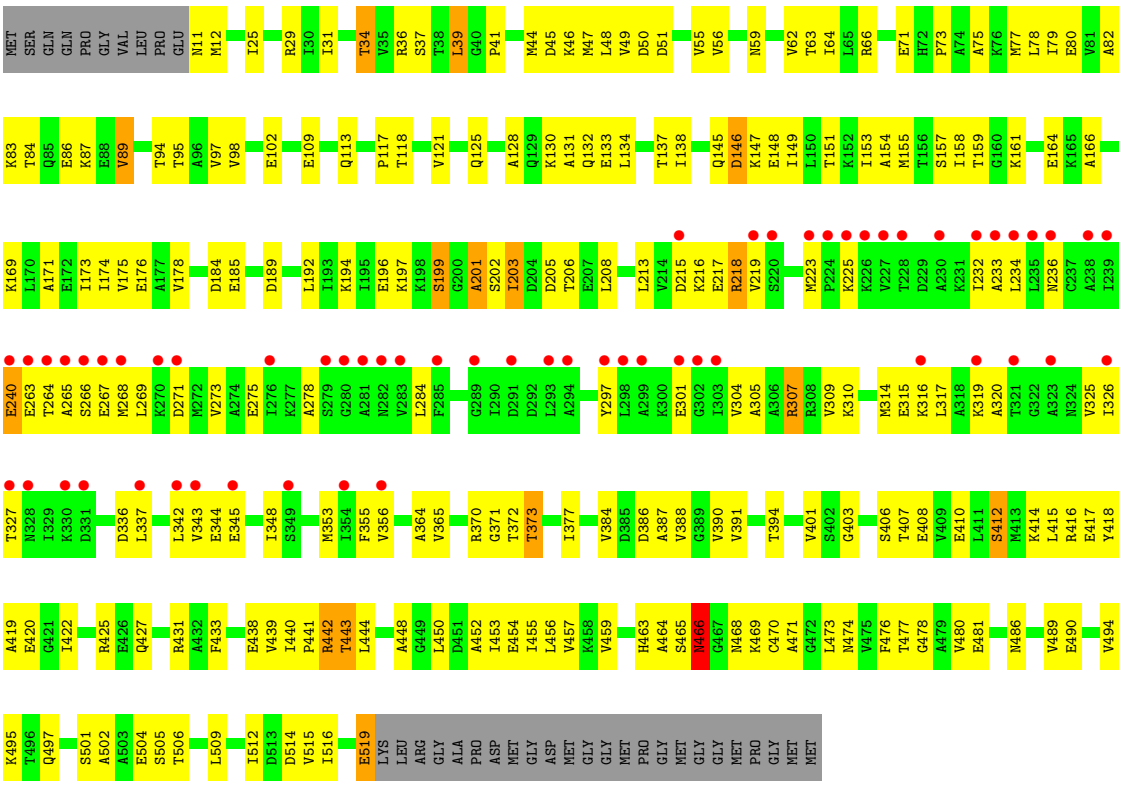
Chain D:





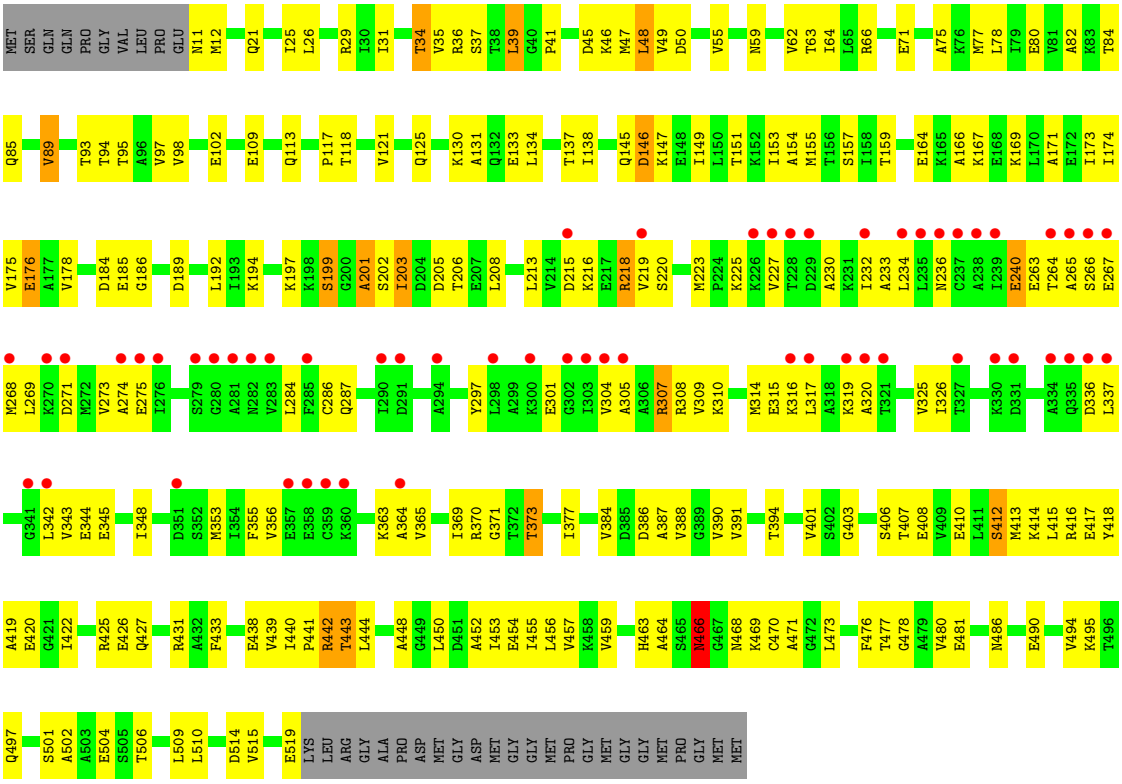
• Molecule 1: Chaperonin

Chain E:



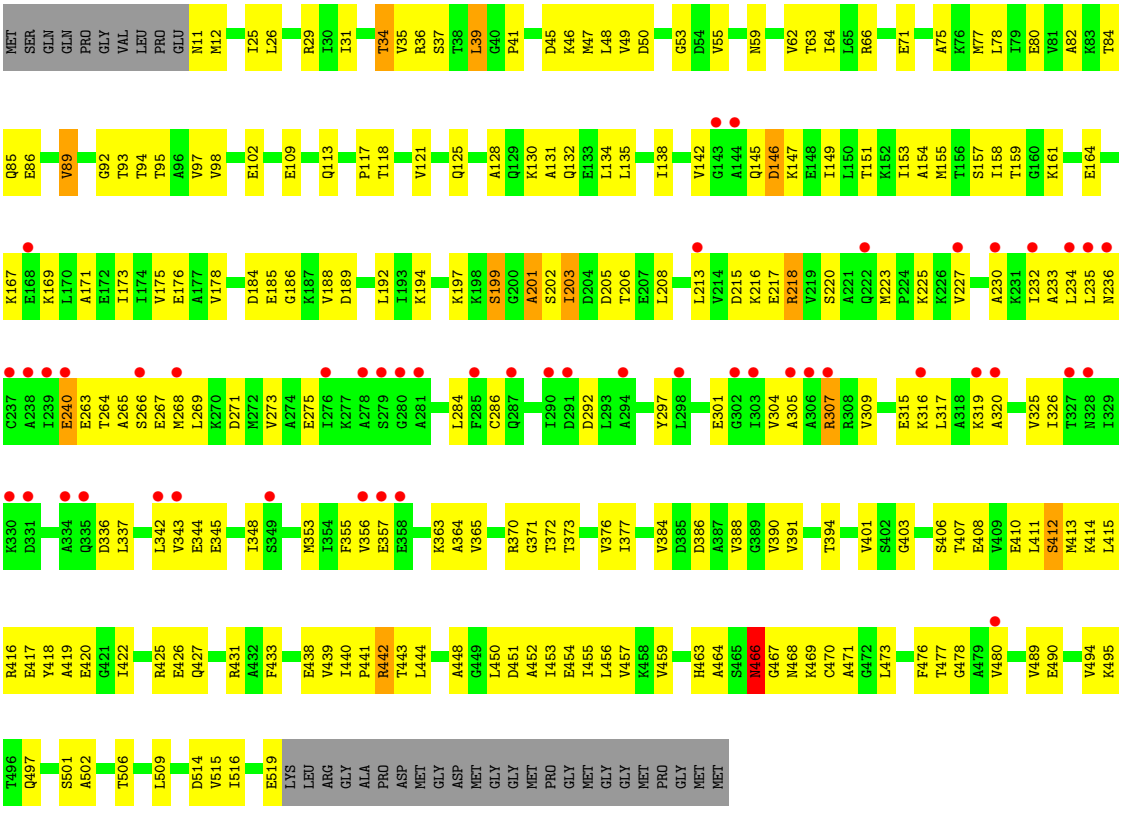
• Molecule 1: Chaperonin

Chain F:



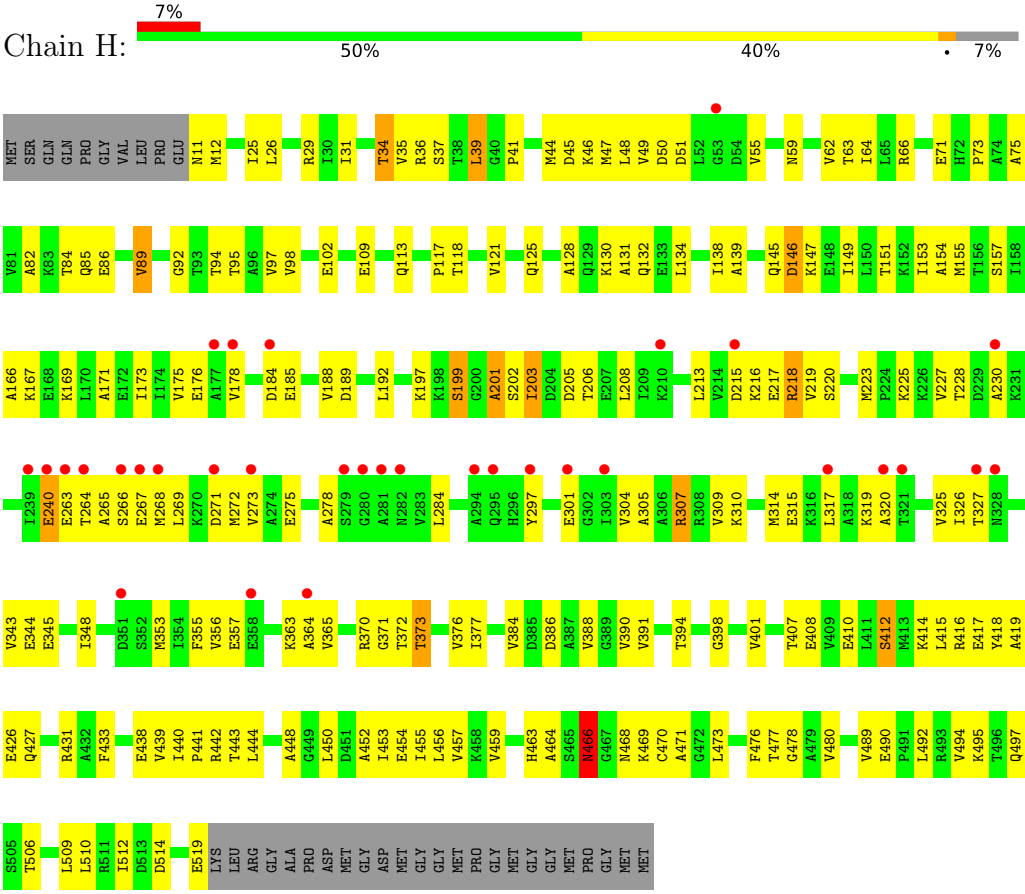
• Molecule 1: Chaperonin

Chain G:



• Molecule 1: Chaperonin

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.45Å 161.92Å 147.37Å 90.00° 124.12° 90.00°	Depositor
Resolution (Å)	54.49 – 3.50 54.49 – 3.50	Depositor EDS
% Data completeness (in resolution range)	77.1 (54.49-3.50) 86.5 (54.49-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.232 , 0.269 0.225 , 0.255	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)	0.30 , 77.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.053 for -h-2*l,-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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	0/3649	0.64	0/4911
1	B	0.50	1/3649 (0.0%)	0.63	0/4911
1	C	0.50	0/3649	0.63	0/4911
1	D	0.48	0/3649	0.62	0/4911
1	E	0.50	0/3649	0.63	0/4911
1	F	0.48	0/3649	0.62	0/4911
1	G	0.46	0/3649	0.62	0/4911
1	H	0.45	0/3649	0.62	0/4911
All	All	0.48	1/29192 (0.0%)	0.63	0/39288

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

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

All (1) bond length outliers are listed below:

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

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3629	0	3762	198	5
1	B	3629	0	3762	202	1
1	C	3629	0	3762	217	3
1	D	3629	0	3762	232	0
1	E	3629	0	3762	221	3
1	F	3629	0	3762	199	3
1	G	3629	0	3762	206	4
1	H	3629	0	3762	212	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	12	5	0
3	B	27	0	12	6	0
3	C	27	0	12	7	0
3	D	27	0	12	6	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (1616) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:LEU:HD23	1:H:444:LEU:CD2	1.71	1.21
1:G:39:LEU:HD23	1:G:444:LEU:CD2	1.73	1.18
1:D:39:LEU:HD23	1:D:444:LEU:CD2	1.74	1.17
1:F:39:LEU:HD23	1:F:444:LEU:CD2	1.71	1.17
1:C:39:LEU:HD23	1:C:444:LEU:CD2	1.74	1.16
1:E:39:LEU:HD23	1:E:444:LEU:CD2	1.76	1.16
1:A:39:LEU:HD23	1:A:444:LEU:CD2	1.76	1.16
1:B:39:LEU:HD23	1:B:444:LEU:CD2	1.73	1.15
1:C:206:THR:HG22	1:C:370:ARG:H	1.09	1.11
1: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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:LYS:HG3	1:F:134:LEU:HD12	1.60	0.82
1:G:218:ARG:HG3	1:G:345:GLU:OE1	1.79	0.82
1:H:218:ARG:NH2	1:H:223:MET:O	2.12	0.82
1:D:51:ASP:HB2	1:E:519:GLU:HB2	1.61	0.82
1:H:31:ILE:HD13	1:H:75:ALA:HB1	1.61	0.82
1:B:31:ILE:HD13	1:B:75:ALA:HB1	1.62	0.82
1:D:31:ILE:HD13	1:D:75:ALA:HB1	1.60	0.82
1:H:46:LYS:HG3	1:H:64:ILE:HD13	1.60	0.82
1:E:268:MET:O	1:E:269:LEU:HD13	1.80	0.81
1:B:218:ARG:HG3	1:B:345:GLU:OE1	1.81	0.81
1:C:373:THR:HB	1:D:80:GLU:HB3	1.63	0.81
1:E:39:LEU:CD2	1:E:444:LEU:HD21	2.10	0.81
1:H:218:ARG:HG3	1:H:345:GLU:OE1	1.81	0.81
1:B:439:VAL:O	1:B:443:THR:HG23	1.81	0.81
1:F:46:LYS:HG3	1:F:64:ILE:HD13	1.60	0.81
1:C:268:MET:O	1:C:269:LEU:HD13	1.80	0.81
1:D:263:GLU:HA	1:D:269:LEU:HD21	1.62	0.81
1:F:263:GLU:HA	1:F:269:LEU:HD21	1.62	0.81
1:C:46:LYS:HG3	1:C:64:ILE:HD13	1.60	0.81
1:F: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
1:E:31:ILE:HD13	1:E:75:ALA:HB1	1.62	0.80
1:H:439:VAL:O	1:H:443:THR:HG23	1.81	0.80
1:F:199:SER:HA	1:F:377:ILE:HD11	1.63	0.80
1:A:130:LYS:HG3	1:A:134:LEU:HD12	1.63	0.80
1:E:218:ARG:CG	1:E:345:GLU:OE1	2.29	0.80
1:A:263:GLU:HA	1:A:269:LEU:HD21	1.62	0.80
1:H:455:ILE:HG21	1:H:473:LEU:HD22	1.64	0.80
1:B:11:ASN:HA	1:B:12:MET:CG	2.12	0.80
1:C:218:ARG:NH2	1:C:223:MET:O	2.13	0.80
1:F:218:ARG:HG3	1:F:345:GLU:OE1	1.81	0.80
1:A:218:ARG:CG	1:A:345:GLU:OE1	2.30	0.80
1:C:11:ASN:HA	1:C:12:MET:CG	2.11	0.79
1:D:164:GLU:HB2	1:E:125:GLN:OE1	1.82	0.79
1:E:46:LYS:HD3	1:F:514:ASP:HB3	1.63	0.79
1:H:263:GLU:HA	1:H:269:LEU:HD21	1.64	0.79
1:F:201:ALA:HB2	1:G:497:GLN:OE1	1.82	0.79
1:B:468:ASN:HB2	1:B:471:ALA:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:GLU:HA	1:C:269:LEU:HD21	1.64	0.79
1:D:11:ASN:HA	1:D:12:MET:CG	2.13	0.79
1:D:199:SER:HA	1:D:377:ILE:HD11	1.65	0.79
1:A:455:ILE:HG21	1:A:473:LEU:HD22	1.64	0.79
1:F:11:ASN:HA	1:F:12:MET:CG	2.12	0.79
1:E:201:ALA:HB2	1:F:497:GLN:OE1	1.83	0.79
1:C:468:ASN:HB2	1:C:471:ALA:HB2	1.65	0.79
1:G:218:ARG:CG	1:G:345:GLU:OE1	2.31	0.79
1:D:218:ARG:HG3	1:D:345:GLU:OE1	1.81	0.79
1:E:218:ARG:NH2	1:E:223:MET:O	2.14	0.79
1:A:39:LEU:CD2	1:A:444:LEU:HD21	2.11	0.78
1:B:263:GLU:HA	1:B:269:LEU:HD21	1.63	0.78
1:F:218:ARG:CG	1:F:345:GLU:OE1	2.32	0.78
1:G:263:GLU:HA	1:G:269:LEU:HD21	1.63	0.78
1:C:31:ILE:HD13	1:C:75:ALA:HB1	1.64	0.78
1:D:468:ASN:HB2	1:D:471:ALA:HB2	1.64	0.78
1:A:11:ASN:HA	1:A:12:MET:CG	2.12	0.78
1:A:199:SER:HA	1:A:377:ILE:HD11	1.66	0.78
1:G:439:VAL:O	1:G:443:THR:HG23	1.83	0.78
1:H:11:ASN:HA	1:H:12:MET:CG	2.14	0.78
1:A:218:ARG:NH2	1:A:223:MET:O	2.15	0.78
1:E:46:LYS:HG3	1:E:64:ILE:HD13	1.64	0.78
1:B:218:ARG:NH2	1:B:223:MET:O	2.13	0.78
1:G:11:ASN:HA	1:G:12:MET:CG	2.14	0.78
1:A:497:GLN:OE1	1:H:201:ALA:HB2	1.84	0.77
1:B:11:ASN:HA	1:B:12:MET:HG2	1.65	0.77
1:H:218:ARG:CG	1:H:345:GLU:OE1	2.32	0.77
1:E:455:ILE:HG21	1:E:473:LEU:HD22	1.67	0.77
1:G:218:ARG:NH2	1:G:223:MET:O	2.14	0.77
1:E:11:ASN:HA	1:E:12:MET:CG	2.15	0.77
1:H:199:SER:HA	1:H:377:ILE:HD11	1.66	0.77
1:B:46:LYS:HG3	1:B:64:ILE:HD13	1.64	0.77
1:D:130:LYS:HG3	1:D:134:LEU:HD12	1.67	0.77
1:H:320:ALA:HB2	1:H:364:ALA:HB3	1.66	0.77
1:B:199:SER:HA	1:B:377:ILE:HD11	1.65	0.77
1:B:218:ARG:CG	1:B:345:GLU:OE1	2.33	0.77
1:H:11:ASN:HA	1:H:12:MET:HG2	1.67	0.77
1:D:320:ALA:HB2	1:D:364:ALA:HB3	1.66	0.77
1:A:501:SER:HB3	1:H:372:THR:HB	1.65	0.77
1:C:206:THR:CG2	1:C:370:ARG:H	1.94	0.77
1:D:455:ILE:HG21	1:D:473:LEU:HD22	1.67	0.77

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:448:ALA:HB3	1:F:450:LEU:HD12	1.76	0.67
1:G:442:ARG: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
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:E:173:ILE:HG23	1:E:208:LEU:HB2	1.78	0.65
1:F:440:ILE:O	1:F:444:LEU:HG	1.95	0.65
1:D:502:ALA:O	1:D:506:THR:HG23	1.95	0.65
1:D:202:SER:OG	1:D:205:ASP:HB2	1.96	0.65
1:D:442:ARG:HG2	1:D:442:ARG:NH1	2.06	0.65
1:G:131:ALA:HB2	1:G:415:LEU:HD11	1.78	0.65
1:B:39:LEU:CD2	1:B:444:LEU:HD23	2.19	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:545:ADP:PB	4:C:546:SO4:O2	2.55	0.65
1:D:131:ALA:HB2	1:D:415:LEU:HD11	1.79	0.65
1:G:376:VAL:HG11	1:H:504:GLU:OE1	1.96	0.65
1:H:173:ILE:HG23	1:H:208:LEU:HB2	1.77	0.65
1:A:356:VAL:HG12	1:A:356:VAL:O	1.97	0.65
1:B: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
1:H:39:LEU:HD11	1:H:95:THR:HG22	1.79	0.65
1:B:178:VAL:HG11	1:B:391:VAL:HG12	1.78	0.65
3:F:545:ADP:O1B	4:F:546:SO4:O2	2.15	0.65
1:C:208:LEU:HD11	1:C:365:VAL:CG1	2.27	0.64
1:F:233:ALA:O	1:F:284:LEU:HD12	1.97	0.64
1:B:401:VAL:HB	1:B:407:THR:HG21	1.77	0.64
1:F:468:ASN:O	1:F:469:LYS:HG2	1.98	0.64
1:H:440:ILE:O	1:H:444:LEU:HG	1.96	0.64
1:A:63:THR:HG22	1:A:66:ARG:NH2	2.12	0.64
1:C:63:THR:HG22	1:C:66:ARG:NH2	2.12	0.64
1:F:189:ASP:HB3	1:F:192:LEU:HG	1.78	0.64
1:G:31:ILE:HD13	1:G:75:ALA:CB	2.27	0.64
1:C:202:SER:OG	1:C:205:ASP:HB2	1.98	0.64
1:B:46:LYS:HD3	1:C:514:ASP:HB3	1.79	0.64
1:E:440:ILE:O	1:E:444:LEU:HG	1.98	0.64
1:G:468:ASN:O	1:G:469:LYS:HG2	1.97	0.64
1:A:401:VAL:HB	1:A:407:THR:HG21	1.80	0.64
1:E:164:GLU:HB2	1:F:125:GLN:OE1	1.97	0.64
1:H:468:ASN:O	1:H:469:LYS:HG2	1.97	0.64
1:A:202:SER:OG	1:A:205:ASP:HB2	1.98	0.64
1:A:416:ARG:O	1:A:419:ALA:HB3	1.97	0.64
1:E:420:GLU:HG2	1:E:431:ARG:HH22	1.62	0.64
1:A:173:ILE:HG23	1:A:208:LEU:HB2	1.80	0.64
1:A:502:ALA:O	1:A:506:THR:HG23	1.98	0.64
1:F:178:VAL:HG11	1:F:391:VAL:HG12	1.80	0.64
1:G:202:SER:OG	1:G:205:ASP:HB2	1.98	0.64
1:A:189:ASP:HB3	1:A:192:LEU:HG	1.80	0.63
1:C:233:ALA:O	1:C:284:LEU:HD12	1.98	0.63
1:C:502:ALA:O	1:C:506:THR:HG23	1.97	0.63
1:C:189:ASP:HB3	1:C:192:LEU:HG	1.80	0.63
1:C:440:ILE:O	1:C:444:LEU:HG	1.98	0.63
1:A:420:GLU:HG2	1:A:431:ARG:HH22	1.63	0.63
1:G:89:VAL:HG11	1:G:494:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ARG:HG2	1:B:442:ARG:NH1	2.05	0.63
1:C:178:VAL:HG11	1:C:391:VAL:HG12	1.79	0.63
1:D:233:ALA:O	1:D:284:LEU:HD12	1.99	0.63
1:E:373:THR:HB	1:F:80:GLU:HB3	1.80	0.63
1:E:94:THR:O	1:E:98:VAL:HG23	1.99	0.63
1:F:271:ASP:O	1:F:275:GLU:HG3	1.99	0.63
1:D:89:VAL:HG11	1:D:494:VAL:HG22	1.81	0.63
1:E:95:THR:HG23	3:E:545:ADP:O2B	1.99	0.63
1:B:271:ASP:O	1:B:275:GLU:HG3	1.98	0.62
1:F:62:VAL:HG13	1:F:63:THR:N	2.14	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:44:MET:HE1	1:E:118:THR:HG23	1.80	0.62
1:D:271:ASP:O	1:D:275:GLU:HG3	1.99	0.62
1: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
3:G:545:ADP:PB	4:G:546:SO4:O2	2.58	0.62
1:H:401:VAL:HB	1:H:407:THR:HG21	1.81	0.62
1:A:440:ILE:O	1:A:444:LEU:HG	1.99	0.62
1:G:271:ASP:O	1:G:275:GLU:HG3	2.00	0.62
1:C:408:GLU:O	1:C:412:SER:HB3	2.00	0.62
1:E:468:ASN:O	1:E:469:LYS:HG2	2.00	0.62
1:F:202:SER:OG	1:F:205:ASP:HB2	1.99	0.62
1:H:408:GLU:O	1:H:412:SER:HB3	1.99	0.62
1:C:271:ASP:O	1:C:275:GLU:HG3	2.00	0.62
1:E:416:ARG:O	1:E:419:ALA:HB3	1.99	0.62
1:B:39:LEU:HD11	1:B:95:THR:HG22	1.82	0.61
1:D: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:SER:OG	1:E:205:ASP:HB2	2.00	0.61
1:H:178:VAL:HG11	1:H:391:VAL:HG12	1.81	0.61
1:G:425:ARG:O	1:G:427:GLN:N	2.33	0.61
1:A:468:ASN:O	1:A:469:LYS:HG2	2.00	0.61
1:C:401:VAL:HB	1:C:407:THR:HG21	1.81	0.61
1:E:203:ILE:HA	1:E:370:ARG:O	2.01	0.61
1:D:440:ILE:O	1:D:444:LEU:HG	2.01	0.61
1:H:202:SER:CB	1:H:205:ASP:HB2	2.31	0.61
1:B:356:VAL:HG12	1:B:356:VAL:O	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: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: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:B:408:GLU:O	1:B:412:SER:HB3	2.01	0.60
1:D:201:ALA:HB2	1:E:497:GLN:OE1	2.01	0.60
1:D:401:VAL:HB	1:D:407:THR:HG21	1.82	0.60
3:G:545:ADP:O3B	4:G:546:SO4:S	2.59	0.60
1:H:416:ARG:O	1:H:419:ALA:HB3	2.00	0.60
1:C:273:VAL:HG11	1:C:297:TYR:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:545:ADP:O1B	4:E:546:SO4:O2	2.18	0.60
1:H:342:LEU:HD21	1:H:344:GLU:HB2	1.83	0.60
1:B:31:ILE:HD13	1:B:75:ALA:CB	2.30	0.60
1:C:49:VAL:HG21	1:D:73:PRO:HG3	1.84	0.60
1:D:273:VAL:HG11	1:D:297:TYR:HB3	1.82	0.60
1:E:218:ARG:HG2	1:E:345:GLU:OE1	2.02	0.60
1:F:273:VAL:HG11	1:F:297:TYR:HB3	1.84	0.60
1:D:31:ILE:HD11	1:D:78:LEU:HB2	1.84	0.60
1:F:203:ILE:HA	1:F:370:ARG:O	2.02	0.60
1:G:342:LEU:HD21	1:G:344:GLU:HB2	1.84	0.60
1:A:31:ILE:HD13	1:A:75:ALA:CB	2.31	0.60
3:D:545:ADP:O1B	3:D:545:ADP:O2A	2.19	0.60
1:E:77:MET:CE	1:E:509:LEU:HD21	2.31	0.60
1:F:89:VAL:HG11	1:F:494:VAL:HG22	1.84	0.60
1:G:233:ALA:O	1:G:284:LEU:HD12	2.01	0.60
1:C: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:HG12	1:D:356:VAL:O	2.02	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:C:131:ALA:HB2	1:C:415:LEU:HD11	1.83	0.59
1:D:145:GLN:O	1:D:147:LYS:N	2.34	0.59
1:G:82:ALA:HB2	1:G:97:VAL:CG2	2.33	0.59
1:H: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:408:GLU:O	1:D:412:SER:HB3	2.02	0.59
1:E:25:ILE:O	1:E:29:ARG:HG3	2.02	0.59
1:H:157:SER:HB2	1:H:390:VAL:HG21	1.84	0.59
1:E:233:ALA:O	1:E:284:LEU:HD12	2.02	0.59
1:E:315:GLU:O	1:E:319:LYS:HG3	2.02	0.59

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:HG11	1:A:494:VAL:HG22	1.85	0.57
1:B:145:GLN:O	1:B:147:LYS:N	2.37	0.57
1:H:138:ILE:HD12	1:H:410:GLU:HG2	1.86	0.57
1:H:425:ARG:O	1:H:427:GLN:N	2.37	0.57
1:B:442:ARG: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: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:G:267:GLU:C	1:G:269:LEU:H	2.07	0.57
1:A:376:VAL:HG11	1:B:504:GLU:OE1	2.05	0.57
1:D:202:SER:CB	1:D:205:ASP:HB2	2.35	0.57
1:D:342:LEU:HD21	1:D:344:GLU:HB2	1.87	0.57
1:E: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
1:F:267:GLU:C	1:F:269:LEU:H	2.09	0.57
1:C:62:VAL:HG13	1:C:63:THR:N	2.21	0.56
1:D:267:GLU:C	1:D:269:LEU:H	2.09	0.56
1:E:145:GLN:O	1:E:147:LYS:N	2.38	0.56
1:F:342:LEU:HD21	1:F:344:GLU:HB2	1.86	0.56
1:F:408:GLU:O	1:F:412:SER:HB3	2.05	0.56
1:A:267:GLU:C	1:A:269:LEU:H	2.08	0.56
1:B:77:MET:HA	1:B:80:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:267:GLU:C	1:B:269:LEU:H	2.07	0.56
1:B:425:ARG:O	1:B:427:GLN:N	2.38	0.56
1: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:151:THR:OG1	1:D:175:VAL:HG21	2.05	0.56
1:H:95:THR:HG23	3:H:545:ADP:O2B	2.06	0.56
1:B:372:THR:CB	1:C:501:SER:HB3	2.35	0.56
3:B:545:ADP:O3B	4:B:546:SO4:S	2.64	0.56
1:C:267:GLU:C	1:C:269:LEU:H	2.08	0.56
1:D:218:ARG:HG2	1:D:345:GLU:OE1	2.06	0.56
1:F:25:ILE:O	1:F:29:ARG:HG3	2.05	0.56
1:F:77:MET:HA	1:F:80:GLU:HG2	1.87	0.56
1:G:138:ILE:HD12	1:G:410:GLU:HG2	1.87	0.56
1:H:267:GLU:C	1:H:269:LEU:H	2.09	0.56
1:H:386:ASP:O	1:H:390:VAL:HG22	2.05	0.56
1:B:218:ARG:HG2	1:B:345:GLU:OE1	2.05	0.56
1:G:94:THR:O	1:G:98:VAL:HG23	2.05	0.56
1:A:77:MET:HA	1:A:80:GLU:HG2	1.88	0.55
1:D:138:ILE:HD12	1:D:410:GLU:HG2	1.88	0.55
1:G:153:ILE:HD13	1:G:394:THR:OG1	2.05	0.55
1:D:51:ASP:HB2	1:E:519:GLU:CB	2.36	0.55
1:E:267:GLU:C	1:E:269:LEU:H	2.09	0.55
1:H:268:MET:C	1:H:269:LEU:HD13	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HA	1:A:370:ARG:O	2.05	0.55
1:D:425:ARG:O	1:D:427:GLN:N	2.40	0.55
1:F:94:THR:O	1:F:98:VAL:HG23	2.06	0.55
1:H:218:ARG:HG2	1:H:345:GLU:OE1	2.04	0.55
1:D:117:PRO:O	1:D:121:VAL:HG12	2.06	0.55
1:F:39:LEU:CD2	1:F:444:LEU:HD23	2.21	0.55
1:H:197:LYS:HB3	1:H:377:ILE:HG21	1.88	0.55
1:H:384:VAL:O	1:H:388:VAL:HG23	2.06	0.55
1:A:39:LEU:HD11	1:A:95:THR:HG22	1.89	0.55
3:E:545:ADP:O3B	4:E:546:SO4:S	2.65	0.55
1:G:157:SER:HB2	1:G:390:VAL:HG21	1.88	0.55
1:G:268:MET:C	1:G:269:LEU:HD13	2.27	0.55
3:H:545:ADP:O1B	3:H:545:ADP:O2A	2.24	0.55
1:H: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:D:268:MET:C	1:D:269:LEU:HD13	2.27	0.55
3:H:545:ADP:PB	4:H:546:SO4:O2	2.65	0.55
1:B:157:SER:HB2	1:B:390:VAL:HG21	1.89	0.55
1:H:153:ILE:HD13	1:H:394:THR:OG1	2.07	0.55
1:B:62:VAL:HG13	1:B:63:THR:N	2.21	0.54
1:D:39:LEU:HD11	1:D:95:THR:HG22	1.88	0.54
1:C:77:MET:HA	1:C:80:GLU:HG2	1.90	0.54
1:D:39:LEU:HD21	1:D:444:LEU:HD21	1.90	0.54
1:F:266:SER:HB3	1:F:268:MET:CE	2.37	0.54
1:G:356:VAL:HG12	1:G:356:VAL:O	2.06	0.54
1:A:95:THR:HG23	3:A:545:ADP:O2B	2.08	0.54
1:A:442:ARG:NH1	1:A:442:ARG:CG	2.67	0.54
1:B:268:MET:C	1:B:269:LEU:HD13	2.27	0.54
1:B:450:LEU:HD22	1:B:455:ILE:HD11	1.89	0.54
1:H:203:ILE:H	1:H:371:GLY:HA2	1.71	0.54
1:A:80:GLU:HB3	1:H:373:THR:HB	1.90	0.54
1:D:416:ARG:O	1:D:419:ALA:HB3	2.08	0.54
1:E:384:VAL:O	1:E:388:VAL:HG23	2.08	0.54
3:F:545:ADP:PB	4:F:546:SO4:O2	2.65	0.54
1:A:215:ASP:HA	1:A:353:MET:HG2	1.89	0.54
1:B:118:THR:HA	1:B:121:VAL:CG1	2.38	0.54
1:C:145:GLN:O	1:C:147:LYS:N	2.40	0.54
1:D:197:LYS:HB3	1:D:377:ILE:HG21	1.90	0.54
1:F:151:THR:OG1	1:F:175:VAL:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:ARG:HH11	1:F:442:ARG:CG	2.12	0.54
1:A:62:VAL:HG13	1:A:63:THR:N	2.23	0.54
1:D:464:ALA:O	1:D:466:ASN:OD1	2.26	0.54
1:G:216:LYS:HE2	1:G:307:ARG:O	2.07	0.54
1:A:464:ALA:O	1:A:466:ASN:OD1	2.25	0.54
1:C:51:ASP:HB2	1:D:519:GLU:HB2	1.89	0.54
1:D:157:SER:HB2	1:D:390:VAL:HG21	1.90	0.54
1:D:215:ASP:HA	1:D:353:MET:HG2	1.90	0.54
1:A:315:GLU:O	1:A:319:LYS:HG3	2.06	0.54
1:E:46:LYS:HG3	1:E:64:ILE:CD1	2.36	0.54
1:F: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:G:39:LEU:HD11	1:G:95:THR:HG22	1.88	0.54
1:E:202:SER:CB	1:E:205:ASP:HB2	2.38	0.54
3:F:545:ADP:O3B	4:F:546:SO4:S	2.66	0.54
1:G:440:ILE:HB	1:G:441:PRO:HD3	1.90	0.54
1:H:450:LEU:HD22	1:H:455:ILE:HD11	1.89	0.54
1:B:216:LYS:HE2	1:B:307:ARG:O	2.08	0.53
1:C:197:LYS:HB3	1:C:377:ILE:HG21	1.90	0.53
1:F:208:LEU:HD11	1:F:365:VAL:HG11	1.89	0.53
1:G:420:GLU:C	1:G:422:ILE:H	2.10	0.53
3:A:545:ADP:PB	4:A:546:SO4:O2	2.66	0.53
1:B:95:THR:HG23	3:B:545:ADP:O2B	2.08	0.53
1:F:154:ALA:HB2	1:F:391:VAL:CG2	2.38	0.53
3:F:545:ADP: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:A:268:MET:C	1:A:269:LEU:HD13	2.28	0.53
1:B:117:PRO:O	1:B:121:VAL:HG12	2.08	0.53
1:C: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:F:11:ASN:HA	1:F:12:MET:HG3	1.90	0.53
1:F:440:ILE:HB	1:F:441:PRO:HD3	1.90	0.53
1:F:450:LEU:HD22	1:F:455:ILE:HD11	1.90	0.53
1:H:202:SER:HB2	1:H:205:ASP:HB2	1.90	0.53
1:H:37:SER:OG	1:H:46:LYS:NZ	2.38	0.53
1:H:464:ALA:O	1:H:466:ASN:OD1	2.25	0.53
1:B:284:LEU:O	1:B:305:ALA:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ASN:HA	1:C:12:MET:HG3	1.91	0.53
3:E:545:ADP:O1B	3:E:545:ADP:O2A	2.25	0.53
1:H:448:ALA:CB	1:H:450:LEU:HD12	2.39	0.53
1: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
1:D:202:SER:OG	1:D:203:ILE:N	2.42	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: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:B:268:MET:C	1:B:269:LEU:HD22	2.29	0.53
1:C:48:LEU:HG	1:D:516:ILE:HB	1.90	0.53
3:D:545:ADP:PB	4:D:546:SO4:O2	2.67	0.53
1:E:268:MET:C	1:E:269:LEU:HD13	2.29	0.53
1:E:284:LEU:O	1:E:305:ALA:HA	2.09	0.53
1:G:203:ILE:H	1:G:371:GLY:HA2	1.73	0.53
1:C:450:LEU:HD22	1:C:455:ILE:HD11	1.91	0.52
1:C:464:ALA:O	1:C:466:ASN:OD1	2.27	0.52
1:E: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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
3:E:545:ADP:PB	4:E:546:SO4:O2	2.68	0.51
1:F:266:SER:HB3	1:F:268:MET:HE3	1.91	0.51
1:G:197:LYS:HB3	1:G:377:ILE:CG2	2.40	0.51
1:G:197:LYS:HB3	1:G:377:ILE:HG21	1.92	0.51
1:H:118:THR:HA	1:H:121:VAL:HG12	1.93	0.51
1:B:419:ALA:O	1:B:427:GLN:HG3	2.10	0.51
1:D:273:VAL:HG21	1:D:297:TYR:HB2	1.92	0.51
1:D:442:ARG: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: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: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:F:268:MET:C	1:F:269:LEU:HD22	2.31	0.51
1:A:82:ALA:HB2	1:A:97:VAL:CG2	2.40	0.51
1:E: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:B:273:VAL:HG21	1:B:297:TYR:HB2	1.91	0.51
1:B:468:ASN:C	1:B:470:CYS:H	2.13	0.51
1:C:36:ARG:NH2	1:C:443:THR:HG22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LEU:HD11	1:C:365:VAL:HG11	1.92	0.51
1:E:155:MET:HE3	1:E:171:ALA:HB2	1.93	0.51
1:F:438:GLU:C	1:F:441:PRO:HD2	2.31	0.51
1:F:468:ASN:C	1:F:470:CYS:H	2.14	0.51
1:G:419:ALA:O	1:G:427:GLN:HG3	2.11	0.51
1:A:326:ILE:HD11	1:A:336:ASP:OD1	2.10	0.51
1:C:49:VAL:CG2	1:D:73:PRO:HG3	2.41	0.51
1:E:154:ALA:HB2	1:E:391:VAL:CG2	2.41	0.51
3:H:545:ADP:O3B	4:H:546:SO4:S	2.68	0.51
1:B:227:VAL:CG1	1:B:230:ALA:HB2	2.41	0.50
1:B:438:GLU:C	1:B:441:PRO:HD2	2.32	0.50
1:C:118:THR:HA	1:C:121:VAL:CG1	2.41	0.50
1:C:215:ASP:HA	1:C:353:MET:HG2	1.93	0.50
1:B:403:GLY:O	1:B:406:SER:HB2	2.11	0.50
1:D:268:MET:C	1:D:269:LEU:HD22	2.31	0.50
1:D:442:ARG:HG3	1:D:452:ALA:HB1	1.93	0.50
1:H:236:ASN:HB2	1:H:325:VAL:CG1	2.40	0.50
1:A:420:GLU:C	1:A:422:ILE:H	2.15	0.50
1: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:H:420:GLU:C	1:H:422:ILE:H	2.15	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:G:425:ARG:C	1:G:427:GLN:N	2.64	0.50
1:H:268:MET:C	1:H:269:LEU:HD22	2.31	0.50
1:C: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:F:420:GLU:C	1:F:422:ILE:H	2.14	0.50
1:B:25:ILE:HG23	1:B:104:LEU:HB3	1.94	0.50
1:D:208:LEU:HD11	1:D:365:VAL:HG11	1.93	0.50
1:D:232:ILE:HG22	1:D:234:LEU:HD12	1.94	0.50
1:F:47:MET:O	1:G:515:VAL:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:MET:O	1:H:80:GLU:HB2	2.12	0.50
1:A:268:MET:C	1:A:269:LEU:HD22	2.32	0.50
1:A:284:LEU:O	1:A:305:ALA:HA	2.11	0.50
1:B:269:LEU:HD22	1:B:269:LEU:N	2.27	0.50
1:C: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:F:425:ARG:C	1:F:427:GLN:N	2.63	0.50
1:G:135:LEU:HD21	1:G:411:LEU:HD22	1.94	0.50
1:H:269:LEU:O	1:H:273:VAL:HG23	2.12	0.50
1:A:425:ARG:C	1:A:427:GLN:N	2.65	0.50
3:A:545:ADP:O3B	4:A:546:SO4:S	2.70	0.50
1:B:202:SER:OG	1:B:203:ILE:N	2.44	0.50
3:B:545:ADP:O3B	4:B:546:SO4:O3	2.30	0.50
1:C:418:TYR:CE2	1:C:422:ILE:HD11	2.46	0.50
1:D:82:ALA:HB2	1:D:97:VAL:HG23	1.93	0.50
1:B:49:VAL:HG12	1:B:50:ASP:N	2.26	0.50
1:B:201:ALA:HB2	1:C:497:GLN:CD	2.28	0.50
1:B:440:ILE:HB	1:B:441:PRO:HD3	1.93	0.50
1:G:202:SER:OG	1:G:370:ARG:HB2	2.12	0.50
1:G:268:MET:C	1:G:269:LEU:HD22	2.31	0.50
1:H:208:LEU:HD11	1:H:365:VAL:HG11	1.91	0.50
1:A:450:LEU:HD21	1:A:478:GLY:HA2	1.94	0.49
1:C:269:LEU:HD22	1:C:269:LEU:N	2.27	0.49
1:C:420:GLU:C	1:C:422:ILE:H	2.14	0.49
1:D:57:VAL:CG2	1:E:512:ILE:HD11	2.42	0.49
1:E: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:E:425:ARG:C	1:E:427:GLN:N	2.64	0.49
1:G:425:ARG:C	1:G:427:GLN:H	2.15	0.49
1: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:216:LYS:HG3	1:G:309:VAL:HG22	1.93	0.49
1:B:77:MET:CE	1:B:509:LEU:HD21	2.42	0.49
1:C:468:ASN:C	1:C:470:CYS:H	2.15	0.49
1:D:36:ARG:NH2	1:D:443:THR:HG22	2.27	0.49
1:F:197:LYS:HB3	1:F:377:ILE:CG2	2.41	0.49

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:LYS:HB3	1:E:377:ILE:HG21	1.93	0.49
1:E:438:GLU:C	1:E:441:PRO:HD2	2.33	0.49
1:E:440:ILE:HB	1:E:441:PRO:HD3	1.95	0.49
1:F:450:LEU:HD21	1:F:478:GLY:HA2	1.95	0.49
1:A:438:GLU:C	1:A:441:PRO:HD2	2.32	0.48
1:C:232:ILE:HG22	1:C:234:LEU:HD12	1.95	0.48
1:E:117:PRO:O	1:E:121:VAL:HG12	2.13	0.48
1:F:490:GLU:OE1	1:F:495:LYS:HE3	2.12	0.48
1:G:468:ASN:C	1:G:470:CYS:H	2.16	0.48
1:H:189:ASP:HB3	1:H:192:LEU:CG	2.42	0.48
1:H:442:ARG:NH1	1:H:442:ARG:CG	2.71	0.48
1:B:425:ARG:C	1:B:427:GLN:N	2.65	0.48
1:E:414:LYS:O	1:E:417:GLU:HG2	2.13	0.48
1:E:442:ARG: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
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:C:419:ALA:O	1:C:427:GLN:HG3	2.14	0.48
1:D:118:THR:HA	1:D:121:VAL:HG12	1.96	0.48
1:D:453:ILE:O	1:D:457:VAL:HG23	2.13	0.48
1:E:133:GLU:O	1:E:137:THR:HG23	2.12	0.48
1:H:363:LYS:HD3	1:H:363:LYS:HA	1.57	0.48
1:A:216:LYS:HG3	1:A:309:VAL:HG22	1.95	0.48
1:B:442:ARG:HG3	1:B:452:ALA:HB1	1.96	0.48
1:C: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:C:438:GLU:C	1:C:441:PRO:HD2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:O	1:D:305:ALA:HA	2.13	0.48
1:E:225:LYS:NZ	1:E:225:LYS:HB3	2.28	0.48
1:E:450:LEU:HD21	1:E:478:GLY:HA2	1.95	0.48
1:F:236:ASN:HB2	1:F:325:VAL:CG1	2.43	0.48
1:G:263:GLU:HA	1:G:269:LEU:CD2	2.38	0.48
1:H:453:ILE:O	1:H:457:VAL:HG23	2.13	0.48
1:A: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:F:225:LYS:NZ	1:F:225:LYS:HB3	2.28	0.48
1:A:225:LYS:NZ	1:A:225:LYS:HB3	2.28	0.48
1:A:263:GLU:HA	1:A:269:LEU:CD2	2.37	0.48
1:A:512:ILE:HD13	1:H:47:MET:HB2	1.96	0.48
1:C:59:ASN:OD1	1:C:59:ASN:O	2.32	0.48
1:E:157:SER:HB2	1:E:390:VAL:HG21	1.94	0.48
1:H:450:LEU:HD21	1:H:478:GLY:HA2	1.95	0.48
1:A:232:ILE:HG22	1:A:234:LEU:HD12	1.95	0.48
1:D:386:ASP:O	1:D:390:VAL:HG22	2.14	0.48
1:E:232:ILE:HG22	1:E:234:LEU:HD12	1.95	0.48
1:F:363:LYS:HA	1:F:363:LYS:HD3	1.59	0.48
1:G:448:ALA:CB	1:G:450:LEU:HD12	2.43	0.48
1:F:442:ARG:NH1	1:F:442:ARG:CG	2.70	0.48
1:A:504:GLU:OE1	1:H:376:VAL:HG11	2.14	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: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:HG12	1:F:388:VAL:O	2.14	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:E:268:MET:C	1:E:269:LEU:HD22	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:ARG:C	1:E:427:GLN:H	2.18	0.47
1:H: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
1:C:154:ALA:HB2	1:C:391:VAL:CG2	2.45	0.47
1:C:155:MET:HE3	1:C:171:ALA:HB2	1.96	0.47
1:D:227:VAL:CG1	1:D:230:ALA:HB2	2.45	0.47
1:D:420:GLU:C	1:D:422:ILE:H	2.16	0.47
1:F:82:ALA:HB2	1:F:97:VAL:CG2	2.45	0.47
1:H:343:VAL:HG13	1:H:356:VAL:HG22	1.96	0.47
1:B:203:ILE:H	1:B:371:GLY:HA2	1.78	0.47
1:D:213:LEU:HD11	1:D:355:PHE:CE2	2.49	0.47
1:G:269:LEU: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: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:C:425:ARG:C	1:C:427:GLN:H	2.17	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:HA	1:G:363:LYS:HD3	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:155:MET:HE3	1:B:171:ALA:HB2	1.97	0.47
1:B:236:ASN:HB2	1:B:325:VAL:CG1	2.44	0.47
1:B:384:VAL:O	1:B:388:VAL:HG23	2.15	0.47
1:F:216:LYS:HG3	1:F:309:VAL:HG22	1.96	0.47
1:B:25:ILE:O	1:B:29:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:HD11	1:C:355:PHE:CE2	2.50	0.47
1:E: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
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: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:D:459:VAL:O	1:D:463:HIS:HD2	1.98	0.46
1:E:468:ASN:C	1:E:470:CYS:H	2.18	0.46
1:F:269:LEU:O	1:F:273:VAL:HG23	2.14	0.46
1:F:425:ARG:C	1:F:427:GLN:H	2.17	0.46
1:H:218:ARG:NH1	1:H:225:LYS:HD3	2.30	0.46
1:B: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:B:425:ARG:C	1:B:427:GLN:H	2.19	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:OD1	1:F:59:ASN:O	2.34	0.46
1:F:218:ARG:NH1	1:F:225:LYS:HD3	2.31	0.46
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TYR:O	1:C:301:GLU:HG2	2.16	0.46
1:D:363:LYS: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:F:155:MET:HE3	1:F:171:ALA:HB2	1.96	0.46
1:G:415:LEU:HD23	1:G:415:LEU:HA	1.65	0.46
1:H:11:ASN:HA	1:H:12:MET:HG3	1.96	0.46
1:H:433:PHE:O	1:H:433:PHE:CD2	2.69	0.46
1:A:297:TYR:O	1:A:301:GLU:HG2	2.16	0.46
1:B:146:ASP:OD1	1:B:149:ILE:HD12	2.14	0.46
1:C:450:LEU:HD21	1:C:478:GLY:HA2	1.98	0.46
1:D:189:ASP:HB3	1:D:192:LEU:CG	2.45	0.46
1:E:232:ILE:O	1:E:337:LEU:HA	2.16	0.46
1:E:420:GLU:C	1:E:422:ILE:H	2.19	0.46
1:H: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:A:425:ARG:C	1:A:427:GLN:H	2.18	0.46
1:B:388:VAL:HG12	1:B:388:VAL:O	2.14	0.46
1:D:297:TYR:O	1:D:301:GLU:HG2	2.16	0.46
1:E:189:ASP:HB3	1:E:192:LEU:CG	2.45	0.46
1:F:414:LYS:O	1:F:417:GLU:HG2	2.16	0.46
1:G:109:GLU:O	1:G:113:GLN:HG3	2.15	0.46
1:H:146:ASP:OD1	1:H:149:ILE:HD12	2.16	0.46
1:H:169:LYS:O	1:H:173:ILE:HG13	2.15	0.46
1:H:275:GLU:O	1:H:278:ALA:HB3	2.16	0.46
1:A:118:THR:HA	1:A:121:VAL:CG1	2.46	0.46
1:C:343:VAL:HG13	1:C:356:VAL:HG22	1.96	0.46
1:E: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:H:178:VAL:HG13	1:H:188:VAL:HG11	1.97	0.46
1:H:438:GLU:C	1:H:441:PRO:HD2	2.36	0.46
1:A:234:LEU:HD21	1:A:317:LEU:HB2	1.98	0.46
1:B:109:GLU:O	1:B:113:GLN:HG3	2.15	0.46
1:C:82:ALA:HB2	1:C:97:VAL:HG23	1.98	0.46
1:D:275:GLU:O	1:D:278:ALA:HB3	2.16	0.46
1:E:194:LYS:HB2	1:E:316:LYS:NZ	2.31	0.46
1:H:213:LEU:HD11	1:H:355:PHE:CD2	2.51	0.46
1:A:151:THR:OG1	1:A:175:VAL:HG21	2.16	0.46
1:A:234:LEU:HD21	1:A:317:LEU:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ARG:NH1	1:C:225:LYS:HD3	2.31	0.46
1:C:236:ASN:HB2	1:C:325:VAL:CG1	2.46	0.46
1:C:269:LEU:O	1:C:273:VAL:HG23	2.16	0.46
1:E:202:SER:OG	1:E:370:ARG:HB2	2.16	0.46
1:E:297:TYR:O	1:E:301:GLU:HG2	2.16	0.46
1:E:453:ILE:O	1:E:457:VAL:HG23	2.16	0.46
1:G: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:310:LYS:O	1:H:314:MET:HG2	2.16	0.46
1:B:233:ALA:HB2	1:B:337:LEU:HD22	1.98	0.45
1:B:234:LEU:HD21	1:B:317:LEU:HB2	1.98	0.45
1:D:218:ARG:NH1	1:D:225:LYS:HD3	2.31	0.45
1:D:240:GLU:O	1:D:269:LEU:HG	2.16	0.45
1:E:34:THR:O	1:E:46:LYS:HE2	2.16	0.45
1:G:45:ASP:O	1:H:512:ILE:HA	2.16	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: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: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:E:118:THR:HA	1:E:121:VAL:HG12	1.96	0.45
1:E:234:LEU:HD21	1:E:317:LEU:HB2	1.98	0.45
1:F:403:GLY:O	1:F:406:SER:HB2	2.16	0.45
1:G:269:LEU:O	1:G:273:VAL:HG23	2.16	0.45
1:G:342:LEU:CD2	1:G:344:GLU:HB2	2.45	0.45
1:G:454:GLU:O	1:G:457:VAL:N	2.47	0.45
1:C:233:ALA:HB2	1:C:337:LEU:HD22	1.99	0.45
1:B:41:PRO:HG3	1:B:159:THR:HG22	1.98	0.45
1:C:219:VAL:CG2	1:C:307:ARG:HD3	2.47	0.45
1:C:433:PHE:O	1:C:433:PHE:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:425:ARG:C	1:D:427:GLN:H	2.19	0.45
1:D:442:ARG:HD3	1:D:456:LEU:HD22	1.99	0.45
1: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:HA	1:B:415:LEU:HD23	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:D:25:ILE:O	1:D:29:ARG:HG3	2.17	0.45
1:E:213:LEU:HD11	1:E:355:PHE:CE2	2.51	0.45
1:F:202:SER:OG	1:F:370:ARG:HB2	2.16	0.45
1:F:476:PHE:O	1:F:477:THR:C	2.55	0.45
1:G:234:LEU:HD21	1:G:317:LEU:CB	2.46	0.45
1:H:459:VAL:O	1:H:463:HIS:HD2	1.99	0.45
1:A:403:GLY:O	1:A:406:SER:HB2	2.16	0.45
1:B:154:ALA:HB2	1:B:391:VAL:CG2	2.47	0.45
1:B:266:SER:HB3	1:B:268:MET:CE	2.46	0.45
1:D: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:F:117:PRO:O	1:F:121:VAL:HG12	2.16	0.45
1:H:49:VAL:HG12	1:H:50:ASP:N	2.31	0.45
1:A:189:ASP:HB3	1:A:192:LEU:CG	2.46	0.45
1:A:417:GLU:C	1:A:419:ALA:N	2.70	0.45
1:D: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: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:519:GLU:HB2	1:H:51:ASP:HB2	1.99	0.45
1:H:425:ARG:C	1:H:427:GLN:H	2.20	0.45
1:A:453:ILE:O	1:A:457:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C: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: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:G:476:PHE:O	1:G:477:THR:C	2.55	0.44
1:H:189:ASP:HB3	1:H:192:LEU:CD1	2.47	0.44
1: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:468:ASN:C	1:D:470:CYS:H	2.20	0.44
1:F:297:TYR:O	1:F:301:GLU:HG2	2.16	0.44
1:F:453:ILE:O	1:F:457:VAL:HG23	2.17	0.44
1:G:227:VAL:CG1	1:G:230:ALA:HB2	2.48	0.44
1:G:233:ALA:HB2	1:G:337:LEU:HD22	1.99	0.44
1:A:459:VAL:O	1:A:463:HIS:HD2	1.99	0.44
1:C:49:VAL:HG22	1:D:73:PRO:HB3	1.99	0.44
1:C:85:GLN:HG2	1:C:93:THR:HA	1.99	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:HG12	1:D:388:VAL:O	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:202:SER:OG	1:G:203:ILE:N	2.50	0.44
1:G:213:LEU:HD11	1:G:355:PHE:CE2	2.53	0.44
1:G:403:GLY:O	1:G:406:SER:HB2	2.18	0.44
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.69	0.44
1:B:178:VAL:HG22	1:B:388:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:GLY:O	1:C:406:SER:HB2	2.17	0.44
1:D: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:A:169:LYS:O	1:A:173:ILE:HG13	2.18	0.44
1:B:240:GLU:O	1:B:269:LEU:HG	2.18	0.44
1:C:234:LEU:HD21	1:C:317:LEU:HB2	1.99	0.44
1:A:342:LEU:HD23	1:A:343:VAL:N	2.32	0.44
1:B:342:LEU:CD2	1:B:344:GLU:HB2	2.48	0.44
1:C:194:LYS:HB2	1:C:316:LYS:NZ	2.32	0.44
1:E:169:LYS:O	1:E:173:ILE:HG13	2.17	0.44
1:E:342:LEU:CD2	1:E:344:GLU:HB2	2.47	0.44
1:E:442:ARG:HG3	1:E:452:ALA:HB1	1.99	0.44
1:F:102:GLU:HG2	1:F:439:VAL:HB	1.98	0.44
3:F:545:ADP:O3B	4:F:546:SO4:O3	2.35	0.44
1:H:234:LEU:HD21	1:H:317:LEU:CB	2.48	0.44
1:H:348:ILE: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:F:47:MET:HG3	1:F:55:VAL:HG23	2.00	0.44
1:A:85:GLN:HG2	1:A:92:GLY:O	2.17	0.44
1:A:213:LEU:HD11	1:A:355:PHE:CE2	2.52	0.44
1: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:71:GLU:OE1	1:G:71:GLU:HA	2.18	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:C:178:VAL:HG22	1:C:388:VAL:HG13	2.00	0.44
1:C:453:ILE:O	1:C:457:VAL:HG23	2.18	0.44
1:E:11:ASN:HA	1:E:12:MET:HG3	1.96	0.44
1:F:348:ILE:O	1:F:348:ILE:CG2	2.66	0.44
1:F:459:VAL:O	1:F:463:HIS:HD2	2.01	0.44
1:G:240:GLU:O	1:G:269:LEU:HG	2.18	0.44
1:B:232:ILE:HG22	1:B:234:LEU:HD12	1.99	0.43
1:C:234:LEU:HD21	1:C:317:LEU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E: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
1:H:433:PHE:CD2	1:H:433:PHE:C	2.91	0.43
1:A:135:LEU:HD21	1:A:411:LEU:HD22	2.00	0.43
1:B:414:LYS:O	1:B:417:GLU:HG2	2.18	0.43
1:C:292:ASP:C	1:D:327:THR:HG21	2.38	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:202:SER:OG	1:H:203:ILE:N	2.48	0.43
1:H:234:LEU:HD21	1:H:317:LEU:HB2	2.00	0.43
1: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:37:SER:OG	1:C:46:LYS:NZ	2.44	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:E:473:LEU:HD12	1:E:474:ASN:N	2.33	0.43
1:F:342:LEU:CD2	1:F:344:GLU:HB2	2.48	0.43
1:G:459:VAL:O	1:G:463:HIS:HD2	2.02	0.43
1:H:232:ILE:O	1:H:337:LEU:HA	2.18	0.43
1:A:153:ILE:HD13	1:A:394:THR:OG1	2.17	0.43
1:A:201:ALA:HB2	1:B:497:GLN:CD	2.34	0.43
1:A:442:ARG:HD3	1:A:456:LEU:HD22	2.00	0.43

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:438:GLU:C	1:G:441:PRO:HD2	2.38	0.43
1:A:82:ALA:HB2	1:A:97:VAL:HG23	2.00	0.42
1:A:456:LEU:HD12	1:A:456:LEU:HA	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: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:C:417:GLU:C	1:C:419:ALA:N	2.72	0.42
1:D:342:LEU:CD2	1:D:344:GLU:HB2	2.49	0.42
1:D:481:GLU:OE1	1:D:486:ASN:ND2	2.52	0.42
1:E:217:GLU:O	1:E:218:ARG:C	2.58	0.42
1:E:476:PHE:O	1:E:477:THR:C	2.57	0.42
1:E:481:GLU:OE1	1:E:486:ASN:ND2	2.52	0.42
1:F:220:SER:HB3	1:F:223:MET:HG3	2.00	0.42
1:G:34:THR:O	1:G:46:LYS:HE2	2.19	0.42
1:H:227:VAL:CG1	1:H:230:ALA:HB2	2.49	0.42
1:A:217:GLU:O	1:A:218:ARG:C	2.58	0.42
1:B:453:ILE:O	1:B:457:VAL:HG23	2.19	0.42
1:C:189:ASP:HB3	1:C:192:LEU:CD1	2.49	0.42
1:C:490:GLU:OE1	1:C:495:LYS:HE3	2.18	0.42
1:E:233:ALA:HB2	1:E:337:LEU:HD22	2.00	0.42
1:E:388:VAL:HG12	1:E:388:VAL:O	2.18	0.42
1:G:202:SER:HB2	1:G:205:ASP:HB2	2.01	0.42
1:H:59:ASN:OD1	1:H:59:ASN:O	2.37	0.42
1:H:414:LYS:O	1:H:417:GLU:HG2	2.19	0.42
1:A:490:GLU:OE1	1:A:495:LYS:HE3	2.19	0.42
1:C:232:ILE:O	1:C:337:LEU:HA	2.19	0.42
1:C:509:LEU:HD23	1:C:509:LEU:HA	1.76	0.42
1:E:273:VAL:HG11	1:E:297:TYR:CB	2.47	0.42
1:A:37:SER:OG	1:A:46:LYS:NZ	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG23	1:H:44:MET:HE1	2.02	0.42
1:B:52:LEU:C	1:B:54:ASP:H	2.23	0.42
1:B:217:GLU:O	1:B:218:ARG:C	2.57	0.42
1:D:85:GLN:HG2	1:D:93:THR:HA	2.01	0.42
1:F:343:VAL:HG13	1:F:356:VAL:HG22	2.02	0.42
1:G:178:VAL:HG13	1:G:188:VAL:HG11	2.00	0.42
1:G:227:VAL:HG12	1:G:230:ALA:HB2	2.02	0.42
1:G:342:LEU:HD23	1:G:343:VAL:N	2.35	0.42
1:H:50:ASP:OD1	1:H:51:ASP:N	2.53	0.42
1:A:189:ASP:HB3	1:A:192:LEU:CD1	2.49	0.42
1:B:142:VAL:HG12	1:B:143:GLY:N	2.34	0.42
1:B:194:LYS:HB2	1:B:316:LYS:NZ	2.34	0.42
1:D:227:VAL:HG12	1:D:230:ALA:HB2	2.00	0.42
1:D:342:LEU:HD23	1:D:343:VAL:N	2.34	0.42
1:E:417:GLU:C	1:E:419:ALA:N	2.69	0.42
1:F:219:VAL:CG2	1:F:307:ARG:HD3	2.49	0.42
1:B:267:GLU:C	1:B:269:LEU:N	2.72	0.42
1:B:456:LEU: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
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:C:433:PHE:CD2	1:C:433:PHE:C	2.92	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:H:476:PHE:O	1:H:477:THR:C	2.57	0.42
1:A:213:LEU:HD11	1:A:355:PHE:CD2	2.55	0.42
1:A:368:LEU:HD12	1:A:368:LEU:HA	1.87	0.42
1:D:158:ILE:O	1:D:161:LYS:HB2	2.20	0.42
1:E:50:ASP:OD1	1:E:51:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:LYS:HB2	1:F:316:LYS:NZ	2.35	0.42
1:G:185:GLU:HA	1:G:186:GLY:HA2	1.81	0.42
1:G:232:ILE:O	1:G:337:LEU:HA	2.20	0.42
1:H:468:ASN:C	1:H:470:CYS:H	2.22	0.42
1:A:154:ALA:HB2	1:A:391:VAL:CG2	2.50	0.42
1:A:296:HIS:CE1	1:B:331:ASP:OD2	2.73	0.42
1:E:158:ILE:O	1:E:161:LYS:HB2	2.20	0.42
1: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:O	1:F:433:PHE:CD2	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: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:C:217:GLU:O	1:C:218:ARG:C	2.58	0.41
1:E:118:THR:HA	1:E:121:VAL:CG1	2.49	0.41
1:E:403:GLY:O	1:E:406:SER:HB2	2.18	0.41
1:F:62:VAL:CG1	1:F:63:THR:N	2.81	0.41
1:G:184:ASP:HA	1:G:185:GLU:HA	1.52	0.41
1:H:199:SER:HA	1:H:377:ILE:CD1	2.45	0.41
1:A:343:VAL:HG13	1:A:356:VAL:HG22	2.02	0.41
1:C:34:THR:O	1:C:46:LYS:HE2	2.20	0.41
1:C:52:LEU:C	1:C:54:ASP:H	2.22	0.41
1:C:414:LYS:O	1:C:417:GLU:HG2	2.20	0.41
1:D:51:ASP:C	1:D:51:ASP:OD1	2.59	0.41
1:D:71:GLU:OE1	1:D:71:GLU:HA	2.19	0.41
1:D:197:LYS:HD2	1:D:377:ILE:HG22	2.01	0.41
1:E:202:SER:HG	1:E:203:ILE:N	2.18	0.41
1:F:48:LEU:HG	1:G:516:ILE:HB	2.02	0.41
1:F:49:VAL:HG12	1:F:50:ASP:N	2.35	0.41
1:G:273:VAL:HG11	1:G:297:TYR:CB	2.49	0.41
1:G:433:PHE:CD2	1:G:433:PHE:C	2.93	0.41
1:H:128:ALA:O	1:H:132:GLN:HG2	2.19	0.41
1:H:269:LEU:HD12	1:H:272:MET:SD	2.61	0.41
1:H:506:THR:O	1:H:510:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG12	1:A:230:ALA:HB2	2.02	0.41
1:B:417:GLU:C	1:B:419:ALA:N	2.71	0.41
1:C:506:THR:O	1:C:510:LEU:HG	2.21	0.41
1:D:199:SER:HA	1:D:377:ILE:CD1	2.43	0.41
1:D:373:THR:HB	1:E:80:GLU:HB3	2.03	0.41
1:F:185:GLU:HA	1:F:186:GLY:HA2	1.81	0.41
1:A:25:ILE:HG23	1:A:104:LEU:HB3	2.02	0.41
1:B:197:LYS:HD2	1:B:377:ILE:HG22	2.03	0.41
1:B: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: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:E:267:GLU:C	1:E:269:LEU:N	2.74	0.41
1:F:273:VAL:HG11	1:F:297:TYR:CB	2.49	0.41
1:H: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:85:GLN:HG2	1:G:92:GLY:O	2.21	0.41
1:H:273:VAL:HG11	1:H:297:TYR:CB	2.50	0.41
1:A:267:GLU:C	1:A:269:LEU:N	2.74	0.41
1:B:269:LEU:HD12	1:B:272:MET:SD	2.61	0.41
1:D: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: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:H:217:GLU:O	1:H:218:ARG:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.95	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:433:PHE:CD2	1:F:433:PHE:C	2.94	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
1:G:167:LYS:HD2	1:G:167:LYS:HA	1.85	0.41
1:G:217:GLU:O	1:G:218:ARG:C	2.59	0.41
1:G:235:LEU:HD23	1:G:235:LEU:HA	1.92	0.41
1:H:441:PRO:HB2	1:H:456:LEU:CD1	2.51	0.41
1:A:310:LYS:O	1:A:314:MET:HG2	2.21	0.41
1:B:433:PHE:C	1:B:433:PHE:CD2	2.95	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:E:44:MET:HA	1:E:44:MET:CE	2.51	0.41
1:G:130:LYS:HG3	1:G:134:LEU:CD1	2.42	0.41
1:H:167:LYS:HD2	1:H:167:LYS:HA	1.82	0.41
1:H:227:VAL:HG12	1:H:230:ALA:HB2	2.03	0.41
1:A:202:SER:HG	1:A:370:ARG:HB2	1.87	0.40
1:B:189:ASP:HB3	1:B:192:LEU:CD1	2.51	0.40
1:B:342:LEU:HD23	1:B:343:VAL:N	2.36	0.40
1:C:130:LYS:HG3	1:C:134:LEU:CD1	2.41	0.40
1:C:412:SER:HB2	1:C:434:ALA:O	2.20	0.40
1:G: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:H:44:MET:HA	1:H:44:MET:CE	2.51	0.40
1:A:273:VAL:HG11	1:A:297:TYR:CB	2.48	0.40
1:B:348:ILE:O	1:B:348:ILE:CG2	2.70	0.40
1:C:267:GLU:C	1:C:269:LEU:N	2.73	0.40
1:C:369:ILE:O	1:C:370:ARG:HG2	2.21	0.40
1:D:25:ILE:HG23	1:D:104:LEU:HB3	2.03	0.40
1:D:155:MET:HE3	1:D:171:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:SER:OG	1:D:370:ARG:HB2	2.20	0.40
1:D:403:GLY:O	1:D:406:SER:HB2	2.22	0.40
1:E:56:VAL:O	1:E:56:VAL:HG13	2.21	0.40
1:F:227:VAL:CG1	1:F:230:ALA:HB2	2.52	0.40
1:G:225:LYS:CG	1:G:345:GLU:HB3	2.51	0.40
1:G:225:LYS:HG3	1:G:345:GLU:HB3	2.03	0.40
1:G:266:SER:HB3	1:G:268:MET:CE	2.51	0.40
1:G:267:GLU:C	1:G:269:LEU:N	2.73	0.40
1:G:433:PHE:CD2	1:G:433:PHE:O	2.75	0.40
1:A:197:LYS:HD2	1:A:377:ILE:HG22	2.03	0.40
1:B:174:ILE:HD13	1:B:387:ALA:CB	2.51	0.40
1:D:225:LYS:HG3	1:D:345:GLU:HB3	2.04	0.40
1:D:476:PHE:O	1:D:477:THR:C	2.60	0.40
1:E:79:ILE:O	1:E:83:LYS:HB2	2.21	0.40
1:F:21:GLN:O	1:F:25:ILE:HG13	2.22	0.40
1:G:153:ILE:HG13	1:G:489:VAL:HG23	2.03	0.40
1:G:155:MET:HE3	1:G:171:ALA:HB2	2.03	0.40
1:G:158:ILE:O	1:G:161:LYS:HB2	2.21	0.40
1:G:357:GLU: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:225:LYS:CG	1:A:345:GLU:HB3	2.51	0.40
1:A:476:PHE:O	1:A:477:THR:C	2.59	0.40
1:C:474:ASN:HD22	1:C:486:ASN:HD22	1.70	0.40
1:D: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:178:VAL:HG22	1:H:388:VAL:HG13	2.02	0.40
1:H:197:LYS:HD2	1:H:377:ILE:HG22	2.03	0.40
1:C:225:LYS:HG3	1:C:345:GLU:HB3	2.03	0.40
1:E:174:ILE:HD13	1:E:387:ALA:CB	2.52	0.40
1:F:34:THR:O	1:F:46:LYS:HE2	2.21	0.40
1:G:202:SER:HG	1:G:203:ILE:N	2.19	0.40
1:H:102:GLU:HG2	1:H:439:VAL:HB	2.02	0.40
1:H:490:GLU:OE1	1:H:495:LYS:HE3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:O	1:C:185:GLU:OE2[4_556]	1.91	0.29
1:E:148:GLU:OE1	1:G:130:LYS:NZ[4_445]	1.99	0.21
1:A:451:ASP:OD1	1:G:425:ARG:NH2[2_556]	2.03	0.17
1: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/521 (93%)	424 (87%)	53 (11%)	8 (2%)	9	43
1	B	485/521 (93%)	423 (87%)	55 (11%)	7 (1%)	11	46
1	C	485/521 (93%)	422 (87%)	56 (12%)	7 (1%)	11	46
1	D	485/521 (93%)	423 (87%)	54 (11%)	8 (2%)	9	43
1	E	485/521 (93%)	426 (88%)	52 (11%)	7 (1%)	11	46
1	F	485/521 (93%)	427 (88%)	50 (10%)	8 (2%)	9	43
1	G	485/521 (93%)	424 (87%)	54 (11%)	7 (1%)	11	46
1	H	485/521 (93%)	425 (88%)	52 (11%)	8 (2%)	9	43
All	All	3880/4168 (93%)	3394 (88%)	426 (11%)	60 (2%)	10	45

All (60) Ramachandran outliers are listed below:

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

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

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Mol	Chain	Res	Type
1	B	426	GLU
1	D	426	GLU
1	E	89	VAL
1	E	166	ALA
1	H	426	GLU
1	A	89	VAL
1	D	89	VAL
1	D	166	ALA
1	F	166	ALA
1	G	89	VAL
1	H	166	ALA
1	B	89	VAL
1	F	426	GLU
1	C	89	VAL
1	H	89	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/413 (94%)	371 (96%)	17 (4%)	28	62
1	B	388/413 (94%)	369 (95%)	19 (5%)	25	59
1	C	388/413 (94%)	370 (95%)	18 (5%)	27	61
1	D	388/413 (94%)	370 (95%)	18 (5%)	27	61
1	E	388/413 (94%)	371 (96%)	17 (4%)	28	62
1	F	388/413 (94%)	370 (95%)	18 (5%)	27	61
1	G	388/413 (94%)	369 (95%)	19 (5%)	25	59
1	H	388/413 (94%)	372 (96%)	16 (4%)	30	63
All	All	3104/3304 (94%)	2962 (95%)	142 (5%)	27	61

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

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

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

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	F	545	2	24,29,29	0.96	0	29,45,45	1.70	6 (20%)
4	SO4	E	546	2	4,4,4	0.25	0	6,6,6	0.32	0
3	ADP	C	545	2	24,29,29	0.97	1 (4%)	29,45,45	1.70	7 (24%)
4	SO4	B	546	2	4,4,4	0.17	0	6,6,6	0.29	0
4	SO4	F	546	2	4,4,4	0.13	0	6,6,6	0.25	0
3	ADP	D	545	2	24,29,29	1.02	1 (4%)	29,45,45	1.75	6 (20%)
3	ADP	A	545	2	24,29,29	1.01	1 (4%)	29,45,45	1.74	7 (24%)
3	ADP	B	545	2	24,29,29	1.07	2 (8%)	29,45,45	1.67	5 (17%)
4	SO4	A	546	2	4,4,4	0.19	0	6,6,6	0.21	0
4	SO4	C	546	2	4,4,4	0.17	0	6,6,6	0.25	0
4	SO4	D	546	2	4,4,4	0.24	0	6,6,6	0.32	0
3	ADP	G	545	2	24,29,29	1.11	3 (12%)	29,45,45	1.72	7 (24%)
4	SO4	G	546	2	4,4,4	0.15	0	6,6,6	0.32	0
3	ADP	H	545	2	24,29,29	1.06	2 (8%)	29,45,45	1.69	7 (24%)
4	SO4	H	546	2	4,4,4	0.20	0	6,6,6	0.24	0
3	ADP	E	545	2	24,29,29	0.94	1 (4%)	29,45,45	1.68	6 (20%)

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	F	545	2	-	5/12/32/32	0/3/3/3
3	ADP	C	545	2	-	5/12/32/32	0/3/3/3
3	ADP	D	545	2	-	5/12/32/32	0/3/3/3
3	ADP	A	545	2	-	5/12/32/32	0/3/3/3
3	ADP	B	545	2	-	5/12/32/32	0/3/3/3
3	ADP	G	545	2	-	5/12/32/32	0/3/3/3
3	ADP	H	545	2	-	5/12/32/32	0/3/3/3
3	ADP	E	545	2	-	5/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	545	ADP	C2-N3	2.61	1.36	1.32
3	H	545	ADP	O4'-C1'	2.39	1.44	1.41
3	G	545	ADP	C5-C4	2.32	1.47	1.40
3	G	545	ADP	O4'-C1'	2.31	1.44	1.41
3	H	545	ADP	C5-C4	2.25	1.46	1.40
3	G	545	ADP	C2-N3	2.24	1.35	1.32
3	B	545	ADP	C5-C4	2.13	1.46	1.40
3	E	545	ADP	C5-C4	2.07	1.46	1.40
3	A	545	ADP	C5-C4	2.05	1.46	1.40
3	C	545	ADP	C2-N3	2.04	1.35	1.32
3	D	545	ADP	C2-N3	2.04	1.35	1.32

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	545	ADP	N3-C2-N1	-4.54	121.58	128.68
3	G	545	ADP	N3-C2-N1	-4.23	122.06	128.68
3	A	545	ADP	N3-C2-N1	-4.20	122.11	128.68
3	H	545	ADP	N3-C2-N1	-4.12	122.24	128.68
3	D	545	ADP	N3-C2-N1	-4.04	122.36	128.68
3	F	545	ADP	N3-C2-N1	-4.03	122.38	128.68
3	B	545	ADP	PA-O3A-PB	-3.95	119.26	132.83
3	C	545	ADP	N3-C2-N1	-3.95	122.51	128.68
3	G	545	ADP	PA-O3A-PB	-3.82	119.70	132.83
3	C	545	ADP	PA-O3A-PB	-3.80	119.80	132.83
3	D	545	ADP	PA-O3A-PB	-3.75	119.96	132.83
3	E	545	ADP	PA-O3A-PB	-3.63	120.38	132.83
3	B	545	ADP	N3-C2-N1	-3.51	123.20	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	545	ADP	PA-O3A-PB	-3.50	120.81	132.83
3	H	545	ADP	O3'-C3'-C2'	-3.45	100.67	111.82
3	A	545	ADP	PA-O3A-PB	-3.44	121.03	132.83
3	F	545	ADP	PA-O3A-PB	-3.40	121.16	132.83
3	D	545	ADP	O3'-C3'-C2'	-3.39	100.87	111.82
3	A	545	ADP	O2'-C2'-C3'	-3.34	101.02	111.82
3	A	545	ADP	O3'-C3'-C2'	-3.33	101.03	111.82
3	F	545	ADP	O3'-C3'-C2'	-3.03	102.03	111.82
3	G	545	ADP	O3'-C3'-C2'	-2.97	102.23	111.82
3	B	545	ADP	O3'-C3'-C2'	-2.93	102.35	111.82
3	B	545	ADP	O2'-C2'-C3'	-2.91	102.41	111.82
3	C	545	ADP	C4-C5-N7	-2.87	106.40	109.40
3	C	545	ADP	O2'-C2'-C3'	-2.85	102.59	111.82
3	B	545	ADP	C4-C5-N7	-2.83	106.45	109.40
3	C	545	ADP	O3'-C3'-C2'	-2.81	102.73	111.82
3	F	545	ADP	O2'-C2'-C3'	-2.77	102.86	111.82
3	D	545	ADP	O2'-C2'-C3'	-2.59	103.44	111.82
3	D	545	ADP	C2'-C3'-C4'	2.59	107.67	102.64
3	H	545	ADP	C2'-C3'-C4'	2.58	107.66	102.64
3	A	545	ADP	C2'-C3'-C4'	2.56	107.62	102.64
3	G	545	ADP	C2'-C3'-C4'	2.55	107.59	102.64
3	E	545	ADP	O2'-C2'-C3'	-2.55	103.58	111.82
3	E	545	ADP	O3'-C3'-C2'	-2.47	103.84	111.82
3	A	545	ADP	N6-C6-N1	2.39	123.53	118.57
3	G	545	ADP	O2'-C2'-C3'	-2.34	104.24	111.82
3	E	545	ADP	C2-N1-C6	2.30	122.68	118.75
3	G	545	ADP	O2A-PA-O1A	2.29	123.55	112.24
3	H	545	ADP	O2'-C2'-C3'	-2.26	104.51	111.82
3	H	545	ADP	O2A-PA-O1A	2.25	123.38	112.24
3	D	545	ADP	C4-C5-N7	-2.24	107.06	109.40
3	E	545	ADP	C2'-C3'-C4'	2.21	106.93	102.64
3	C	545	ADP	C2'-C3'-C4'	2.18	106.87	102.64
3	H	545	ADP	C2-N1-C6	2.17	122.47	118.75
3	A	545	ADP	C2-N1-C6	2.10	122.34	118.75
3	F	545	ADP	C2'-C3'-C4'	2.08	106.69	102.64
3	F	545	ADP	C4-C5-N7	-2.02	107.29	109.40
3	C	545	ADP	O2A-PA-O1A	2.00	122.15	112.24
3	G	545	ADP	C2-N1-C6	2.00	122.18	118.75

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	C3'-C4'-C5'-O5'
3	B	545	ADP	C5'-O5'-PA-O1A
3	B	545	ADP	C5'-O5'-PA-O2A
3	B	545	ADP	C3'-C4'-C5'-O5'
3	C	545	ADP	C5'-O5'-PA-O1A
3	C	545	ADP	C5'-O5'-PA-O2A
3	C	545	ADP	C3'-C4'-C5'-O5'
3	D	545	ADP	C5'-O5'-PA-O1A
3	D	545	ADP	C5'-O5'-PA-O2A
3	D	545	ADP	C3'-C4'-C5'-O5'
3	E	545	ADP	C5'-O5'-PA-O1A
3	E	545	ADP	C5'-O5'-PA-O2A
3	E	545	ADP	C3'-C4'-C5'-O5'
3	F	545	ADP	C5'-O5'-PA-O1A
3	F	545	ADP	C5'-O5'-PA-O2A
3	F	545	ADP	C3'-C4'-C5'-O5'
3	G	545	ADP	C5'-O5'-PA-O1A
3	G	545	ADP	C5'-O5'-PA-O2A
3	G	545	ADP	C3'-C4'-C5'-O5'
3	H	545	ADP	C5'-O5'-PA-O1A
3	H	545	ADP	C5'-O5'-PA-O2A
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'
3	A	545	ADP	C5'-O5'-PA-O3A
3	B	545	ADP	C5'-O5'-PA-O3A
3	C	545	ADP	C5'-O5'-PA-O3A
3	D	545	ADP	C5'-O5'-PA-O3A
3	E	545	ADP	C5'-O5'-PA-O3A
3	F	545	ADP	C5'-O5'-PA-O3A
3	G	545	ADP	C5'-O5'-PA-O3A
3	H	545	ADP	C5'-O5'-PA-O3A

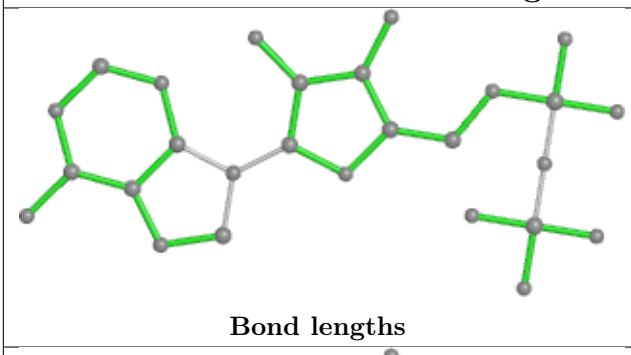
There are no ring outliers.

16 monomers are involved in 48 short contacts:

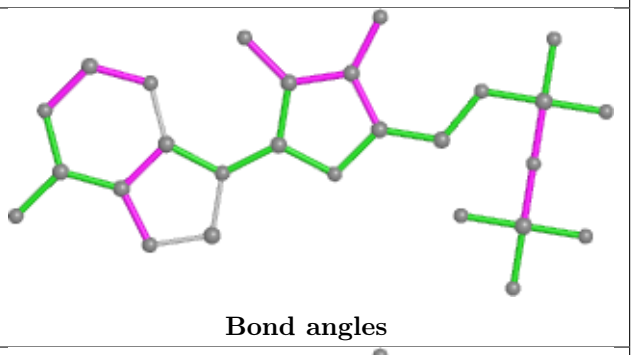
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	545	ADP	6	0
4	E	546	SO4	4	0
3	C	545	ADP	7	0
4	B	546	SO4	4	0
4	F	546	SO4	4	0
3	D	545	ADP	6	0
3	A	545	ADP	5	0
3	B	545	ADP	6	0
4	A	546	SO4	3	0
4	C	546	SO4	5	0
4	D	546	SO4	4	0
3	G	545	ADP	6	0
4	G	546	SO4	4	0
3	H	545	ADP	6	0
4	H	546	SO4	4	0
3	E	545	ADP	6	0

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 then 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.

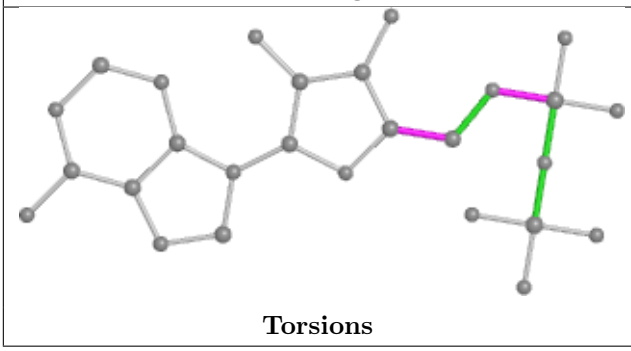
Ligand ADP F 545



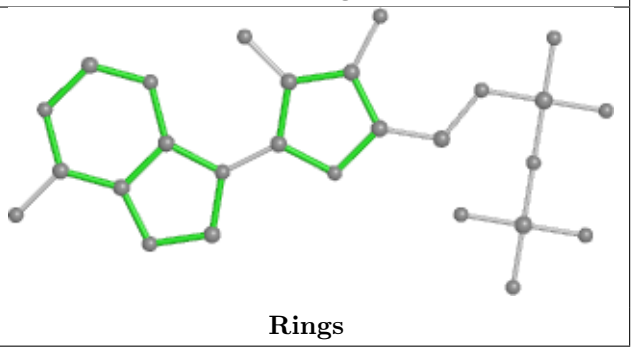
Bond lengths



Bond angles

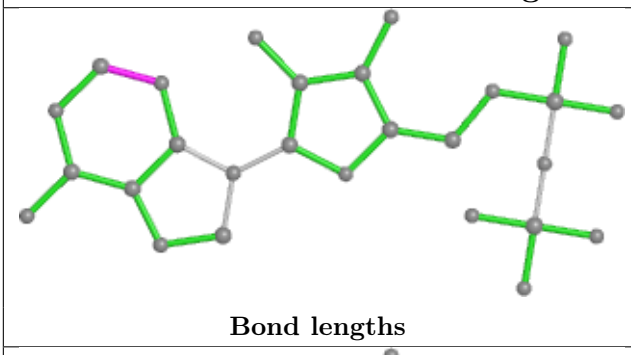


Torsions

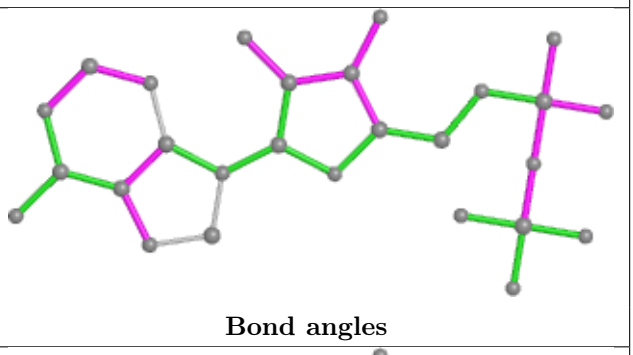


Rings

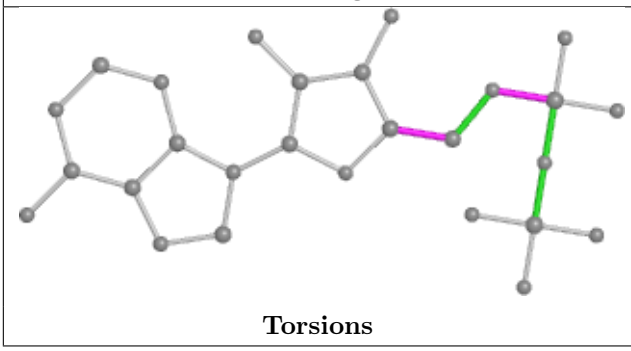
Ligand ADP C 545



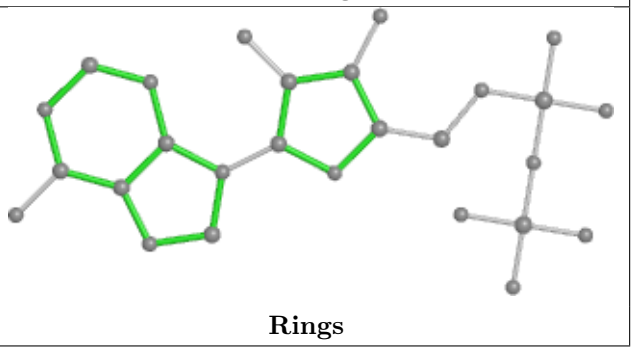
Bond lengths



Bond angles

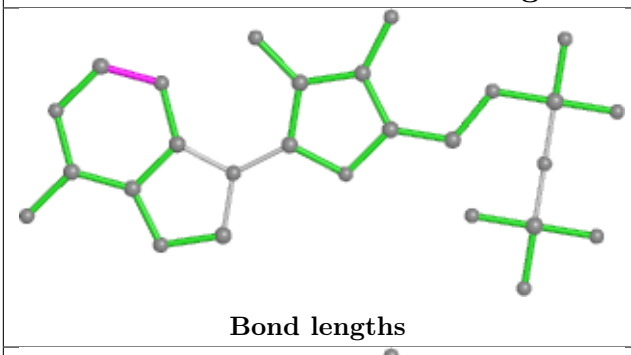


Torsions

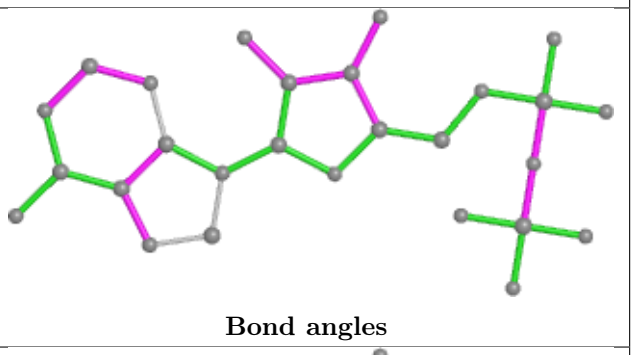


Rings

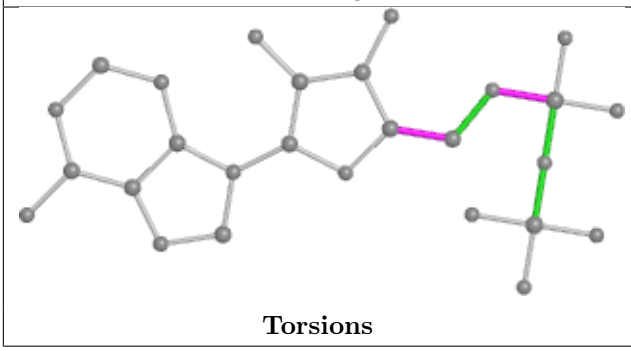
Ligand ADP D 545



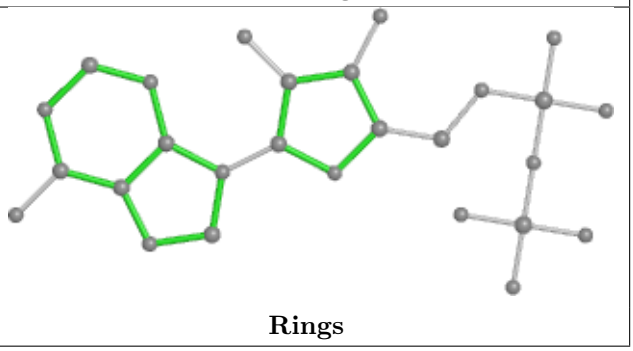
Bond lengths



Bond angles

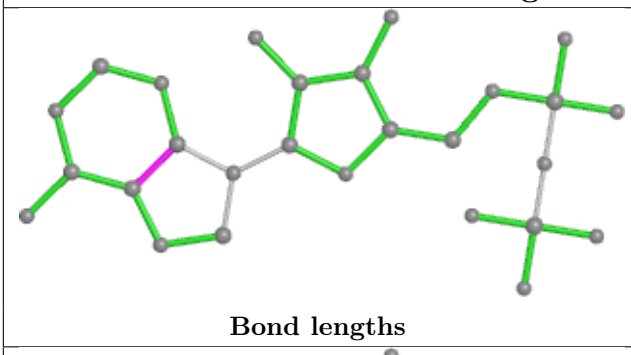


Torsions

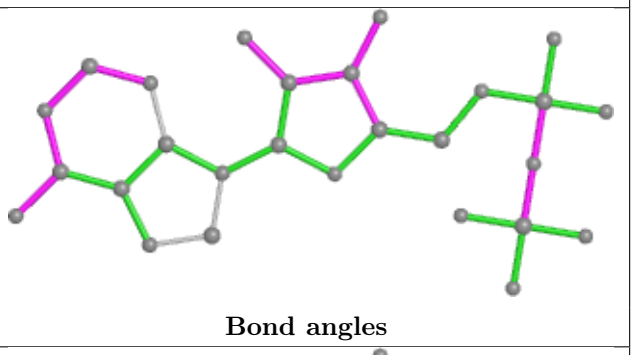


Rings

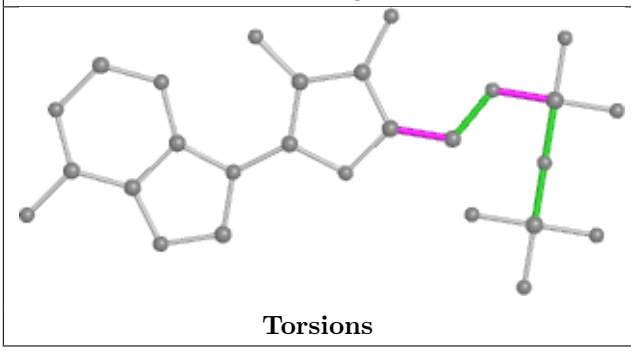
Ligand ADP A 545



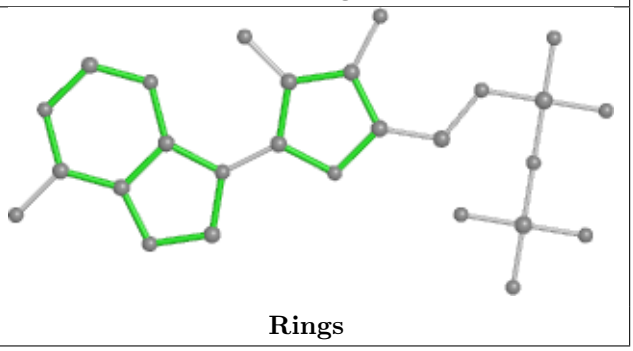
Bond lengths



Bond angles

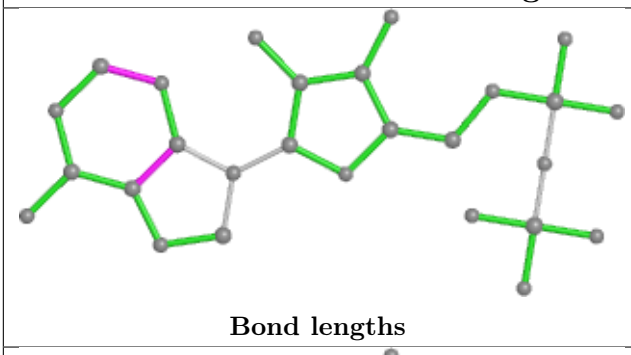


Torsions

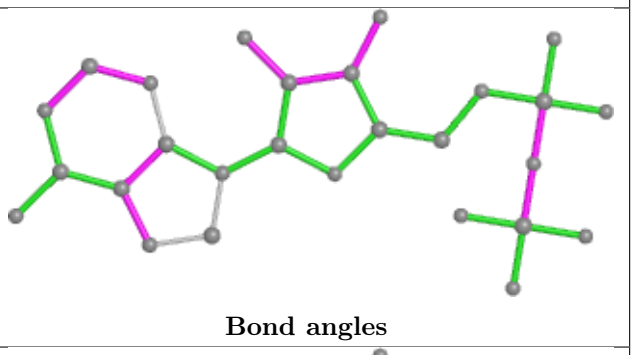


Rings

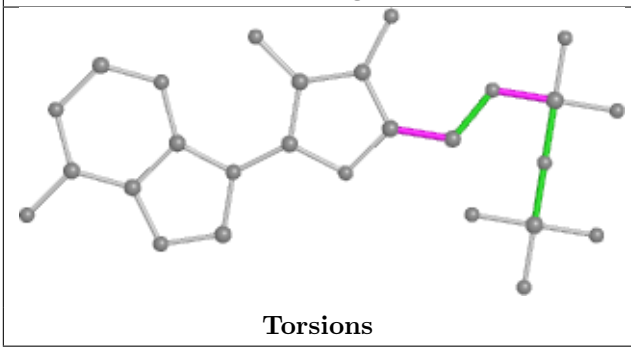
Ligand ADP B 545



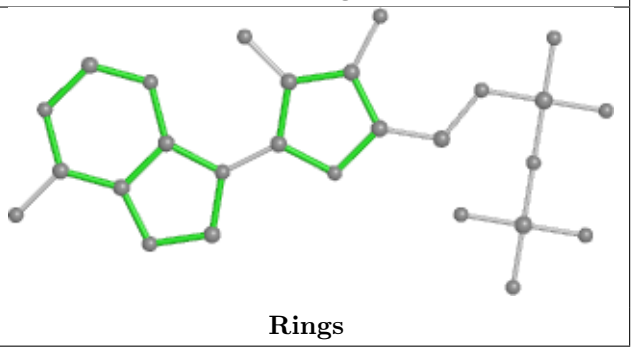
Bond lengths



Bond angles

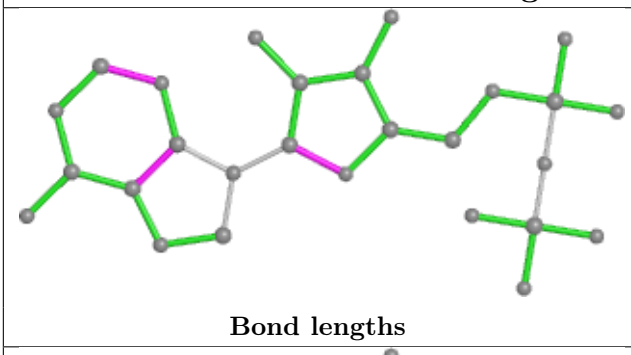


Torsions

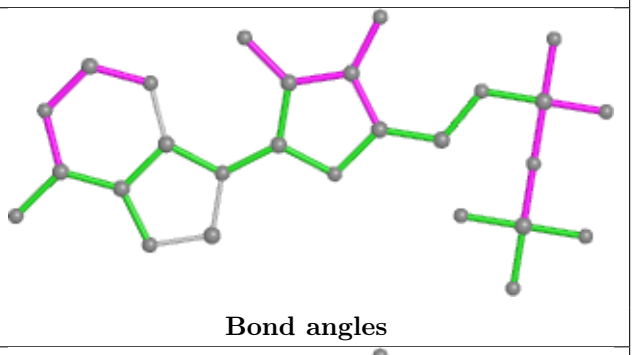


Rings

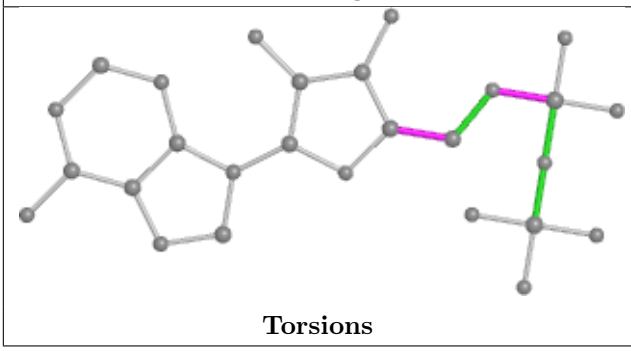
Ligand ADP G 545



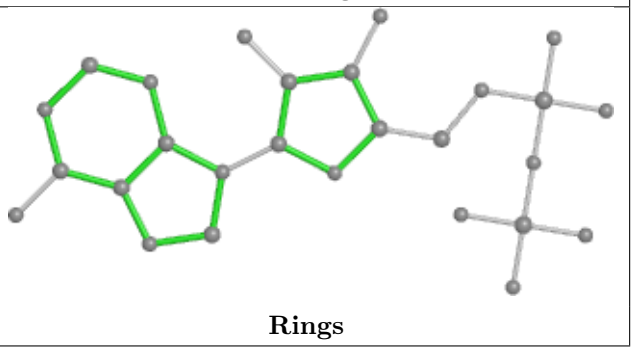
Bond lengths



Bond angles

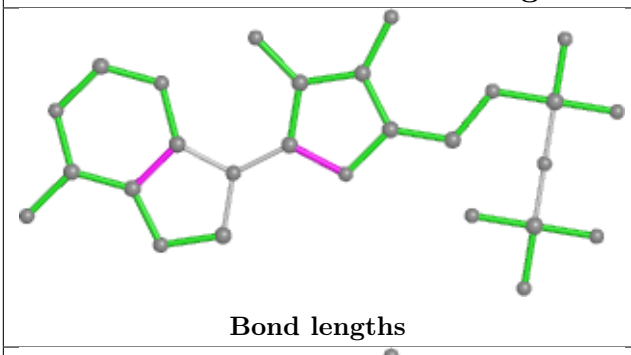


Torsions

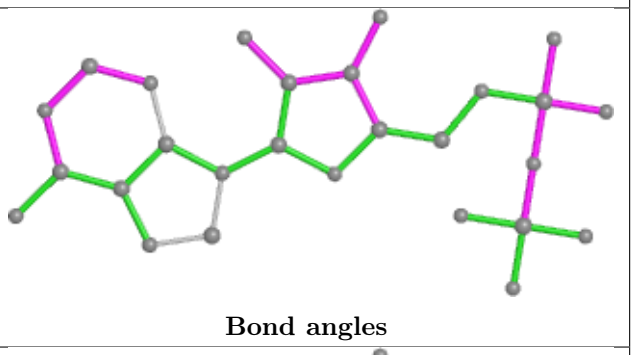


Rings

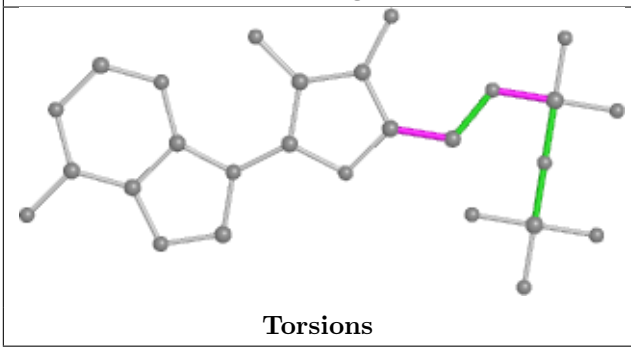
Ligand ADP H 545



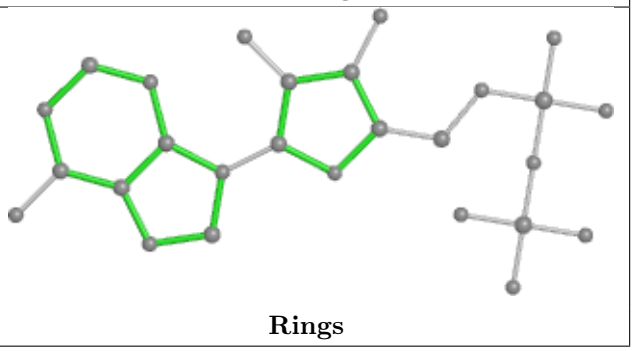
Bond lengths



Bond angles

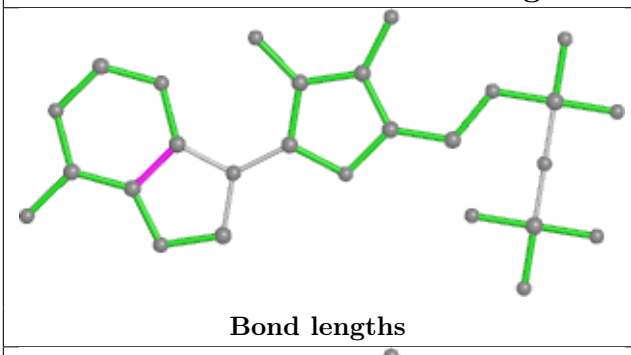


Torsions

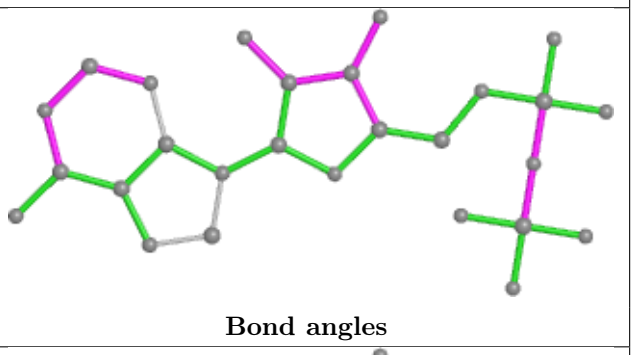


Rings

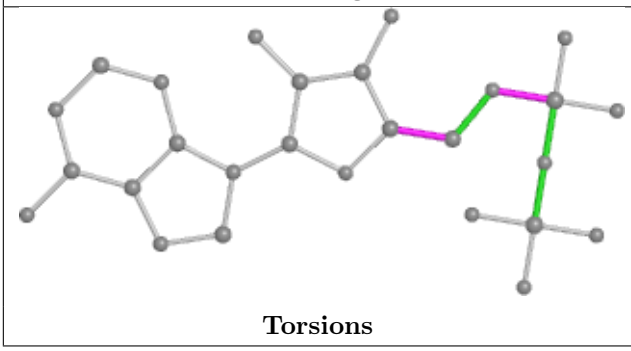
Ligand ADP E 545



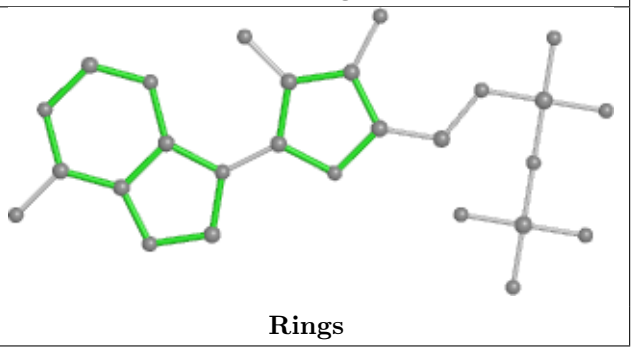
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.08	41 (8%) 11 11	26, 88, 242, 287	0
1	B	487/521 (93%)	-0.12	16 (3%) 46 41	38, 90, 196, 247	0
1	C	487/521 (93%)	0.25	44 (9%) 9 10	39, 88, 282, 341	0
1	D	487/521 (93%)	0.18	50 (10%) 6 7	42, 103, 243, 287	0
1	E	487/521 (93%)	0.22	59 (12%) 4 5	34, 94, 252, 294	0
1	F	487/521 (93%)	0.32	58 (11%) 4 5	41, 100, 258, 295	0
1	G	487/521 (93%)	0.35	49 (10%) 7 7	41, 122, 245, 291	0
1	H	487/521 (93%)	0.24	35 (7%) 15 15	64, 127, 229, 274	0
All	All	3896/4168 (93%)	0.19	352 (9%) 9 10	26, 102, 250, 341	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	239	ILE	15.5
1	C	327	THR	15.4
1	C	238	ALA	15.1
1	F	281	ALA	12.3
1	C	239	ILE	10.8
1	E	281	ALA	10.7
1	G	238	ALA	10.7
1	D	266	SER	10.6
1	E	327	THR	10.1
1	D	281	ALA	9.9
1	C	289	GLY	9.5
1	C	264	THR	9.3
1	E	303	ILE	9.2
1	E	298	LEU	8.9
1	C	281	ALA	8.6
1	F	282	ASN	7.9

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Mol	Chain	Res	Type	RSRZ
1	F	268	MET	7.9
1	A	239	ILE	7.8
1	D	267	GLU	7.7
1	F	335	GLN	7.4
1	C	279	SER	7.4
1	A	327	THR	7.3
1	C	303	ILE	7.3
1	F	228	THR	7.2
1	F	302	GLY	7.2
1	G	279	SER	7.2
1	G	240	GLU	6.9
1	A	281	ALA	6.8
1	F	290	ILE	6.7
1	H	294	ALA	6.7
1	F	303	ILE	6.6
1	F	275	GLU	6.6
1	C	302	GLY	6.4
1	F	219	VAL	6.4
1	F	327	THR	6.2
1	F	266	SER	6.0
1	F	270	LYS	6.0
1	C	267	GLU	6.0
1	A	228	THR	5.8
1	C	335	GLN	5.8
1	G	303	ILE	5.7
1	E	240	GLU	5.7
1	A	303	ILE	5.7
1	E	302	GLY	5.7
1	E	264	THR	5.6
1	E	230	ALA	5.6
1	A	279	SER	5.6
1	E	225	LYS	5.5
1	D	239	ILE	5.5
1	C	263	GLU	5.4
1	G	236	ASN	5.4
1	F	271	ASP	5.4
1	E	328	ASN	5.2
1	E	343	VAL	5.2
1	H	279	SER	5.2
1	G	327	THR	5.2
1	H	281	ALA	5.1
1	F	239	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	237	CYS	5.0
1	D	303	ILE	5.0
1	F	265	ALA	5.0
1	G	237	CYS	4.9
1	A	235	LEU	4.9
1	G	235	LEU	4.8
1	C	270	LYS	4.8
1	E	276	ILE	4.8
1	E	294	ALA	4.8
1	F	285	PHE	4.8
1	G	266	SER	4.7
1	C	282	ASN	4.7
1	E	266	SER	4.7
1	C	326	ILE	4.6
1	E	227	VAL	4.6
1	C	271	ASP	4.5
1	F	320	ALA	4.5
1	C	276	ILE	4.5
1	F	238	ALA	4.5
1	C	290	ILE	4.5
1	A	240	GLU	4.5
1	A	302	GLY	4.4
1	H	230	ALA	4.4
1	E	267	GLU	4.4
1	A	236	ASN	4.4
1	C	268	MET	4.4
1	G	268	MET	4.4
1	A	276	ILE	4.4
1	G	276	ILE	4.4
1	A	326	ILE	4.3
1	E	219	VAL	4.3
1	C	230	ALA	4.3
1	C	343	VAL	4.3
1	H	178	VAL	4.3
1	G	358	GLU	4.3
1	D	263	GLU	4.3
1	F	236	ASN	4.3
1	A	238	ALA	4.2
1	D	294	ALA	4.2
1	E	297	TYR	4.2
1	G	281	ALA	4.2
1	A	267	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	330	LYS	4.1
1	C	273	VAL	4.1
1	G	290	ILE	4.1
1	G	234	LEU	4.1
1	F	291	ASP	4.1
1	D	358	GLU	4.0
1	C	291	ASP	4.0
1	D	236	ASN	4.0
1	D	298	LEU	4.0
1	G	343	VAL	4.0
1	C	237	CYS	4.0
1	G	330	LYS	4.0
1	D	280	GLY	4.0
1	B	264	THR	3.9
1	F	294	ALA	3.9
1	H	266	SER	3.9
1	E	285	PHE	3.9
1	F	215	ASP	3.9
1	D	282	ASN	3.8
1	C	340	ALA	3.8
1	F	358	GLU	3.8
1	C	336	ASP	3.8
1	A	227	VAL	3.7
1	D	296	HIS	3.7
1	C	227	VAL	3.7
1	E	232	ILE	3.7
1	C	240	GLU	3.7
1	F	334	ALA	3.7
1	H	263	GLU	3.7
1	D	349	SER	3.7
1	E	223	MET	3.7
1	F	279	SER	3.6
1	E	349	SER	3.6
1	B	327	THR	3.6
1	A	280	GLY	3.6
1	D	268	MET	3.6
1	F	274	ALA	3.6
1	D	215	ASP	3.6
1	E	228	THR	3.5
1	A	273	VAL	3.5
1	A	234	LEU	3.5
1	H	297	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	364	ALA	3.5
1	A	265	ALA	3.5
1	F	276	ILE	3.5
1	E	331	ASP	3.4
1	E	265	ALA	3.4
1	H	264	THR	3.4
1	D	271	ASP	3.4
1	D	238	ALA	3.4
1	E	293	LEU	3.4
1	G	294	ALA	3.4
1	G	232	ILE	3.4
1	H	280	GLY	3.4
1	F	232	ILE	3.4
1	A	294	ALA	3.4
1	E	271	ASP	3.4
1	A	266	SER	3.3
1	D	285	PHE	3.3
1	C	228	THR	3.3
1	F	298	LEU	3.3
1	F	342	LEU	3.3
1	D	240	GLU	3.3
1	C	226	LYS	3.3
1	D	219	VAL	3.3
1	H	321	THR	3.3
1	F	227	VAL	3.3
1	A	225	LYS	3.3
1	F	357	GLU	3.2
1	D	270	LYS	3.2
1	H	268	MET	3.2
1	B	235	LEU	3.2
1	H	317	LEU	3.2
1	G	305	ALA	3.2
1	B	267	GLU	3.2
1	E	220	SER	3.2
1	H	335	GLN	3.1
1	B	239	ILE	3.1
1	A	268	MET	3.1
1	D	276	ILE	3.1
1	D	364	ALA	3.1
1	A	290	ILE	3.1
1	H	267	GLU	3.1
1	A	328	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	237	CYS	3.1
1	G	227	VAL	3.1
1	F	235	LEU	3.1
1	D	264	THR	3.1
1	D	351	ASP	3.0
1	H	210	LYS	3.0
1	F	267	GLU	3.0
1	E	280	GLY	3.0
1	C	232	ILE	3.0
1	F	283	VAL	3.0
1	C	215	ASP	3.0
1	D	287	GLN	3.0
1	D	327	THR	3.0
1	E	289	GLY	3.0
1	D	342	LEU	3.0
1	G	306	ALA	3.0
1	B	337	LEU	3.0
1	D	350	GLY	3.0
1	B	240	GLU	3.0
1	D	232	ILE	3.0
1	H	239	ILE	3.0
1	D	340	ALA	2.9
1	F	280	GLY	2.9
1	H	53	GLY	2.9
1	G	349	SER	2.9
1	C	301	GLU	2.9
1	E	268	MET	2.9
1	D	320	ALA	2.9
1	G	480	VAL	2.9
1	G	334	ALA	2.9
1	A	298	LEU	2.9
1	G	320	ALA	2.9
1	E	337	LEU	2.8
1	C	280	GLY	2.8
1	E	238	ALA	2.8
1	E	330	LYS	2.8
1	F	337	LEU	2.8
1	A	337	LEU	2.8
1	D	53	GLY	2.8
1	G	168	GLU	2.8
1	A	299	ALA	2.8
1	E	283	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	144	ALA	2.7
1	D	265	ALA	2.7
1	C	269	LEU	2.7
1	H	327	THR	2.7
1	E	224	PRO	2.7
1	E	239	ILE	2.7
1	D	272	MET	2.7
1	H	273	VAL	2.6
1	H	215	ASP	2.6
1	E	234	LEU	2.6
1	F	317	LEU	2.6
1	E	233	ALA	2.6
1	F	351	ASP	2.6
1	D	359	CYS	2.6
1	E	215	ASP	2.6
1	G	357	GLU	2.6
1	F	226	LYS	2.6
1	C	220	SER	2.6
1	C	355	PHE	2.6
1	G	356	VAL	2.6
1	G	342	LEU	2.6
1	G	302	GLY	2.6
1	B	298	LEU	2.6
1	D	275	GLU	2.6
1	D	229	ASP	2.6
1	G	298	LEU	2.5
1	G	331	ASP	2.5
1	F	264	THR	2.5
1	H	320	ALA	2.5
1	H	303	ILE	2.5
1	D	279	SER	2.5
1	H	240	GLU	2.5
1	H	295	GLN	2.5
1	B	266	SER	2.5
1	A	232	ILE	2.5
1	G	222	GLN	2.5
1	C	292	ASP	2.5
1	E	282	ASN	2.5
1	F	316	LYS	2.5
1	H	328	ASN	2.5
1	A	329	ILE	2.5
1	D	295	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	519	GLU	2.5
1	E	356	VAL	2.5
1	G	278	ALA	2.5
1	G	287	GLN	2.4
1	H	301	GLU	2.4
1	A	297	TYR	2.4
1	B	290	ILE	2.4
1	F	305	ALA	2.4
1	E	263	GLU	2.4
1	A	330	LYS	2.4
1	C	298	LEU	2.4
1	C	266	SER	2.4
1	G	307	ARG	2.4
1	F	331	ASP	2.4
1	H	351	ASP	2.4
1	E	235	LEU	2.4
1	A	335	GLN	2.4
1	F	360	LYS	2.4
1	E	323	ALA	2.4
1	F	321	THR	2.4
1	B	518	ALA	2.3
1	F	341	GLY	2.3
1	B	238	ALA	2.3
1	F	359	CYS	2.3
1	G	316	LYS	2.3
1	G	144	ALA	2.3
1	G	285	PHE	2.3
1	H	232	ILE	2.3
1	H	177	ALA	2.3
1	E	326	ILE	2.3
1	F	229	ASP	2.3
1	E	279	SER	2.3
1	G	213	LEU	2.3
1	D	316	LYS	2.3
1	G	291	ASP	2.3
1	H	184	ASP	2.3
1	G	230	ALA	2.3
1	F	304	VAL	2.3
1	A	229	ASP	2.3
1	C	234	LEU	2.2
1	G	280	GLY	2.2
1	A	278	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	334	ALA	2.2
1	D	334	ALA	2.2
1	F	336	ASP	2.2
1	D	335	GLN	2.2
1	E	345	GLU	2.2
1	B	295	GLN	2.2
1	C	236	ASN	2.2
1	E	299	ALA	2.2
1	H	282	ASN	2.2
1	E	321	THR	2.2
1	F	319	LYS	2.2
1	D	302	GLY	2.2
1	G	319	LYS	2.2
1	G	328	ASN	2.2
1	G	143	GLY	2.2
1	B	302	GLY	2.2
1	C	328	ASN	2.2
1	E	291	ASP	2.1
1	G	335	GLN	2.1
1	E	354	ILE	2.1
1	E	342	LEU	2.1
1	E	301	GLU	2.1
1	D	290	ILE	2.1
1	A	282	ASN	2.1
1	F	234	LEU	2.1
1	E	226	LYS	2.1
1	E	319	LYS	2.1
1	A	334	ALA	2.1
1	D	297	TYR	2.1
1	B	273	VAL	2.1
1	E	270	LYS	2.1
1	A	336	ASP	2.1
1	F	364	ALA	2.1
1	B	303	ILE	2.0
1	A	291	ASP	2.0
1	E	316	LYS	2.0
1	E	236	ASN	2.0
1	F	300	LYS	2.0
1	H	271	ASP	2.0
1	H	358	GLU	2.0
1	D	341	GLY	2.0
1	D	337	LEU	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 monosaccharides 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, 95^{th} 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.

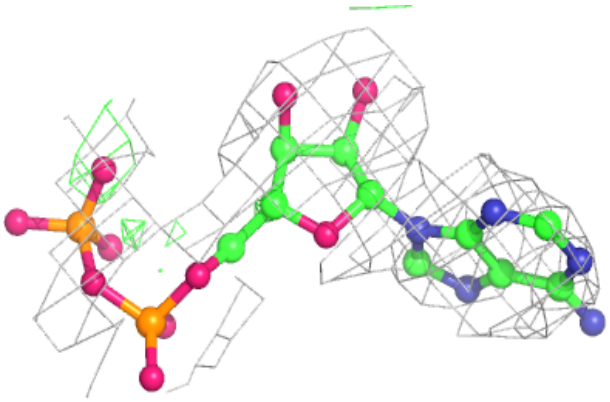
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	H	545	27/27	0.92	0.22	72,100,114,124	0
2	MG	G	544	1/1	0.95	0.26	111,111,111,111	0
2	MG	H	544	1/1	0.95	0.36	111,111,111,111	0
3	ADP	B	545	27/27	0.95	0.20	47,65,83,90	0
3	ADP	C	545	27/27	0.95	0.18	46,68,88,95	0
3	ADP	E	545	27/27	0.95	0.22	49,70,86,98	0
3	ADP	G	545	27/27	0.95	0.20	71,99,116,122	0
2	MG	C	544	1/1	0.95	0.20	57,57,57,57	0
3	ADP	A	545	27/27	0.96	0.19	38,59,78,83	0
3	ADP	F	545	27/27	0.96	0.21	45,69,88,95	0
4	SO4	H	546	5/5	0.96	0.14	96,104,122,137	0
2	MG	D	544	1/1	0.97	0.25	92,92,92,92	0
2	MG	E	544	1/1	0.97	0.23	55,55,55,55	0
2	MG	F	544	1/1	0.97	0.35	83,83,83,83	0
2	MG	B	544	1/1	0.97	0.24	58,58,58,58	0
4	SO4	G	546	5/5	0.97	0.18	75,90,123,124	0
3	ADP	D	545	27/27	0.97	0.20	66,89,104,118	0
4	SO4	B	546	5/5	0.98	0.22	59,71,88,107	0
4	SO4	C	546	5/5	0.98	0.21	71,78,107,110	0
4	SO4	D	546	5/5	0.98	0.19	66,71,89,100	0
4	SO4	E	546	5/5	0.98	0.21	65,72,99,100	0
4	SO4	F	546	5/5	0.98	0.23	100,101,134,137	0
2	MG	A	544	1/1	0.98	0.22	65,65,65,65	0
4	SO4	A	546	5/5	0.98	0.20	76,81,105,106	0

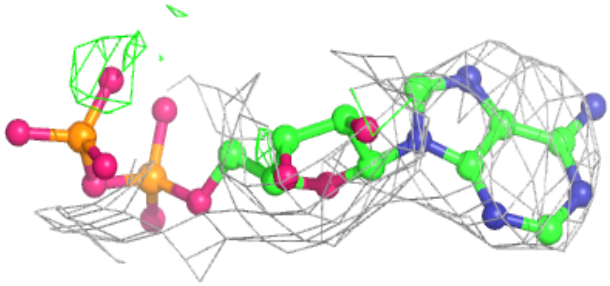
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

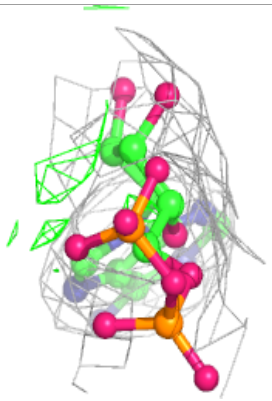
orientation to approximate a three-dimensional view.

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)

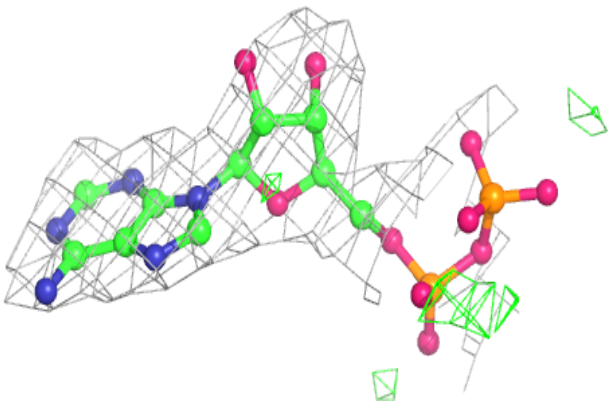


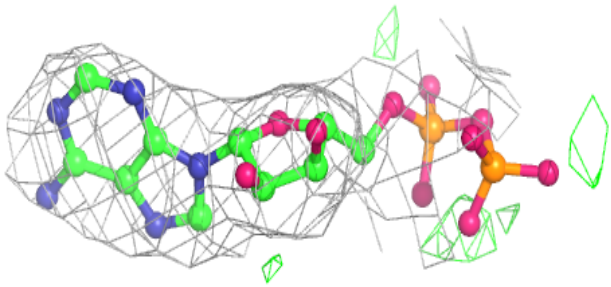


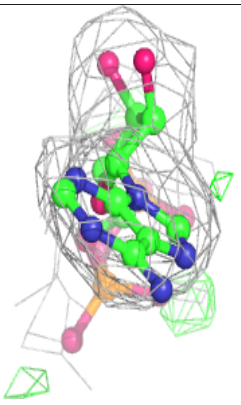


Electron density around ADP B 545:

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

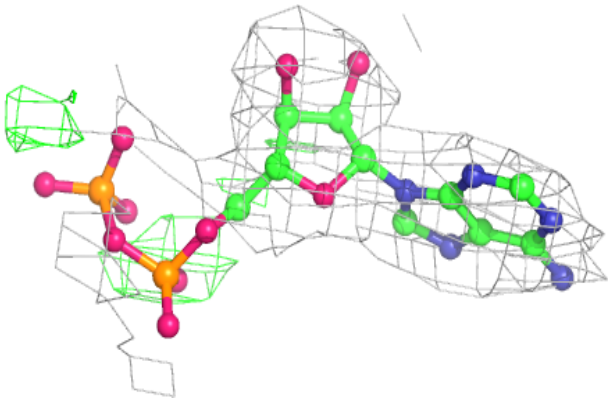


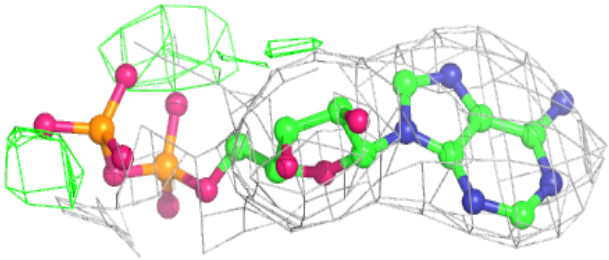


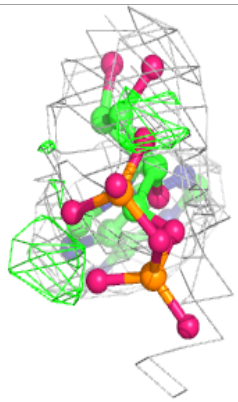


Electron density around ADP C 545:

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

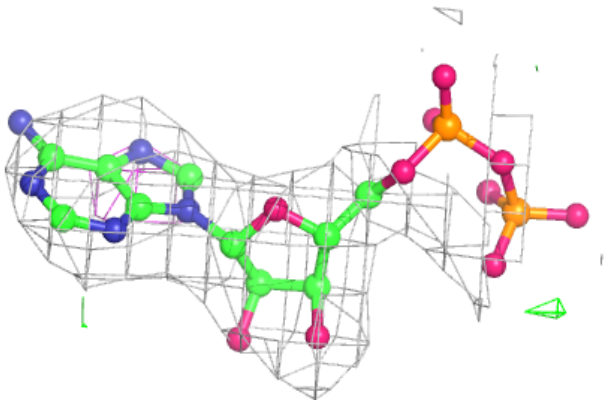


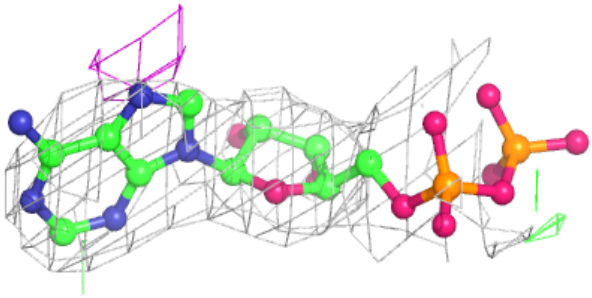


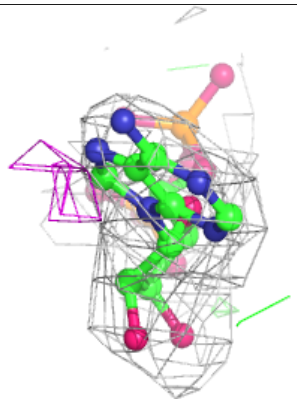


Electron density around ADP E 545:

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

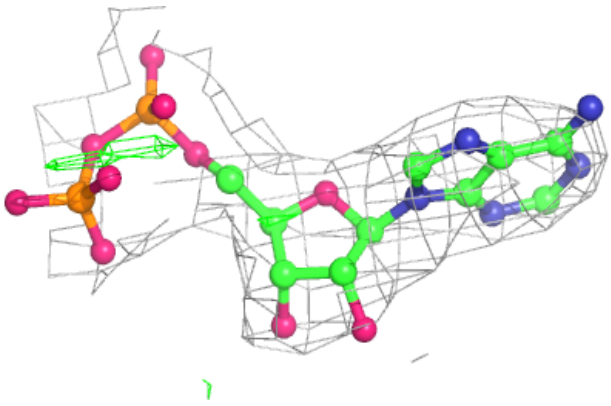


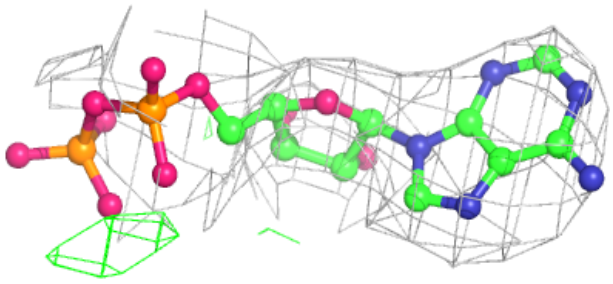


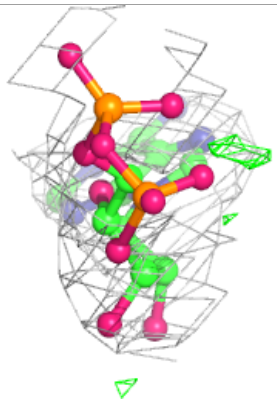


Electron density around ADP G 545:

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

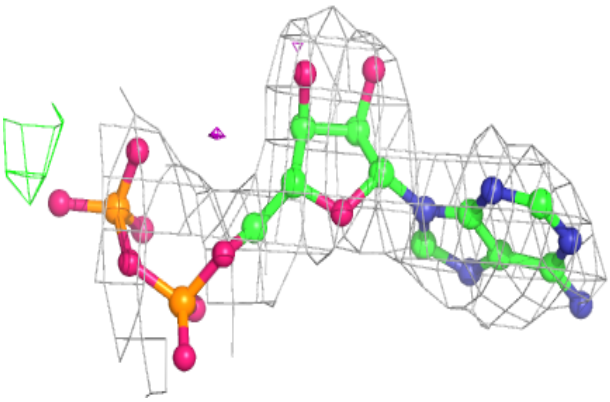


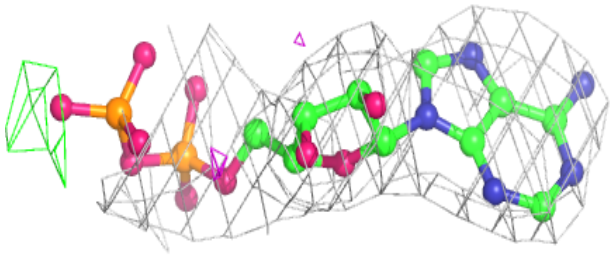


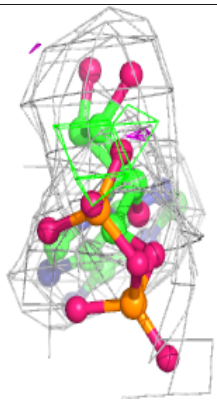


Electron density around ADP A 545:

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

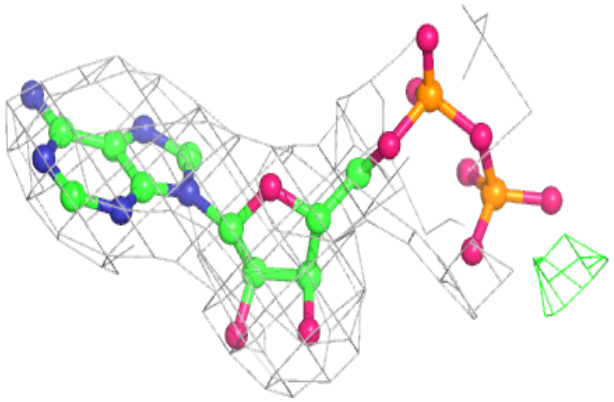


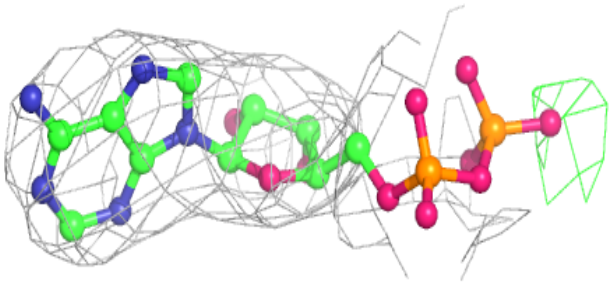


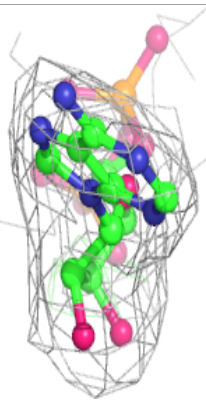


Electron density around ADP F 545:

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

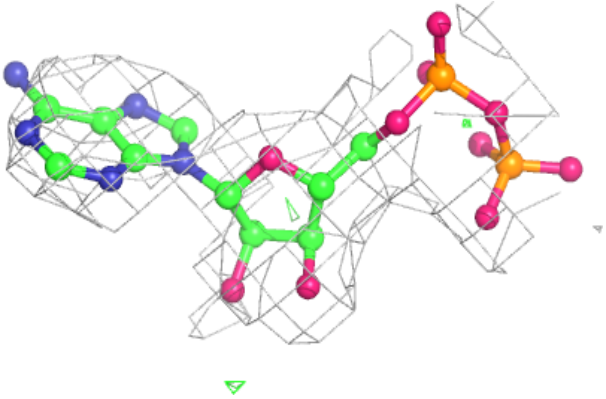


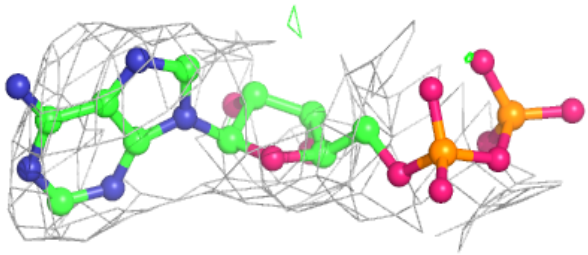


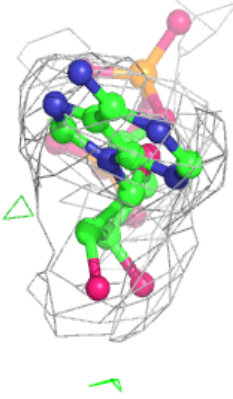


Electron density around ADP D 545:

$2mF_o$-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.