



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 AM GMT

PDB ID : 2PX0  
Title : Crystal structure of FlhF complexed with GMPPNP/Mg(2+)  
Authors : Bange, G.; Wild, K.; Sinning, I.  
Deposited on : 2007-05-14  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

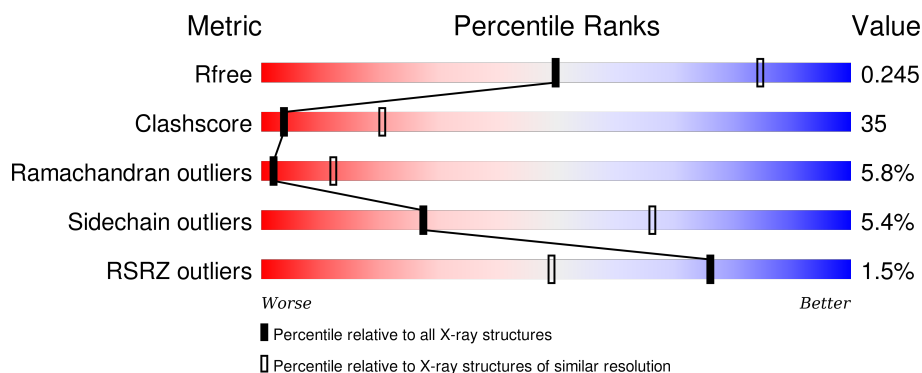
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	296	
1	B	296	
1	C	296	
1	D	296	
1	E	296	

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Mol	Chain	Length	Quality of chain
1	F	296	<div><div></div><div>41%41%5%13%</div></div>
1	G	296	<div><div>2%</div><div>32%49%5%13%</div></div>
1	H	296	<div><div>2%</div><div>39%42%6%13%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16624 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 Flagellar biosynthesis protein flhF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	B	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	C	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	D	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	E	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	F	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	G	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	H	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	MET	-	CLONING ARTIFACT	UNP Q01960
A	72	GLY	-	CLONING ARTIFACT	UNP Q01960
A	73	HIS	-	CLONING ARTIFACT	UNP Q01960
A	74	HIS	-	CLONING ARTIFACT	UNP Q01960
A	75	HIS	-	CLONING ARTIFACT	UNP Q01960
A	76	HIS	-	CLONING ARTIFACT	UNP Q01960
A	77	HIS	-	CLONING ARTIFACT	UNP Q01960
A	78	HIS	-	CLONING ARTIFACT	UNP Q01960
B	71	MET	-	CLONING ARTIFACT	UNP Q01960
B	72	GLY	-	CLONING ARTIFACT	UNP Q01960
B	73	HIS	-	CLONING ARTIFACT	UNP Q01960
B	74	HIS	-	CLONING ARTIFACT	UNP Q01960
B	75	HIS	-	CLONING ARTIFACT	UNP Q01960

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Chain	Residue	Modelled	Actual	Comment	Reference
B	76	HIS	-	CLONING ARTIFACT	UNP Q01960
B	77	HIS	-	CLONING ARTIFACT	UNP Q01960
B	78	HIS	-	CLONING ARTIFACT	UNP Q01960
C	71	MET	-	CLONING ARTIFACT	UNP Q01960
C	72	GLY	-	CLONING ARTIFACT	UNP Q01960
C	73	HIS	-	CLONING ARTIFACT	UNP Q01960
C	74	HIS	-	CLONING ARTIFACT	UNP Q01960
C	75	HIS	-	CLONING ARTIFACT	UNP Q01960
C	76	HIS	-	CLONING ARTIFACT	UNP Q01960
C	77	HIS	-	CLONING ARTIFACT	UNP Q01960
C	78	HIS	-	CLONING ARTIFACT	UNP Q01960
D	71	MET	-	CLONING ARTIFACT	UNP Q01960
D	72	GLY	-	CLONING ARTIFACT	UNP Q01960
D	73	HIS	-	CLONING ARTIFACT	UNP Q01960
D	74	HIS	-	CLONING ARTIFACT	UNP Q01960
D	75	HIS	-	CLONING ARTIFACT	UNP Q01960
D	76	HIS	-	CLONING ARTIFACT	UNP Q01960
D	77	HIS	-	CLONING ARTIFACT	UNP Q01960
D	78	HIS	-	CLONING ARTIFACT	UNP Q01960
E	71	MET	-	CLONING ARTIFACT	UNP Q01960
E	72	GLY	-	CLONING ARTIFACT	UNP Q01960
E	73	HIS	-	CLONING ARTIFACT	UNP Q01960
E	74	HIS	-	CLONING ARTIFACT	UNP Q01960
E	75	HIS	-	CLONING ARTIFACT	UNP Q01960
E	76	HIS	-	CLONING ARTIFACT	UNP Q01960
E	77	HIS	-	CLONING ARTIFACT	UNP Q01960
E	78	HIS	-	CLONING ARTIFACT	UNP Q01960
F	71	MET	-	CLONING ARTIFACT	UNP Q01960
F	72	GLY	-	CLONING ARTIFACT	UNP Q01960
F	73	HIS	-	CLONING ARTIFACT	UNP Q01960
F	74	HIS	-	CLONING ARTIFACT	UNP Q01960
F	75	HIS	-	CLONING ARTIFACT	UNP Q01960
F	76	HIS	-	CLONING ARTIFACT	UNP Q01960
F	77	HIS	-	CLONING ARTIFACT	UNP Q01960
F	78	HIS	-	CLONING ARTIFACT	UNP Q01960
G	71	MET	-	CLONING ARTIFACT	UNP Q01960
G	72	GLY	-	CLONING ARTIFACT	UNP Q01960
G	73	HIS	-	CLONING ARTIFACT	UNP Q01960
G	74	HIS	-	CLONING ARTIFACT	UNP Q01960
G	75	HIS	-	CLONING ARTIFACT	UNP Q01960
G	76	HIS	-	CLONING ARTIFACT	UNP Q01960
G	77	HIS	-	CLONING ARTIFACT	UNP Q01960

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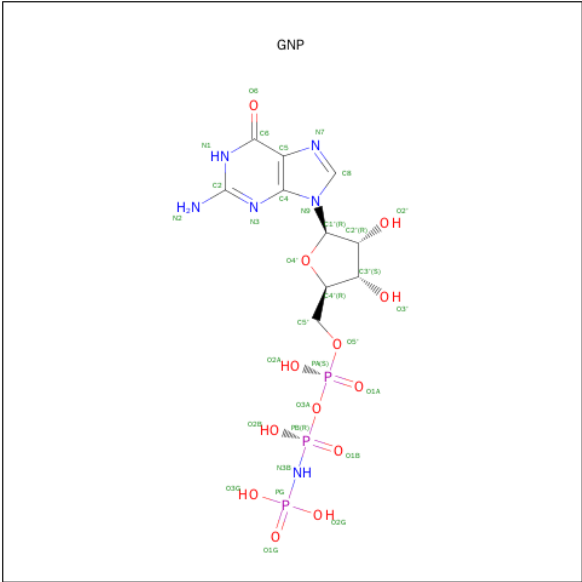
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Chain	Residue	Modelled	Actual	Comment	Reference
G	78	HIS	-	CLONING ARTIFACT	UNP Q01960
H	71	MET	-	CLONING ARTIFACT	UNP Q01960
H	72	GLY	-	CLONING ARTIFACT	UNP Q01960
H	73	HIS	-	CLONING ARTIFACT	UNP Q01960
H	74	HIS	-	CLONING ARTIFACT	UNP Q01960
H	75	HIS	-	CLONING ARTIFACT	UNP Q01960
H	76	HIS	-	CLONING ARTIFACT	UNP Q01960
H	77	HIS	-	CLONING ARTIFACT	UNP Q01960
H	78	HIS	-	CLONING ARTIFACT	UNP Q01960

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

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	G	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	H	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is water.

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

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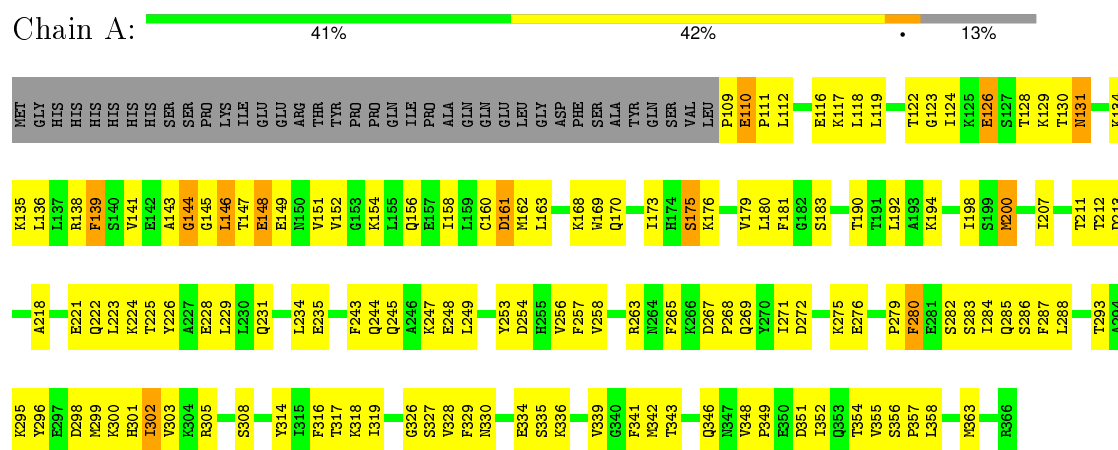
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	3	Total 3	O 3	0	0
4	F	3	Total 3	O 3	0	0
4	G	3	Total 3	O 3	0	0
4	H	3	Total 3	O 3	0	0

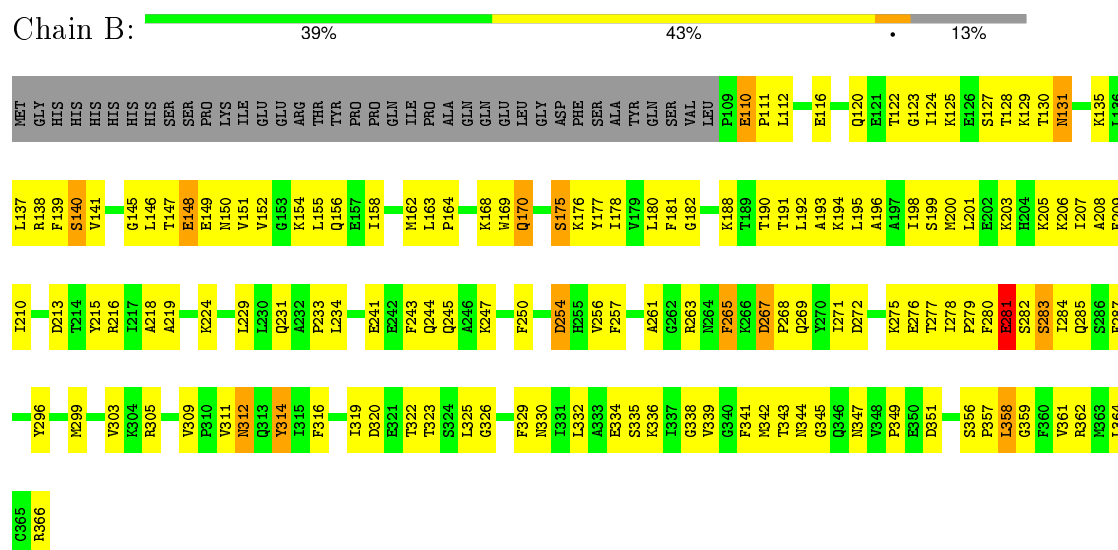
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Flagellar biosynthesis protein flhF

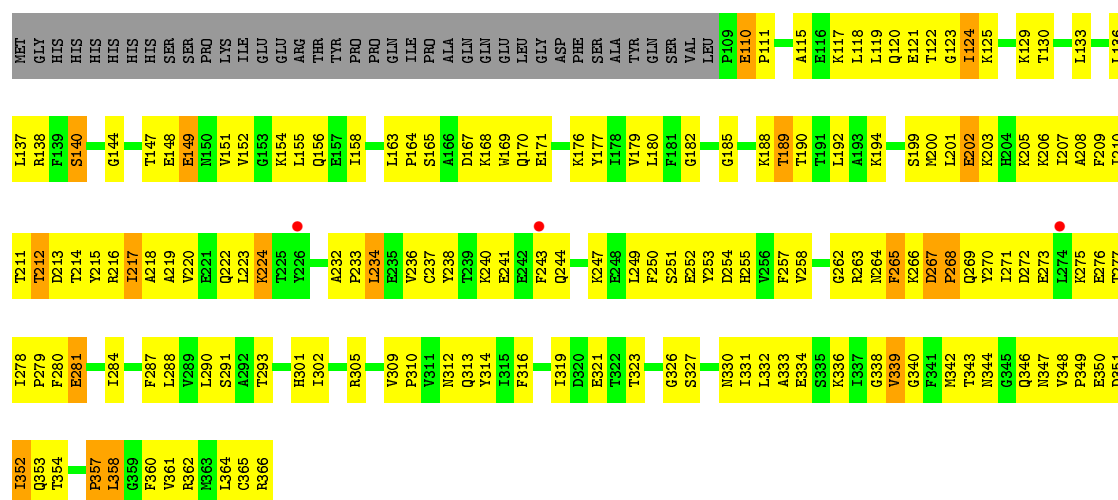


#### • Molecule 1: Flagellar biosynthesis protein flhF

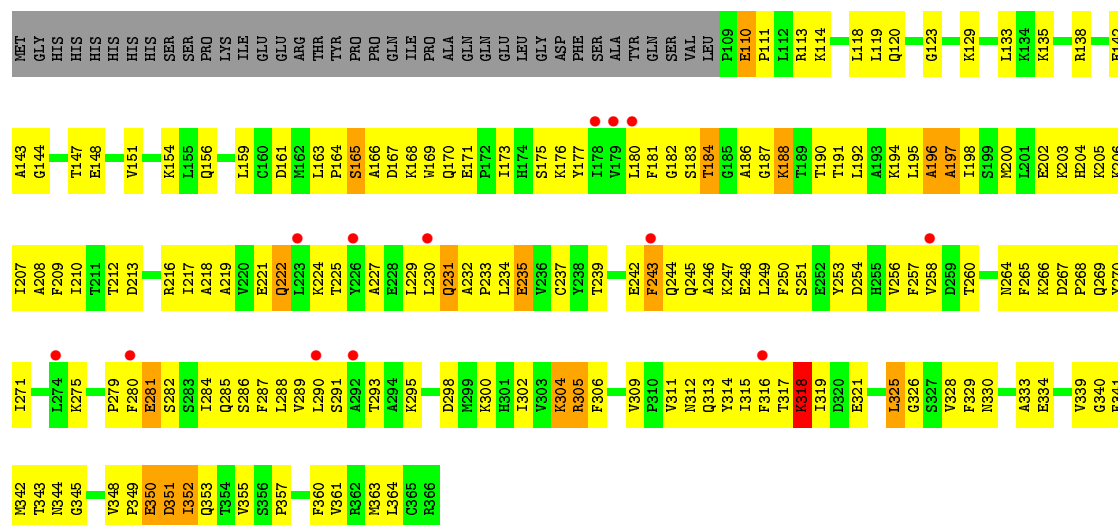


#### • Molecule 1: Flagellar biosynthesis protein flhF

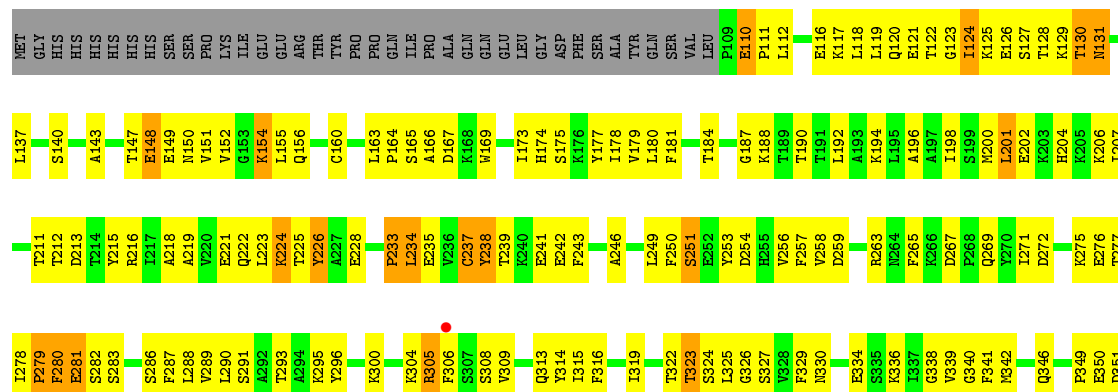


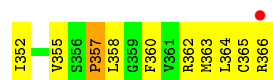


• Molecule 1: Flagellar biosynthesis protein fhfF



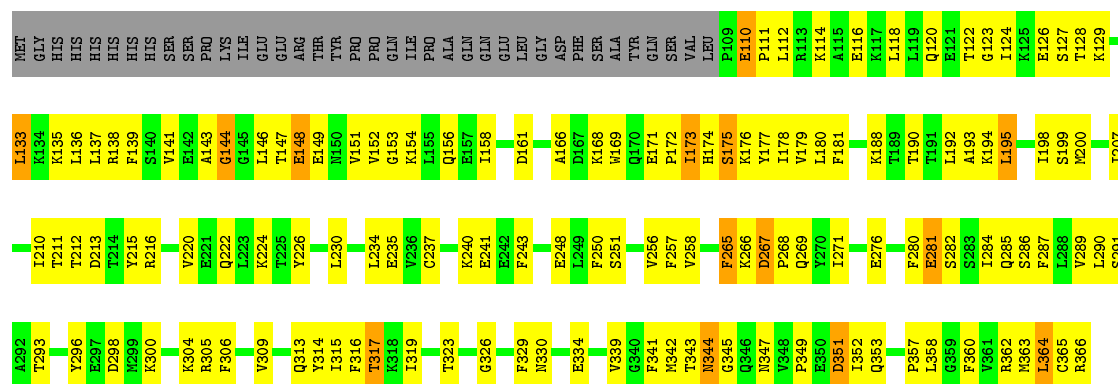
• Molecule 1: Flagellar biosynthesis protein fhfF





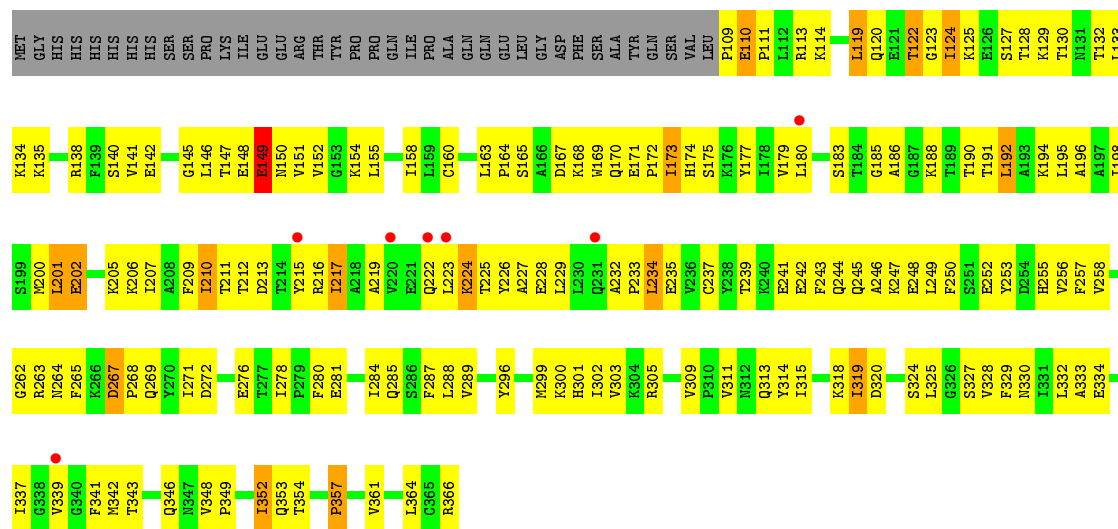
• Molecule 1: Flagellar biosynthesis protein fhfF

Chain F: 41% 41% 5% 13%



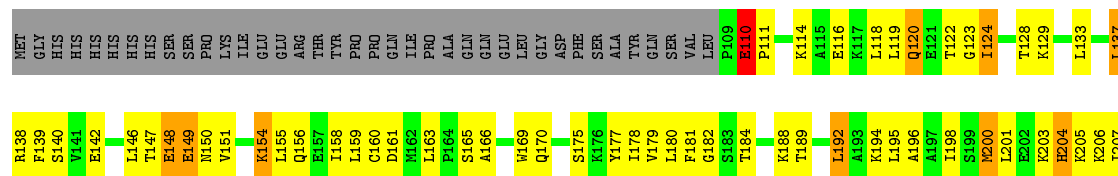
• Molecule 1: Flagellar biosynthesis protein fhfF

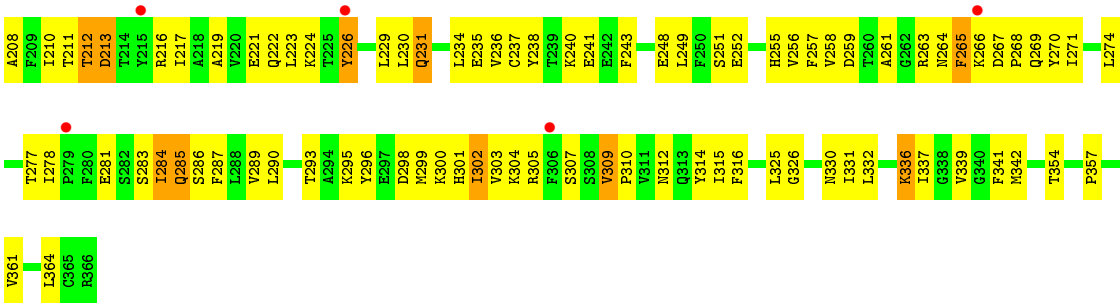
Chain G: 32% 49% 5% 13%



• Molecule 1: Flagellar biosynthesis protein fhfF

Chain H: 39% 42% 6% 13%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.65Å 111.38Å 112.09Å 90.00° 89.78° 90.00°	Depositor
Resolution (Å)	62.97 – 3.00 62.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (62.97-3.00) 97.9 (62.97-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.254 , 0.328 0.252 , 0.245	Depositor DCC
$R_{free}$ test set	2605 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.5	EDS
Estimated twinning fraction	0.019 for -h,l,k 0.028 for -h,-l,-k 0.088 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 51126 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/2079	0.65	0/2805
1	B	0.35	0/2079	0.62	0/2805
1	C	0.33	0/2079	0.61	0/2805
1	D	0.34	0/2079	0.61	0/2805
1	E	0.38	0/2079	0.65	0/2805
1	F	0.38	0/2079	0.63	0/2805
1	G	0.35	0/2079	0.62	0/2805
1	H	0.36	0/2079	0.61	0/2805
All	All	0.36	0/16632	0.62	0/22440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2042	0	2080	126	0
1	B	2042	0	2080	140	0
1	C	2042	0	2080	164	0
1	D	2042	0	2080	179	0
1	E	2042	0	2080	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2042	0	2079	130	0
1	G	2042	0	2080	159	0
1	H	2042	0	2080	158	0
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	32	0	13	0	0
3	B	32	0	13	0	0
3	C	32	0	13	2	0
3	D	32	0	13	2	0
3	E	32	0	13	2	0
3	F	32	0	13	0	0
3	G	32	0	13	0	0
3	H	32	0	13	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	1	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
All	All	16624	0	16743	1166	0

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 35.

All (1166) 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:D:166:ALA:HA	1:D:357:PRO:HG2	1.35	1.09
1:C:211:THR:HG22	1:C:212:THR:H	1.24	1.01
1:G:289:VAL:HG22	1:G:315:ILE:HB	1.44	0.99
1:G:319:ILE:HG21	1:G:342:MET:HE2	1.42	0.99
1:D:289:VAL:HG22	1:D:315:ILE:HB	1.45	0.98
1:C:192:LEU:HD22	1:C:257:PHE:HB3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:GLU:HG3	1:D:111:PRO:HD3	1.48	0.96
1:E:192:LEU:HD11	1:E:258:VAL:O	1.65	0.96
1:E:358:LEU:HG	1:E:362:ARG:HH21	1.28	0.96
1:C:110:GLU:HB3	1:C:111:PRO:HD3	1.50	0.92
1:H:208:ALA:HB3	1:H:256:VAL:HG22	1.52	0.90
1:D:216:ARG:HB3	1:D:219:ALA:HB2	1.52	0.90
1:C:268:PRO:HA	1:C:271:ILE:HB	1.55	0.89
1:B:140:SER:HB2	1:B:146:LEU:HD11	1.54	0.88
1:C:206:LYS:HB2	1:C:254:ASP:H	1.38	0.87
1:E:275:LYS:HD3	1:E:309:VAL:HG12	1.56	0.87
1:G:268:PRO:HD3	1:G:305:ARG:HH21	1.39	0.86
1:G:341:PHE:HB3	1:G:352:ILE:HD11	1.57	0.85
1:F:192:LEU:HD22	1:F:257:PHE:HB3	1.57	0.85
1:E:121:GLU:HB3	1:E:366:ARG:HG3	1.59	0.85
1:F:267:ASP:OD2	1:F:269:GLN:HB3	1.77	0.84
1:A:298:ASP:OD1	1:E:323:THR:HB	1.77	0.84
1:C:211:THR:HG22	1:C:213:ASP:H	1.41	0.83
1:H:268:PRO:HD3	1:H:305:ARG:NH2	1.93	0.83
1:C:216:ARG:HB3	1:C:219:ALA:HB2	1.59	0.82
1:E:163:LEU:HB3	1:E:164:PRO:HD2	1.59	0.82
1:E:164:PRO:HG2	1:E:169:TRP:HE1	1.45	0.82
1:D:302:ILE:HA	1:D:305:ARG:HB2	1.62	0.81
1:H:216:ARG:HB3	1:H:219:ALA:HB2	1.62	0.81
1:E:179:VAL:O	1:E:180:LEU:HD23	1.81	0.80
1:E:211:THR:HG22	1:E:213:ASP:H	1.45	0.80
1:H:224:LYS:HA	1:H:234:LEU:HD13	1.64	0.80
1:F:200:MET:HB2	1:F:207:ILE:HG13	1.63	0.80
1:A:152:VAL:O	1:A:156:GLN:HG3	1.82	0.80
1:B:127:SER:O	1:B:131:ASN:HB2	1.81	0.80
1:G:192:LEU:HD11	1:G:257:PHE:HB3	1.61	0.80
1:D:110:GLU:CG	1:D:111:PRO:HD3	2.12	0.79
1:A:211:THR:HG22	1:A:213:ASP:H	1.46	0.79
1:D:264:ASN:ND2	1:D:266:LYS:H	1.80	0.79
1:D:248:GLU:HA	1:D:251:SER:HB2	1.62	0.79
1:A:110:GLU:HB3	1:A:111:PRO:CD	2.11	0.79
1:D:203:LYS:O	1:D:205:LYS:HG3	1.82	0.79
1:B:281:GLU:HG2	1:B:282:SER:N	1.99	0.78
1:A:327:SER:HA	1:A:330:ASN:HD22	1.49	0.78
1:D:280:PHE:HA	1:D:284:ILE:HD12	1.66	0.78
1:H:180:LEU:HD22	1:H:287:PHE:HB2	1.64	0.78
1:B:180:LEU:CD2	1:B:287:PHE:HB2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:SER:HA	1:B:203:LYS:HB2	1.66	0.77
1:A:180:LEU:HD22	1:A:287:PHE:HB2	1.65	0.77
1:F:171:GLU:HB2	1:F:313:GLN:HG3	1.66	0.77
1:F:319:ILE:HG21	1:F:342:MET:HE3	1.66	0.76
1:C:217:ILE:HD13	1:C:217:ILE:H	1.50	0.76
1:H:221:GLU:HA	1:H:224:LYS:HB2	1.68	0.76
1:H:206:LYS:HD2	1:H:206:LYS:N	2.01	0.76
1:H:122:THR:OG1	1:H:124:ILE:HG12	1.85	0.76
1:C:216:ARG:HH22	1:G:216:ARG:HH22	1.33	0.75
1:E:110:GLU:HB2	1:E:111:PRO:CD	2.17	0.75
1:B:267:ASP:OD2	1:B:269:GLN:HB3	1.86	0.75
1:H:223:LEU:HA	1:H:226:TYR:HB2	1.69	0.75
1:G:122:THR:OG1	1:G:124:ILE:HG12	1.88	0.74
1:H:223:LEU:HD12	1:H:226:TYR:HB3	1.70	0.74
1:B:271:ILE:HD11	1:B:305:ARG:HB3	1.70	0.74
1:C:272:ASP:HA	1:C:275:LYS:HE2	1.70	0.74
1:D:264:ASN:HD21	1:D:266:LYS:H	1.35	0.74
1:F:180:LEU:HD22	1:F:287:PHE:HB2	1.70	0.74
1:G:319:ILE:HG21	1:G:342:MET:CE	2.18	0.73
1:F:207:ILE:HD12	1:F:257:PHE:HE2	1.53	0.73
1:C:218:ALA:HB3	1:G:222:GLN:HG2	1.70	0.73
1:H:170:GLN:HG2	1:H:354:THR:OG1	1.88	0.73
1:E:358:LEU:HG	1:E:362:ARG:NH2	2.03	0.73
1:D:216:ARG:HB3	1:D:219:ALA:CB	2.18	0.73
1:H:137:LEU:HD23	1:H:138:ARG:H	1.53	0.73
1:C:211:THR:HG22	1:C:212:THR:N	2.02	0.73
1:E:192:LEU:HD22	1:E:257:PHE:HB3	1.70	0.73
1:C:206:LYS:HB3	1:C:253:TYR:HD1	1.52	0.73
1:G:211:THR:HG22	1:G:213:ASP:H	1.53	0.73
1:A:110:GLU:HB3	1:A:111:PRO:HD2	1.69	0.72
1:D:147:THR:HG22	1:D:148:GLU:H	1.53	0.72
1:H:192:LEU:CD2	1:H:257:PHE:HB3	2.19	0.72
1:B:347:ASN:ND2	1:F:215:TYR:OH	2.22	0.72
1:F:175:SER:HB2	1:F:285:GLN:HE21	1.54	0.72
1:A:109:PRO:O	1:A:110:GLU:HG2	1.88	0.72
1:D:181:PHE:HE2	1:D:286:SER:HB2	1.54	0.72
1:B:281:GLU:HG2	1:B:282:SER:H	1.55	0.71
1:D:222:GLN:HE22	1:H:216:ARG:HH21	1.35	0.71
1:C:179:VAL:HG22	1:C:258:VAL:HB	1.72	0.71
1:B:110:GLU:HB2	1:B:111:PRO:CD	2.20	0.71
1:H:120:GLN:HE21	1:H:129:LYS:HE3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:LEU:HA	1:H:140:SER:HG	1.56	0.70
1:E:237:CYS:HB3	1:E:242:GLU:HB2	1.74	0.70
1:G:352:ILE:HD13	1:G:353:GLN:N	2.06	0.70
1:B:124:ILE:CG2	1:B:128:THR:HB	2.21	0.70
1:H:268:PRO:HA	1:H:271:ILE:HD13	1.74	0.70
1:D:194:LYS:HG2	1:D:348:VAL:HG13	1.72	0.70
1:E:319:ILE:HG21	1:E:342:MET:HE3	1.73	0.70
1:B:244:GLN:HE22	1:B:247:LYS:NZ	1.90	0.69
1:C:200:MET:HB2	1:C:207:ILE:HG13	1.74	0.69
1:B:275:LYS:HZ1	1:B:309:VAL:HB	1.57	0.69
1:C:122:THR:OG1	1:C:124:ILE:HG12	1.92	0.69
1:H:137:LEU:HA	1:H:140:SER:OG	1.91	0.69
1:A:138:ARG:O	1:A:141:VAL:HG12	1.93	0.69
1:F:268:PRO:HA	1:F:271:ILE:HD13	1.73	0.69
1:F:180:LEU:CD2	1:F:287:PHE:HB2	2.21	0.69
1:B:358:LEU:O	1:B:362:ARG:HG3	1.93	0.69
1:C:110:GLU:CB	1:C:111:PRO:HD3	2.21	0.69
1:F:200:MET:HB2	1:F:207:ILE:CG1	2.22	0.69
1:C:211:THR:CG2	1:C:212:THR:H	2.05	0.69
1:C:123:GLY:CA	1:C:326:GLY:HA3	2.22	0.69
1:E:216:ARG:HB3	1:E:219:ALA:HB2	1.74	0.69
1:D:192:LEU:O	1:D:192:LEU:HD13	1.92	0.69
1:F:152:VAL:O	1:F:156:GLN:HG3	1.93	0.69
1:D:300:LYS:O	1:D:304:LYS:HD3	1.93	0.68
1:F:210:ILE:HB	1:F:258:VAL:HG22	1.74	0.68
1:D:280:PHE:CA	1:D:284:ILE:HD12	2.23	0.68
1:C:323:THR:HG22	1:C:366:ARG:HH22	1.57	0.68
1:G:233:PRO:HB2	1:G:250:PHE:CZ	2.28	0.68
1:A:147:THR:C	1:A:149:GLU:H	1.96	0.68
1:E:194:LYS:HD3	1:E:352:ILE:HB	1.74	0.68
1:B:194:LYS:HG2	1:B:349:PRO:HA	1.76	0.68
1:D:196:ALA:HA	1:D:257:PHE:CE2	2.29	0.68
1:F:179:VAL:O	1:F:180:LEU:HD23	1.93	0.68
1:G:119:LEU:HD11	1:G:132:THR:HG21	1.74	0.68
1:D:191:THR:O	1:D:195:LEU:HD13	1.94	0.67
1:H:192:LEU:HD11	1:H:258:VAL:O	1.94	0.67
1:A:198:ILE:HD11	1:A:349:PRO:HB2	1.74	0.67
1:F:280:PHE:HA	1:F:284:ILE:HD12	1.75	0.67
1:A:279:PRO:O	1:A:280:PHE:HB2	1.94	0.67
1:H:189:THR:HG21	1:H:222:GLN:OE1	1.94	0.67
1:D:182:GLY:N	1:D:188:LYS:HD3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:GLU:HG3	1:H:249:LEU:HD23	1.77	0.67
1:D:177:TYR:OH	1:D:247:LYS:HB3	1.95	0.67
1:B:200:MET:HB2	1:B:207:ILE:HG13	1.76	0.67
1:D:239:THR:OG1	1:D:242:GLU:HG3	1.94	0.67
1:E:147:THR:O	1:E:151:VAL:HG13	1.95	0.67
1:F:169:TRP:CE2	1:F:357:PRO:HG3	2.30	0.67
1:G:244:GLN:HA	1:G:247:LYS:HD3	1.77	0.67
1:B:181:PHE:HZ	1:B:311:VAL:HG12	1.59	0.67
1:F:226:TYR:HE1	1:F:230:LEU:HD13	1.59	0.66
1:A:234:LEU:HD23	1:A:235:GLU:N	2.10	0.66
1:C:208:ALA:O	1:C:209:PHE:HD1	1.79	0.66
1:G:177:TYR:HD1	1:G:256:VAL:HB	1.59	0.66
1:B:152:VAL:HG12	1:B:156:GLN:HE21	1.61	0.66
1:E:147:THR:HG22	1:E:148:GLU:N	2.11	0.66
1:D:186:ALA:O	1:D:318:LYS:HE3	1.96	0.66
1:D:314:TYR:O	1:D:339:VAL:HG23	1.95	0.66
1:G:192:LEU:CD1	1:G:257:PHE:HB3	2.26	0.66
1:C:199:SER:HA	1:C:203:LYS:CG	2.26	0.65
1:A:253:TYR:HE1	1:H:336:LYS:HZ1	1.44	0.65
1:E:272:ASP:O	1:E:276:GLU:HG2	1.97	0.65
1:G:173:ILE:HA	1:G:285:GLN:NE2	2.11	0.65
1:D:286:SER:O	1:D:312:ASN:HB2	1.96	0.65
1:G:280:PHE:HA	1:G:284:ILE:HD12	1.79	0.65
1:E:322:THR:HG21	1:E:325:LEU:CD1	2.27	0.65
1:D:343:THR:HA	1:D:352:ILE:HA	1.78	0.65
1:C:171:GLU:HB2	1:C:313:GLN:HG3	1.78	0.65
1:C:170:GLN:HG2	1:C:354:THR:OG1	1.96	0.65
1:D:110:GLU:HB3	1:D:111:PRO:CD	2.27	0.65
1:A:268:PRO:HD3	1:A:305:ARG:HH22	1.60	0.65
1:H:284:ILE:HG23	1:H:285:GLN:N	2.12	0.65
1:D:167:ASP:C	1:D:169:TRP:H	1.99	0.65
1:D:275:LYS:HA	1:D:280:PHE:HE2	1.61	0.65
1:A:147:THR:O	1:A:149:GLU:N	2.30	0.65
1:E:194:LYS:O	1:E:198:ILE:HG12	1.96	0.64
1:B:194:LYS:O	1:B:198:ILE:HG12	1.96	0.64
1:F:116:GLU:HB2	1:F:133:LEU:HD11	1.79	0.64
1:D:285:GLN:HG3	1:D:312:ASN:ND2	2.12	0.64
1:E:358:LEU:HD12	1:E:358:LEU:O	1.97	0.64
1:G:233:PRO:HB2	1:G:250:PHE:CE1	2.32	0.64
1:A:288:LEU:HD23	1:A:314:TYR:HE1	1.62	0.64
1:E:279:PRO:O	1:E:280:PHE:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:LYS:O	1:H:198:ILE:HG12	1.97	0.64
1:F:349:PRO:O	1:F:352:ILE:HG22	1.97	0.64
1:C:123:GLY:HA3	1:C:326:GLY:HA3	1.79	0.64
1:B:278:ILE:N	1:B:278:ILE:HD12	2.12	0.64
1:E:163:LEU:HB3	1:E:164:PRO:CD	2.28	0.64
1:G:267:ASP:OD2	1:G:269:GLN:HB3	1.97	0.64
1:C:288:LEU:HG	1:C:290:LEU:HD11	1.78	0.64
1:G:155:LEU:O	1:G:158:ILE:HB	1.98	0.63
1:A:112:LEU:HD11	1:A:146:LEU:HD12	1.80	0.63
1:A:271:ILE:O	1:A:275:LYS:HE2	1.98	0.63
1:H:231:GLN:N	1:H:231:GLN:OE1	2.31	0.63
1:E:223:LEU:HA	1:E:226:TYR:HB2	1.78	0.63
1:H:192:LEU:HD22	1:H:257:PHE:HB3	1.80	0.63
1:G:180:LEU:CD2	1:G:287:PHE:HB2	2.29	0.63
1:A:211:THR:HG22	1:A:213:ASP:N	2.13	0.62
1:A:194:LYS:O	1:A:198:ILE:HG12	1.99	0.62
1:B:154:LYS:O	1:B:158:ILE:HG13	1.98	0.62
1:B:180:LEU:HD23	1:B:287:PHE:HB2	1.79	0.62
1:H:302:ILE:O	1:H:302:ILE:HD12	1.99	0.62
1:G:211:THR:OG1	1:G:223:LEU:HD23	1.99	0.62
1:D:110:GLU:CB	1:D:111:PRO:HD3	2.28	0.62
1:D:181:PHE:CE2	1:D:286:SER:HB2	2.34	0.62
1:F:169:TRP:CE3	1:F:339:VAL:HG22	2.35	0.62
1:C:237:CYS:SG	1:C:243:PHE:HA	2.40	0.62
1:G:324:SER:HB3	1:G:366:ARG:NH2	2.15	0.62
1:B:175:SER:HB3	1:B:283:SER:O	2.00	0.62
1:E:110:GLU:HB2	1:E:111:PRO:HD3	1.81	0.62
1:E:119:LEU:O	1:E:129:LYS:HE2	2.00	0.62
1:H:119:LEU:HD21	1:H:155:LEU:HD11	1.82	0.62
1:F:319:ILE:HG21	1:F:342:MET:CE	2.29	0.61
1:E:287:PHE:CD2	1:E:315:ILE:HD11	2.36	0.61
1:B:120:GLN:HG2	1:B:129:LYS:HD3	1.82	0.61
1:D:147:THR:HG22	1:D:148:GLU:N	2.14	0.61
1:A:295:LYS:HE2	1:E:327:SER:OG	1.99	0.61
1:G:224:LYS:HG2	1:G:234:LEU:HD22	1.82	0.61
1:F:111:PRO:O	1:F:114:LYS:HB3	2.00	0.61
1:G:211:THR:HG22	1:G:212:THR:N	2.13	0.61
1:D:166:ALA:HA	1:D:357:PRO:CG	2.22	0.61
1:F:266:LYS:HA	1:F:305:ARG:HE	1.65	0.61
1:F:265:PHE:O	1:F:305:ARG:HD2	2.01	0.61
1:E:200:MET:HG2	1:E:201:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:THR:C	1:A:149:GLU:N	2.54	0.60
1:D:210:ILE:HG21	1:D:243:PHE:HE1	1.65	0.60
1:B:200:MET:HB2	1:B:207:ILE:CG1	2.31	0.60
1:G:224:LYS:O	1:G:228:GLU:HG3	2.01	0.60
1:G:328:VAL:HG12	1:G:332:LEU:HD12	1.82	0.60
1:G:194:LYS:O	1:G:198:ILE:HG12	2.01	0.60
1:F:266:LYS:HG3	1:F:305:ARG:HH21	1.66	0.60
1:C:240:LYS:O	1:C:244:GLN:HB2	2.01	0.60
1:G:177:TYR:CD1	1:G:256:VAL:HB	2.36	0.60
1:B:357:PRO:O	1:B:361:VAL:HG23	2.00	0.60
1:G:196:ALA:HA	1:G:257:PHE:CE2	2.35	0.60
1:G:239:THR:OG1	1:G:242:GLU:HG3	2.02	0.60
1:H:210:ILE:O	1:H:258:VAL:HA	2.02	0.60
1:D:319:ILE:HD11	1:D:344:ASN:HB3	1.82	0.60
1:C:314:TYR:HB2	1:C:338:GLY:O	2.02	0.60
1:G:337:ILE:O	1:G:337:ILE:HD12	2.02	0.60
1:A:342:MET:O	1:A:352:ILE:HD12	2.01	0.60
1:H:192:LEU:HD21	1:H:257:PHE:HB3	1.83	0.60
1:H:206:LYS:H	1:H:206:LYS:HD2	1.67	0.60
1:G:173:ILE:HA	1:G:285:GLN:HE22	1.65	0.59
1:G:170:GLN:HG2	1:G:354:THR:OG1	2.02	0.59
1:G:296:TYR:OH	1:G:300:LYS:HE2	2.01	0.59
1:E:319:ILE:O	1:E:322:THR:HG22	2.02	0.59
1:H:265:PHE:O	1:H:271:ILE:HD11	2.03	0.59
1:B:177:TYR:CZ	1:B:247:LYS:HG3	2.37	0.59
1:H:160:CYS:HA	1:H:163:LEU:HD23	1.84	0.59
1:A:200:MET:HB2	1:A:207:ILE:HG13	1.84	0.59
1:F:234:LEU:O	1:F:235:GLU:HG2	2.02	0.59
1:G:194:LYS:HG2	1:G:348:VAL:HG13	1.83	0.59
1:B:316:PHE:O	1:B:342:MET:HA	2.02	0.59
1:A:346:GLN:HE22	1:E:263:ARG:HD3	1.67	0.59
1:H:182:GLY:N	1:H:188:LYS:HD3	2.18	0.59
1:B:110:GLU:HB2	1:B:111:PRO:HD2	1.84	0.59
1:H:221:GLU:HA	1:H:224:LYS:CB	2.33	0.59
1:H:299:MET:O	1:H:303:VAL:HG23	2.02	0.59
1:D:289:VAL:HG22	1:D:315:ILE:CB	2.27	0.59
1:E:147:THR:HG22	1:E:148:GLU:H	1.66	0.59
1:D:176:LYS:HA	1:D:254:ASP:O	2.03	0.59
1:F:330:ASN:O	1:F:334:GLU:HG2	2.03	0.59
1:H:114:LYS:O	1:H:118:LEU:HG	2.02	0.59
1:G:133:LEU:C	1:G:135:LYS:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:THR:HG22	1:G:213:ASP:N	2.18	0.58
1:F:122:THR:HB	1:F:364:LEU:HD22	1.85	0.58
1:E:322:THR:HG21	1:E:325:LEU:HD11	1.85	0.58
1:D:280:PHE:N	1:D:284:ILE:HD12	2.19	0.58
1:F:139:PHE:CE2	1:F:154:LYS:HE3	2.38	0.58
1:E:122:THR:OG1	1:E:124:ILE:HG12	2.03	0.58
1:D:194:LYS:CG	1:D:348:VAL:HG13	2.32	0.58
1:G:138:ARG:O	1:G:142:GLU:HG2	2.01	0.58
1:D:110:GLU:HB3	1:D:111:PRO:HD3	1.86	0.58
1:A:145:GLY:O	1:A:147:THR:N	2.36	0.58
1:D:206:LYS:HB2	1:D:254:ASP:H	1.68	0.58
1:A:263:ARG:HA	1:E:346:GLN:HE22	1.67	0.58
1:G:119:LEU:O	1:G:122:THR:HG23	2.03	0.58
1:H:137:LEU:HD23	1:H:138:ARG:N	2.17	0.58
1:F:177:TYR:HD1	1:F:256:VAL:HB	1.68	0.58
1:G:190:THR:HG22	1:G:194:LYS:HE3	1.84	0.58
1:G:138:ARG:O	1:G:141:VAL:HG12	2.04	0.58
1:D:280:PHE:H	1:D:284:ILE:HD12	1.69	0.58
1:H:357:PRO:O	1:H:361:VAL:HG23	2.03	0.58
1:C:240:LYS:HG2	1:C:241:GLU:OE2	2.04	0.58
1:F:211:THR:HG21	1:F:220:VAL:HG22	1.86	0.58
1:B:199:SER:HA	1:B:203:LYS:HD2	1.85	0.58
1:H:177:TYR:O	1:H:178:ILE:HD13	2.04	0.58
1:D:247:LYS:HE3	1:D:279:PRO:HG3	1.85	0.58
1:C:147:THR:C	1:C:149:GLU:H	2.08	0.58
1:D:156:GLN:HA	1:D:159:LEU:HD12	1.84	0.58
1:F:226:TYR:CE1	1:F:230:LEU:HD13	2.39	0.57
1:D:176:LYS:HG2	1:D:256:VAL:HG23	1.86	0.57
1:B:244:GLN:HE22	1:B:247:LYS:HZ3	1.52	0.57
1:B:277:THR:HB	1:B:278:ILE:HD12	1.86	0.57
1:H:289:VAL:O	1:H:290:LEU:HD23	2.04	0.57
1:C:224:LYS:HE2	1:C:224:LYS:O	2.04	0.57
1:A:343:THR:HG22	1:A:352:ILE:HD13	1.87	0.57
1:G:163:LEU:HB3	1:G:164:PRO:HD2	1.87	0.57
1:E:124:ILE:H	1:E:326:GLY:HA3	1.68	0.57
1:B:265:PHE:O	1:B:305:ARG:HG3	2.03	0.57
1:G:330:ASN:O	1:G:334:GLU:HG2	2.04	0.57
1:A:192:LEU:HD21	1:A:257:PHE:HB3	1.87	0.57
1:F:317:THR:HB	1:F:343:THR:OG1	2.05	0.57
1:B:272:ASP:O	1:B:276:GLU:HG2	2.05	0.57
1:F:175:SER:CB	1:F:285:GLN:HE21	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:O	1:B:140:SER:N	2.32	0.57
1:C:217:ILE:HD13	1:C:217:ILE:N	2.19	0.57
1:C:199:SER:O	1:C:203:LYS:HB2	2.04	0.57
1:D:316:PHE:HB2	1:D:342:MET:HG3	1.87	0.57
1:H:278:ILE:HD12	1:H:278:ILE:N	2.20	0.57
1:H:196:ALA:HA	1:H:257:PHE:CE2	2.40	0.57
1:G:299:MET:O	1:G:303:VAL:HG23	2.05	0.57
1:E:330:ASN:O	1:E:334:GLU:HG2	2.04	0.56
1:A:342:MET:HE1	1:A:355:VAL:HG11	1.87	0.56
1:A:272:ASP:O	1:A:276:GLU:HG2	2.04	0.56
1:B:110:GLU:CB	1:B:111:PRO:CD	2.83	0.56
1:H:120:GLN:NE2	1:H:129:LYS:HE3	2.20	0.56
1:D:315:ILE:HA	1:D:341:PHE:O	2.05	0.56
1:E:196:ALA:HA	1:E:257:PHE:CE2	2.40	0.56
1:G:119:LEU:HD11	1:G:132:THR:CG2	2.34	0.56
1:C:164:PRO:HG2	1:C:169:TRP:HE1	1.70	0.56
1:F:235:GLU:HG3	1:F:250:PHE:CE2	2.40	0.56
1:G:325:LEU:N	1:G:325:LEU:HD12	2.21	0.56
1:G:127:SER:O	1:G:130:THR:HB	2.05	0.56
1:F:154:LYS:O	1:F:158:ILE:HG13	2.05	0.56
1:E:188:LYS:NZ	3:E:5:GNP:O1B	2.38	0.56
1:E:355:VAL:HG11	1:E:363:MET:HE1	1.87	0.56
1:A:318:LYS:NZ	1:E:184:THR:O	2.38	0.56
1:D:210:ILE:HD12	1:D:258:VAL:HG22	1.86	0.56
1:D:295:LYS:HG3	1:H:293:THR:O	2.06	0.56
1:B:305:ARG:HG2	1:B:305:ARG:HH11	1.69	0.56
1:B:192:LEU:HD11	1:B:257:PHE:HB3	1.88	0.56
1:E:147:THR:HG22	1:E:149:GLU:H	1.69	0.56
1:D:357:PRO:O	1:D:361:VAL:HG23	2.05	0.56
1:B:192:LEU:HD13	1:B:192:LEU:O	2.05	0.56
1:G:272:ASP:O	1:G:276:GLU:HG2	2.06	0.56
1:D:110:GLU:OE1	1:D:110:GLU:HA	2.05	0.56
1:C:314:TYR:O	1:C:339:VAL:HG23	2.06	0.56
1:H:147:THR:C	1:H:149:GLU:H	2.07	0.56
1:E:233:PRO:HB2	1:E:250:PHE:HE1	1.71	0.56
1:G:140:SER:HB2	1:G:146:LEU:HD11	1.88	0.56
1:C:199:SER:HA	1:C:203:LYS:HG3	1.87	0.56
1:D:233:PRO:HB2	1:D:250:PHE:CE1	2.41	0.56
1:G:163:LEU:HD13	1:G:333:ALA:HA	1.88	0.56
1:E:239:THR:HB	1:E:241:GLU:OE1	2.06	0.56
1:G:343:THR:HA	1:G:352:ILE:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:NH1	1:G:222:GLN:HE22	2.04	0.55
1:A:268:PRO:HD3	1:A:305:ARG:NH2	2.20	0.55
1:F:173:ILE:HD11	1:F:195:LEU:HG	1.88	0.55
1:H:154:LYS:O	1:H:158:ILE:HG13	2.06	0.55
1:E:275:LYS:CD	1:E:309:VAL:HG12	2.31	0.55
1:C:216:ARG:HB3	1:C:219:ALA:CB	2.35	0.55
1:F:173:ILE:HG23	1:F:178:ILE:HD11	1.87	0.55
1:D:164:PRO:O	1:D:165:SER:O	2.24	0.55
1:H:169:TRP:O	1:H:170:GLN:HB2	2.07	0.55
1:E:152:VAL:O	1:E:156:GLN:HG3	2.06	0.55
1:G:225:THR:O	1:G:229:LEU:HG	2.06	0.55
1:G:175:SER:HB3	1:G:285:GLN:HB2	1.88	0.55
1:H:268:PRO:HD3	1:H:305:ARG:HH21	1.70	0.55
1:A:176:LYS:HE2	1:A:253:TYR:O	2.07	0.55
1:C:125:LYS:HG2	1:C:330:ASN:OD1	2.06	0.55
1:F:358:LEU:O	1:F:362:ARG:HG3	2.07	0.55
1:B:218:ALA:HB3	1:F:222:GLN:HG2	1.88	0.55
1:G:319:ILE:O	1:G:319:ILE:HG13	2.06	0.55
1:G:341:PHE:CB	1:G:352:ILE:HD11	2.33	0.55
1:G:223:LEU:HA	1:G:226:TYR:HD2	1.71	0.55
1:G:309:VAL:O	1:G:309:VAL:HG22	2.05	0.55
1:B:195:LEU:HD11	1:B:341:PHE:CE2	2.41	0.55
1:D:325:LEU:HD23	1:D:328:VAL:HG21	1.87	0.55
1:B:216:ARG:HB3	1:B:219:ALA:HB2	1.89	0.55
1:A:299:MET:HA	1:A:302:ILE:HG12	1.87	0.55
1:G:194:LYS:CG	1:G:348:VAL:HG13	2.37	0.55
1:C:169:TRP:CD2	1:C:357:PRO:HG3	2.42	0.55
1:F:234:LEU:HG	1:F:235:GLU:N	2.22	0.55
1:D:120:GLN:NE2	1:D:129:LYS:HE3	2.20	0.55
1:C:270:TYR:HA	1:C:273:GLU:HB3	1.89	0.55
1:B:112:LEU:HD21	1:B:137:LEU:HD13	1.89	0.55
1:B:281:GLU:CG	1:B:282:SER:N	2.67	0.55
1:G:265:PHE:HD1	1:G:271:ILE:HD12	1.72	0.55
1:B:241:GLU:HB3	1:B:245:GLN:NE2	2.23	0.54
1:A:355:VAL:HG11	1:A:363:MET:HE1	1.88	0.54
1:C:223:LEU:HG	1:C:234:LEU:HD11	1.88	0.54
1:C:122:THR:HG21	1:C:364:LEU:HD13	1.89	0.54
1:A:126:GLU:CD	1:A:129:LYS:HZ1	2.10	0.54
1:B:208:ALA:HB3	1:B:256:VAL:HA	1.89	0.54
1:G:200:MET:HG2	1:G:201:LEU:HD23	1.89	0.54
1:E:358:LEU:CG	1:E:362:ARG:HH21	2.13	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:PHE:HB3	1:H:315:ILE:HG12	1.90	0.54
1:E:119:LEU:HD21	1:E:155:LEU:HD11	1.87	0.54
1:A:176:LYS:O	1:A:256:VAL:N	2.39	0.54
1:B:164:PRO:HG2	1:B:169:TRP:HE1	1.72	0.54
1:F:289:VAL:O	1:F:290:LEU:HD23	2.08	0.54
1:B:229:LEU:HD13	1:B:229:LEU:O	2.07	0.54
1:G:120:GLN:NE2	1:G:129:LYS:HE3	2.22	0.54
1:B:339:VAL:HG23	1:B:339:VAL:O	2.06	0.54
1:G:183:SER:HB2	1:G:186:ALA:HB2	1.88	0.54
1:G:314:TYR:HB2	1:G:339:VAL:HA	1.90	0.54
1:C:263:ARG:HA	1:G:346:GLN:HE22	1.72	0.54
1:F:291:SER:OG	1:F:293:THR:HB	2.07	0.54
1:D:181:PHE:HZ	1:D:311:VAL:HG22	1.72	0.54
1:D:198:ILE:HD12	1:D:202:GLU:OE2	2.07	0.54
1:G:332:LEU:HD21	1:G:339:VAL:HG13	1.90	0.54
1:D:110:GLU:CB	1:D:111:PRO:CD	2.85	0.54
1:F:194:LYS:O	1:F:198:ILE:HG12	2.08	0.54
1:F:136:LEU:O	1:F:136:LEU:HG	2.08	0.54
1:H:179:VAL:O	1:H:180:LEU:HD23	2.08	0.54
1:H:216:ARG:HB3	1:H:219:ALA:CB	2.35	0.54
1:B:332:LEU:HD21	1:B:339:VAL:HG13	1.88	0.54
1:H:111:PRO:HB2	1:H:151:VAL:CG2	2.38	0.54
1:C:358:LEU:O	1:C:362:ARG:HG3	2.08	0.54
1:H:263:ARG:HB2	1:H:265:PHE:CE1	2.43	0.54
1:F:110:GLU:HB2	1:F:111:PRO:CD	2.37	0.54
1:H:296:TYR:OH	1:H:300:LYS:HE2	2.08	0.54
1:D:291:SER:C	1:D:293:THR:H	2.12	0.54
1:G:287:PHE:CD2	1:G:315:ILE:HD11	2.43	0.53
1:B:190:THR:O	1:B:193:ALA:HB3	2.07	0.53
1:F:235:GLU:HG3	1:F:250:PHE:HE2	1.73	0.53
1:E:355:VAL:HG11	1:E:363:MET:CE	2.38	0.53
1:E:234:LEU:HD23	1:E:235:GLU:N	2.23	0.53
1:D:194:LYS:HG2	1:D:349:PRO:HA	1.91	0.53
1:A:147:THR:O	1:A:151:VAL:HG23	2.07	0.53
1:A:234:LEU:HD23	1:A:234:LEU:C	2.27	0.53
1:C:203:LYS:O	1:C:205:LYS:HG2	2.08	0.53
1:B:176:LYS:HA	1:B:254:ASP:O	2.08	0.53
1:H:316:PHE:HE2	1:H:332:LEU:HD21	1.73	0.53
1:H:211:THR:HG22	1:H:212:THR:N	2.23	0.53
1:A:180:LEU:CD2	1:A:287:PHE:HB2	2.37	0.53
1:B:178:ILE:HB	1:B:257:PHE:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:LEU:HD11	1:F:146:LEU:CD1	2.38	0.53
1:C:217:ILE:H	1:C:217:ILE:CD1	2.20	0.53
1:G:124:ILE:HG22	1:G:128:THR:OG1	2.08	0.53
1:A:198:ILE:CD1	1:A:349:PRO:HB2	2.39	0.53
1:A:288:LEU:HD23	1:A:314:TYR:CE1	2.44	0.53
1:F:344:ASN:HD21	1:F:351:ASP:HA	1.73	0.53
1:F:147:THR:C	1:F:149:GLU:N	2.61	0.53
1:C:319:ILE:HG12	1:C:344:ASN:HB3	1.90	0.53
1:F:124:ILE:CG2	1:F:128:THR:HB	2.39	0.53
1:C:211:THR:HG22	1:C:213:ASP:N	2.17	0.53
1:H:287:PHE:HB3	1:H:315:ILE:CG1	2.38	0.53
1:F:234:LEU:HG	1:F:235:GLU:H	1.73	0.53
1:E:290:LEU:O	1:E:316:PHE:HA	2.09	0.53
1:E:206:LYS:HB2	1:E:254:ASP:H	1.73	0.53
1:B:200:MET:HG2	1:B:201:LEU:HD23	1.90	0.53
1:H:240:LYS:HG3	1:H:241:GLU:OE2	2.09	0.53
1:G:318:LYS:C	1:G:320:ASP:H	2.11	0.53
1:F:122:THR:HB	1:F:364:LEU:CD2	2.39	0.53
1:D:165:SER:OG	1:D:168:LYS:HB2	2.09	0.53
1:F:147:THR:HG22	1:F:149:GLU:H	1.73	0.53
1:G:122:THR:OG1	1:G:123:GLY:N	2.42	0.53
1:B:196:ALA:HA	1:B:257:PHE:CE2	2.44	0.53
1:E:250:PHE:O	1:E:253:TYR:HD1	1.92	0.53
1:H:285:GLN:HG3	1:H:312:ASN:ND2	2.24	0.53
1:C:209:PHE:O	1:C:234:LEU:HA	2.08	0.53
1:D:196:ALA:HA	1:D:257:PHE:HE2	1.72	0.53
1:G:148:GLU:O	1:G:148:GLU:HG3	2.09	0.53
1:B:231:GLN:N	1:B:231:GLN:OE1	2.42	0.53
1:H:211:THR:HG22	1:H:213:ASP:H	1.74	0.53
1:F:147:THR:C	1:F:149:GLU:H	2.10	0.53
1:B:285:GLN:HG3	1:B:312:ASN:ND2	2.24	0.53
1:F:175:SER:HB2	1:F:285:GLN:HB2	1.90	0.52
1:G:237:CYS:SG	1:G:243:PHE:HA	2.49	0.52
1:A:249:LEU:HD23	1:H:336:LYS:HE2	1.91	0.52
1:C:177:TYR:CE1	1:C:247:LYS:HG2	2.43	0.52
1:C:152:VAL:O	1:C:156:GLN:HG3	2.09	0.52
1:A:143:ALA:O	1:A:144:GLY:O	2.26	0.52
1:G:200:MET:HB2	1:G:207:ILE:HG13	1.90	0.52
1:B:129:LYS:C	1:B:131:ASN:H	2.12	0.52
1:D:300:LYS:NZ	1:D:304:LYS:NZ	2.58	0.52
1:H:213:ASP:HA	1:H:261:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ILE:HD12	1:B:257:PHE:HE2	1.75	0.52
1:F:114:LYS:HE2	1:F:148:GLU:O	2.10	0.52
1:B:169:TRP:CE3	1:B:339:VAL:HG22	2.44	0.52
1:D:119:LEU:HB3	1:D:129:LYS:CG	2.39	0.52
1:E:281:GLU:O	1:E:283:SER:N	2.42	0.52
1:E:296:TYR:OH	1:E:300:LYS:HD2	2.09	0.52
1:E:126:GLU:O	1:E:127:SER:C	2.47	0.52
1:C:264:ASN:C	1:C:266:LYS:H	2.13	0.52
1:D:264:ASN:ND2	1:D:266:LYS:N	2.53	0.52
1:B:169:TRP:CD1	1:B:338:GLY:HA3	2.45	0.52
1:A:319:ILE:HG12	1:A:343:THR:O	2.10	0.52
1:H:267:ASP:OD1	1:H:269:GLN:HB2	2.09	0.52
1:H:274:LEU:O	1:H:274:LEU:HD23	2.10	0.52
1:C:247:LYS:O	1:C:251:SER:HB3	2.10	0.52
1:A:224:LYS:O	1:A:228:GLU:HG3	2.10	0.52
1:A:200:MET:HB2	1:A:207:ILE:CG1	2.39	0.52
1:G:329:PHE:HB2	1:G:364:LEU:HD11	1.92	0.52
1:C:214:THR:HG21	1:C:238:TYR:CE2	2.45	0.52
1:G:341:PHE:HB3	1:G:352:ILE:CD1	2.35	0.52
1:C:147:THR:C	1:C:149:GLU:N	2.61	0.52
1:G:179:VAL:HG22	1:G:258:VAL:HB	1.91	0.52
1:F:306:PHE:HD1	1:F:309:VAL:HG11	1.75	0.52
1:H:266:LYS:C	1:H:305:ARG:HH12	2.11	0.51
1:H:124:ILE:CG2	1:H:128:THR:HB	2.40	0.51
1:D:182:GLY:HA2	1:D:288:LEU:CD1	2.40	0.51
1:G:250:PHE:C	1:G:252:GLU:H	2.12	0.51
1:H:111:PRO:O	1:H:114:LYS:HB3	2.09	0.51
1:C:182:GLY:N	1:C:188:LYS:HD3	2.24	0.51
1:D:287:PHE:CE1	1:D:313:GLN:HB2	2.46	0.51
1:G:207:ILE:HD12	1:G:257:PHE:HE2	1.76	0.51
1:D:264:ASN:ND2	1:D:265:PHE:N	2.58	0.51
1:D:300:LYS:NZ	1:D:304:LYS:HZ1	2.07	0.51
1:B:218:ALA:CB	1:F:222:GLN:HG2	2.41	0.51
1:G:160:CYS:SG	1:G:361:VAL:HG21	2.50	0.51
1:A:218:ALA:CB	1:E:222:GLN:HA	2.39	0.51
1:H:179:VAL:HG13	1:H:258:VAL:HB	1.92	0.51
1:D:264:ASN:HD21	1:D:266:LYS:N	2.04	0.51
1:D:188:LYS:NZ	1:D:188:LYS:HB2	2.25	0.51
1:C:122:THR:HG22	1:C:364:LEU:O	2.11	0.51
1:C:156:GLN:HG2	1:C:365:CYS:SG	2.49	0.51
1:E:291:SER:OG	1:E:293:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:HG3	1:C:254:ASP:OD2	2.10	0.51
1:B:281:GLU:OE2	1:B:284:ILE:HG13	2.11	0.51
1:D:280:PHE:H	1:D:284:ILE:CD1	2.23	0.51
1:H:166:ALA:HA	1:H:357:PRO:HG2	1.90	0.51
1:B:314:TYR:HB2	1:B:339:VAL:HA	1.92	0.51
1:D:224:LYS:HA	1:D:227:ALA:HB3	1.92	0.51
1:D:114:LYS:O	1:D:118:LEU:HG	2.10	0.51
1:E:364:LEU:O	1:E:366:ARG:N	2.43	0.51
1:C:216:ARG:CZ	1:G:222:GLN:HE22	2.23	0.51
1:G:198:ILE:HG23	1:G:202:GLU:OE1	2.11	0.51
1:E:224:LYS:HD3	1:E:224:LYS:C	2.30	0.51
1:A:244:GLN:HG3	1:A:248:GLU:OE2	2.10	0.51
1:E:152:VAL:O	1:E:155:LEU:HB3	2.10	0.51
1:D:167:ASP:C	1:D:169:TRP:N	2.63	0.51
1:F:147:THR:HG22	1:F:149:GLU:HB3	1.92	0.51
1:E:322:THR:HG21	1:E:325:LEU:HD12	1.92	0.51
1:C:217:ILE:O	1:C:217:ILE:HG12	2.10	0.51
1:A:211:THR:HG22	1:A:212:THR:N	2.25	0.51
1:B:181:PHE:CZ	1:B:311:VAL:HG12	2.45	0.51
1:E:278:ILE:HG23	1:E:279:PRO:HD2	1.93	0.51
1:C:188:LYS:HE2	4:C:3001:HOH:O	2.09	0.51
1:F:120:GLN:NE2	1:F:129:LYS:HE3	2.25	0.51
1:H:192:LEU:HD12	1:H:259:ASP:HB2	1.93	0.50
1:E:124:ILE:HA	1:E:330:ASN:HD21	1.76	0.50
1:C:222:GLN:OE1	1:G:222:GLN:HG3	2.11	0.50
1:C:171:GLU:OE1	1:C:312:ASN:HB3	2.09	0.50
1:F:248:GLU:C	1:F:250:PHE:H	2.15	0.50
1:G:114:LYS:HE2	1:G:148:GLU:HB2	1.93	0.50
1:B:233:PRO:HB2	1:B:250:PHE:CE1	2.46	0.50
1:D:207:ILE:HD12	1:D:257:PHE:CE2	2.46	0.50
1:F:266:LYS:O	1:F:305:ARG:NE	2.45	0.50
1:A:317:THR:HA	1:A:343:THR:OG1	2.12	0.50
1:C:349:PRO:HD2	1:C:350:GLU:OE1	2.12	0.50
1:H:181:PHE:HZ	1:H:286:SER:HG	1.57	0.50
1:G:147:THR:HB	1:G:150:ASN:ND2	2.26	0.50
1:C:268:PRO:HD3	1:C:305:ARG:HH21	1.77	0.50
1:A:154:LYS:O	1:A:158:ILE:HG13	2.10	0.50
1:F:300:LYS:O	1:F:304:LYS:HD3	2.11	0.50
1:E:112:LEU:HD21	1:E:137:LEU:HD13	1.94	0.50
1:G:140:SER:CB	1:G:146:LEU:HD11	2.42	0.50
1:D:230:LEU:O	1:D:231:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:PHE:O	1:G:210:ILE:HG13	2.12	0.50
1:D:181:PHE:O	1:D:288:LEU:HA	2.11	0.50
1:A:192:LEU:CD2	1:A:257:PHE:HB3	2.42	0.50
1:B:206:LYS:HD2	1:B:254:ASP:OD1	2.12	0.50
1:A:335:SER:C	1:A:336:LYS:HD2	2.32	0.50
1:D:212:THR:HB	1:D:260:THR:HG22	1.93	0.50
1:H:271:ILE:N	1:H:271:ILE:HD12	2.26	0.50
1:A:279:PRO:O	1:A:280:PHE:CB	2.59	0.50
1:G:309:VAL:CG2	1:G:309:VAL:O	2.59	0.50
1:H:111:PRO:HB2	1:H:151:VAL:HG21	1.94	0.50
1:G:173:ILE:HG21	1:G:195:LEU:HD23	1.94	0.50
1:G:285:GLN:HG2	1:G:287:PHE:HE1	1.77	0.50
1:F:152:VAL:HG23	1:F:153:GLY:N	2.27	0.50
1:E:190:THR:HG22	1:E:190:THR:O	2.11	0.50
1:F:280:PHE:CA	1:F:284:ILE:HD12	2.40	0.50
1:H:316:PHE:O	1:H:342:MET:HA	2.12	0.50
1:F:289:VAL:C	1:F:290:LEU:HD23	2.32	0.50
1:C:137:LEU:C	1:C:137:LEU:HD23	2.32	0.50
1:H:206:LYS:CD	1:H:206:LYS:N	2.74	0.50
1:A:176:LYS:HG3	1:A:254:ASP:O	2.11	0.50
1:G:169:TRP:CE2	1:G:357:PRO:HG3	2.47	0.50
1:F:138:ARG:HG2	1:F:138:ARG:HH11	1.77	0.50
1:C:212:THR:HG23	1:C:277:THR:HG21	1.92	0.49
1:F:192:LEU:CD2	1:F:257:PHE:HB3	2.37	0.49
1:E:123:GLY:CA	1:E:326:GLY:HA3	2.41	0.49
1:A:300:LYS:O	1:A:303:VAL:HG12	2.11	0.49
1:B:199:SER:CA	1:B:203:LYS:HB2	2.41	0.49
1:H:133:LEU:O	1:H:137:LEU:HD22	2.12	0.49
1:E:233:PRO:HB2	1:E:250:PHE:CE1	2.47	0.49
1:G:114:LYS:CE	1:G:148:GLU:HB2	2.42	0.49
1:B:233:PRO:HB2	1:B:250:PHE:HE1	1.78	0.49
1:B:162:MET:HG2	1:H:248:GLU:OE1	2.12	0.49
1:H:175:SER:HB3	1:H:283:SER:O	2.12	0.49
1:D:166:ALA:CA	1:D:357:PRO:HG2	2.25	0.49
1:B:271:ILE:HG22	1:B:275:LYS:HZ2	1.76	0.49
1:H:169:TRP:CE2	1:H:357:PRO:HG3	2.48	0.49
1:B:345:GLY:HA3	1:B:351:ASP:OD2	2.13	0.49
1:A:293:THR:O	1:E:295:LYS:HG3	2.12	0.49
1:D:111:PRO:HB3	1:D:148:GLU:HA	1.93	0.49
1:C:288:LEU:HG	1:C:290:LEU:CD1	2.42	0.49
1:C:220:VAL:CG1	1:C:236:VAL:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:THR:O	1:F:193:ALA:HB3	2.13	0.49
1:H:179:VAL:C	1:H:180:LEU:HD23	2.33	0.49
1:E:211:THR:HG23	1:E:259:ASP:HB3	1.94	0.49
1:B:281:GLU:OE2	1:B:283:SER:N	2.46	0.49
1:F:133:LEU:C	1:F:135:LYS:H	2.15	0.49
1:H:159:LEU:O	1:H:163:LEU:HD22	2.13	0.49
1:G:133:LEU:C	1:G:135:LYS:N	2.66	0.49
1:G:205:LYS:HD3	1:G:255:HIS:CE1	2.48	0.49
1:G:171:GLU:HB3	1:G:313:GLN:HG3	1.93	0.49
1:B:182:GLY:N	1:B:188:LYS:HD3	2.28	0.49
1:E:123:GLY:HA3	1:E:326:GLY:HA3	1.94	0.49
1:B:280:PHE:HA	1:B:284:ILE:HD12	1.93	0.49
1:F:171:GLU:HB2	1:F:313:GLN:CG	2.39	0.49
1:H:140:SER:HB2	1:H:146:LEU:HG	1.95	0.49
1:D:348:VAL:CG1	1:D:349:PRO:HA	2.43	0.49
1:F:212:THR:O	1:F:212:THR:HG22	2.13	0.49
1:G:243:PHE:CE2	1:G:247:LYS:HD2	2.48	0.49
1:A:243:PHE:CE2	1:A:247:LYS:HD2	2.48	0.49
1:B:320:ASP:OD1	1:B:344:ASN:HA	2.13	0.49
1:C:110:GLU:HB3	1:C:111:PRO:CD	2.32	0.49
1:G:268:PRO:HD3	1:G:305:ARG:NH2	2.20	0.49
1:F:175:SER:H	1:F:285:GLN:NE2	2.10	0.49
1:D:169:TRP:O	1:D:171:GLU:N	2.46	0.49
1:G:303:VAL:O	1:G:303:VAL:HG12	2.12	0.49
1:E:233:PRO:O	1:E:234:LEU:HB2	2.13	0.49
1:C:118:LEU:HD23	1:C:155:LEU:HD23	1.95	0.49
1:G:180:LEU:HD22	1:G:287:PHE:HB2	1.94	0.49
1:H:160:CYS:HA	1:H:163:LEU:CD2	2.43	0.49
1:F:344:ASN:HD21	1:F:351:ASP:CA	2.26	0.49
1:D:234:LEU:C	1:D:234:LEU:HD23	2.33	0.49
1:F:194:LYS:HG2	1:F:349:PRO:HA	1.95	0.48
1:C:165:SER:HB2	1:C:167:ASP:OD1	2.13	0.48
1:E:180:LEU:CD2	1:E:287:PHE:HB2	2.43	0.48
1:H:129:LYS:HB3	1:H:129:LYS:NZ	2.27	0.48
1:B:205:LYS:HB3	1:B:254:ASP:OD2	2.13	0.48
1:B:147:THR:HG22	1:B:148:GLU:OE2	2.12	0.48
1:C:278:ILE:HG23	1:C:279:PRO:HD2	1.95	0.48
1:A:130:THR:O	1:A:134:LYS:HG2	2.13	0.48
1:B:163:LEU:HD11	1:B:329:PHE:CE1	2.48	0.48
1:E:309:VAL:O	1:E:309:VAL:HG23	2.13	0.48
1:A:269:GLN:O	1:A:272:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:O	1:A:110:GLU:CG	2.59	0.48
1:G:124:ILE:HA	1:G:330:ASN:OD1	2.13	0.48
1:C:244:GLN:NE2	1:C:247:LYS:HD2	2.27	0.48
1:C:244:GLN:O	1:C:247:LYS:HB2	2.13	0.48
1:C:177:TYR:HB2	1:C:284:ILE:HG12	1.94	0.48
1:G:325:LEU:C	1:G:364:LEU:HD21	2.33	0.48
1:C:194:LYS:HG2	1:C:349:PRO:HA	1.95	0.48
1:D:306:PHE:HD2	1:D:309:VAL:HG11	1.77	0.48
1:H:309:VAL:HG22	1:H:309:VAL:O	2.12	0.48
1:D:111:PRO:O	1:D:114:LYS:HB3	2.14	0.48
1:D:352:ILE:HG12	1:D:353:GLN:N	2.28	0.48
1:E:151:VAL:HG23	1:E:152:VAL:H	1.79	0.48
1:F:148:GLU:HA	1:F:151:VAL:CG2	2.44	0.48
1:G:288:LEU:HB2	1:G:311:VAL:HG11	1.95	0.48
1:H:147:THR:C	1:H:149:GLU:N	2.67	0.48
1:B:335:SER:C	1:B:336:LYS:HD2	2.33	0.48
1:B:322:THR:HA	1:F:298:ASP:OD2	2.14	0.48
1:H:169:TRP:CE3	1:H:339:VAL:HG22	2.47	0.48
1:B:241:GLU:HB3	1:B:245:GLN:HE22	1.79	0.48
1:C:151:VAL:HG23	1:C:152:VAL:H	1.77	0.48
1:A:336:LYS:N	1:A:336:LYS:HD2	2.29	0.48
1:E:173:ILE:HG23	1:E:178:ILE:CD1	2.43	0.48
1:C:224:LYS:HA	1:C:234:LEU:HD13	1.95	0.48
1:A:109:PRO:O	1:A:110:GLU:CB	2.62	0.48
1:D:173:ILE:HD13	1:D:257:PHE:HZ	1.77	0.48
1:C:247:LYS:NZ	1:C:281:GLU:OE2	2.46	0.48
1:E:250:PHE:O	1:E:253:TYR:N	2.45	0.48
1:D:119:LEU:HB3	1:D:129:LYS:HG3	1.96	0.48
1:E:288:LEU:HD23	1:E:314:TYR:CE1	2.49	0.48
1:H:258:VAL:HG12	1:H:259:ASP:N	2.29	0.48
1:C:208:ALA:C	1:C:209:PHE:HD1	2.17	0.48
1:B:194:LYS:HA	1:B:349:PRO:HB3	1.95	0.48
1:C:199:SER:HA	1:C:203:LYS:HB2	1.96	0.48
1:C:210:ILE:O	1:C:258:VAL:HG13	2.14	0.48
1:H:210:ILE:CD1	1:H:256:VAL:HG11	2.44	0.48
1:H:263:ARG:H	1:H:265:PHE:HE1	1.60	0.48
1:E:350:GLU:N	1:E:350:GLU:OE1	2.47	0.48
1:A:296:TYR:CE2	1:A:300:LYS:HD2	2.48	0.48
1:D:279:PRO:HG2	1:D:284:ILE:HD11	1.95	0.48
1:D:183:SER:OG	1:D:184:THR:N	2.46	0.48
1:B:193:ALA:O	1:B:194:LYS:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:PHE:O	1:D:210:ILE:HG13	2.13	0.48
1:D:329:PHE:CD2	1:D:364:LEU:HD11	2.49	0.48
1:E:265:PHE:HD1	1:E:271:ILE:HD12	1.78	0.48
1:C:223:LEU:HG	1:C:234:LEU:CD1	2.44	0.47
1:F:281:GLU:OE2	1:F:284:ILE:HG13	2.14	0.47
1:B:208:ALA:HB3	1:B:256:VAL:HG22	1.95	0.47
1:H:325:LEU:N	1:H:325:LEU:HD12	2.29	0.47
1:D:265:PHE:C	1:D:267:ASP:H	2.16	0.47
1:F:287:PHE:CE2	1:F:313:GLN:HB2	2.49	0.47
1:G:212:THR:O	1:G:212:THR:HG22	2.13	0.47
1:G:211:THR:CG2	1:G:212:THR:N	2.77	0.47
1:E:151:VAL:HG23	1:E:152:VAL:N	2.29	0.47
1:A:170:GLN:HG2	1:A:354:THR:OG1	2.13	0.47
1:B:215:TYR:HB2	1:B:263:ARG:NH2	2.29	0.47
1:C:110:GLU:CB	1:C:111:PRO:CD	2.92	0.47
1:C:250:PHE:HD1	1:C:253:TYR:HE2	1.62	0.47
1:D:200:MET:CE	1:D:207:ILE:HB	2.44	0.47
1:A:190:THR:O	1:A:194:LYS:HG3	2.15	0.47
1:E:116:GLU:HG2	1:E:120:GLN:NE2	2.29	0.47
1:F:111:PRO:HB2	1:F:151:VAL:HG21	1.96	0.47
1:D:268:PRO:C	1:D:270:TYR:H	2.17	0.47
1:D:194:LYS:O	1:D:198:ILE:HG12	2.15	0.47
1:C:263:ARG:HA	1:G:346:GLN:NE2	2.29	0.47
1:G:109:PRO:O	1:G:113:ARG:HB2	2.14	0.47
1:B:265:PHE:C	1:B:267:ASP:H	2.18	0.47
1:H:295:LYS:O	1:H:298:ASP:HB2	2.14	0.47
1:A:358:LEU:O	1:A:358:LEU:HD12	2.14	0.47
1:E:179:VAL:HG12	1:E:180:LEU:N	2.29	0.47
1:G:211:THR:CG2	1:G:213:ASP:H	2.24	0.47
1:D:194:LYS:HE2	1:D:351:ASP:O	2.13	0.47
1:A:245:GLN:O	1:A:249:LEU:N	2.48	0.47
1:F:114:LYS:O	1:F:118:LEU:HG	2.14	0.47
1:D:147:THR:O	1:D:151:VAL:HG22	2.15	0.47
1:E:123:GLY:O	1:E:124:ILE:O	2.32	0.47
1:E:289:VAL:HG22	1:E:315:ILE:HB	1.97	0.47
1:E:287:PHE:HB3	1:E:315:ILE:CD1	2.45	0.47
3:D:4:GNP:O4'	1:H:184:THR:HB	2.14	0.47
1:F:271:ILE:N	1:F:271:ILE:HD12	2.29	0.47
1:D:314:TYR:HB2	1:D:339:VAL:HB	1.97	0.47
1:F:211:THR:HG22	1:F:213:ASP:H	1.80	0.47
1:B:254:ASP:OD1	1:B:254:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PHE:CE2	1:A:286:SER:HB2	2.50	0.47
1:D:190:THR:HG22	1:D:190:THR:O	2.15	0.47
1:C:136:LEU:HD23	1:C:136:LEU:O	2.14	0.47
1:C:154:LYS:O	1:C:158:ILE:HG13	2.15	0.47
1:G:253:TYR:CD1	1:G:253:TYR:N	2.82	0.47
1:E:325:LEU:HD23	1:E:360:PHE:HE1	1.79	0.47
1:H:268:PRO:C	1:H:270:TYR:H	2.19	0.47
1:E:147:THR:CG2	1:E:148:GLU:N	2.77	0.47
1:C:182:GLY:H	1:C:188:LYS:HD3	1.79	0.47
1:A:163:LEU:HD21	1:A:329:PHE:CE2	2.50	0.47
1:C:267:ASP:O	1:C:269:GLN:N	2.48	0.47
1:H:264:ASN:C	1:H:266:LYS:H	2.19	0.47
1:D:317:THR:HA	1:D:343:THR:OG1	2.15	0.47
1:D:350:GLU:O	1:D:352:ILE:HG22	2.15	0.47
1:D:237:CYS:SG	1:D:243:PHE:HA	2.55	0.47
1:G:110:GLU:HB2	1:G:111:PRO:CD	2.45	0.47
1:E:267:ASP:OD1	1:E:269:GLN:HB2	2.15	0.47
1:D:315:ILE:HG12	1:D:341:PHE:HB2	1.97	0.46
1:B:209:PHE:HB2	1:B:233:PRO:O	2.15	0.46
1:B:169:TRP:CZ3	1:B:339:VAL:HG22	2.50	0.46
1:C:357:PRO:O	1:C:360:PHE:N	2.47	0.46
1:A:355:VAL:HG11	1:A:363:MET:CE	2.45	0.46
1:D:176:LYS:O	1:D:256:VAL:N	2.43	0.46
1:F:345:GLY:HA3	1:F:351:ASP:OD2	2.13	0.46
1:G:171:GLU:HB3	1:G:313:GLN:CG	2.45	0.46
1:C:115:ALA:O	1:C:119:LEU:HG	2.14	0.46
1:B:147:THR:O	1:B:151:VAL:HG23	2.14	0.46
1:C:216:ARG:HD3	1:C:219:ALA:HB2	1.97	0.46
1:B:116:GLU:O	1:B:120:GLN:HG3	2.15	0.46
1:C:147:THR:O	1:C:149:GLU:N	2.47	0.46
1:A:163:LEU:HD11	1:A:329:PHE:CD2	2.50	0.46
1:G:227:ALA:HB1	1:G:232:ALA:O	2.14	0.46
1:F:123:GLY:C	1:F:326:GLY:HA3	2.36	0.46
1:A:131:ASN:HD21	1:G:249:LEU:HA	1.79	0.46
1:D:330:ASN:O	1:D:334:GLU:HG2	2.16	0.46
1:C:210:ILE:HB	1:C:258:VAL:HG22	1.98	0.46
1:A:285:GLN:HE21	1:A:287:PHE:HZ	1.64	0.46
1:G:224:LYS:HA	1:G:224:LYS:HE2	1.96	0.46
1:A:126:GLU:HA	1:A:129:LYS:HZ3	1.81	0.46
1:H:210:ILE:HB	1:H:258:VAL:HG22	1.97	0.46
1:C:264:ASN:OD1	1:C:264:ASN:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:THR:O	1:E:129:LYS:C	2.54	0.46
1:C:199:SER:OG	1:C:255:HIS:ND1	2.45	0.46
1:F:266:LYS:HA	1:F:305:ARG:NE	2.29	0.46
1:F:147:THR:CG2	1:F:149:GLU:HB3	2.45	0.46
1:H:211:THR:CG2	1:H:212:THR:N	2.79	0.46
1:E:164:PRO:HG2	1:E:169:TRP:NE1	2.24	0.46
1:D:268:PRO:C	1:D:270:TYR:N	2.68	0.46
1:F:175:SER:H	1:F:285:GLN:HE22	1.62	0.46
1:A:138:ARG:NH1	1:A:139:PHE:CD2	2.83	0.46
1:A:222:GLN:HG2	1:E:218:ALA:HB1	1.97	0.46
1:D:246:ALA:O	1:D:249:LEU:HB3	2.16	0.46
1:B:147:THR:HG22	1:B:149:GLU:H	1.79	0.46
1:E:288:LEU:HD13	1:E:306:PHE:CD2	2.50	0.46
1:A:221:GLU:O	1:A:225:THR:HG23	2.16	0.46
1:G:125:LYS:H	1:G:330:ASN:HD21	1.63	0.46
1:G:145:GLY:O	1:G:146:LEU:HD23	2.16	0.46
1:E:221:GLU:O	1:E:225:THR:HG23	2.15	0.46
1:D:216:ARG:CB	1:D:219:ALA:HB2	2.35	0.46
1:H:266:LYS:HE3	1:H:301:HIS:ND1	2.31	0.46
1:C:217:ILE:O	1:G:222:GLN:HG2	2.16	0.46
1:B:244:GLN:O	1:B:247:LYS:HB3	2.16	0.46
1:F:266:LYS:CG	1:F:305:ARG:HH21	2.29	0.46
1:C:188:LYS:N	3:C:3:GNP:O1B	2.45	0.46
1:A:123:GLY:CA	1:A:326:GLY:HA3	2.44	0.46
1:D:213:ASP:OD2	1:D:219:ALA:HB1	2.16	0.46
1:H:223:LEU:HD12	1:H:226:TYR:CB	2.43	0.46
1:A:267:ASP:OD2	1:A:269:GLN:HB3	2.16	0.46
1:C:120:GLN:OE1	1:C:129:LYS:HE3	2.16	0.46
1:A:160:CYS:C	1:A:162:MET:H	2.20	0.46
1:E:122:THR:HB	1:E:364:LEU:CD2	2.46	0.46
1:E:211:THR:HG22	1:E:213:ASP:N	2.21	0.46
1:C:170:GLN:HE21	1:C:354:THR:HG23	1.81	0.46
1:C:117:LYS:HE3	1:C:121:GLU:OE2	2.16	0.46
1:A:301:HIS:O	1:A:303:VAL:N	2.49	0.45
1:H:206:LYS:H	1:H:206:LYS:CD	2.28	0.45
1:H:129:LYS:HZ3	1:H:129:LYS:HB3	1.79	0.45
1:A:249:LEU:C	1:A:249:LEU:HD23	2.37	0.45
1:C:171:GLU:HB2	1:C:313:GLN:CG	2.46	0.45
1:F:315:ILE:HG12	1:F:341:PHE:HB2	1.98	0.45
1:D:210:ILE:HG21	1:D:243:PHE:CE1	2.49	0.45
1:B:147:THR:C	1:B:149:GLU:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:THR:HG22	1:C:190:THR:N	2.31	0.45
1:B:110:GLU:C	1:B:112:LEU:H	2.19	0.45
1:G:250:PHE:C	1:G:252:GLU:N	2.69	0.45
1:G:169:TRP:CE3	1:G:339:VAL:HG22	2.51	0.45
1:F:323:THR:CG2	1:F:366:ARG:HH22	2.29	0.45
1:F:147:THR:O	1:F:149:GLU:N	2.49	0.45
1:E:349:PRO:HD2	1:E:350:GLU:OE1	2.17	0.45
1:B:210:ILE:HG21	1:B:243:PHE:CE1	2.51	0.45
1:A:296:TYR:CE1	1:A:330:ASN:HB3	2.51	0.45
1:G:244:GLN:O	1:G:248:GLU:HG3	2.17	0.45
1:F:296:TYR:OH	1:F:300:LYS:HD2	2.17	0.45
1:C:119:LEU:HD21	1:C:155:LEU:HD11	1.98	0.45
1:H:315:ILE:CD1	1:H:341:PHE:HB2	2.47	0.45
1:A:279:PRO:HG2	1:A:280:PHE:H	1.82	0.45
1:E:147:THR:CG2	1:E:148:GLU:H	2.30	0.45
1:E:224:LYS:O	1:E:228:GLU:HG3	2.15	0.45
1:B:296:TYR:OH	1:B:334:GLU:OE2	2.31	0.45
1:D:123:GLY:CA	1:D:326:GLY:HA3	2.47	0.45
1:C:346:GLN:HE22	1:G:263:ARG:HA	1.80	0.45
1:E:128:THR:O	1:E:131:ASN:N	2.50	0.45
1:D:319:ILE:HG21	1:D:342:MET:HE3	1.99	0.45
1:A:341:PHE:HB3	1:A:352:ILE:HD11	1.98	0.45
1:H:200:MET:HB2	1:H:207:ILE:HG13	1.98	0.45
1:D:350:GLU:H	1:D:350:GLU:CD	2.20	0.45
1:C:200:MET:C	1:C:202:GLU:H	2.19	0.45
1:C:323:THR:CG2	1:C:366:ARG:HH22	2.27	0.45
1:F:111:PRO:HG2	1:F:112:LEU:HD12	1.99	0.45
1:A:126:GLU:HA	1:A:129:LYS:NZ	2.32	0.45
1:A:124:ILE:CG2	1:A:128:THR:HB	2.47	0.45
1:F:143:ALA:O	1:F:144:GLY:O	2.34	0.45
1:C:232:ALA:HB1	1:C:233:PRO:HD2	1.99	0.45
1:C:133:LEU:H	1:C:133:LEU:HD12	1.81	0.45
1:H:305:ARG:NH1	1:H:305:ARG:HG3	2.31	0.45
1:B:147:THR:H	1:B:150:ASN:HD21	1.64	0.45
1:A:356:SER:O	1:A:357:PRO:C	2.55	0.45
1:H:205:LYS:HD2	1:H:255:HIS:CE1	2.51	0.45
1:A:179:VAL:O	1:A:180:LEU:HD23	2.16	0.45
1:D:183:SER:O	1:D:188:LYS:HE3	2.17	0.45
1:C:123:GLY:O	1:C:124:ILE:C	2.55	0.45
1:D:342:MET:HE1	1:D:355:VAL:HG11	1.99	0.45
1:H:296:TYR:CE1	1:H:330:ASN:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:VAL:HA	1:C:310:PRO:HD3	1.79	0.45
1:E:341:PHE:CD1	1:E:341:PHE:N	2.84	0.45
1:A:229:LEU:C	1:A:231:GLN:H	2.19	0.45
1:D:302:ILE:C	1:D:305:ARG:H	2.20	0.45
1:B:192:LEU:HD21	1:B:257:PHE:HB3	1.99	0.45
1:E:177:TYR:CD1	1:E:256:VAL:HB	2.52	0.45
1:E:243:PHE:O	1:E:246:ALA:HB3	2.17	0.45
1:E:275:LYS:NZ	1:E:308:SER:HB2	2.32	0.44
1:H:123:GLY:H	1:H:326:GLY:HA3	1.82	0.44
1:D:345:GLY:HA3	1:D:351:ASP:HB3	1.98	0.44
1:G:235:GLU:CG	1:G:250:PHE:HE2	2.30	0.44
1:G:167:ASP:C	1:G:169:TRP:N	2.70	0.44
1:B:169:TRP:CE2	1:B:357:PRO:HG3	2.52	0.44
1:E:238:TYR:CD1	1:E:238:TYR:N	2.84	0.44
1:A:316:PHE:CE1	1:A:328:VAL:HG13	2.52	0.44
1:F:237:CYS:SG	1:F:243:PHE:HA	2.57	0.44
1:C:302:ILE:HA	1:C:305:ARG:CG	2.47	0.44
1:B:278:ILE:HG22	1:B:280:PHE:H	1.81	0.44
1:D:348:VAL:HG13	1:D:349:PRO:HA	1.98	0.44
1:D:350:GLU:O	1:D:352:ILE:N	2.50	0.44
1:E:120:GLN:HA	1:E:129:LYS:NZ	2.32	0.44
1:C:169:TRP:CD1	1:C:338:GLY:HA3	2.53	0.44
1:F:127:SER:OG	1:F:128:THR:N	2.51	0.44
1:G:200:MET:HB2	1:G:207:ILE:CG1	2.47	0.44
1:E:192:LEU:HD11	1:E:258:VAL:C	2.33	0.44
1:H:200:MET:HB2	1:H:207:ILE:CG1	2.47	0.44
1:D:321:GLU:HG3	1:H:264:ASN:CG	2.36	0.44
1:H:314:TYR:HB2	1:H:339:VAL:HA	1.99	0.44
1:H:336:LYS:HD2	1:H:336:LYS:N	2.33	0.44
1:G:167:ASP:CG	1:G:168:LYS:N	2.70	0.44
1:D:235:GLU:HB2	1:D:250:PHE:HZ	1.81	0.44
1:E:224:LYS:HA	1:E:234:LEU:HD13	1.98	0.44
1:C:316:PHE:O	1:C:342:MET:HA	2.17	0.44
1:E:314:TYR:HB2	1:E:339:VAL:HG12	1.99	0.44
1:D:302:ILE:O	1:D:305:ARG:N	2.49	0.44
1:D:345:GLY:HA3	1:D:351:ASP:OD2	2.18	0.44
1:G:169:TRP:CD2	1:G:357:PRO:HG3	2.52	0.44
1:C:177:TYR:CB	1:C:284:ILE:HG12	2.48	0.44
1:A:224:LYS:C	1:A:226:TYR:H	2.20	0.44
1:G:172:PRO:O	1:G:174:HIS:N	2.50	0.44
1:A:117:LYS:CE	1:A:118:LEU:HD23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LYS:HA	1:C:254:ASP:O	2.17	0.44
1:E:130:THR:CG2	1:E:131:ASN:N	2.80	0.44
1:G:278:ILE:HG22	1:G:280:PHE:H	1.82	0.44
1:F:110:GLU:CB	1:F:111:PRO:CD	2.95	0.44
1:H:229:LEU:HD12	1:H:229:LEU:N	2.32	0.44
1:A:330:ASN:O	1:A:334:GLU:HG2	2.17	0.44
1:A:222:GLN:HG2	1:E:218:ALA:CB	2.47	0.44
1:C:151:VAL:HG23	1:C:152:VAL:N	2.33	0.44
1:E:117:LYS:HB3	1:E:117:LYS:HE2	1.77	0.44
1:H:210:ILE:O	1:H:258:VAL:HG13	2.17	0.44
1:F:192:LEU:HA	1:F:192:LEU:HD23	1.90	0.44
1:D:208:ALA:O	1:D:257:PHE:N	2.46	0.44
1:G:265:PHE:HD1	1:G:271:ILE:CD1	2.30	0.44
1:G:215:TYR:HB2	1:G:263:ARG:NH2	2.32	0.44
1:E:305:ARG:HD2	1:E:305:ARG:HA	1.68	0.44
1:D:110:GLU:HG3	1:D:111:PRO:CD	2.34	0.44
1:H:281:GLU:O	1:H:284:ILE:HB	2.18	0.44
1:D:290:LEU:CD2	1:D:302:ILE:HD11	2.48	0.44
1:B:268:PRO:HA	1:B:271:ILE:HD12	2.00	0.44
1:D:239:THR:HG1	1:D:242:GLU:HG3	1.81	0.44
1:D:221:GLU:O	1:D:225:THR:HG23	2.17	0.44
1:H:212:THR:O	1:H:212:THR:CG2	2.66	0.44
1:C:265:PHE:O	1:C:271:ILE:HD11	2.17	0.44
1:B:199:SER:HA	1:B:203:LYS:CB	2.43	0.44
1:A:284:ILE:CG2	1:A:285:GLN:N	2.80	0.44
1:H:129:LYS:CB	1:H:129:LYS:NZ	2.81	0.44
1:G:233:PRO:HB2	1:G:250:PHE:HZ	1.82	0.44
1:D:243:PHE:O	1:D:246:ALA:N	2.51	0.44
1:D:206:LYS:HB3	1:D:253:TYR:CD2	2.53	0.44
1:H:278:ILE:H	1:H:278:ILE:HD12	1.81	0.44
1:C:262:GLY:HA3	3:C:3:GNP:O3G	2.17	0.44
1:E:165:SER:O	1:E:167:ASP:N	2.51	0.44
1:A:175:SER:HB3	1:A:283:SER:O	2.18	0.44
1:B:325:LEU:HD22	1:B:325:LEU:N	2.33	0.44
1:D:163:LEU:HG	1:D:164:PRO:HD2	2.00	0.43
1:C:220:VAL:HG13	1:C:236:VAL:HG21	1.99	0.43
1:A:163:LEU:N	1:A:163:LEU:HD22	2.32	0.43
1:A:169:TRP:NE1	1:A:357:PRO:HG3	2.33	0.43
1:A:117:LYS:HE3	1:A:118:LEU:HD23	1.98	0.43
1:C:267:ASP:HA	1:C:268:PRO:HD2	1.88	0.43
1:D:268:PRO:O	1:D:270:TYR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ILE:CD1	1:D:305:ARG:HD2	2.48	0.43
1:E:287:PHE:HB3	1:E:315:ILE:HD11	2.00	0.43
1:D:300:LYS:HZ1	1:D:304:LYS:NZ	2.16	0.43
1:G:151:VAL:HG23	1:G:152:VAL:N	2.32	0.43
1:C:287:PHE:CD1	1:C:287:PHE:N	2.86	0.43
1:E:329:PHE:C	1:E:329:PHE:CD1	2.92	0.43
1:C:272:ASP:O	1:C:276:GLU:HG2	2.18	0.43
1:B:135:LYS:O	1:B:138:ARG:N	2.51	0.43
1:B:191:THR:C	1:B:193:ALA:N	2.71	0.43
1:C:347:ASN:HB2	1:C:351:ASP:OD2	2.19	0.43
1:B:213:ASP:OD2	1:B:261:ALA:HA	2.18	0.43
1:B:124:ILE:HG22	1:B:125:LYS:N	2.34	0.43
1:F:352:ILE:HG13	1:F:353:GLN:N	2.33	0.43
1:G:288:LEU:HD23	1:G:314:TYR:CE1	2.53	0.43
1:G:309:VAL:O	1:G:311:VAL:HG23	2.19	0.43
1:C:180:LEU:HD12	1:C:192:LEU:HG	2.00	0.43
1:D:222:GLN:NE2	1:H:219:ALA:HA	2.34	0.43
1:D:169:TRP:CZ3	1:D:355:VAL:HG23	2.53	0.43
1:B:164:PRO:HB2	1:B:168:LYS:HD2	1.99	0.43
1:A:119:LEU:HB3	1:A:129:LYS:HG2	2.00	0.43
1:D:268:PRO:HA	1:D:271:ILE:CG1	2.48	0.43
1:H:147:THR:O	1:H:149:GLU:N	2.52	0.43
1:D:113:ARG:NH1	1:E:224:LYS:HE3	2.34	0.43
1:F:123:GLY:CA	1:F:326:GLY:HA3	2.49	0.43
1:C:327:SER:O	1:C:331:ILE:HG12	2.18	0.43
1:B:145:GLY:C	1:B:146:LEU:HD12	2.39	0.43
1:D:248:GLU:CD	1:D:248:GLU:H	2.22	0.43
1:A:173:ILE:HA	1:A:285:GLN:HE22	1.84	0.43
1:F:112:LEU:HD11	1:F:146:LEU:HD13	2.00	0.43
1:H:243:PHE:CZ	1:H:278:ILE:HG13	2.53	0.43
1:H:285:GLN:HG2	1:H:287:PHE:HE1	1.84	0.43
1:E:169:TRP:CD1	1:E:338:GLY:HA3	2.52	0.43
1:D:196:ALA:O	1:D:197:ALA:C	2.57	0.43
1:D:206:LYS:HB2	1:D:253:TYR:HA	2.00	0.43
1:F:323:THR:HG23	1:F:366:ARG:HH12	1.84	0.43
1:D:138:ARG:O	1:D:142:GLU:HG2	2.19	0.43
1:H:192:LEU:HD11	1:H:258:VAL:C	2.39	0.43
1:C:267:ASP:C	1:C:269:GLN:H	2.22	0.43
1:H:305:ARG:HD2	1:H:305:ARG:N	2.34	0.43
1:H:123:GLY:O	1:H:124:ILE:C	2.56	0.43
1:D:286:SER:OG	1:D:311:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:LEU:C	1:E:234:LEU:HD23	2.38	0.43
1:C:319:ILE:HD13	1:C:342:MET:HE3	2.01	0.43
1:C:291:SER:C	1:C:293:THR:H	2.22	0.43
1:C:208:ALA:HB2	1:C:253:TYR:CD2	2.54	0.43
1:B:120:GLN:HG2	1:B:129:LYS:CE	2.48	0.43
1:B:271:ILE:HG22	1:B:275:LYS:NZ	2.34	0.43
1:B:305:ARG:HH11	1:B:305:ARG:CG	2.32	0.43
1:B:244:GLN:HE22	1:B:247:LYS:HZ2	1.62	0.43
1:C:361:VAL:O	1:C:364:LEU:HB3	2.19	0.43
1:A:148:GLU:HA	1:A:151:VAL:CG2	2.49	0.43
1:E:198:ILE:O	1:E:202:GLU:HB2	2.19	0.43
1:D:233:PRO:HB2	1:D:250:PHE:HE1	1.81	0.43
1:C:215:TYR:HB2	1:C:263:ARG:NH2	2.34	0.43
1:D:268:PRO:HA	1:D:271:ILE:HD12	2.00	0.42
1:D:339:VAL:CG2	1:D:340:GLY:N	2.82	0.42
1:F:352:ILE:HD12	1:F:353:GLN:H	1.84	0.42
1:E:188:LYS:NZ	3:E:5:GNP:O3G	2.51	0.42
1:C:264:ASN:OD1	1:C:266:LYS:HB3	2.19	0.42
1:B:120:GLN:HG2	1:B:129:LYS:CD	2.49	0.42
1:G:235:GLU:HG3	1:G:250:PHE:HE2	1.84	0.42
1:E:190:THR:O	1:E:194:LYS:HG3	2.18	0.42
1:A:268:PRO:HA	1:A:271:ILE:HD12	2.01	0.42
1:D:250:PHE:HA	1:D:253:TYR:CD1	2.54	0.42
1:A:229:LEU:C	1:A:231:GLN:N	2.72	0.42
1:C:343:THR:HA	1:C:352:ILE:HA	2.01	0.42
1:D:147:THR:O	1:D:151:VAL:CG2	2.67	0.42
1:H:266:LYS:HA	1:H:305:ARG:NH1	2.34	0.42
1:B:209:PHE:O	1:B:210:ILE:HG13	2.19	0.42
1:E:110:GLU:C	1:E:112:LEU:H	2.22	0.42
1:G:147:THR:O	1:G:149:GLU:N	2.48	0.42
1:A:122:THR:OG1	1:A:124:ILE:HG12	2.19	0.42
1:G:213:ASP:OD1	1:G:219:ALA:CB	2.67	0.42
1:F:341:PHE:HB3	1:F:352:ILE:HD11	2.00	0.42
1:F:111:PRO:O	1:F:114:LYS:N	2.51	0.42
1:C:163:LEU:HD23	1:C:169:TRP:CZ2	2.55	0.42
1:E:250:PHE:O	1:E:251:SER:C	2.57	0.42
1:C:330:ASN:O	1:C:334:GLU:HG2	2.20	0.42
1:A:169:TRP:CE2	1:A:357:PRO:HG3	2.54	0.42
1:C:179:VAL:HG12	1:C:180:LEU:N	2.34	0.42
1:E:180:LEU:HD22	1:E:287:PHE:HB2	2.02	0.42
1:B:243:PHE:CE2	1:B:279:PRO:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:PRO:O	1:D:280:PHE:HB2	2.18	0.42
1:D:349:PRO:HD2	1:D:350:GLU:OE2	2.18	0.42
1:B:319:ILE:HG12	1:B:343:THR:O	2.20	0.42
1:D:217:ILE:O	1:D:218:ALA:HB3	2.19	0.42
1:B:122:THR:HB	1:B:364:LEU:HD22	2.02	0.42
1:F:176:LYS:NZ	1:F:251:SER:O	2.39	0.42
1:G:207:ILE:HD12	1:G:257:PHE:CE2	2.55	0.42
1:H:212:THR:N	1:H:259:ASP:O	2.50	0.42
1:A:211:THR:OG1	1:A:223:LEU:HD23	2.20	0.42
1:A:146:LEU:HB3	1:A:151:VAL:HG22	2.01	0.42
1:F:169:TRP:NE1	1:F:357:PRO:HG3	2.34	0.42
1:F:135:LYS:C	1:F:137:LEU:H	2.23	0.42
1:A:163:LEU:HD21	1:A:329:PHE:HE2	1.83	0.42
1:E:313:GLN:OE1	1:E:340:GLY:HA2	2.19	0.42
1:G:188:LYS:HZ3	1:G:262:GLY:HA2	1.84	0.42
1:H:266:LYS:O	1:H:305:ARG:NH1	2.44	0.42
1:H:305:ARG:C	1:H:307:SER:H	2.22	0.42
1:B:314:TYR:HB2	1:B:338:GLY:O	2.19	0.42
1:G:146:LEU:HB3	1:G:151:VAL:CG1	2.50	0.42
1:G:114:LYS:HZ2	1:G:152:VAL:HG22	1.85	0.42
1:G:179:VAL:HG22	1:G:258:VAL:CG2	2.49	0.42
1:C:137:LEU:O	1:C:140:SER:OG	2.34	0.42
1:C:138:ARG:O	1:C:140:SER:N	2.52	0.42
1:C:185:GLY:HA3	1:G:185:GLY:O	2.19	0.42
1:H:207:ILE:HD12	1:H:257:PHE:HE2	1.83	0.42
1:C:234:LEU:HD23	1:C:234:LEU:C	2.40	0.42
1:H:305:ARG:HG3	1:H:305:ARG:HH11	1.85	0.42
1:D:232:ALA:HA	1:D:233:PRO:HD3	1.83	0.42
1:F:138:ARG:HG2	1:F:138:ARG:NH1	2.34	0.42
1:G:110:GLU:HB2	1:G:111:PRO:HD3	2.01	0.42
1:G:188:LYS:NZ	1:G:262:GLY:HA2	2.34	0.42
1:F:181:PHE:CZ	1:F:286:SER:HB3	2.55	0.42
1:E:118:LEU:O	1:E:122:THR:HG23	2.20	0.42
1:C:366:ARG:HD3	1:C:366:ARG:HA	1.89	0.42
1:H:110:GLU:CB	1:H:111:PRO:CD	2.98	0.42
1:H:110:GLU:HB3	1:H:111:PRO:CD	2.50	0.42
1:H:110:GLU:HB3	1:H:111:PRO:HD3	2.00	0.42
1:B:224:LYS:HA	1:B:234:LEU:HD13	2.01	0.42
1:H:208:ALA:O	1:H:256:VAL:HA	2.20	0.42
1:H:210:ILE:HD11	1:H:256:VAL:HG11	2.02	0.42
1:B:111:PRO:HG3	1:B:146:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ASP:OD2	1:D:269:GLN:HB3	2.20	0.42
1:E:286:SER:O	1:E:287:PHE:CD1	2.72	0.42
1:A:179:VAL:C	1:A:180:LEU:HD23	2.40	0.42
1:A:179:VAL:HG22	1:A:258:VAL:HB	2.02	0.42
1:H:156:GLN:HA	1:H:159:LEU:HD12	2.02	0.42
1:D:163:LEU:HD12	1:D:333:ALA:HA	2.02	0.42
1:C:348:VAL:HA	1:C:349:PRO:HA	1.86	0.42
1:G:191:THR:HG21	1:G:315:ILE:HG21	2.02	0.41
1:B:243:PHE:CE2	1:B:278:ILE:HG23	2.55	0.41
1:B:124:ILE:HA	1:B:330:ASN:HD21	1.84	0.41
1:E:279:PRO:HG2	1:E:280:PHE:H	1.85	0.41
1:D:293:THR:O	1:D:293:THR:HG22	2.20	0.41
1:F:344:ASN:HD22	1:F:351:ASP:HB3	1.84	0.41
1:A:244:GLN:HE22	1:A:247:LYS:NZ	2.18	0.41
1:H:204:HIS:O	1:H:205:LYS:HG3	2.19	0.41
1:E:360:PHE:C	1:E:362:ARG:N	2.73	0.41
1:C:267:ASP:OD2	1:C:269:GLN:HG3	2.20	0.41
1:C:268:PRO:HA	1:C:271:ILE:CB	2.39	0.41
1:E:112:LEU:CD2	1:E:137:LEU:HD13	2.50	0.41
1:F:175:SER:N	1:F:285:GLN:HE22	2.18	0.41
1:A:222:GLN:HG2	1:E:218:ALA:O	2.20	0.41
1:E:130:THR:HG22	1:E:131:ASN:N	2.34	0.41
1:D:209:PHE:O	1:D:210:ILE:CG1	2.68	0.41
1:E:206:LYS:N	1:E:254:ASP:OD2	2.37	0.41
1:A:169:TRP:CD1	1:A:357:PRO:HG3	2.55	0.41
1:G:206:LYS:O	1:G:207:ILE:HD13	2.20	0.41
1:D:267:ASP:HA	1:D:268:PRO:HD2	1.91	0.41
1:H:116:GLU:O	1:H:120:GLN:HB2	2.20	0.41
1:B:359:GLY:O	1:B:362:ARG:HB2	2.20	0.41
1:H:277:THR:HG22	1:H:278:ILE:HD12	2.03	0.41
1:F:290:LEU:O	1:F:316:PHE:HA	2.20	0.41
1:C:319:ILE:CG1	1:C:344:ASN:HB3	2.50	0.41
1:G:179:VAL:HG22	1:G:258:VAL:CB	2.50	0.41
1:E:212:THR:HG23	1:E:277:THR:HG21	2.03	0.41
1:E:200:MET:HB2	1:E:207:ILE:HG13	2.01	0.41
1:H:296:TYR:CE2	1:H:300:LYS:HE2	2.55	0.41
1:H:274:LEU:HD23	1:H:274:LEU:C	2.41	0.41
1:E:177:TYR:HD1	1:E:256:VAL:HB	1.85	0.41
1:H:229:LEU:C	1:H:230:LEU:HD12	2.40	0.41
1:B:323:THR:O	1:B:366:ARG:NH2	2.53	0.41
1:C:321:GLU:HG3	1:G:264:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:C	1:D:135:LYS:N	2.74	0.41
1:D:245:GLN:HA	1:D:248:GLU:OE1	2.20	0.41
1:D:188:LYS:NZ	3:D:4:GNP:O1B	2.46	0.41
1:A:222:GLN:NE2	1:E:219:ALA:HA	2.35	0.41
1:C:199:SER:O	1:C:205:LYS:HB2	2.20	0.41
1:H:196:ALA:HA	1:H:257:PHE:CZ	2.56	0.41
1:C:176:LYS:NZ	1:C:176:LYS:HB2	2.36	0.41
1:H:265:PHE:CA	1:H:271:ILE:HD11	2.50	0.41
1:H:234:LEU:C	1:H:234:LEU:HD23	2.41	0.41
1:F:326:GLY:O	1:F:329:PHE:HB3	2.20	0.41
1:H:236:VAL:HG12	1:H:238:TYR:CE1	2.55	0.41
1:B:278:ILE:H	1:B:278:ILE:HD12	1.81	0.41
1:A:194:LYS:HA	1:A:348:VAL:HG13	2.01	0.41
1:C:330:ASN:O	1:C:333:ALA:HB3	2.21	0.41
1:H:331:ILE:HG22	1:H:332:LEU:N	2.35	0.41
1:D:264:ASN:CG	1:D:265:PHE:N	2.74	0.41
1:H:314:TYR:CE2	1:H:337:ILE:HG13	2.56	0.41
1:F:224:LYS:HA	1:F:234:LEU:HD22	2.03	0.41
1:B:122:THR:HG22	1:B:364:LEU:O	2.21	0.41
1:E:154:LYS:HD3	1:E:154:LYS:O	2.21	0.41
1:H:315:ILE:HD13	1:H:341:PHE:HB2	2.02	0.41
1:C:264:ASN:O	1:C:266:LYS:N	2.53	0.41
1:B:138:ARG:O	1:B:141:VAL:HG12	2.20	0.41
1:G:352:ILE:HD13	1:G:352:ILE:C	2.41	0.41
1:C:217:ILE:O	1:C:218:ALA:HB3	2.20	0.41
1:D:339:VAL:HG22	1:D:340:GLY:N	2.36	0.41
1:F:137:LEU:O	1:F:141:VAL:HB	2.20	0.41
1:C:169:TRP:CZ2	1:C:332:LEU:HD13	2.55	0.41
1:E:314:TYR:CB	1:E:339:VAL:HG12	2.51	0.41
1:A:131:ASN:O	1:A:135:LYS:HG2	2.20	0.41
1:D:225:THR:O	1:D:229:LEU:HG	2.21	0.41
1:F:360:PHE:O	1:F:363:MET:HB3	2.21	0.41
1:B:170:GLN:HE22	1:B:356:SER:HA	1.86	0.41
1:D:213:ASP:OD2	1:D:219:ALA:CB	2.69	0.41
1:E:164:PRO:CG	1:E:169:TRP:HE1	2.25	0.41
1:G:132:THR:HG23	1:G:158:ILE:HG21	2.03	0.41
1:B:244:GLN:HA	1:B:247:LYS:HB3	2.02	0.41
1:F:364:LEU:O	1:F:366:ARG:N	2.53	0.41
1:F:240:LYS:HG3	1:F:241:GLU:OE2	2.20	0.41
1:G:301:HIS:O	1:G:305:ARG:HD3	2.21	0.40
1:H:268:PRO:C	1:H:270:TYR:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:ALA:O	1:G:250:PHE:HD2	2.04	0.40
1:A:148:GLU:HA	1:A:151:VAL:HG23	2.02	0.40
1:C:199:SER:HA	1:C:203:LYS:CB	2.51	0.40
1:F:347:ASN:HB2	1:F:351:ASP:CG	2.41	0.40
1:B:123:GLY:CA	1:B:326:GLY:HA3	2.51	0.40
1:G:180:LEU:HG	1:G:192:LEU:HD23	2.02	0.40
1:D:321:GLU:HG3	1:H:264:ASN:OD1	2.22	0.40
1:D:281:GLU:O	1:D:284:ILE:N	2.37	0.40
1:G:125:LYS:HD2	1:G:330:ASN:ND2	2.36	0.40
1:E:116:GLU:HG2	1:E:120:GLN:HE21	1.84	0.40
1:A:249:LEU:HD23	1:A:249:LEU:O	2.22	0.40
1:D:295:LYS:O	1:D:298:ASP:HB2	2.21	0.40
1:D:212:THR:CB	1:D:260:THR:HG22	2.52	0.40
1:B:151:VAL:O	1:B:155:LEU:HB2	2.21	0.40
1:D:306:PHE:CD2	1:D:309:VAL:HG11	2.56	0.40
1:E:267:ASP:OD1	1:E:269:GLN:CB	2.69	0.40
1:H:203:LYS:O	1:H:204:HIS:C	2.59	0.40
1:G:241:GLU:HB3	1:G:245:GLN:NE2	2.36	0.40
1:H:217:ILE:HG12	1:H:217:ILE:H	1.67	0.40
1:C:266:LYS:HG3	1:C:305:ARG:HH12	1.86	0.40
1:D:281:GLU:OE2	1:D:284:ILE:HG13	2.22	0.40
1:F:152:VAL:HG23	1:F:153:GLY:H	1.86	0.40
1:A:176:LYS:HA	1:A:254:ASP:O	2.20	0.40
1:F:323:THR:HG22	1:F:366:ARG:HH22	1.86	0.40
1:A:267:ASP:O	1:A:269:GLN:N	2.54	0.40
1:B:299:MET:O	1:B:303:VAL:HG23	2.20	0.40
1:C:271:ILE:HG22	1:C:272:ASP:N	2.36	0.40
1:E:160:CYS:HA	1:E:163:LEU:HD23	2.03	0.40
1:B:272:ASP:O	1:B:275:LYS:HB2	2.21	0.40
1:H:339:VAL:HG23	1:H:339:VAL:O	2.21	0.40
1:C:313:GLN:HB3	1:C:340:GLY:H	1.86	0.40
1:B:122:THR:CG2	1:B:364:LEU:HD22	2.52	0.40
1:F:172:PRO:O	1:F:174:HIS:N	2.54	0.40
1:D:360:PHE:O	1:D:363:MET:HB2	2.21	0.40
1:G:154:LYS:HD2	1:G:154:LYS:HA	1.96	0.40
1:G:289:VAL:HA	1:G:315:ILE:O	2.21	0.40
1:E:364:LEU:HD23	1:E:364:LEU:O	2.21	0.40
1:H:264:ASN:O	1:H:266:LYS:N	2.54	0.40
1:D:268:PRO:HA	1:D:271:ILE:HG13	2.02	0.40
1:B:193:ALA:O	1:B:196:ALA:N	2.55	0.40
1:F:314:TYR:HB2	1:F:339:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:LEU:CD1	1:F:146:LEU:HD13	2.51	0.40
1:B:332:LEU:HD21	1:B:339:VAL:CG1	2.51	0.40
1:G:133:LEU:O	1:G:135:LYS:N	2.54	0.40
1:F:139:PHE:CD2	1:F:154:LYS:HE3	2.56	0.40
1:H:237:CYS:SG	1:H:243:PHE:HA	2.61	0.40
1:D:168:LYS:HG3	1:D:168:LYS:O	2.20	0.40
1:D:325:LEU:HD23	1:D:328:VAL:CG2	2.52	0.40
1:C:344:ASN:ND2	1:C:353:GLN:HE21	2.19	0.40
1:H:267:ASP:C	1:H:269:GLN:H	2.24	0.40
1:F:212:THR:O	1:F:212:THR:CG2	2.69	0.40
1:B:326:GLY:O	1:B:329:PHE:HB3	2.22	0.40
1:C:249:LEU:O	1:C:252:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

## 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	256/296 (86%)	209 (82%)	35 (14%)	12 (5%)	3	17
1	B	256/296 (86%)	201 (78%)	46 (18%)	9 (4%)	4	24
1	C	256/296 (86%)	200 (78%)	38 (15%)	18 (7%)	1	7
1	D	256/296 (86%)	186 (73%)	49 (19%)	21 (8%)	1	5
1	E	256/296 (86%)	192 (75%)	42 (16%)	22 (9%)	1	4
1	F	256/296 (86%)	208 (81%)	37 (14%)	11 (4%)	3	19
1	G	256/296 (86%)	198 (77%)	47 (18%)	11 (4%)	3	19
1	H	256/296 (86%)	190 (74%)	52 (20%)	14 (6%)	2	13
All	All	2048/2368 (86%)	1584 (77%)	346 (17%)	118 (6%)	2	12

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLU
1	A	144	GLY
1	A	146	LEU
1	B	110	GLU
1	B	139	PHE
1	B	175	SER
1	D	110	GLU
1	D	165	SER
1	D	170	GLN
1	D	318	LYS
1	D	351	ASP
1	E	110	GLU
1	E	124	ILE
1	E	143	ALA
1	E	215	TYR
1	E	282	SER
1	F	110	GLU
1	H	165	SER
1	H	200	MET
1	H	201	LEU
1	H	204	HIS
1	A	148	GLU
1	A	175	SER
1	A	265	PHE
1	A	351	ASP
1	C	110	GLU
1	C	140	SER
1	C	202	GLU
1	C	212	THR
1	D	204	HIS
1	D	282	SER
1	E	140	SER
1	E	166	ALA
1	E	204	HIS
1	E	251	SER
1	E	365	CYS
1	F	144	GLY
1	F	265	PHE
1	F	282	SER
1	F	351	ASP
1	F	365	CYS
1	G	165	SER
1	G	217	ILE

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Mol	Chain	Res	Type
1	H	124	ILE
1	H	150	ASN
1	H	265	PHE
1	H	302	ILE
1	A	280	PHE
1	A	302	ILE
1	B	130	THR
1	B	140	SER
1	B	281	GLU
1	B	283	SER
1	B	312	ASN
1	C	201	LEU
1	C	265	PHE
1	C	268	PRO
1	C	280	PHE
1	C	301	HIS
1	C	357	PRO
1	D	143	ALA
1	D	144	GLY
1	D	161	ASP
1	D	175	SER
1	D	243	PHE
1	E	351	ASP
1	E	357	PRO
1	F	126	GLU
1	F	166	ALA
1	F	188	LYS
1	G	202	GLU
1	G	210	ILE
1	H	110	GLU
1	H	213	ASP
1	H	285	GLN
1	A	282	SER
1	C	234	LEU
1	E	249	LEU
1	F	173	ILE
1	G	110	GLU
1	H	148	GLU
1	H	251	SER
1	A	161	ASP
1	A	200	MET
1	B	265	PHE

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Mol	Chain	Res	Type
1	C	189	THR
1	C	358	LEU
1	D	188	LYS
1	D	196	ALA
1	D	222	GLN
1	D	231	GLN
1	D	244	GLN
1	E	150	ASN
1	E	175	SER
1	E	201	LEU
1	E	234	LEU
1	G	134	LYS
1	G	149	GLU
1	D	187	GLY
1	D	197	ALA
1	D	350	GLU
1	E	125	LYS
1	E	279	PRO
1	E	280	PHE
1	F	175	SER
1	G	319	ILE
1	C	124	ILE
1	C	144	GLY
1	E	187	GLY
1	E	233	PRO
1	C	267	ASP
1	G	173	ILE
1	C	339	VAL
1	C	352	ILE
1	G	357	PRO
1	H	310	PRO
1	D	352	ILE
1	G	302	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	228/262 (87%)	218 (96%)	10 (4%)	35	74
1	B	228/262 (87%)	220 (96%)	8 (4%)	43	80
1	C	228/262 (87%)	220 (96%)	8 (4%)	43	80
1	D	228/262 (87%)	219 (96%)	9 (4%)	39	77
1	E	228/262 (87%)	211 (92%)	17 (8%)	17	51
1	F	228/262 (87%)	215 (94%)	13 (6%)	25	64
1	G	228/262 (87%)	214 (94%)	14 (6%)	23	61
1	H	228/262 (87%)	208 (91%)	20 (9%)	12	42
All	All	1824/2096 (87%)	1725 (95%)	99 (5%)	27	66

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	126	GLU
1	A	131	ASN
1	A	136	LEU
1	A	139	PHE
1	A	161	ASP
1	A	168	LYS
1	A	183	SER
1	A	308	SER
1	A	339	VAL
1	B	131	ASN
1	B	148	GLU
1	B	170	GLN
1	B	254	ASP
1	B	267	ASP
1	B	281	GLU
1	B	314	TYR
1	B	358	LEU
1	C	130	THR
1	C	148	GLU
1	C	149	GLU
1	C	168	LYS
1	C	217	ILE
1	C	224	LYS
1	C	281	GLU
1	C	336	LYS
1	D	154	LYS

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Mol	Chain	Res	Type
1	D	180	LEU
1	D	184	THR
1	D	235	GLU
1	D	281	GLU
1	D	304	LYS
1	D	305	ARG
1	D	318	LYS
1	D	325	LEU
1	E	130	THR
1	E	131	ASN
1	E	148	GLU
1	E	154	LYS
1	E	174	HIS
1	E	181	PHE
1	E	224	LYS
1	E	226	TYR
1	E	237	CYS
1	E	238	TYR
1	E	281	GLU
1	E	304	LYS
1	E	305	ARG
1	E	323	THR
1	E	324	SER
1	E	336	LYS
1	E	357	PRO
1	F	133	LEU
1	F	148	GLU
1	F	161	ASP
1	F	168	LYS
1	F	195	LEU
1	F	199	SER
1	F	216	ARG
1	F	267	ASP
1	F	276	GLU
1	F	281	GLU
1	F	317	THR
1	F	344	ASN
1	F	364	LEU
1	G	119	LEU
1	G	122	THR
1	G	124	ILE
1	G	149	GLU

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Mol	Chain	Res	Type
1	G	192	LEU
1	G	201	LEU
1	G	217	ILE
1	G	224	LYS
1	G	234	LEU
1	G	267	ASP
1	G	281	GLU
1	G	327	SER
1	G	349	PRO
1	G	352	ILE
1	H	110	GLU
1	H	120	GLN
1	H	137	LEU
1	H	139	PHE
1	H	142	GLU
1	H	148	GLU
1	H	149	GLU
1	H	154	LYS
1	H	161	ASP
1	H	192	LEU
1	H	195	LEU
1	H	212	THR
1	H	226	TYR
1	H	231	GLN
1	H	252	GLU
1	H	284	ILE
1	H	304	LYS
1	H	309	VAL
1	H	336	LYS
1	H	364	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	150	ASN
1	A	170	GLN
1	A	222	GLN
1	A	244	GLN
1	A	330	ASN
1	A	346	GLN
1	B	156	GLN

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Mol	Chain	Res	Type
1	B	244	GLN
1	B	245	GLN
1	B	269	GLN
1	B	312	ASN
1	B	346	GLN
1	B	347	ASN
1	C	170	GLN
1	C	244	GLN
1	C	344	ASN
1	C	346	GLN
1	D	120	GLN
1	D	222	GLN
1	D	264	ASN
1	D	269	GLN
1	D	312	ASN
1	D	346	GLN
1	E	120	GLN
1	E	156	GLN
1	E	244	GLN
1	E	330	ASN
1	E	346	GLN
1	E	347	ASN
1	F	120	GLN
1	F	285	GLN
1	F	344	ASN
1	F	346	GLN
1	F	347	ASN
1	F	353	GLN
1	G	120	GLN
1	G	222	GLN
1	G	231	GLN
1	G	245	GLN
1	G	285	GLN
1	G	346	GLN
1	G	347	ASN
1	H	120	GLN
1	H	170	GLN
1	H	285	GLN
1	H	313	GLN
1	H	346	GLN
1	H	347	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	GNP	A	1	2	28,34,34	2.03	11 (39%)	33,54,54	2.66	9 (27%)
3	GNP	B	2	2	28,34,34	1.99	11 (39%)	33,54,54	2.68	8 (24%)
3	GNP	C	3	2	28,34,34	2.16	10 (35%)	33,54,54	2.61	10 (30%)
3	GNP	D	4	2	28,34,34	1.98	9 (32%)	33,54,54	2.73	10 (30%)
3	GNP	E	5	2	28,34,34	2.02	10 (35%)	33,54,54	2.60	9 (27%)
3	GNP	F	6	2	28,34,34	1.93	9 (32%)	33,54,54	2.74	10 (30%)
3	GNP	G	7	2	28,34,34	1.99	8 (28%)	33,54,54	2.62	8 (24%)
3	GNP	H	8	2	28,34,34	2.04	11 (39%)	33,54,54	2.66	9 (27%)

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	GNP	A	1	2	-	0/12/38/38	0/3/3/3
3	GNP	B	2	2	-	0/12/38/38	0/3/3/3
3	GNP	C	3	2	-	0/12/38/38	0/3/3/3
3	GNP	D	4	2	-	0/12/38/38	0/3/3/3
3	GNP	E	5	2	-	0/12/38/38	0/3/3/3
3	GNP	F	6	2	-	0/12/38/38	0/3/3/3
3	GNP	G	7	2	-	0/12/38/38	0/3/3/3
3	GNP	H	8	2	-	0/12/38/38	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	GNP	O6-C6	-3.43	1.16	1.24
3	C	3	GNP	PG-O3G	-3.25	1.47	1.56
3	C	3	GNP	O6-C6	-3.19	1.17	1.24
3	A	1	GNP	O6-C6	-3.13	1.17	1.24
3	H	8	GNP	PG-O3G	-3.11	1.48	1.56
3	D	4	GNP	O4'-C4'	-3.09	1.37	1.45
3	F	6	GNP	O6-C6	-3.07	1.17	1.24
3	B	2	GNP	O6-C6	-3.04	1.17	1.24
3	G	7	GNP	PG-O3G	-3.03	1.48	1.56
3	E	5	GNP	PG-O3G	-3.02	1.48	1.56
3	F	6	GNP	PG-O3G	-2.96	1.48	1.56
3	D	4	GNP	PG-O3G	-2.95	1.48	1.56
3	C	3	GNP	O4'-C4'	-2.86	1.38	1.45
3	D	4	GNP	O6-C6	-2.85	1.18	1.24
3	B	2	GNP	PG-O3G	-2.83	1.48	1.56
3	H	8	GNP	O6-C6	-2.80	1.18	1.24
3	E	5	GNP	PB-O2B	-2.78	1.48	1.56
3	A	1	GNP	PG-O3G	-2.72	1.49	1.56
3	G	7	GNP	O6-C6	-2.71	1.18	1.24
3	G	7	GNP	O4'-C4'	-2.71	1.38	1.45
3	B	2	GNP	O4'-C4'	-2.51	1.39	1.45
3	H	8	GNP	O4'-C4'	-2.49	1.39	1.45
3	G	7	GNP	PB-O2B	-2.47	1.49	1.56
3	C	3	GNP	PB-O2B	-2.46	1.49	1.56
3	F	6	GNP	PB-O2B	-2.46	1.49	1.56
3	E	5	GNP	O4'-C4'	-2.45	1.39	1.45
3	A	1	GNP	O4'-C4'	-2.45	1.39	1.45
3	B	2	GNP	PB-O2B	-2.27	1.50	1.56
3	A	1	GNP	PB-O2B	-2.26	1.50	1.56
3	H	8	GNP	PB-O2B	-2.24	1.50	1.56
3	A	1	GNP	C5-C4	-2.18	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	GNP	PB-O2B	-2.06	1.50	1.56
3	E	5	GNP	C5-C4	-2.05	1.35	1.40
3	B	2	GNP	C5-C4	-2.03	1.35	1.40
3	D	4	GNP	C2-N1	2.16	1.39	1.35
3	H	8	GNP	C2-N1	2.17	1.39	1.35
3	B	2	GNP	PG-O1G	2.25	1.48	1.46
3	A	1	GNP	C6-C5	2.33	1.45	1.41
3	F	6	GNP	PG-N3B	2.34	1.69	1.63
3	A	1	GNP	C2-N1	2.40	1.39	1.35
3	E	5	GNP	PG-O1G	2.48	1.48	1.46
3	H	8	GNP	PG-N3B	2.51	1.70	1.63
3	B	2	GNP	C6-C5	2.53	1.46	1.41
3	C	3	GNP	PG-O1G	2.55	1.49	1.46
3	B	2	GNP	PG-N3B	2.56	1.70	1.63
3	H	8	GNP	C6-C5	2.57	1.46	1.41
3	F	6	GNP	PB-O3A	2.58	1.62	1.59
3	H	8	GNP	PG-O1G	2.59	1.49	1.46
3	C	3	GNP	C6-C5	2.60	1.46	1.41
3	G	7	GNP	PG-N3B	2.64	1.70	1.63
3	E	5	GNP	C6-C5	2.79	1.46	1.41
3	F	6	GNP	C6-C5	2.80	1.46	1.41
3	D	4	GNP	PG-O1G	2.85	1.49	1.46
3	A	1	GNP	PG-O1G	2.87	1.49	1.46
3	D	4	GNP	C6-C5	2.92	1.47	1.41
3	E	5	GNP	C6-N1	2.92	1.38	1.33
3	E	5	GNP	PG-N3B	2.96	1.71	1.63
3	F	6	GNP	PG-O1G	3.03	1.49	1.46
3	G	7	GNP	C6-C5	3.08	1.47	1.41
3	C	3	GNP	PB-O3A	3.16	1.63	1.59
3	H	8	GNP	PB-O3A	3.25	1.63	1.59
3	C	3	GNP	C6-N1	3.25	1.39	1.33
3	B	2	GNP	C6-N1	3.28	1.39	1.33
3	C	3	GNP	PG-N3B	3.30	1.72	1.63
3	A	1	GNP	PB-O3A	3.33	1.63	1.59
3	F	6	GNP	C6-N1	3.36	1.39	1.33
3	H	8	GNP	C6-N1	3.45	1.39	1.33
3	A	1	GNP	C6-N1	3.49	1.39	1.33
3	D	4	GNP	C6-N1	3.60	1.39	1.33
3	B	2	GNP	PB-O3A	3.72	1.63	1.59
3	G	7	GNP	C6-N1	3.79	1.40	1.33
3	F	6	GNP	C2-N2	4.35	1.42	1.34
3	B	2	GNP	C2-N2	4.51	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8	GNP	C2-N2	4.64	1.43	1.34
3	A	1	GNP	C2-N2	4.66	1.43	1.34
3	G	7	GNP	C2-N2	4.67	1.43	1.34
3	D	4	GNP	C2-N2	4.73	1.43	1.34
3	C	3	GNP	C2-N2	4.77	1.43	1.34
3	E	5	GNP	C2-N2	5.29	1.44	1.34

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	GNP	C5-C6-N1	-9.27	110.92	123.59
3	H	8	GNP	C5-C6-N1	-9.27	110.92	123.59
3	G	7	GNP	C5-C6-N1	-9.17	111.05	123.59
3	A	1	GNP	C5-C6-N1	-9.17	111.05	123.59
3	C	3	GNP	C5-C6-N1	-9.03	111.25	123.59
3	F	6	GNP	C5-C6-N1	-8.96	111.33	123.59
3	B	2	GNP	C5-C6-N1	-8.90	111.42	123.59
3	E	5	GNP	C5-C6-N1	-8.80	111.56	123.59
3	B	2	GNP	O1G-PG-N3B	-7.99	99.64	111.90
3	F	6	GNP	O1G-PG-N3B	-7.74	100.03	111.90
3	A	1	GNP	O1G-PG-N3B	-7.42	100.52	111.90
3	H	8	GNP	O1G-PG-N3B	-7.33	100.65	111.90
3	E	5	GNP	O1G-PG-N3B	-7.21	100.84	111.90
3	C	3	GNP	O1G-PG-N3B	-6.93	101.27	111.90
3	D	4	GNP	O1G-PG-N3B	-6.71	101.61	111.90
3	G	7	GNP	O1G-PG-N3B	-6.51	101.91	111.90
3	F	6	GNP	N2-C2-N1	-4.99	108.94	117.20
3	G	7	GNP	N2-C2-N1	-4.93	109.03	117.20
3	C	3	GNP	N2-C2-N1	-4.82	109.23	117.20
3	B	2	GNP	N2-C2-N1	-4.71	109.40	117.20
3	H	8	GNP	N2-C2-N1	-4.54	109.68	117.20
3	D	4	GNP	N2-C2-N1	-4.54	109.68	117.20
3	E	5	GNP	N2-C2-N1	-4.42	109.88	117.20
3	A	1	GNP	N2-C2-N1	-4.21	110.23	117.20
3	G	7	GNP	O3A-PB-N3B	-4.12	95.09	106.44
3	D	4	GNP	O3A-PB-N3B	-4.02	95.37	106.44
3	A	1	GNP	O3A-PB-N3B	-3.83	95.90	106.44
3	H	8	GNP	O3A-PB-N3B	-3.25	97.49	106.44
3	F	6	GNP	O3A-PB-N3B	-3.09	97.94	106.44
3	B	2	GNP	O3A-PB-N3B	-2.99	98.20	106.44
3	F	6	GNP	C2'-C1'-N9	-2.99	109.73	114.29
3	C	3	GNP	O3A-PB-N3B	-2.83	98.66	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	GNP	O3A-PB-N3B	-2.76	98.85	106.44
3	E	5	GNP	C2'-C1'-N9	-2.64	110.25	114.29
3	A	1	GNP	C2'-C1'-N9	-2.61	110.30	114.29
3	C	3	GNP	C2'-C1'-N9	-2.31	110.77	114.29
3	D	4	GNP	PA-O3A-PB	-2.25	125.13	132.67
3	H	8	GNP	C2'-C1'-N9	-2.18	110.96	114.29
3	C	3	GNP	O4'-C4'-C5'	2.01	116.51	109.32
3	A	1	GNP	C6-N1-C2	2.04	118.77	115.94
3	F	6	GNP	O4'-C1'-N9	2.10	112.49	108.10
3	B	2	GNP	O4'-C4'-C5'	2.10	116.84	109.32
3	F	6	GNP	C6-N1-C2	2.12	118.89	115.94
3	E	5	GNP	C6-N1-C2	2.14	118.90	115.94
3	H	8	GNP	O4'-C4'-C5'	2.17	117.08	109.32
3	D	4	GNP	O4'-C4'-C5'	2.18	117.12	109.32
3	A	1	GNP	O4'-C4'-C5'	2.18	117.13	109.32
3	E	5	GNP	O4'-C4'-C5'	2.22	117.26	109.32
3	B	2	GNP	C6-N1-C2	2.27	119.08	115.94
3	C	3	GNP	C4'-O4'-C1'	2.29	112.24	109.72
3	C	3	GNP	C6-N1-C2	2.41	119.29	115.94
3	H	8	GNP	C6-N1-C2	2.42	119.29	115.94
3	F	6	GNP	O4'-C4'-C5'	2.46	118.11	109.32
3	G	7	GNP	C6-N1-C2	2.50	119.41	115.94
3	G	7	GNP	O4'-C4'-C5'	2.51	118.29	109.32
3	D	4	GNP	C6-N1-C2	2.55	119.48	115.94
3	D	4	GNP	C4'-O4'-C1'	3.47	113.53	109.72
3	E	5	GNP	N3-C2-N1	3.93	133.43	127.44
3	A	1	GNP	N3-C2-N1	3.94	133.44	127.44
3	C	3	GNP	N3-C2-N1	3.94	133.45	127.44
3	D	4	GNP	N3-C2-N1	3.95	133.47	127.44
3	G	7	GNP	N3-C2-N1	4.00	133.54	127.44
3	H	8	GNP	N3-C2-N1	4.05	133.62	127.44
3	B	2	GNP	N3-C2-N1	4.09	133.68	127.44
3	F	6	GNP	N3-C2-N1	4.21	133.86	127.44
3	B	2	GNP	O2B-PB-O1B	4.29	118.96	110.00
3	A	1	GNP	O2B-PB-O1B	4.30	118.98	110.00
3	C	3	GNP	O2B-PB-O1B	4.36	119.09	110.00
3	G	7	GNP	O2B-PB-O1B	4.41	119.21	110.00
3	D	4	GNP	O2B-PB-O1B	4.45	119.30	110.00
3	H	8	GNP	O2B-PB-O1B	4.47	119.33	110.00
3	E	5	GNP	O2B-PB-O1B	4.51	119.42	110.00
3	F	6	GNP	O2B-PB-O1B	4.60	119.61	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	GNP	2	0
3	D	4	GNP	2	0
3	E	5	GNP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	258/296 (87%)	-0.25	0 <span>100</span> <span>100</span>	31, 61, 86, 94	0
1	B	258/296 (87%)	-0.22	0 <span>100</span> <span>100</span>	39, 75, 104, 112	0
1	C	258/296 (87%)	-0.14	3 (1%) <span>81</span> <span>55</span>	54, 89, 111, 119	0
1	D	258/296 (87%)	0.04	13 (5%) <span>32</span> <span>13</span>	55, 96, 115, 125	0
1	E	258/296 (87%)	-0.19	2 (0%) <span>87</span> <span>67</span>	40, 72, 96, 109	0
1	F	258/296 (87%)	-0.21	0 <span>100</span> <span>100</span>	40, 67, 90, 116	0
1	G	258/296 (87%)	0.03	7 (2%) <span>58</span> <span>28</span>	55, 84, 102, 118	0
1	H	258/296 (87%)	-0.05	5 (1%) <span>70</span> <span>41</span>	50, 85, 108, 114	0
All	All	2064/2368 (87%)	-0.12	30 (1%) <span>76</span> <span>49</span>	31, 79, 108, 125	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	TYR	4.7
1	D	178	ILE	4.4
1	G	231	GLN	3.6
1	G	222	GLN	3.4
1	C	243	PHE	3.3
1	D	243	PHE	3.0
1	D	230	LEU	3.0
1	D	179	VAL	2.8
1	G	215	TYR	2.7
1	H	226	TYR	2.5
1	H	215	TYR	2.5
1	G	180	LEU	2.4
1	E	306	PHE	2.4
1	G	220	VAL	2.4
1	D	290	LEU	2.3
1	D	316	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	258	VAL	2.2
1	G	339	VAL	2.2
1	H	279	PRO	2.2
1	H	306	PHE	2.2
1	E	366	ARG	2.1
1	C	226	TYR	2.1
1	D	292	ALA	2.1
1	D	180	LEU	2.1
1	D	274	LEU	2.1
1	C	274	LEU	2.1
1	D	223	LEU	2.0
1	G	223	LEU	2.0
1	H	266	LYS	2.0
1	D	280	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GNP	A	1	32/32	0.97	0.21	0.32	41,47,50,52	0
3	GNP	E	5	32/32	0.98	0.18	-0.59	43,48,53,54	0
3	GNP	G	7	32/32	0.95	0.17	-0.68	55,66,69,70	0
3	GNP	F	6	32/32	0.98	0.17	-0.74	42,46,58,60	0
3	GNP	C	3	32/32	0.96	0.17	-0.76	66,71,76,77	0
3	GNP	B	2	32/32	0.98	0.17	-0.85	47,54,57,59	0
3	GNP	D	4	32/32	0.93	0.19	-0.86	67,75,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GNP	H	8	32/32	0.94	0.15	-0.98	65,67,73,74	0
2	MG	F	6000	1/1	0.94	0.11	-1.95	47,47,47,47	0
2	MG	G	7000	1/1	0.82	0.14	-2.15	59,59,59,59	0
2	MG	B	2000	1/1	0.95	0.16	-2.30	51,51,51,51	0
2	MG	E	5000	1/1	0.98	0.13	-2.62	50,50,50,50	0
2	MG	C	3000	1/1	0.86	0.07	-2.62	72,72,72,72	0
2	MG	H	8000	1/1	0.81	0.06	-4.09	74,74,74,74	0
2	MG	A	1000	1/1	0.90	0.25	-	47,47,47,47	0
2	MG	D	4000	1/1	0.77	0.09	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.