



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:25 am BST

PDB ID : 3NM1  
Title : The Crystal Structure of Candida glabrata THI6, a Bifunctional Enzyme involved in Thiamin Biosynthesis of Eukaryotes  
Authors : Paul, D.; Chatterjee, A.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2010-06-21  
Resolution : 3.21 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

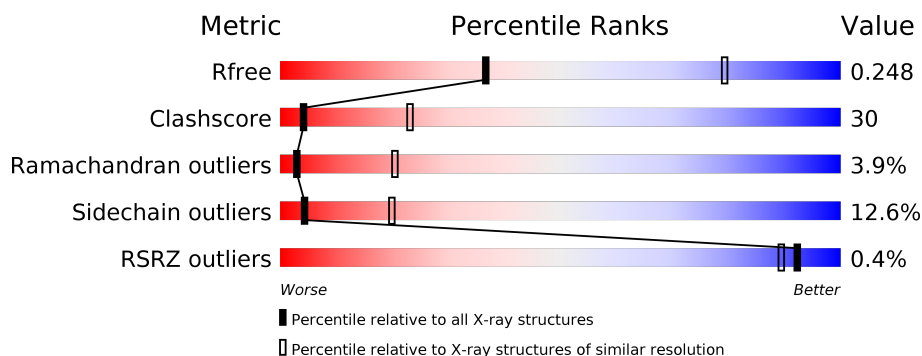
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	<div> <div></div> <div>47% 40% 6% 6%</div> </div>
1	B	540	<div> <div></div> <div>47% 40% 6% 6%</div> </div>
1	C	540	<div> <div></div> <div>46% 40% 7% 6%</div> </div>
1	D	540	<div> <div></div> <div>50% 36% 7% 6%</div> </div>
1	E	540	<div> <div></div> <div>49% 36% 8% 6%</div> </div>
1	F	540	<div> <div></div> <div>49% 38% 6% 6%</div> </div>

## 2 Entry composition [i](#)

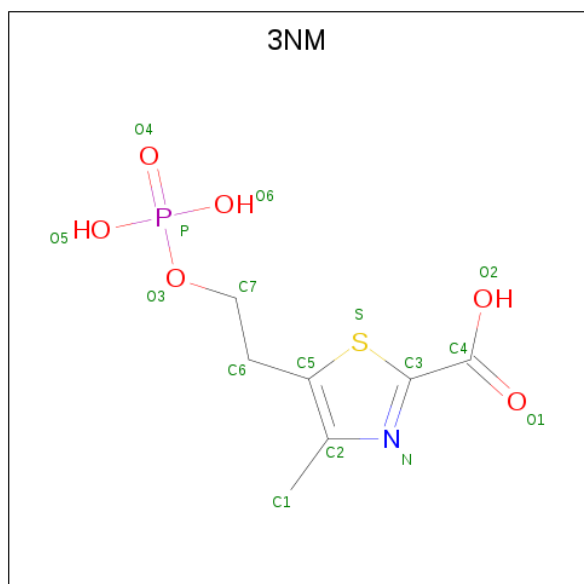
There are 5 unique types of molecules in this entry. The entry contains 22801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thiamine biosynthetic bifunctional enzyme.

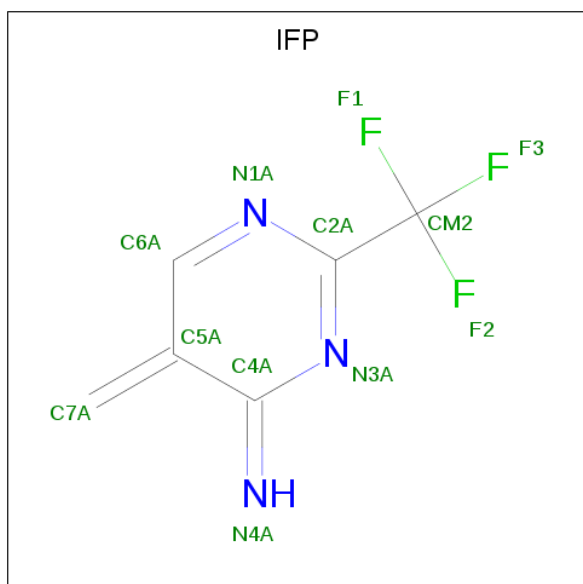
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	B	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	C	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	D	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	E	505	Total	C	N	O	S	0	0	0
			3748	2375	629	723	21			
1	F	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			

- Molecule 2 is 4-methyl-5-[2-(phosphonooxy)ethyl]-1,3-thiazole-2-carboxylic acid (three-letter code: 3NM) (formula: C<sub>7</sub>H<sub>10</sub>NO<sub>6</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	E	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	F	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		

- Molecule 3 is 2-TRIFLUOROMETHYL-5-METHYLENE-5H-PYRIMIDIN-4-YLIDENEA MINE (three-letter code: IFP) (formula: C<sub>6</sub>H<sub>4</sub>F<sub>3</sub>N<sub>3</sub>).



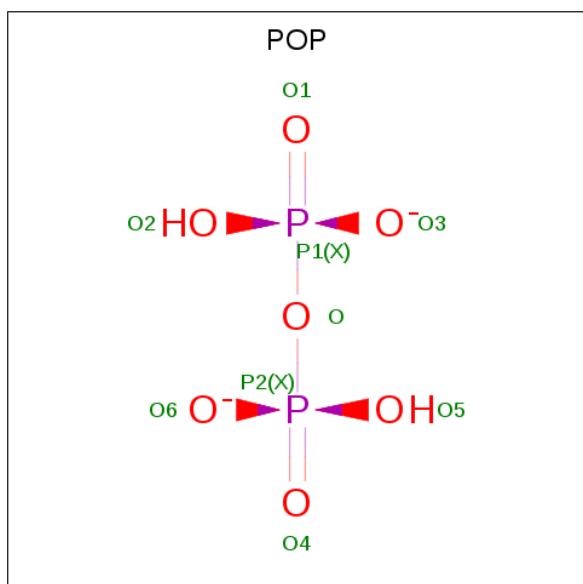
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 6	F 3	N 3	0	0
3	B	1	Total 12	C 6	F 3	N 3	0	0
3	C	1	Total 12	C 6	F 3	N 3	0	0
3	D	1	Total 12	C 6	F 3	N 3	0	0
3	E	1	Total 12	C 6	F 3	N 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	F	N	0	0
			12	6	3	3		

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		
4	C	1	Total	O	P	0	0
			9	7	2		
4	D	1	Total	O	P	0	0
			9	7	2		
4	E	1	Total	O	P	0	0
			9	7	2		
4	F	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

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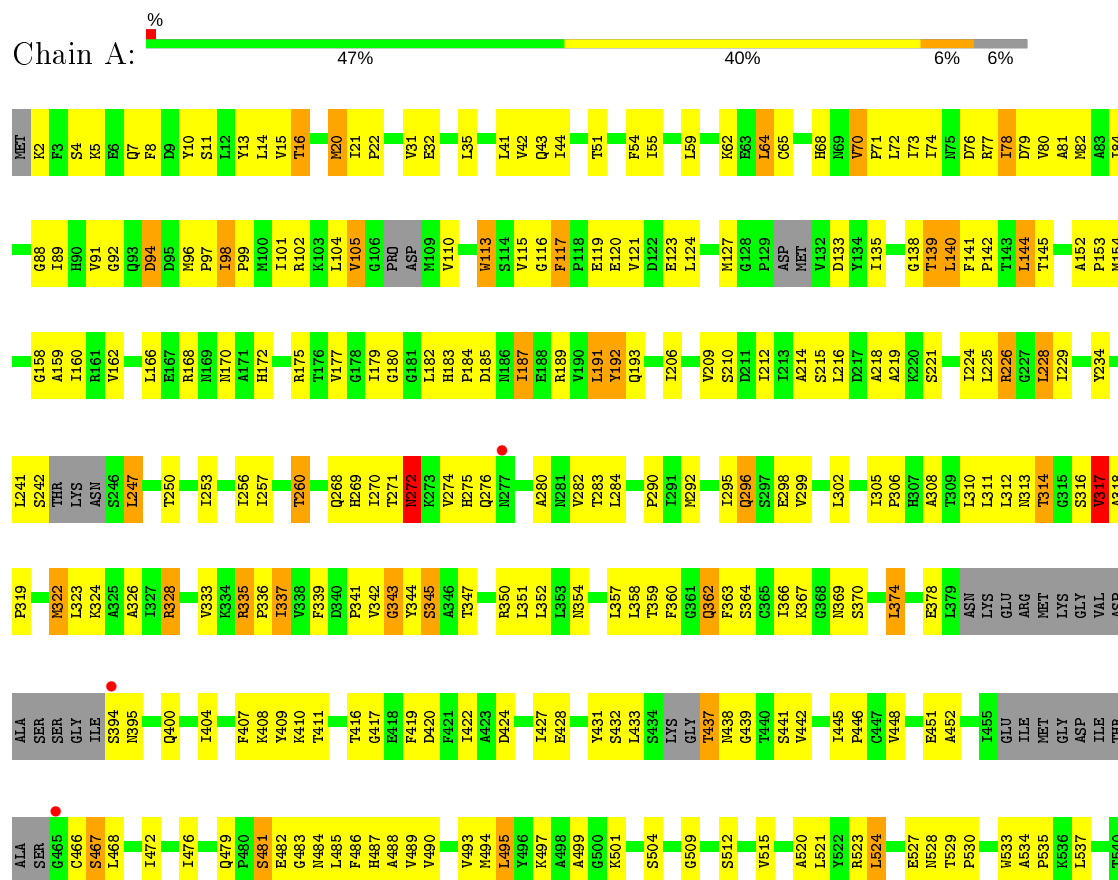
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0

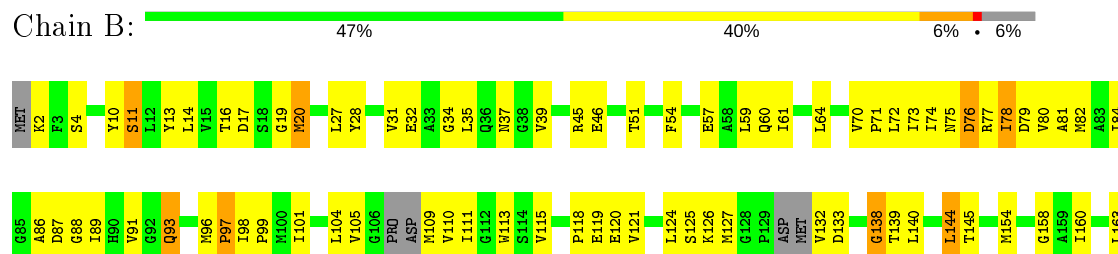
### 3 Residue-property plots

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

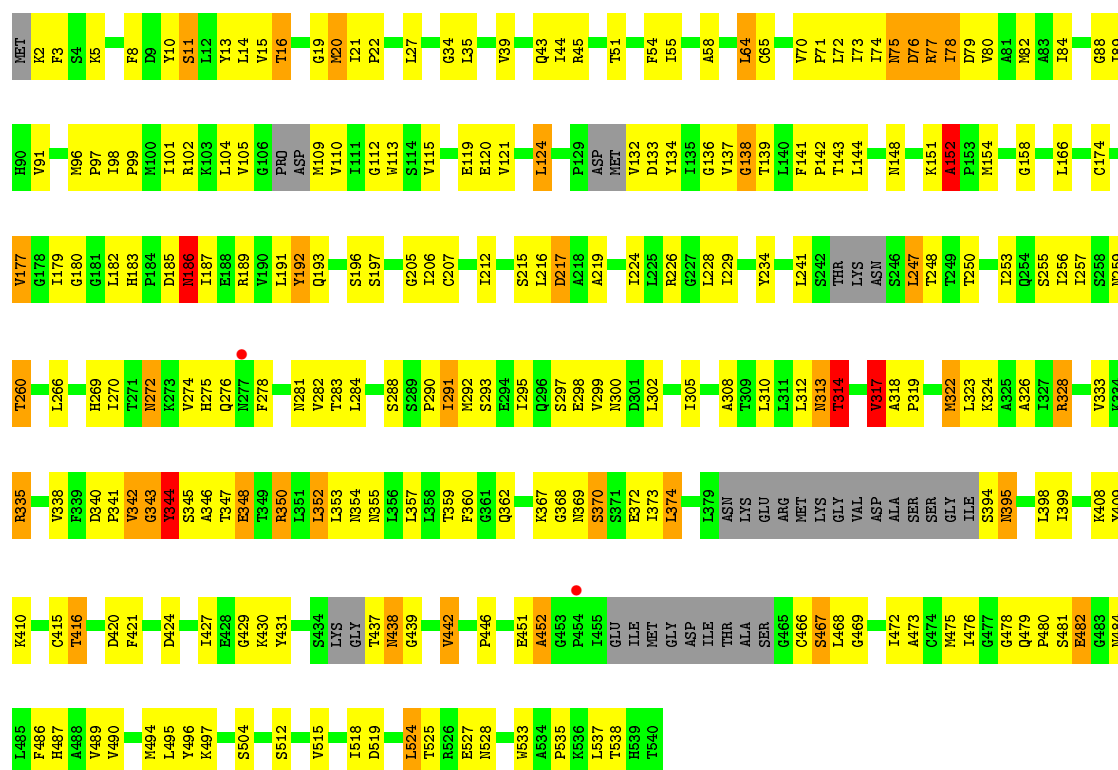
- Molecule 1: Thiamine biosynthetic bifunctional enzyme



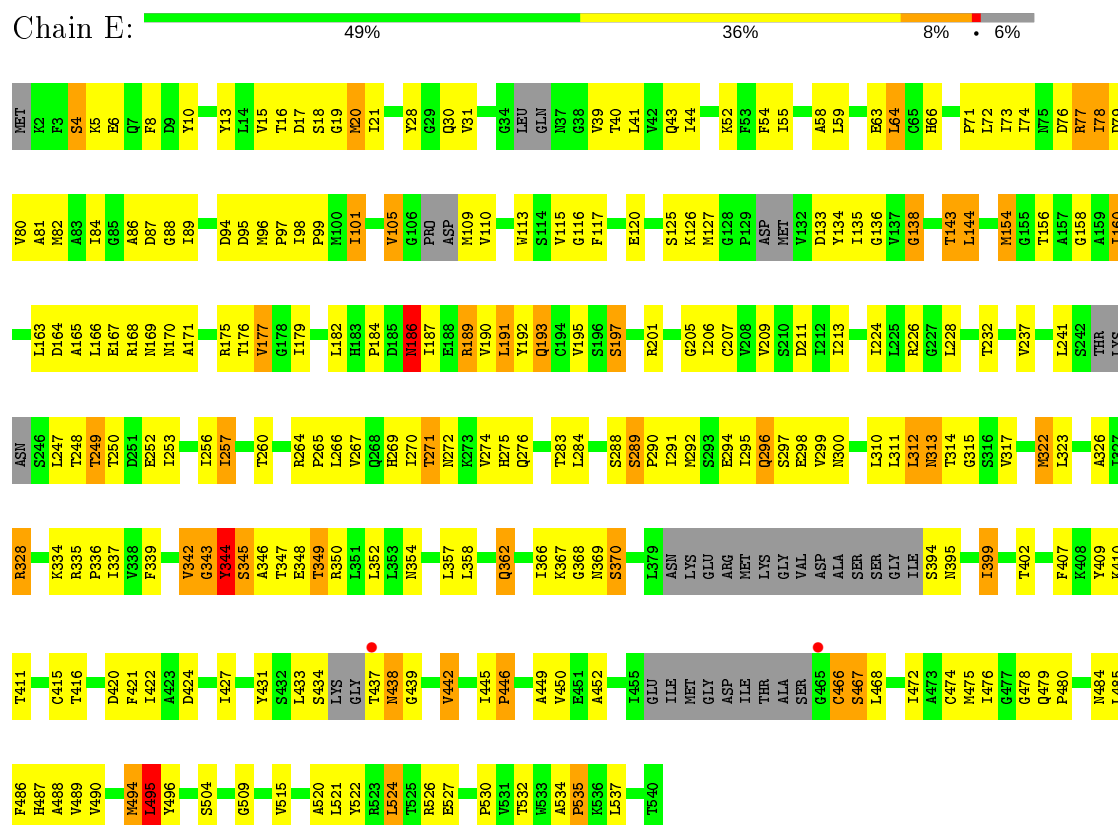
- Molecule 1: Thiamine biosynthetic bifunctional enzyme





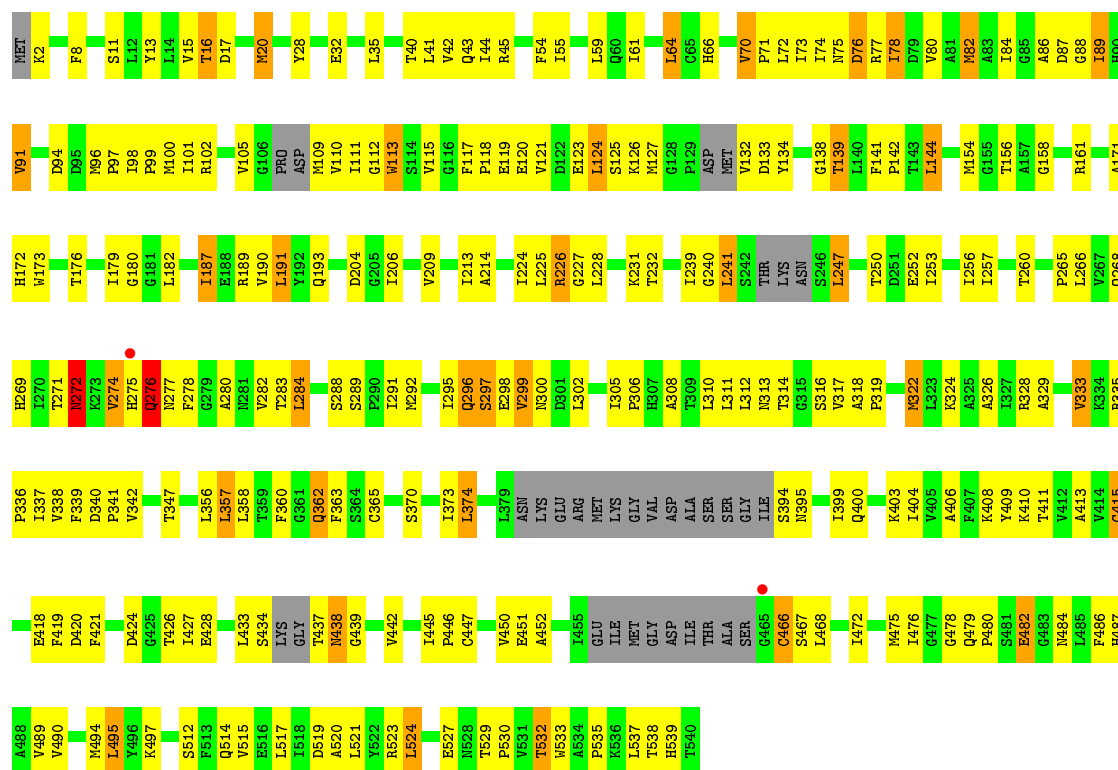


### • Molecule 1: Thiamine biosynthetic bifunctional enzyme



### • Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.94Å 154.21Å 148.70Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	38.55 – 3.21 38.55 – 3.21	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.55-3.21) 97.9 (38.55-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.65 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.201 , 0.232 0.193 , 0.248	Depositor DCC
$R_{free}$ test set	3731 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.8	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3NM, IFP, POP

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	0.48	0/3824	0.70	2/5190 (0.0%)
1	B	0.46	0/3824	0.67	2/5190 (0.0%)
1	C	0.49	0/3824	0.70	3/5190 (0.1%)
1	D	0.50	0/3824	0.74	4/5190 (0.1%)
1	E	0.48	0/3806	0.70	2/5164 (0.0%)
1	F	0.47	0/3824	0.65	0/5190
All	All	0.48	0/22926	0.69	13/31114 (0.0%)

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	B	1	0
1	D	0	1
All	All	1	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	317	VAL	CB-CA-C	-15.99	81.02	111.40
1	C	345	SER	N-CA-CB	-13.34	90.49	110.50
1	A	345	SER	N-CA-CB	-12.85	91.22	110.50
1	E	345	SER	N-CA-CB	-12.75	91.38	110.50
1	E	344	TYR	CB-CA-C	12.68	135.76	110.40
1	C	344	TYR	CB-CA-C	12.31	135.03	110.40
1	B	345	SER	N-CA-CB	-12.21	92.19	110.50
1	A	344	TYR	CB-CA-C	11.09	132.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	TYR	CB-CA-C	10.65	131.69	110.40
1	D	344	TYR	CB-CA-C	10.58	131.56	110.40
1	D	345	SER	N-CA-CB	-8.33	98.00	110.50
1	D	152	ALA	CB-CA-C	5.17	117.85	110.10
1	C	76	ASP	N-CA-C	5.02	124.55	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	344	TYR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	317	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3765	0	3750	262	0
1	B	3765	0	3750	230	0
1	C	3765	0	3750	221	0
1	D	3765	0	3750	218	0
1	E	3748	0	3730	223	0
1	F	3765	0	3750	226	0
2	A	16	0	7	3	0
2	B	16	0	7	3	0
2	C	16	0	7	0	0
2	D	16	0	7	1	0
2	E	16	0	7	2	0
2	F	16	0	7	2	0
3	A	12	0	4	1	0
3	B	12	0	4	1	0
3	C	12	0	4	0	0
3	D	12	0	4	0	0
3	E	12	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	12	0	4	0	0
4	A	9	0	0	1	0
4	B	9	0	0	2	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
4	E	9	0	0	0	0
4	F	9	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	22801	0	22546	1342	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 30.

All (1342) 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:B:78:ILE:HG21	1:B:96:MET:HE1	1.33	1.10
1:F:78:ILE:HG21	1:F:96:MET:HE1	1.34	1.09
1:B:343:GLY:HA3	1:B:350:ARG:HD3	1.29	1.09
1:F:8:PHE:CE2	1:F:110:VAL:HG21	1.91	1.06
1:A:313:ASN:ND2	1:A:342:VAL:HG21	1.71	1.06
1:E:77:ARG:HG2	1:E:77:ARG:HH11	1.18	1.04
1:D:317:VAL:O	1:D:317:VAL:CG1	1.91	1.03
1:D:299:VAL:HG21	1:D:326:ALA:HA	1.40	1.03
1:C:96:MET:HE3	1:C:101:ILE:HG12	1.37	1.03
1:D:317:VAL:HG12	1:D:317:VAL:O	1.19	1.01
1:A:78:ILE:HG21	1:A:96:MET:HE1	1.43	0.99
1:B:366:ILE:HD12	1:B:411:THR:HG21	1.43	0.99
1:A:187:ILE:HG12	1:A:206:ILE:HD13	1.41	0.99
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.26	0.97
1:C:274:VAL:HG23	1:C:275:HIS:HD2	1.25	0.96
1:C:299:VAL:HG21	1:C:326:ALA:HA	1.48	0.96
1:A:8:PHE:CE2	1:A:110:VAL:HG11	2.00	0.95
1:A:313:ASN:HD21	1:A:342:VAL:HG21	1.31	0.95
1:C:343:GLY:HA3	1:C:350:ARG:HD3	1.47	0.93
1:A:343:GLY:HA3	1:A:350:ARG:HD3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:THR:HG21	1:E:354:ASN:HD21	1.34	0.93
1:C:144:LEU:HD12	1:C:144:LEU:H	1.33	0.92
1:A:154:MET:HG2	1:A:158:GLY:HA3	1.51	0.91
1:B:115:VAL:HG13	1:B:120:GLU:HB2	1.53	0.91
1:E:366:ILE:HD12	1:E:411:THR:HG21	1.50	0.90
1:B:484:ASN:ND2	1:B:487:HIS:H	1.69	0.90
1:C:78:ILE:HG21	1:C:96:MET:CE	2.01	0.89
1:A:339:PHE:CE2	1:A:341:PRO:HG3	2.07	0.89
1:E:110:VAL:HG23	1:E:133:ASP:HB2	1.55	0.88
1:A:299:VAL:HG21	1:A:326:ALA:HA	1.55	0.88
1:F:250:THR:HG23	1:F:530:PRO:HB2	1.55	0.88
1:F:8:PHE:HE2	1:F:110:VAL:HG21	1.37	0.88
1:D:192:TYR:HD1	1:D:234:TYR:HD2	1.20	0.88
1:E:299:VAL:HG21	1:E:326:ALA:HA	1.54	0.88
1:D:276:GLN:HG3	1:D:292:MET:HE2	1.57	0.87
1:F:339:PHE:CE2	1:F:341:PRO:HG3	2.10	0.87
1:A:367:LYS:NZ	1:A:466:CYS:HA	1.88	0.87
1:D:187:ILE:HG12	1:D:206:ILE:HD13	1.58	0.86
1:D:183:HIS:H	1:D:186:ASN:HD21	1.19	0.86
1:E:343:GLY:HA3	1:E:350:ARG:HD3	1.58	0.85
1:F:78:ILE:HG21	1:F:96:MET:CE	2.06	0.85
1:E:101:ILE:O	1:E:105:VAL:HG22	1.76	0.85
1:A:35:LEU:HD22	1:A:70:VAL:HG11	1.59	0.85
1:A:313:ASN:ND2	1:A:342:VAL:CG2	2.39	0.85
1:B:35:LEU:HD21	1:B:70:VAL:HG11	1.59	0.85
1:C:274:VAL:HG23	1:C:275:HIS:CD2	2.10	0.85
1:F:370:SER:O	1:F:374:LEU:HB2	1.76	0.84
1:C:367:LYS:NZ	1:C:466:CYS:HA	1.94	0.83
1:D:14:LEU:HD13	1:D:212:ILE:HD12	1.59	0.83
1:F:91:VAL:HG11	1:F:101:ILE:HD13	1.60	0.83
1:E:160:ILE:HD11	1:E:193:GLN:O	1.81	0.81
1:D:192:TYR:CD1	1:D:234:TYR:HD2	1.97	0.81
1:A:272:ASN:ND2	1:A:272:ASN:H	1.75	0.81
1:B:274:VAL:HG23	1:B:275:HIS:HD2	1.46	0.81
1:E:58:ALA:HB1	1:E:84:ILE:HD13	1.63	0.81
1:F:276:GLN:HG3	1:F:292:MET:CE	2.11	0.81
1:A:282:VAL:HG21	1:A:467:SER:HB3	1.63	0.80
1:D:512:SER:HA	1:D:515:VAL:HG12	1.63	0.80
1:F:35:LEU:HD22	1:F:70:VAL:HG11	1.63	0.80
1:B:495:LEU:HD22	1:B:521:LEU:HD23	1.64	0.80
1:F:15:VAL:HB	1:F:209:VAL:HG22	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:VAL:HG23	1:D:343:GLY:H	1.44	0.80
1:D:154:MET:HG2	1:D:158:GLY:HA3	1.62	0.79
1:F:74:ILE:HD11	1:F:84:ILE:HD11	1.64	0.79
1:D:77:ARG:CG	1:D:77:ARG:HH11	1.96	0.79
1:E:78:ILE:HD13	1:E:96:MET:HE1	1.64	0.79
1:F:271:THR:HA	1:F:313:ASN:HB3	1.64	0.79
1:B:274:VAL:HG23	1:B:275:HIS:CD2	2.17	0.79
1:E:328:ARG:HH11	1:E:328:ARG:CG	1.95	0.79
1:B:339:PHE:CE2	1:B:341:PRO:HG3	2.19	0.78
1:B:154:MET:HG2	1:B:158:GLY:HA3	1.66	0.78
1:C:282:VAL:HG21	1:C:467:SER:HB3	1.65	0.78
1:A:20:MET:HG2	1:A:214:ALA:HB2	1.66	0.78
1:B:343:GLY:CA	1:B:350:ARG:HD3	2.13	0.78
1:C:78:ILE:HG21	1:C:96:MET:HE1	1.64	0.78
1:C:79:ASP:HB3	1:D:79:ASP:HB3	1.65	0.77
1:A:367:LYS:HZ1	1:A:466:CYS:HA	1.48	0.77
1:C:44:ILE:HG13	1:C:72:LEU:HD11	1.64	0.77
1:E:467:SER:HB2	1:E:496:TYR:CE1	2.17	0.77
1:F:154:MET:HG2	1:F:158:GLY:HA3	1.66	0.77
1:F:252:GLU:O	1:F:256:ILE:HD13	1.84	0.77
1:A:192:TYR:HD1	1:A:234:TYR:HD2	1.33	0.77
1:A:253:ILE:HD11	1:A:494:MET:HE2	1.67	0.77
1:A:337:ILE:N	1:A:337:ILE:HD12	2.00	0.77
1:C:328:ARG:HG3	1:C:328:ARG:HH11	1.49	0.76
1:D:281:ASN:HB3	1:D:518:ILE:HD13	1.67	0.76
1:E:186:ASN:HD22	1:E:186:ASN:C	1.89	0.76
1:F:276:GLN:HG3	1:F:292:MET:HE2	1.65	0.76
1:F:274:VAL:HG23	1:F:275:HIS:HD2	1.50	0.76
1:B:314:THR:HG21	1:B:354:ASN:HD21	1.48	0.75
1:B:475:MET:CE	1:B:495:LEU:HD12	2.17	0.75
1:B:191:LEU:HD22	1:B:206:ILE:HD11	1.68	0.75
1:B:78:ILE:HG21	1:B:96:MET:CE	2.14	0.75
1:C:187:ILE:HG23	1:C:206:ILE:CD1	2.16	0.75
1:B:253:ILE:O	1:B:257:ILE:HG13	1.87	0.75
1:D:437:THR:O	1:D:439:GLY:N	2.20	0.75
1:B:495:LEU:CD2	1:B:521:LEU:HD23	2.16	0.74
1:E:77:ARG:HG2	1:E:77:ARG:NH1	1.84	0.74
1:F:268:GLN:HB3	1:F:310:LEU:HD12	1.67	0.74
1:D:272:ASN:H	1:D:272:ASN:ND2	1.86	0.74
1:E:44:ILE:HG13	1:E:72:LEU:HD11	1.68	0.74
1:C:154:MET:HG2	1:C:158:GLY:HA3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD13	1:A:409:TYR:CE2	2.23	0.73
1:A:89:ILE:HD11	1:A:101:ILE:CG2	2.17	0.73
1:B:475:MET:HE1	1:B:495:LEU:HD12	1.70	0.73
1:A:78:ILE:HG21	1:A:96:MET:CE	2.17	0.73
1:F:124:LEU:HA	1:F:127:MET:HE2	1.70	0.73
1:F:424:ASP:HB2	1:F:486:PHE:CD1	2.23	0.73
1:A:115:VAL:HG13	1:A:120:GLU:HB2	1.70	0.73
1:E:98:ILE:N	1:E:99:PRO:HD2	2.04	0.73
1:F:527:GLU:HG3	1:F:527:GLU:O	1.87	0.73
1:A:479:GLN:NE2	1:A:483:GLY:HA3	2.03	0.73
1:F:73:ILE:HA	1:F:88:GLY:O	1.89	0.73
1:C:367:LYS:HZ1	1:C:466:CYS:HA	1.54	0.72
1:E:41:LEU:HD11	1:E:73:ILE:HD11	1.69	0.72
1:F:98:ILE:HD11	1:F:113:TRP:CD1	2.25	0.72
1:C:40:THR:HG21	1:C:226:ARG:HH21	1.53	0.72
1:D:282:VAL:HG21	1:D:467:SER:HB3	1.69	0.72
1:F:299:VAL:HG21	1:F:326:ALA:HA	1.70	0.72
1:B:111:ILE:CG2	1:B:132:VAL:HA	2.19	0.72
1:E:274:VAL:HG23	1:E:275:HIS:HD2	1.52	0.72
1:F:437:THR:O	1:F:439:GLY:N	2.22	0.72
1:B:115:VAL:HA	1:B:120:GLU:OE1	1.90	0.72
1:C:256:ILE:HG22	1:C:475:MET:HE1	1.71	0.72
1:F:59:LEU:HD21	1:F:84:ILE:HB	1.70	0.72
1:C:437:THR:O	1:C:439:GLY:N	2.22	0.72
1:E:77:ARG:HH11	1:E:77:ARG:CG	2.00	0.72
1:F:257:ILE:HD11	1:F:533:TRP:HH2	1.53	0.71
1:E:184:PRO:HD3	1:E:211:ASP:OD1	1.90	0.71
1:A:8:PHE:CE2	1:A:110:VAL:CG1	2.72	0.71
1:E:8:PHE:CE2	1:E:110:VAL:HG11	2.25	0.71
1:E:274:VAL:HG23	1:E:275:HIS:CD2	2.26	0.71
1:C:484:ASN:ND2	1:C:487:HIS:H	1.89	0.71
1:B:266:LEU:HD23	1:B:305:ILE:HG21	1.71	0.71
1:C:96:MET:CE	1:C:101:ILE:HG12	2.19	0.70
1:D:270:ILE:HD12	1:D:310:LEU:HD11	1.71	0.70
1:E:276:GLN:HG3	1:E:292:MET:HE3	1.73	0.70
1:F:373:ILE:HG13	1:F:415:CYS:HB2	1.73	0.70
1:A:342:VAL:HG23	1:A:342:VAL:O	1.91	0.70
1:D:16:THR:O	1:D:45:ARG:HB3	1.91	0.70
1:E:271:THR:HA	1:E:313:ASN:HB3	1.73	0.70
1:C:21:ILE:HD11	1:C:27:LEU:HD12	1.74	0.70
1:A:89:ILE:HD11	1:A:101:ILE:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:TYR:HE1	1:B:64:LEU:HB2	1.55	0.70
1:A:370:SER:O	1:A:374:LEU:HB2	1.91	0.70
1:B:484:ASN:HD21	1:B:487:HIS:H	1.40	0.70
1:E:314:THR:HG21	1:E:354:ASN:ND2	2.06	0.70
1:B:314:THR:HG21	1:B:354:ASN:ND2	2.07	0.69
1:C:271:THR:HA	1:C:313:ASN:HB3	1.72	0.69
1:C:241:LEU:O	1:C:428:GLU:HA	1.92	0.69
1:F:420:ASP:OD2	1:F:497:LYS:HD3	1.92	0.69
1:F:520:ALA:O	1:F:524:LEU:HB2	1.92	0.69
1:A:420:ASP:OD2	1:A:497:LYS:HD3	1.92	0.69
1:D:98:ILE:HG21	1:D:132:VAL:HG22	1.73	0.69
1:A:44:ILE:HG13	1:A:72:LEU:HD11	1.73	0.69
1:F:124:LEU:HA	1:F:127:MET:CE	2.22	0.69
1:D:97:PRO:O	1:D:101:ILE:HG13	1.93	0.69
1:A:91:VAL:HG11	1:A:101:ILE:HD13	1.73	0.69
1:C:377:ALA:HB2	1:C:405:VAL:HG23	1.75	0.69
1:C:40:THR:HG21	1:C:226:ARG:NH2	2.08	0.69
1:F:156:THR:HG21	1:F:193:GLN:HG3	1.75	0.69
1:B:78:ILE:HB	1:B:89:ILE:HD13	1.73	0.68
1:C:358:LEU:HD23	1:C:363:PHE:HE1	1.58	0.68
1:D:367:LYS:NZ	1:D:466:CYS:HA	2.08	0.68
1:F:247:LEU:HG	1:F:539:HIS:NE2	2.08	0.68
1:D:373:ILE:HG13	1:D:415:CYS:HB2	1.73	0.68
1:A:343:GLY:CA	1:A:350:ARG:HD3	2.23	0.68
1:B:407:PHE:CE2	1:B:410:LYS:HE3	2.27	0.68
1:C:101:ILE:O	1:C:105:VAL:HG22	1.93	0.68
1:A:35:LEU:HD12	1:A:64:LEU:HD13	1.74	0.68
1:D:183:HIS:H	1:D:186:ASN:ND2	1.89	0.68
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.06	0.68
1:D:367:LYS:HZ3	1:D:466:CYS:HA	1.59	0.68
1:E:74:ILE:HD11	1:E:84:ILE:HD11	1.76	0.68
1:A:274:VAL:HG23	1:A:275:HIS:HD2	1.57	0.68
1:D:313:ASN:C	1:D:313:ASN:HD22	1.96	0.68
1:B:192:TYR:HD1	1:B:234:TYR:HD2	1.42	0.68
1:F:337:ILE:HG21	1:F:363:PHE:CD2	2.29	0.68
1:A:347:THR:HG21	1:C:298:GLU:HG3	1.75	0.67
1:F:486:PHE:O	1:F:490:VAL:HG23	1.93	0.67
1:A:400:GLN:O	1:A:404:ILE:HG13	1.94	0.67
1:D:44:ILE:HG13	1:D:72:LEU:HD11	1.76	0.67
1:F:337:ILE:HG21	1:F:363:PHE:HD2	1.58	0.67
1:B:77:ARG:HH11	1:F:77:ARG:NH1	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:MET:HG3	1:E:158:GLY:HA3	1.75	0.67
1:A:8:PHE:HE2	1:A:110:VAL:CG1	2.07	0.67
1:E:256:ILE:HD13	1:E:488:ALA:HA	1.76	0.67
1:C:294:GLU:OE1	1:C:318:ALA:HB2	1.95	0.67
1:D:484:ASN:HD22	1:D:487:HIS:H	1.41	0.67
1:F:8:PHE:CE2	1:F:110:VAL:CG2	2.76	0.67
1:C:527:GLU:O	1:C:527:GLU:HG3	1.95	0.67
1:E:520:ALA:O	1:E:524:LEU:HB2	1.94	0.67
1:F:98:ILE:HD13	1:F:101:ILE:HD12	1.77	0.67
1:D:192:TYR:HD1	1:D:234:TYR:CD2	2.08	0.67
1:E:467:SER:HB2	1:E:496:TYR:HE1	1.58	0.67
1:D:308:ALA:O	1:D:335:ARG:HD3	1.95	0.67
1:E:110:VAL:HG23	1:E:133:ASP:CB	2.25	0.67
1:F:15:VAL:HB	1:F:209:VAL:CG2	2.24	0.67
1:D:298:GLU:HG2	1:F:347:THR:HG21	1.75	0.67
1:B:144:LEU:H	1:B:144:LEU:HD12	1.59	0.67
1:F:125:SER:C	1:F:127:MET:H	1.98	0.66
1:A:96:MET:CE	1:A:101:ILE:HG12	2.26	0.66
1:B:322:MET:HG3	1:B:323:LEU:N	2.10	0.66
1:A:512:SER:HA	1:A:515:VAL:HG12	1.77	0.66
1:E:472:ILE:O	1:E:476:ILE:HG13	1.95	0.66
1:B:433:LEU:O	1:B:434:SER:HB2	1.95	0.66
1:D:394:SER:OG	1:D:395:ASN:N	2.28	0.66
1:F:427:ILE:O	1:F:427:ILE:HG22	1.94	0.66
1:B:250:THR:HG23	1:B:530:PRO:HB2	1.77	0.66
1:F:115:VAL:HG13	1:F:120:GLU:HB2	1.77	0.66
1:F:358:LEU:HD13	1:F:409:TYR:CE2	2.31	0.66
1:E:328:ARG:HG2	1:E:328:ARG:HH11	1.61	0.66
1:B:14:LEU:HD11	1:B:213:ILE:HD11	1.77	0.65
1:F:8:PHE:HE2	1:F:110:VAL:CG2	2.07	0.65
1:E:342:VAL:HG23	1:E:343:GLY:H	1.61	0.65
1:F:74:ILE:CD1	1:F:84:ILE:HD11	2.27	0.65
1:B:28:TYR:CE1	1:B:64:LEU:HG	2.30	0.65
1:B:420:ASP:OD2	1:B:497:LYS:HD3	1.97	0.65
1:E:125:SER:C	1:E:127:MET:H	1.99	0.65
1:E:276:GLN:HG3	1:E:292:MET:CE	2.25	0.65
1:A:145:THR:HB	2:A:541:3NM:H7	1.77	0.65
1:B:467:SER:HB2	1:B:496:TYR:CE1	2.31	0.65
1:B:520:ALA:O	1:B:524:LEU:HB2	1.96	0.65
1:E:256:ILE:HG22	1:E:475:MET:HE1	1.79	0.65
1:C:495:LEU:HD11	1:C:525:THR:CG2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG22	1:A:43:GLN:HB3	1.78	0.65
1:A:74:ILE:HD12	1:A:81:ALA:HA	1.78	0.65
1:B:197:SER:O	1:B:442:VAL:HG23	1.96	0.65
1:F:442:VAL:O	1:F:445:ILE:HG12	1.97	0.65
1:A:318:ALA:HB1	1:A:322:MET:HG2	1.79	0.65
1:A:322:MET:HG3	1:A:323:LEU:HD23	1.78	0.65
1:B:485:LEU:O	1:B:489:VAL:HG23	1.95	0.65
1:B:276:GLN:HG3	1:B:292:MET:CE	2.26	0.65
1:E:366:ILE:CD1	1:E:411:THR:HG21	2.26	0.65
1:A:292:MET:HE2	1:B:274:VAL:HG11	1.76	0.65
1:E:269:HIS:HB3	1:E:271:THR:HG22	1.79	0.65
1:A:433:LEU:HD12	1:A:433:LEU:N	2.11	0.64
1:C:358:LEU:HD23	1:C:363:PHE:CE1	2.31	0.64
1:F:89:ILE:HD11	1:F:101:ILE:CG2	2.27	0.64
1:A:187:ILE:HG12	1:A:206:ILE:CD1	2.23	0.64
1:B:77:ARG:HH11	1:B:77:ARG:HG2	1.62	0.64
1:C:264:ARG:N	1:C:265:PRO:HD3	2.12	0.64
1:C:298:GLU:HG2	1:C:302:LEU:HD11	1.78	0.64
1:B:20:MET:HE3	1:B:213:ILE:HB	1.78	0.64
1:D:78:ILE:HG21	1:D:96:MET:CE	2.27	0.64
1:A:253:ILE:HD11	1:A:494:MET:CE	2.27	0.64
1:E:256:ILE:HG12	1:E:479:GLN:OE1	1.98	0.64
1:A:74:ILE:HD11	1:A:84:ILE:HD11	1.79	0.64
1:A:78:ILE:O	1:A:81:ALA:HB3	1.97	0.64
1:B:328:ARG:CG	1:B:328:ARG:HH11	2.10	0.64
1:B:366:ILE:CD1	1:B:411:THR:HG21	2.25	0.64
1:D:283:THR:HB	1:D:290:PRO:HG3	1.80	0.64
1:B:88:GLY:HA3	1:B:110:VAL:CG1	2.28	0.64
1:A:299:VAL:HG21	1:A:326:ALA:CA	2.25	0.64
1:B:17:ASP:HB3	1:B:20:MET:HE1	1.79	0.64
1:B:192:TYR:CD1	1:B:234:TYR:HD2	2.16	0.64
1:C:339:PHE:CE2	1:C:341:PRO:HG3	2.33	0.64
1:C:427:ILE:O	1:C:427:ILE:HG22	1.98	0.64
1:C:484:ASN:HD22	1:C:487:HIS:H	1.44	0.64
1:B:183:HIS:O	1:B:187:ILE:HD12	1.97	0.64
1:B:267:VAL:HG12	1:B:269:HIS:CE1	2.32	0.63
1:E:187:ILE:HG23	1:E:206:ILE:CD1	2.28	0.63
1:E:299:VAL:CG2	1:E:326:ALA:HA	2.28	0.63
1:C:249:THR:OG1	1:C:252:GLU:HG3	1.98	0.63
1:F:269:HIS:HB2	1:F:292:MET:SD	2.38	0.63
1:A:274:VAL:HG23	1:A:275:HIS:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:LYS:HZ2	1:D:469:GLY:H	1.45	0.63
1:E:20:MET:HG2	1:E:20:MET:O	1.98	0.63
1:E:79:ASP:OD1	1:E:80:VAL:N	2.32	0.63
1:A:172:HIS:O	1:A:175:ARG:NH2	2.32	0.63
1:B:145:THR:HB	2:B:541:3NM:H7	1.81	0.63
1:C:187:ILE:HG23	1:C:206:ILE:HD13	1.79	0.63
1:C:256:ILE:HG22	1:C:475:MET:CE	2.27	0.63
1:A:256:ILE:O	1:A:260:THR:HG22	1.97	0.63
1:D:420:ASP:OD2	1:D:497:LYS:HD3	1.98	0.63
1:A:479:GLN:HE21	1:A:483:GLY:HA3	1.61	0.63
1:B:35:LEU:CD2	1:B:70:VAL:HG11	2.29	0.63
1:B:72:LEU:HD12	1:B:73:ILE:N	2.14	0.63
1:D:299:VAL:CG2	1:D:326:ALA:HA	2.22	0.63
1:E:168:ARG:HG2	1:E:168:ARG:O	1.98	0.63
1:C:275:HIS:CD2	1:C:275:HIS:H	2.17	0.62
1:C:38:GLY:O	1:C:40:THR:HG23	1.98	0.62
1:A:366:ILE:HD12	1:A:411:THR:HG21	1.80	0.62
1:A:88:GLY:HA3	1:A:110:VAL:HG13	1.79	0.62
1:A:77:ARG:NH1	1:E:77:ARG:NH1	2.48	0.62
1:B:189:ARG:O	1:B:193:GLN:HG2	1.99	0.62
1:F:97:PRO:O	1:F:101:ILE:HG13	1.99	0.62
1:A:187:ILE:HD13	1:A:225:LEU:CD2	2.29	0.62
1:A:476:ILE:HD13	1:A:485:LEU:HD11	1.80	0.62
1:B:275:HIS:N	1:B:275:HIS:CD2	2.67	0.62
1:E:495:LEU:HD22	1:E:521:LEU:HD23	1.80	0.62
1:F:187:ILE:HG23	1:F:206:ILE:HD12	1.80	0.62
1:F:484:ASN:HD22	1:F:487:HIS:H	1.47	0.62
1:A:269:HIS:HB2	1:A:292:MET:SD	2.40	0.62
1:B:533:TRP:HB3	1:B:535:PRO:HD2	1.80	0.62
1:B:513:PHE:C	1:B:513:PHE:CD2	2.73	0.62
1:A:96:MET:HE2	1:A:101:ILE:HG12	1.82	0.61
1:B:195:VAL:HG12	1:B:202:SER:HB2	1.80	0.61
1:B:310:LEU:HD23	1:B:337:ILE:HG23	1.82	0.61
1:B:498:ALA:O	1:B:502:ILE:HG13	2.00	0.61
1:D:399:ILE:HD13	1:D:421:PHE:CD2	2.35	0.61
1:C:78:ILE:HG21	1:C:96:MET:HE2	1.78	0.61
1:D:8:PHE:HE2	1:D:110:VAL:HB	1.65	0.61
1:B:364:SER:HB3	1:B:485:LEU:HD21	1.83	0.61
1:D:276:GLN:HG3	1:D:292:MET:CE	2.29	0.61
1:D:51:THR:O	1:D:55:ILE:HG13	2.00	0.61
1:E:484:ASN:HD22	1:E:487:HIS:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:O	1:A:187:ILE:HD12	2.01	0.61
1:F:308:ALA:O	1:F:335:ARG:HD3	2.01	0.61
1:A:272:ASN:HD21	1:A:313:ASN:HD22	1.49	0.61
1:A:468:LEU:O	1:A:472:ILE:HG13	2.01	0.61
1:D:399:ILE:HD11	1:D:421:PHE:CE2	2.36	0.61
1:E:89:ILE:O	1:E:89:ILE:HG13	1.99	0.61
1:A:272:ASN:N	1:A:272:ASN:ND2	2.44	0.60
1:A:324:LYS:HB2	1:A:360:PHE:CE1	2.36	0.60
1:A:59:LEU:HD21	1:A:84:ILE:HB	1.83	0.60
1:B:286:LEU:HD11	1:B:471:THR:HG23	1.83	0.60
1:B:193:GLN:NE2	1:B:362:GLN:HE21	1.99	0.60
1:A:144:LEU:HD12	1:A:144:LEU:H	1.65	0.60
1:B:299:VAL:HG21	1:B:326:ALA:HA	1.84	0.60
1:C:365:CYS:HA	1:C:412:VAL:O	2.01	0.60
1:E:136:GLY:HA2	1:E:177:VAL:HG23	1.84	0.60
1:B:79:ASP:OD1	1:B:80:VAL:N	2.35	0.60
1:F:35:LEU:HD12	1:F:64:LEU:HD13	1.83	0.60
1:A:424:ASP:HB3	1:A:446:PRO:HG2	1.83	0.60
1:D:424:ASP:HB2	1:D:486:PHE:CD1	2.36	0.60
1:F:59:LEU:CD2	1:F:84:ILE:HB	2.32	0.60
1:A:509:GLY:HA2	1:C:522:TYR:CD2	2.36	0.60
1:D:79:ASP:OD1	1:D:80:VAL:N	2.35	0.60
1:E:437:THR:O	1:E:439:GLY:N	2.35	0.60
1:A:313:ASN:HD21	1:A:342:VAL:CG2	2.07	0.60
1:D:298:GLU:OE1	1:F:347:THR:HG21	2.00	0.60
1:F:296:GLN:HG2	1:F:322:MET:HB2	1.83	0.60
1:A:305:ILE:HG23	1:A:306:PRO:HD2	1.83	0.60
1:C:40:THR:CG2	1:C:226:ARG:HH21	2.15	0.60
1:A:337:ILE:H	1:A:337:ILE:HD12	1.67	0.59
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.67	0.59
1:D:328:ARG:HG3	1:D:328:ARG:HH11	1.67	0.59
1:D:74:ILE:HD11	1:D:84:ILE:HD11	1.84	0.59
1:E:135:ILE:CG1	1:E:176:THR:HG22	2.32	0.59
1:D:408:LYS:HD3	1:D:409:TYR:CZ	2.37	0.59
1:D:180:GLY:HA2	2:D:541:3NM:H7A	1.84	0.59
1:A:192:TYR:HD1	1:A:234:TYR:CD2	2.18	0.59
1:D:137:VAL:O	1:D:138:GLY:O	2.20	0.59
1:F:91:VAL:HG11	1:F:101:ILE:CD1	2.31	0.59
1:A:42:VAL:O	1:A:72:LEU:HD12	2.02	0.59
1:A:77:ARG:NH1	1:E:77:ARG:HH11	2.01	0.59
1:D:342:VAL:HG23	1:D:343:GLY:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:PRO:HD2	1:E:288:SER:OG	2.02	0.59
1:C:250:THR:HG23	1:C:530:PRO:HB2	1.85	0.59
1:F:451:GLU:HG2	1:F:452:ALA:N	2.17	0.59
1:B:20:MET:HG2	1:B:20:MET:O	2.02	0.59
1:A:416:THR:HG21	1:A:468:LEU:HD23	1.85	0.59
1:C:370:SER:O	1:C:374:LEU:HB2	2.02	0.59
1:D:278:PHE:O	1:D:281:ASN:HB2	2.02	0.59
1:C:89:ILE:HD11	1:C:101:ILE:HD13	1.84	0.59
1:A:358:LEU:HD23	1:A:363:PHE:HE1	1.68	0.58
1:B:125:SER:C	1:B:127:MET:H	2.07	0.58
1:C:276:GLN:NE2	1:C:292:MET:HB3	2.18	0.58
1:D:187:ILE:HG23	1:D:206:ILE:CD1	2.32	0.58
1:F:394:SER:OG	1:F:395:ASN:N	2.35	0.58
1:A:79:ASP:OD1	1:A:80:VAL:N	2.36	0.58
1:A:73:ILE:HG23	1:A:88:GLY:C	2.24	0.58
1:C:15:VAL:HB	1:C:209:VAL:HG22	1.84	0.58
1:C:8:PHE:CE2	1:C:110:VAL:HG21	2.38	0.58
1:D:274:VAL:HG23	1:D:275:HIS:CD2	2.38	0.58
1:E:295:ILE:HG22	1:E:298:GLU:HB2	1.85	0.58
1:A:283:THR:HB	1:A:290:PRO:HG3	1.86	0.58
1:C:342:VAL:HG23	1:C:343:GLY:H	1.69	0.58
1:F:109:MET:HG2	1:F:110:VAL:N	2.19	0.58
1:F:424:ASP:HB3	1:F:446:PRO:HG2	1.85	0.58
1:F:479:GLN:HE21	1:F:484:ASN:H	1.50	0.58
1:B:87:ASP:O	1:B:110:VAL:HG12	2.04	0.58
1:B:343:GLY:HA3	1:B:350:ARG:CD	2.20	0.58
1:E:468:LEU:O	1:E:472:ILE:HG13	2.04	0.58
1:E:74:ILE:HD12	1:E:81:ALA:HA	1.84	0.58
1:E:347:THR:HG21	1:F:298:GLU:HG2	1.85	0.58
1:A:96:MET:O	1:A:101:ILE:HD11	2.03	0.58
1:C:35:LEU:HD22	1:C:70:VAL:HG11	1.85	0.58
1:E:187:ILE:HG12	1:E:206:ILE:HD13	1.85	0.58
1:E:266:LEU:HD11	1:E:291:ILE:HG13	1.86	0.58
1:F:533:TRP:C	1:F:535:PRO:HD2	2.23	0.58
1:A:367:LYS:HZ2	1:A:466:CYS:HA	1.68	0.58
1:A:298:GLU:CG	1:B:347:THR:HG21	2.33	0.58
1:D:248:THR:HG23	1:D:487:HIS:ND1	2.18	0.58
1:E:250:THR:HG23	1:E:530:PRO:HB2	1.86	0.58
1:E:328:ARG:HG2	1:E:328:ARG:NH1	2.19	0.58
1:C:328:ARG:CG	1:C:328:ARG:HH11	2.13	0.57
1:E:116:GLY:C	1:E:117:PHE:HD2	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:TYR:HE2	1:B:362:GLN:HG3	1.69	0.57
1:B:77:ARG:NH1	1:F:77:ARG:NH1	2.52	0.57
1:A:117:PHE:CD2	1:A:117:PHE:N	2.72	0.57
1:A:534:ALA:N	1:A:535:PRO:CD	2.67	0.57
1:B:115:VAL:HG13	1:B:120:GLU:CB	2.31	0.57
1:B:422:ILE:HG22	1:B:486:PHE:HE1	1.69	0.57
1:B:367:LYS:NZ	1:B:466:CYS:HA	2.19	0.57
1:E:15:VAL:HB	1:E:209:VAL:HG22	1.84	0.57
1:B:89:ILE:O	1:B:89:ILE:HG13	2.05	0.57
1:D:451:GLU:HG2	1:D:452:ALA:N	2.19	0.57
1:A:272:ASN:HD21	1:A:313:ASN:ND2	2.01	0.57
1:B:271:THR:HA	1:B:313:ASN:HB3	1.85	0.57
1:F:276:GLN:HG3	1:F:292:MET:HE3	1.85	0.57
1:B:109:MET:HG2	1:B:110:VAL:H	1.70	0.57
1:B:256:ILE:O	1:B:260:THR:HG22	2.05	0.57
1:D:348:GLU:HA	1:D:348:GLU:OE1	2.05	0.57
1:B:322:MET:HE2	1:B:326:ALA:HB2	1.86	0.57
1:C:20:MET:HG2	1:C:214:ALA:HB2	1.87	0.57
1:D:89:ILE:HD11	1:D:101:ILE:HG21	1.86	0.57
1:C:21:ILE:HD11	1:C:27:LEU:CD1	2.34	0.57
1:D:98:ILE:HG21	1:D:132:VAL:CG2	2.35	0.57
1:A:119:GLU:OE1	1:A:119:GLU:N	2.28	0.57
1:A:495:LEU:HD22	1:A:521:LEU:CD2	2.34	0.57
1:A:250:THR:HG23	1:A:530:PRO:HB2	1.86	0.57
1:B:276:GLN:HG3	1:B:292:MET:HE3	1.84	0.57
1:C:308:ALA:O	1:C:335:ARG:NH1	2.37	0.57
1:C:125:SER:CB	1:C:169:ASN:HD22	2.18	0.57
1:E:20:MET:CG	1:E:20:MET:O	2.53	0.57
1:F:187:ILE:HG23	1:F:206:ILE:CD1	2.34	0.57
1:A:192:TYR:CD1	1:A:234:TYR:HD2	2.17	0.56
1:D:151:LYS:O	1:D:152:ALA:HB3	2.04	0.56
1:F:274:VAL:HG23	1:F:275:HIS:CD2	2.37	0.56
1:F:468:LEU:O	1:F:472:ILE:HG13	2.05	0.56
1:F:475:MET:CE	1:F:495:LEU:HD12	2.35	0.56
1:A:247:LEU:HD22	1:A:537:LEU:HG	1.86	0.56
1:A:407:PHE:HE2	1:A:427:ILE:HD11	1.70	0.56
1:B:475:MET:HE2	1:B:495:LEU:HD12	1.88	0.56
1:D:65:CYS:HB3	1:D:70:VAL:O	2.06	0.56
1:F:89:ILE:HD11	1:F:101:ILE:HG21	1.87	0.56
1:A:89:ILE:O	1:A:89:ILE:HG13	2.04	0.56
1:D:101:ILE:O	1:D:105:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:HD22	1:D:64:LEU:O	2.04	0.56
1:E:283:THR:HG23	1:E:474:CYS:SG	2.45	0.56
1:E:59:LEU:HD21	1:E:84:ILE:HB	1.87	0.56
1:B:190:VAL:O	1:B:194:CYS:HB2	2.05	0.56
1:C:17:ASP:HB3	1:C:20:MET:CE	2.35	0.56
1:C:269:HIS:HB2	1:C:292:MET:SD	2.45	0.56
1:C:367:LYS:HZ2	1:C:466:CYS:HA	1.67	0.56
1:C:520:ALA:O	1:C:524:LEU:HB2	2.04	0.56
1:D:333:VAL:HG12	1:D:333:VAL:O	2.04	0.56
1:A:280:ALA:HB2	1:A:292:MET:CE	2.36	0.56
1:B:10:TYR:CE1	1:B:175:ARG:HG3	2.41	0.56
1:D:115:VAL:O	1:D:138:GLY:N	2.32	0.56
1:A:225:LEU:O	1:A:229:ILE:HG13	2.04	0.56
1:C:211:ASP:OD1	1:C:225:LEU:HD21	2.05	0.56
1:A:32:GLU:HG3	1:A:64:LEU:HD11	1.87	0.56
1:A:77:ARG:HH12	1:E:77:ARG:HH11	1.52	0.56
1:D:14:LEU:CD1	1:D:212:ILE:HD12	2.33	0.56
1:B:534:ALA:N	1:B:535:PRO:HD2	2.20	0.56
1:D:272:ASN:N	1:D:272:ASN:ND2	2.54	0.56
1:D:347:THR:OG1	1:D:350:ARG:HB2	2.06	0.56
1:D:75:ASN:O	1:D:77:ARG:N	2.34	0.56
1:B:318:ALA:HB1	1:B:322:MET:HG2	1.86	0.56
1:B:468:LEU:O	1:B:472:ILE:HG13	2.06	0.56
1:C:44:ILE:HD11	1:C:61:ILE:CG2	2.35	0.56
1:F:15:VAL:HG22	1:F:43:GLN:NE2	2.19	0.56
1:F:55:ILE:HG23	1:F:84:ILE:CG2	2.36	0.56
1:B:76:ASP:HA	1:B:91:VAL:HG12	1.88	0.55
1:C:249:THR:HG23	1:C:252:GLU:OE1	2.06	0.55
1:E:116:GLY:O	1:E:117:PHE:HD2	1.89	0.55
1:E:275:HIS:HB3	1:E:466:CYS:SG	2.46	0.55
1:F:59:LEU:HD21	1:F:84:ILE:CB	2.36	0.55
1:A:192:TYR:CE2	1:A:410:LYS:HG3	2.42	0.55
1:C:115:VAL:HG13	1:C:120:GLU:HB2	1.88	0.55
1:C:51:THR:O	1:C:55:ILE:HG13	2.04	0.55
1:D:343:GLY:HA3	1:D:350:ARG:HD3	1.88	0.55
1:D:486:PHE:O	1:D:490:VAL:HG23	2.06	0.55
1:D:8:PHE:CD1	1:D:71:PRO:HG2	2.42	0.55
1:E:294:GLU:HA	1:E:322:MET:HE1	1.88	0.55
1:F:400:GLN:O	1:F:404:ILE:HG13	2.06	0.55
1:A:8:PHE:CZ	1:A:110:VAL:HG11	2.40	0.55
1:A:117:PHE:N	1:A:117:PHE:HD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:O	1:A:35:LEU:HG	2.06	0.55
1:B:257:ILE:HB	1:B:528:ASN:ND2	2.21	0.55
1:D:247:LEU:HD21	1:D:538:THR:O	2.05	0.55
1:E:269:HIS:HB3	1:E:271:THR:CG2	2.36	0.55
1:F:495:LEU:HD22	1:F:521:LEU:CD2	2.37	0.55
1:A:98:ILE:HD11	1:A:113:TRP:NE1	2.22	0.55
1:A:274:VAL:CG1	1:C:292:MET:HG3	2.37	0.55
1:C:74:ILE:HD12	1:C:86:ALA:HB2	1.89	0.55
1:F:16:THR:O	1:F:45:ARG:HB3	2.05	0.55
1:A:179:ILE:HG12	1:A:180:GLY:N	2.22	0.55
1:A:35:LEU:HD12	1:A:64:LEU:CD1	2.37	0.55
1:B:323:LEU:HD13	1:B:357:LEU:HD21	1.88	0.55
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.72	0.55
1:E:59:LEU:CD2	1:E:84:ILE:HB	2.36	0.55
1:A:257:ILE:HA	1:A:260:THR:CG2	2.37	0.55
1:A:407:PHE:CE2	1:A:427:ILE:HD11	2.41	0.55
1:D:313:ASN:HD21	1:D:342:VAL:HG21	1.71	0.55
1:E:78:ILE:O	1:E:81:ALA:HB3	2.06	0.55
1:A:121:VAL:CG1	1:A:166:LEU:HD23	2.36	0.55
1:A:337:ILE:CD1	1:A:337:ILE:N	2.70	0.55
1:E:164:ASP:OD2	1:E:197:SER:HB2	2.07	0.55
1:C:302:LEU:N	1:C:302:LEU:CD1	2.69	0.55
1:D:299:VAL:HG13	1:D:300:ASN:N	2.22	0.55
1:E:266:LEU:HD11	1:E:291:ILE:CG1	2.36	0.55
1:E:310:LEU:HD23	1:E:337:ILE:HD13	1.89	0.55
1:F:96:MET:HE3	1:F:101:ILE:HG12	1.89	0.55
1:C:191:LEU:HB3	1:C:431:TYR:CD2	2.42	0.54
1:E:116:GLY:C	1:E:117:PHE:CD2	2.80	0.54
1:F:257:ILE:HD11	1:F:533:TRP:CH2	2.40	0.54
1:F:55:ILE:HG12	1:F:80:VAL:HG13	1.88	0.54
1:B:88:GLY:HA3	1:B:110:VAL:HG12	1.89	0.54
1:D:77:ARG:CG	1:D:77:ARG:NH1	2.63	0.54
1:A:328:ARG:HH11	1:A:328:ARG:HG3	1.72	0.54
1:A:62:LYS:HB2	1:A:72:LEU:HD23	1.89	0.54
1:B:183:HIS:C	1:B:187:ILE:HD12	2.27	0.54
1:B:97:PRO:O	1:B:101:ILE:HG13	2.08	0.54
1:C:394:SER:OG	1:C:395:ASN:N	2.40	0.54
1:A:484:ASN:HD22	1:A:487:HIS:H	1.56	0.54
1:B:10:TYR:HE1	1:B:175:ARG:HG3	1.73	0.54
1:D:11:SER:HB2	1:D:226:ARG:HH12	1.71	0.54
1:E:135:ILE:HG13	1:E:176:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:GLU:HA	1:E:322:MET:CE	2.37	0.54
1:B:10:TYR:O	1:B:11:SER:C	2.46	0.54
1:E:186:ASN:HD22	1:E:187:ILE:N	2.05	0.54
1:B:187:ILE:HG12	1:B:206:ILE:HD13	1.89	0.54
1:B:28:TYR:OH	1:B:64:LEU:HD23	2.08	0.54
1:B:78:ILE:CG2	1:B:96:MET:HE1	2.24	0.54
1:E:424:ASP:HB3	1:E:446:PRO:HG2	1.89	0.54
1:C:437:THR:C	1:C:439:GLY:N	2.60	0.54
1:E:314:THR:OG1	1:E:354:ASN:OD1	2.24	0.54
1:C:296:GLN:HG3	1:C:322:MET:HB2	1.90	0.54
1:F:189:ARG:O	1:F:193:GLN:HG2	2.08	0.54
1:F:282:VAL:HG21	1:F:467:SER:HB3	1.90	0.54
1:A:378:GLU:OE2	1:A:408:LYS:HE2	2.08	0.54
1:B:210:SER:O	1:B:214:ALA:HB3	2.07	0.54
1:C:296:GLN:O	1:C:299:VAL:HG12	2.07	0.54
1:C:58:ALA:HB1	1:C:84:ILE:HD13	1.90	0.54
1:E:449:ALA:O	1:E:537:LEU:HD12	2.08	0.54
1:E:78:ILE:O	1:E:82:MET:HG3	2.08	0.54
1:D:318:ALA:HB1	1:D:322:MET:HG2	1.88	0.53
1:F:43:GLN:HA	1:F:73:ILE:O	2.07	0.53
1:C:235:LYS:HE2	1:C:237:VAL:O	2.08	0.53
1:C:55:ILE:HG23	1:C:84:ILE:CG2	2.38	0.53
1:D:424:ASP:HB3	1:D:446:PRO:HG2	1.88	0.53
1:E:362:GLN:HE21	1:E:362:GLN:HA	1.72	0.53
1:F:299:VAL:HG21	1:F:326:ALA:CA	2.38	0.53
1:B:187:ILE:HG23	1:B:206:ILE:CD1	2.38	0.53
1:B:294:GLU:OE1	1:B:318:ALA:HB2	2.09	0.53
1:B:342:VAL:HG23	1:B:343:GLY:H	1.73	0.53
1:D:197:SER:O	1:D:442:VAL:HG23	2.08	0.53
1:F:125:SER:C	1:F:127:MET:N	2.61	0.53
1:F:358:LEU:HD23	1:F:363:PHE:CE1	2.44	0.53
1:F:358:LEU:HD23	1:F:363:PHE:HE1	1.71	0.53
1:A:422:ILE:HD12	1:A:490:VAL:HG22	1.90	0.53
1:B:433:LEU:O	1:B:434:SER:CB	2.56	0.53
1:D:74:ILE:HD13	1:D:80:VAL:HG12	1.90	0.53
1:E:163:LEU:HD22	1:E:201:ARG:HD3	1.89	0.53
1:E:224:ILE:O	1:E:228:LEU:HD13	2.09	0.53
1:E:323:LEU:HD13	1:E:357:LEU:HD11	1.89	0.53
1:E:295:ILE:CG2	1:E:298:GLU:HB2	2.39	0.53
1:E:427:ILE:O	1:E:427:ILE:HG22	2.09	0.53
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ILE:HD13	1:F:225:LEU:HD22	1.89	0.53
1:F:324:LYS:HB2	1:F:360:PHE:CE1	2.43	0.53
1:B:109:MET:HG2	1:B:110:VAL:N	2.24	0.53
1:F:337:ILE:CG2	1:F:363:PHE:HD2	2.22	0.53
1:A:299:VAL:HG21	1:A:326:ALA:CB	2.39	0.53
1:A:55:ILE:HG23	1:A:84:ILE:CG2	2.39	0.53
1:C:482:GLU:H	1:C:482:GLU:CD	2.12	0.53
1:D:260:THR:HA	1:D:478:GLY:HA3	1.91	0.53
1:A:110:VAL:HA	1:A:133:ASP:OD2	2.08	0.53
1:A:98:ILE:N	1:A:99:PRO:HD2	2.23	0.53
1:E:232:THR:HG22	1:E:431:TYR:O	2.09	0.53
1:F:209:VAL:HB	2:F:541:3NM:O5	2.09	0.53
1:B:119:GLU:CD	1:B:119:GLU:H	2.12	0.53
1:C:437:THR:O	1:C:438:ASN:C	2.47	0.53
1:D:121:VAL:HG13	1:D:166:LEU:HD23	1.90	0.53
1:D:437:THR:C	1:D:439:GLY:N	2.61	0.53
1:D:78:ILE:HD11	1:D:104:LEU:HD12	1.91	0.53
1:F:144:LEU:H	1:F:144:LEU:HD12	1.73	0.53
1:D:257:ILE:HD11	1:D:533:TRP:HH2	1.73	0.52
1:E:8:PHE:CE2	1:E:110:VAL:CG1	2.91	0.52
1:E:394:SER:OG	1:E:395:ASN:N	2.42	0.52
1:B:533:TRP:C	1:B:535:PRO:HD2	2.29	0.52
1:F:20:MET:HE3	1:F:214:ALA:HB2	1.91	0.52
1:F:472:ILE:HG23	1:F:489:VAL:HG22	1.91	0.52
1:A:333:VAL:HG12	1:A:333:VAL:O	2.10	0.52
1:B:27:LEU:O	1:B:31:VAL:HG23	2.10	0.52
1:B:437:THR:O	1:B:438:ASN:C	2.46	0.52
1:B:46:GLU:OE2	1:B:46:GLU:HA	2.08	0.52
1:A:91:VAL:HG11	1:A:101:ILE:CD1	2.38	0.52
1:B:16:THR:HG23	1:B:27:LEU:HD11	1.91	0.52
1:B:283:THR:HB	1:B:290:PRO:HG3	1.90	0.52
1:C:123:GLU:O	1:C:127:MET:HG3	2.09	0.52
1:D:115:VAL:HG13	1:D:120:GLU:CB	2.39	0.52
1:F:176:THR:O	1:F:204:ASP:HB2	2.09	0.52
1:F:433:LEU:O	1:F:434:SER:OG	2.21	0.52
1:F:42:VAL:HG12	1:F:72:LEU:CD1	2.39	0.52
1:A:121:VAL:HG13	1:A:166:LEU:HD23	1.92	0.52
1:C:141:PHE:HB3	1:C:142:PRO:CD	2.40	0.52
1:A:442:VAL:O	1:A:445:ILE:HG12	2.10	0.52
1:C:104:LEU:O	1:C:105:VAL:HG13	2.10	0.52
1:C:260:THR:HA	1:C:478:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:ASP:O	1:F:445:ILE:HB	2.09	0.52
1:B:427:ILE:HG22	1:B:427:ILE:O	2.09	0.52
1:E:144:LEU:HD12	1:E:144:LEU:H	1.74	0.52
1:F:495:LEU:HD22	1:F:521:LEU:HD23	1.91	0.52
1:A:10:TYR:O	1:A:11:SER:C	2.48	0.52
1:C:220:LYS:O	1:C:224:ILE:HG13	2.10	0.52
1:E:115:VAL:HG13	1:E:120:GLU:HB2	1.92	0.52
1:E:256:ILE:HG22	1:E:475:MET:CE	2.40	0.52
1:D:21:ILE:HD11	1:D:27:LEU:HD13	1.92	0.52
1:F:119:GLU:O	1:F:123:GLU:HG3	2.09	0.52
1:B:138:GLY:HA3	1:B:154:MET:CE	2.39	0.52
1:C:112:GLY:HA3	1:C:134:TYR:CZ	2.45	0.52
1:C:419:PHE:CE1	1:C:451:GLU:HB2	2.45	0.52
1:F:80:VAL:O	1:F:84:ILE:HG12	2.10	0.52
1:A:272:ASN:N	1:A:272:ASN:HD22	2.07	0.51
1:B:367:LYS:HZ3	1:B:466:CYS:HA	1.75	0.51
1:F:78:ILE:HD12	1:F:96:MET:HE1	1.91	0.51
1:A:221:SER:HA	1:A:224:ILE:HD12	1.92	0.51
1:B:272:ASN:ND2	1:B:315:GLY:O	2.44	0.51
1:C:44:ILE:HD11	1:C:61:ILE:HG21	1.92	0.51
1:E:437:THR:C	1:E:439:GLY:N	2.63	0.51
1:F:44:ILE:HD11	1:F:72:LEU:HD21	1.93	0.51
1:B:35:LEU:HD12	1:B:64:LEU:CD1	2.41	0.51
1:C:17:ASP:HB3	1:C:20:MET:HE1	1.91	0.51
1:E:527:GLU:HG3	1:E:527:GLU:O	2.10	0.51
1:F:77:ARG:HE	1:F:80:VAL:HG23	1.75	0.51
1:F:98:ILE:N	1:F:99:PRO:HD2	2.26	0.51
1:A:192:TYR:HA	1:A:431:TYR:HB3	1.93	0.51
1:A:257:ILE:HD11	1:A:533:TRP:HH2	1.75	0.51
1:B:139:THR:HG23	2:B:541:3NM:O1	2.11	0.51
1:D:55:ILE:HG23	1:D:84:ILE:CG2	2.39	0.51
1:D:8:PHE:CE2	1:D:110:VAL:HB	2.45	0.51
1:D:98:ILE:HD11	1:D:113:TRP:NE1	2.25	0.51
1:F:139:THR:HG23	2:F:541:3NM:O1	2.11	0.51
1:F:209:VAL:O	1:F:213:ILE:HB	2.10	0.51
1:A:319:PRO:O	1:A:322:MET:HB3	2.10	0.51
1:A:484:ASN:HD21	1:A:486:PHE:HB3	1.75	0.51
1:A:347:THR:HG21	1:C:298:GLU:CG	2.41	0.51
1:C:517:LEU:O	1:C:517:LEU:HD23	2.11	0.51
1:E:323:LEU:CD1	1:E:357:LEU:HD11	2.40	0.51
1:A:268:GLN:CD	1:A:302:LEU:HD23	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ARG:HG3	1:D:193:GLN:HE21	1.76	0.51
1:E:165:ALA:HA	1:E:168:ARG:NH2	2.24	0.51
1:A:123:GLU:O	1:A:127:MET:HG3	2.10	0.51
1:A:451:GLU:HG2	1:A:452:ALA:N	2.25	0.51
1:B:32:GLU:HA	1:B:64:LEU:HD11	1.92	0.51
1:D:78:ILE:HG21	1:D:96:MET:HE2	1.92	0.51
1:A:41:LEU:HD11	1:A:73:ILE:HD11	1.93	0.51
1:B:339:PHE:HE1	1:B:357:LEU:HD23	1.76	0.51
1:C:286:LEU:HD21	1:C:521:LEU:HD22	1.93	0.51
1:E:18:SER:O	1:E:21:ILE:HG13	2.10	0.51
1:F:182:LEU:HB3	1:F:187:ILE:HG13	1.92	0.51
1:A:43:GLN:HA	1:A:73:ILE:O	2.11	0.51
1:A:268:GLN:HG2	1:A:310:LEU:CD1	2.41	0.51
1:B:16:THR:HG22	1:B:17:ASP:N	2.26	0.51
1:B:534:ALA:N	1:B:535:PRO:CD	2.74	0.51
1:D:399:ILE:CD1	1:D:421:PHE:CE2	2.94	0.51
1:D:484:ASN:HD21	1:D:486:PHE:HB3	1.76	0.51
1:F:282:VAL:HG21	1:F:467:SER:CB	2.41	0.51
1:C:533:TRP:HB3	1:C:535:PRO:HD2	1.92	0.50
1:E:295:ILE:HG22	1:E:298:GLU:H	1.75	0.50
1:F:305:ILE:HG23	1:F:306:PRO:HD2	1.92	0.50
1:F:268:GLN:HB3	1:F:310:LEU:CD1	2.37	0.50
1:F:419:PHE:HB3	1:F:421:PHE:CE2	2.47	0.50
1:B:272:ASN:N	1:B:272:ASN:ND2	2.60	0.50
1:C:275:HIS:N	1:C:275:HIS:CD2	2.78	0.50
1:D:151:LYS:O	1:D:152:ALA:CB	2.59	0.50
1:D:272:ASN:O	1:D:276:GLN:HB2	2.11	0.50
1:D:476:ILE:HD11	1:D:489:VAL:HG22	1.94	0.50
1:B:184:PRO:HD3	1:B:211:ASP:OD1	2.11	0.50
1:D:328:ARG:CG	1:D:328:ARG:HH11	2.25	0.50
1:A:280:ALA:HB2	1:A:292:MET:HE2	1.93	0.50
1:C:125:SER:HB2	1:C:169:ASN:HD22	1.74	0.50
1:F:406:ALA:HB1	1:F:411:THR:O	2.11	0.50
1:F:475:MET:HE1	1:F:495:LEU:HD12	1.93	0.50
1:A:299:VAL:CG2	1:A:326:ALA:HA	2.34	0.50
1:C:124:LEU:HD23	1:C:124:LEU:C	2.31	0.50
1:C:316:SER:O	1:C:317:VAL:HB	2.11	0.50
1:C:41:LEU:HD21	1:C:73:ILE:HD11	1.93	0.50
1:B:495:LEU:O	1:B:495:LEU:HD23	2.11	0.50
1:D:10:TYR:O	1:D:11:SER:C	2.50	0.50
1:D:257:ILE:HG12	1:D:475:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ILE:HD13	1:D:525:THR:HG22	1.94	0.50
1:E:179:ILE:HG13	1:E:207:CYS:SG	2.51	0.50
1:E:78:ILE:HG21	1:E:96:MET:CE	2.42	0.50
1:A:101:ILE:O	1:A:105:VAL:HG22	2.12	0.50
1:A:209:VAL:HG12	1:A:210:SER:N	2.26	0.50
1:D:533:TRP:O	1:D:535:PRO:HD2	2.12	0.50
1:A:187:ILE:HG23	1:A:206:ILE:HD11	1.94	0.50
1:A:298:GLU:HG3	1:B:347:THR:HG21	1.94	0.50
1:B:365:CYS:HA	1:B:412:VAL:O	2.12	0.50
1:C:125:SER:C	1:C:127:MET:H	2.16	0.50
1:D:430:LYS:CD	1:D:437:THR:HG21	2.41	0.50
1:B:75:ASN:O	1:B:77:ARG:N	2.38	0.49
1:C:276:GLN:HG3	1:C:292:MET:CE	2.42	0.49
1:C:73:ILE:HA	1:C:88:GLY:O	2.12	0.49
1:F:241:LEU:O	1:F:428:GLU:HA	2.12	0.49
1:C:188:GLU:HG3	1:C:228:LEU:HG	1.94	0.49
1:A:509:GLY:HA2	1:C:522:TYR:HD2	1.75	0.49
1:D:35:LEU:HD12	1:D:64:LEU:HD13	1.93	0.49
1:E:299:VAL:CG1	1:E:300:ASN:N	2.75	0.49
1:F:482:GLU:H	1:F:482:GLU:CD	2.16	0.49
1:B:424:ASP:HB3	1:B:446:PRO:HG2	1.94	0.49
1:B:209:VAL:HG21	2:B:541:3NM:H6A	1.94	0.49
1:D:283:THR:HG22	1:D:288:SER:HB2	1.92	0.49
1:D:192:TYR:CE2	1:D:410:LYS:HG3	2.47	0.49
1:E:192:TYR:HA	1:E:431:TYR:HB3	1.94	0.49
1:F:228:LEU:N	1:F:228:LEU:CD1	2.75	0.49
1:A:437:THR:O	1:A:439:GLY:N	2.45	0.49
1:B:265:PRO:HB3	1:B:307:HIS:O	2.12	0.49
1:C:275:HIS:HD2	1:C:275:HIS:H	1.58	0.49
1:D:19:GLY:O	1:D:20:MET:HB2	2.12	0.49
1:D:247:LEU:HD22	1:D:537:LEU:HG	1.95	0.49
1:A:417:GLY:O	1:A:497:LYS:NZ	2.45	0.49
1:A:51:THR:HB	1:E:95:ASP:HA	1.94	0.49
1:B:267:VAL:CG1	1:B:269:HIS:CE1	2.96	0.49
1:C:144:LEU:N	1:C:144:LEU:HD12	2.09	0.49
1:D:347:THR:HG21	1:E:298:GLU:HG2	1.94	0.49
1:B:495:LEU:HD22	1:B:521:LEU:CD2	2.38	0.49
1:C:76:ASP:HA	1:C:91:VAL:HG12	1.95	0.49
1:F:171:ALA:HA	1:F:173:TRP:CZ3	2.48	0.49
1:C:208:VAL:HG11	1:C:225:LEU:HD13	1.93	0.49
1:D:480:PRO:O	1:D:482:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLY:O	1:B:39:VAL:HG23	2.12	0.49
1:C:78:ILE:O	1:C:81:ALA:HB3	2.13	0.49
1:D:341:PRO:O	1:D:342:VAL:C	2.51	0.49
1:F:182:LEU:HD12	1:F:190:VAL:HG21	1.94	0.49
1:A:419:PHE:CE1	1:A:451:GLU:HB2	2.48	0.49
1:C:345:SER:HA	1:C:351:LEU:HD13	1.94	0.49
1:D:124:LEU:HD23	1:D:124:LEU:C	2.33	0.49
1:A:274:VAL:HG11	1:C:292:MET:HG3	1.95	0.48
1:A:78:ILE:HD11	1:A:104:LEU:HD12	1.95	0.48
1:B:111:ILE:HG23	1:B:132:VAL:HA	1.94	0.48
1:B:275:HIS:N	1:B:275:HIS:HD2	2.11	0.48
1:B:61:ILE:HG22	1:B:72:LEU:HD22	1.95	0.48
1:C:472:ILE:HD13	1:C:489:VAL:HG13	1.95	0.48
1:E:362:GLN:NE2	1:E:362:GLN:HA	2.28	0.48
1:F:125:SER:O	1:F:127:MET:N	2.46	0.48
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.27	0.48
1:C:109:MET:HG2	1:C:110:VAL:N	2.27	0.48
1:C:424:ASP:HB2	1:C:486:PHE:CD1	2.48	0.48
1:C:64:LEU:O	1:C:64:LEU:HD22	2.11	0.48
1:E:73:ILE:N	1:E:73:ILE:HD12	2.27	0.48
1:A:187:ILE:HG23	1:A:206:ILE:CD1	2.43	0.48
1:A:484:ASN:ND2	1:A:487:HIS:H	2.12	0.48
1:C:226:ARG:HD3	1:C:226:ARG:HA	1.63	0.48
1:D:430:LYS:HD2	1:D:437:THR:HG21	1.94	0.48
1:E:160:ILE:HD13	1:E:195:VAL:O	2.12	0.48
1:A:527:GLU:O	1:A:529:THR:N	2.46	0.48
1:A:92:GLY:HA3	4:A:543:POP:O4	2.13	0.48
1:D:8:PHE:HD1	1:D:71:PRO:HG2	1.77	0.48
1:F:411:THR:HA	1:F:426:THR:HG22	1.94	0.48
1:C:276:GLN:HG3	1:C:292:MET:HE3	1.96	0.48
1:D:110:VAL:HG23	1:D:133:ASP:HB2	1.94	0.48
1:F:512:SER:HA	1:F:515:VAL:HG12	1.95	0.48
1:A:65:CYS:O	1:A:68:HIS:N	2.47	0.48
1:A:97:PRO:O	1:A:101:ILE:HG13	2.14	0.48
1:D:215:SER:C	1:D:217:ASP:H	2.16	0.48
1:F:403:LYS:HE2	1:F:447:CYS:HB2	1.96	0.48
1:B:84:ILE:HD11	1:B:86:ALA:HB2	1.95	0.48
1:B:88:GLY:HA3	1:B:110:VAL:HG13	1.95	0.48
1:D:256:ILE:HG22	1:D:475:MET:HE1	1.95	0.48
1:D:313:ASN:C	1:D:313:ASN:ND2	2.66	0.48
1:E:265:PRO:O	1:E:288:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:MET:O	1:E:495:LEU:C	2.52	0.48
1:F:466:CYS:O	1:F:466:CYS:SG	2.72	0.48
1:A:135:ILE:O	1:A:135:ILE:HG13	2.13	0.48
1:A:476:ILE:HD11	1:A:489:VAL:CG2	2.43	0.48
1:B:187:ILE:HG23	1:B:206:ILE:HD11	1.95	0.48
1:D:278:PHE:CE1	1:D:518:ILE:HD11	2.49	0.48
1:F:280:ALA:O	1:F:284:LEU:HD22	2.14	0.48
1:F:41:LEU:HD12	1:F:71:PRO:HD2	1.96	0.48
1:E:192:TYR:CE1	1:E:410:LYS:HB3	2.49	0.48
1:E:479:GLN:HA	1:E:480:PRO:HD3	1.59	0.48
1:E:78:ILE:HD13	1:E:96:MET:CE	2.39	0.48
1:E:522:TYR:O	1:E:526:ARG:HD3	2.14	0.48
1:E:58:ALA:CB	1:E:84:ILE:HD13	2.40	0.48
1:A:422:ILE:CD1	1:A:493:VAL:HG21	2.44	0.47
1:B:89:ILE:HD11	1:B:101:ILE:HG21	1.94	0.47
1:B:98:ILE:HD12	1:B:111:ILE:HD13	1.95	0.47
1:C:197:SER:O	1:C:442:VAL:HG23	2.14	0.47
1:D:275:HIS:CD2	1:D:275:HIS:N	2.80	0.47
1:D:340:ASP:HA	1:D:341:PRO:HD3	1.67	0.47
1:E:484:ASN:ND2	1:E:487:HIS:H	2.11	0.47
1:F:299:VAL:HG21	1:F:326:ALA:CB	2.45	0.47
1:F:335:ARG:NH1	1:F:336:PRO:HD3	2.30	0.47
1:F:517:LEU:HD23	1:F:517:LEU:C	2.34	0.47
1:F:524:LEU:HA	1:F:524:LEU:HD12	1.65	0.47
1:B:224:ILE:O	1:B:228:LEU:HD13	2.13	0.47
1:C:272:ASN:ND2	1:C:272:ASN:N	2.62	0.47
1:C:41:LEU:HD21	1:C:73:ILE:CD1	2.44	0.47
1:D:370:SER:O	1:D:374:LEU:HB2	2.14	0.47
1:D:467:SER:HB2	1:D:496:TYR:HE1	1.79	0.47
1:A:116:GLY:C	1:A:117:PHE:HD2	2.16	0.47
1:A:357:LEU:O	1:A:360:PHE:HB2	2.14	0.47
1:C:472:ILE:O	1:C:476:ILE:HG13	2.14	0.47
1:C:256:ILE:HD13	1:C:488:ALA:HA	1.97	0.47
1:D:253:ILE:O	1:D:257:ILE:HG13	2.13	0.47
1:E:8:PHE:HE1	1:E:71:PRO:HB3	1.80	0.47
1:C:135:ILE:CG1	1:C:176:THR:HG22	2.44	0.47
1:D:295:ILE:HG22	1:D:298:GLU:H	1.80	0.47
1:C:322:MET:HE3	1:C:326:ALA:HB2	1.96	0.47
1:E:191:LEU:HD12	1:E:191:LEU:HA	1.69	0.47
1:E:79:ASP:OD1	1:E:80:VAL:HG23	2.15	0.47
1:B:77:ARG:NH1	1:F:77:ARG:CZ	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ARG:O	1:C:193:GLN:HG2	2.14	0.47
1:C:313:ASN:O	1:C:314:THR:C	2.53	0.47
1:C:3:PHE:CE2	1:C:71:PRO:HA	2.50	0.47
1:E:166:LEU:CD2	1:E:171:ALA:HB3	2.44	0.47
1:E:442:VAL:O	1:E:445:ILE:HG12	2.14	0.47
1:F:179:ILE:HG12	1:F:180:GLY:N	2.29	0.47
1:F:265:PRO:O	1:F:288:SER:HB3	2.14	0.47
1:B:78:ILE:HG12	1:B:79:ASP:N	2.29	0.47
1:D:112:GLY:HA3	1:D:134:TYR:CE2	2.49	0.47
1:D:91:VAL:HG11	1:D:101:ILE:CD1	2.44	0.47
1:F:247:LEU:HD22	1:F:537:LEU:HG	1.97	0.47
1:F:75:ASN:O	1:F:77:ARG:N	2.39	0.47
1:A:308:ALA:O	1:A:335:ARG:HD3	2.15	0.47
1:B:519:ASP:O	1:B:522:TYR:HB3	2.15	0.47
1:D:344:TYR:C	1:D:346:ALA:H	2.18	0.47
1:E:168:ARG:CZ	1:E:168:ARG:HB3	2.44	0.47
1:E:299:VAL:HG13	1:E:300:ASN:N	2.28	0.47
1:A:116:GLY:C	1:A:117:PHE:CD2	2.89	0.47
1:A:308:ALA:O	1:A:335:ARG:NH1	2.41	0.47
1:A:271:THR:HA	1:A:313:ASN:HB3	1.96	0.47
1:B:370:SER:O	1:B:374:LEU:HB2	2.14	0.47
1:D:34:GLY:O	1:D:39:VAL:HG23	2.15	0.47
1:D:324:LYS:HB2	1:D:360:PHE:CE1	2.50	0.47
1:F:283:THR:HG23	1:F:288:SER:HB2	1.97	0.47
1:F:324:LYS:HA	1:F:360:PHE:CD1	2.50	0.47
1:D:484:ASN:ND2	1:D:487:HIS:H	2.11	0.47
1:E:328:ARG:HG3	1:E:328:ARG:HH11	1.75	0.47
1:F:74:ILE:HD12	1:F:86:ALA:HB2	1.97	0.47
1:A:187:ILE:HD13	1:A:225:LEU:HD22	1.96	0.47
1:A:422:ILE:HD13	1:A:493:VAL:HG21	1.96	0.47
1:C:275:HIS:HB3	1:C:466:CYS:SG	2.55	0.47
1:D:299:VAL:CG1	1:D:300:ASN:N	2.78	0.47
1:F:187:ILE:HG12	1:F:206:ILE:CD1	2.45	0.47
1:F:191:LEU:HD22	1:F:206:ILE:HD11	1.96	0.47
1:F:78:ILE:HB	1:F:89:ILE:HD12	1.96	0.47
1:A:35:LEU:CD2	1:A:70:VAL:HG11	2.39	0.46
1:E:19:GLY:O	1:E:20:MET:CB	2.63	0.46
1:F:239:ILE:HG22	1:F:240:GLY:N	2.31	0.46
1:F:472:ILE:O	1:F:476:ILE:HG13	2.15	0.46
1:A:4:SER:N	1:A:7:GLN:OE1	2.47	0.46
1:C:206:ILE:HB	1:C:229:ILE:HD11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ARG:HB3	1:E:336:PRO:CD	2.45	0.46
1:F:102:ARG:NH1	1:F:109:MET:O	2.38	0.46
1:A:316:SER:C	1:A:317:VAL:HG23	2.36	0.46
1:A:96:MET:HE3	1:A:101:ILE:HG12	1.96	0.46
1:B:79:ASP:OD1	1:B:80:VAL:HG23	2.14	0.46
1:E:20:MET:HE2	1:E:213:ILE:HG21	1.97	0.46
1:E:260:THR:HA	1:E:478:GLY:HA3	1.97	0.46
1:F:193:GLN:NE2	1:F:362:GLN:NE2	2.63	0.46
1:A:159:ALA:O	1:A:162:VAL:HB	2.16	0.46
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.66	0.46
1:A:433:LEU:CD1	1:A:433:LEU:N	2.78	0.46
2:A:541:3NM:N	3:A:542:IFP:C7A	2.79	0.46
1:B:191:LEU:HA	1:B:191:LEU:HD12	1.68	0.46
1:E:399:ILE:HD11	1:E:421:PHE:CE2	2.50	0.46
1:E:41:LEU:HD11	1:E:73:ILE:CD1	2.42	0.46
1:F:338:VAL:HG22	1:F:365:CYS:HB3	1.97	0.46
1:F:406:ALA:HB2	1:F:413:ALA:HB3	1.98	0.46
1:A:534:ALA:H	1:A:535:PRO:CD	2.27	0.46
1:C:302:LEU:HD13	1:C:302:LEU:H	1.80	0.46
1:C:479:GLN:HA	1:C:480:PRO:HD3	1.66	0.46
1:D:416:THR:HG22	1:D:420:ASP:OD1	2.16	0.46
1:E:10:TYR:O	1:E:205:GLY:HA3	2.15	0.46
1:A:8:PHE:CD1	1:A:71:PRO:HG2	2.50	0.46
1:C:339:PHE:HE2	1:C:341:PRO:HG3	1.78	0.46
1:D:283:THR:CG2	1:D:288:SER:HB2	2.46	0.46
1:E:8:PHE:CZ	1:E:110:VAL:HG11	2.50	0.46
1:E:28:TYR:CE1	1:E:64:LEU:HG	2.51	0.46
1:A:298:GLU:HG2	1:A:302:LEU:HD13	1.98	0.46
1:B:240:GLY:C	1:B:241:LEU:HG	2.35	0.46
1:B:422:ILE:CG2	1:B:486:PHE:HE1	2.28	0.46
1:C:129:PRO:HG3	1:C:173:TRP:CD2	2.50	0.46
1:E:312:LEU:HA	1:E:312:LEU:HD13	1.62	0.46
1:E:73:ILE:HG22	1:E:74:ILE:N	2.31	0.46
1:A:142:PRO:HA	1:A:153:PRO:HG3	1.98	0.46
1:A:268:GLN:OE1	1:A:302:LEU:HD23	2.16	0.46
1:B:427:ILE:O	1:B:429:GLY:N	2.49	0.46
1:C:264:ARG:N	1:C:265:PRO:CD	2.78	0.46
1:E:296:GLN:HG2	1:E:322:MET:HB2	1.96	0.46
1:F:8:PHE:CD1	1:F:71:PRO:HG2	2.51	0.46
1:A:394:SER:OG	1:A:395:ASN:N	2.49	0.46
1:A:407:PHE:CD1	1:A:442:VAL:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:VAL:O	1:B:213:ILE:HG12	2.16	0.46
1:A:298:GLU:OE1	1:B:350:ARG:HD2	2.16	0.46
1:D:299:VAL:HG21	1:D:326:ALA:CA	2.29	0.46
1:E:125:SER:O	1:E:127:MET:N	2.49	0.46
1:E:66:HIS:HE1	1:E:87:ASP:OD1	1.99	0.46
1:F:437:THR:C	1:F:439:GLY:N	2.65	0.46
1:A:115:VAL:HA	1:A:120:GLU:OE1	2.16	0.46
1:A:192:TYR:HD2	1:A:192:TYR:O	1.99	0.46
1:C:65:CYS:HB3	1:C:70:VAL:O	2.16	0.46
1:D:278:PHE:HE1	1:D:518:ILE:HD11	1.80	0.46
1:D:78:ILE:HG13	1:D:79:ASP:N	2.24	0.46
1:A:77:ARG:HH12	1:E:77:ARG:CG	2.29	0.46
1:B:422:ILE:N	1:B:422:ILE:HD12	2.31	0.45
1:B:484:ASN:HD21	1:B:486:PHE:HB3	1.81	0.45
1:C:183:HIS:C	1:C:187:ILE:HD12	2.36	0.45
1:C:298:GLU:HG2	1:C:302:LEU:CD1	2.44	0.45
1:C:322:MET:HG3	1:C:323:LEU:N	2.28	0.45
1:A:509:GLY:CA	1:C:522:TYR:HD2	2.29	0.45
1:D:89:ILE:HD12	1:D:91:VAL:HG13	1.98	0.45
1:A:280:ALA:O	1:A:284:LEU:HD22	2.16	0.45
1:D:115:VAL:HG13	1:D:120:GLU:HB3	1.98	0.45
1:E:86:ALA:O	1:E:109:MET:CE	2.64	0.45
1:E:98:ILE:N	1:E:99:PRO:CD	2.78	0.45
1:F:450:VAL:HG21	1:F:494:MET:HG2	1.96	0.45
1:A:55:ILE:HG23	1:A:84:ILE:HG21	1.99	0.45
1:C:119:GLU:O	1:C:122:ASP:HB2	2.16	0.45
1:D:298:GLU:CG	1:F:347:THR:HG21	2.43	0.45
1:E:30:GLN:OE1	1:E:30:GLN:HA	2.15	0.45
1:F:373:ILE:HG13	1:F:415:CYS:CB	2.45	0.45
1:A:113:TRP:HB3	1:A:135:ILE:HG22	1.98	0.45
1:B:59:LEU:O	1:B:60:GLN:C	2.53	0.45
1:B:70:VAL:HG23	1:B:71:PRO:HD2	1.98	0.45
1:E:88:GLY:HA3	1:E:110:VAL:HG13	1.98	0.45
1:E:8:PHE:CD1	1:E:71:PRO:HG2	2.52	0.45
1:F:329:ALA:O	1:F:333:VAL:HG23	2.16	0.45
1:F:529:THR:O	1:F:532:THR:HG23	2.17	0.45
1:A:495:LEU:HD22	1:A:521:LEU:HD23	1.98	0.45
1:B:118:PRO:HA	1:B:121:VAL:HG23	1.99	0.45
1:D:136:GLY:HA2	1:D:177:VAL:HG23	1.99	0.45
1:D:369:ASN:O	1:D:370:SER:C	2.54	0.45
1:F:226:ARG:HA	1:F:226:ARG:HD3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:CG	1:C:328:ARG:NH1	2.73	0.45
1:D:192:TYR:HD2	1:D:192:TYR:O	2.00	0.45
1:D:276:GLN:CG	1:D:292:MET:HE2	2.38	0.45
1:D:399:ILE:CD1	1:D:421:PHE:CD2	3.00	0.45
1:E:186:ASN:C	1:E:186:ASN:ND2	2.62	0.45
1:F:109:MET:CG	1:F:110:VAL:N	2.79	0.45
1:F:224:ILE:O	1:F:228:LEU:HD13	2.17	0.45
1:A:212:ILE:O	1:A:215:SER:HB3	2.17	0.45
1:A:328:ARG:NH1	1:A:328:ARG:CG	2.74	0.45
1:B:339:PHE:CD2	1:B:341:PRO:HG3	2.52	0.45
1:B:427:ILE:C	1:B:429:GLY:H	2.20	0.45
1:D:102:ARG:NH1	1:D:109:MET:O	2.47	0.45
1:D:10:TYR:O	1:D:205:GLY:HA3	2.17	0.45
1:E:182:LEU:HD12	1:E:190:VAL:HG21	1.99	0.45
1:E:437:THR:O	1:E:438:ASN:C	2.54	0.45
1:F:226:ARG:O	1:F:227:GLY:C	2.55	0.45
1:A:189:ARG:NH1	1:A:359:THR:O	2.50	0.45
1:A:4:SER:O	1:A:5:LYS:C	2.55	0.45
1:C:433:LEU:O	1:C:434:SER:CB	2.65	0.45
1:C:530:PRO:HA	1:C:533:TRP:CE2	2.52	0.45
1:D:338:VAL:HG21	1:D:473:ALA:HB2	1.99	0.45
1:D:344:TYR:O	1:D:350:ARG:HB3	2.17	0.45
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.65	0.45
1:E:115:VAL:HG13	1:E:120:GLU:CB	2.45	0.45
1:E:55:ILE:HG23	1:E:84:ILE:HG22	1.99	0.45
1:F:15:VAL:HG22	1:F:43:GLN:HE21	1.81	0.45
1:F:64:LEU:HD22	1:F:64:LEU:O	2.16	0.45
1:A:313:ASN:HD22	1:A:342:VAL:HG21	1.72	0.45
1:B:125:SER:C	1:B:127:MET:N	2.71	0.45
1:B:14:LEU:HD11	1:B:213:ILE:CD1	2.44	0.45
1:C:225:LEU:O	1:C:229:ILE:HG13	2.17	0.45
1:D:179:ILE:HG13	1:D:207:CYS:SG	2.57	0.45
1:D:11:SER:CB	1:D:226:ARG:HH12	2.30	0.45
1:D:274:VAL:HG13	1:E:276:GLN:HG2	1.98	0.45
1:E:166:LEU:HD22	1:E:171:ALA:HB3	1.99	0.45
1:E:484:ASN:HD21	1:E:486:PHE:HB3	1.82	0.45
1:A:416:THR:HG22	1:A:420:ASP:OD1	2.17	0.45
1:B:394:SER:OG	1:B:395:ASN:N	2.48	0.45
1:C:74:ILE:HD11	1:C:84:ILE:HD11	1.99	0.45
1:C:97:PRO:O	1:C:101:ILE:HG13	2.17	0.45
1:E:509:GLY:HA3	1:F:519:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:534:ALA:N	1:E:535:PRO:HD3	2.32	0.45
1:E:8:PHE:HE1	1:E:71:PRO:CB	2.30	0.45
1:B:239:ILE:HG22	1:B:240:GLY:N	2.32	0.44
1:C:169:ASN:O	1:C:170:ASN:C	2.56	0.44
1:F:231:LYS:HG2	1:F:232:THR:H	1.82	0.44
1:A:280:ALA:O	1:A:284:LEU:CD2	2.66	0.44
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.74	0.44
1:C:193:GLN:NE2	1:C:362:GLN:HE21	2.15	0.44
1:C:347:THR:OG1	1:C:350:ARG:HB2	2.18	0.44
1:D:305:ILE:H	1:D:305:ILE:HG13	1.59	0.44
1:E:485:LEU:O	1:E:489:VAL:HG23	2.17	0.44
1:F:357:LEU:HA	1:F:357:LEU:HD13	1.67	0.44
1:A:274:VAL:HG11	1:C:292:MET:CG	2.48	0.44
1:A:295:ILE:N	1:A:295:ILE:HD12	2.32	0.44
1:B:27:LEU:HD23	1:B:57:GLU:OE1	2.16	0.44
1:C:109:MET:CG	1:C:110:VAL:N	2.80	0.44
1:C:355:ASN:O	1:C:359:THR:HG23	2.16	0.44
1:D:121:VAL:CG1	1:D:166:LEU:HD23	2.47	0.44
1:A:183:HIS:HB3	1:A:184:PRO:CD	2.48	0.44
1:A:224:ILE:O	1:A:228:LEU:HD13	2.18	0.44
1:C:237:VAL:HA	1:C:334:LYS:O	2.17	0.44
1:D:512:SER:HA	1:D:515:VAL:CG1	2.40	0.44
1:E:19:GLY:O	1:E:20:MET:HB2	2.17	0.44
1:F:193:GLN:NE2	1:F:362:GLN:HE21	2.16	0.44
1:A:59:LEU:CD2	1:A:84:ILE:HB	2.47	0.44
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.79	0.44
1:C:129:PRO:HG3	1:C:173:TRP:CE3	2.52	0.44
1:C:322:MET:CE	1:C:326:ALA:HB2	2.48	0.44
1:C:80:VAL:O	1:C:83:ALA:HB3	2.18	0.44
1:C:59:LEU:HD21	1:C:84:ILE:HB	1.99	0.44
1:D:224:ILE:O	1:D:228:LEU:HD13	2.18	0.44
1:E:407:PHE:HE2	1:E:427:ILE:CD1	2.30	0.44
1:F:253:ILE:O	1:F:257:ILE:HG13	2.18	0.44
1:A:183:HIS:HB3	1:A:184:PRO:HD2	1.99	0.44
1:A:369:ASN:O	1:A:370:SER:C	2.56	0.44
1:A:468:LEU:O	1:A:468:LEU:HD12	2.18	0.44
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.29	0.44
1:C:427:ILE:C	1:C:429:GLY:H	2.20	0.44
1:E:267:VAL:CG1	1:E:269:HIS:CE1	3.00	0.44
1:E:283:THR:HB	1:E:290:PRO:HG3	1.99	0.44
1:E:468:LEU:HD12	1:E:472:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:PHE:CE2	1:F:467:SER:OG	2.70	0.44
1:B:352:LEU:HD22	1:B:352:LEU:HA	1.54	0.44
1:B:369:ASN:O	1:B:370:SER:C	2.56	0.44
1:C:299:VAL:CG2	1:C:326:ALA:HA	2.34	0.44
1:D:119:GLU:H	1:D:119:GLU:CD	2.21	0.44
1:E:237:VAL:HA	1:E:334:LYS:O	2.18	0.44
1:E:422:ILE:HD12	1:E:490:VAL:HG22	1.99	0.44
1:F:112:GLY:HA3	1:F:134:TYR:CZ	2.52	0.44
1:F:403:LYS:HE2	1:F:447:CYS:CB	2.48	0.44
1:F:523:ARG:O	1:F:527:GLU:HG2	2.18	0.44
1:A:437:THR:C	1:A:439:GLY:N	2.71	0.44
1:C:339:PHE:CD2	1:C:341:PRO:HG3	2.53	0.44
1:E:55:ILE:HG23	1:E:84:ILE:CG2	2.47	0.44
1:A:228:LEU:N	1:A:228:LEU:CD1	2.81	0.44
1:A:256:ILE:HD13	1:A:488:ALA:HA	2.00	0.44
1:B:256:ILE:HD13	1:B:488:ALA:HA	2.00	0.44
1:C:341:PRO:HB3	1:C:354:ASN:OD1	2.17	0.44
1:C:394:SER:HB3	1:C:397:LEU:HB3	1.98	0.44
1:C:534:ALA:N	1:C:535:PRO:CD	2.80	0.44
1:D:5:LYS:HE2	1:D:133:ASP:OD2	2.17	0.44
1:E:187:ILE:HG23	1:E:206:ILE:HD13	2.00	0.44
1:F:182:LEU:CD1	1:F:190:VAL:HG21	2.48	0.44
1:F:437:THR:O	1:F:438:ASN:C	2.56	0.44
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.75	0.43
1:B:93:GLN:OE1	1:B:120:GLU:HG2	2.18	0.43
1:C:495:LEU:HA	1:C:495:LEU:HD23	1.83	0.43
1:C:500:GLY:O	1:C:504:SER:HB3	2.18	0.43
1:D:272:ASN:N	1:D:272:ASN:HD22	2.16	0.43
1:D:368:GLY:O	1:D:415:CYS:HA	2.18	0.43
1:F:260:THR:HA	1:F:478:GLY:HA3	2.00	0.43
1:F:495:LEU:O	1:F:495:LEU:HD23	2.17	0.43
1:A:339:PHE:HE2	1:A:341:PRO:HG3	1.72	0.43
1:A:35:LEU:CD1	1:A:64:LEU:HD13	2.46	0.43
1:B:19:GLY:O	1:B:20:MET:HB2	2.17	0.43
1:B:266:LEU:HD23	1:B:305:ILE:CG2	2.45	0.43
1:C:257:ILE:HD11	1:C:533:TRP:HH2	1.83	0.43
1:C:445:ILE:O	1:C:445:ILE:HG13	2.17	0.43
1:D:373:ILE:HD13	1:D:373:ILE:HA	1.78	0.43
1:E:4:SER:O	1:E:5:LYS:C	2.57	0.43
1:E:452:ALA:HB2	1:E:535:PRO:HB3	2.00	0.43
1:F:115:VAL:O	1:F:138:GLY:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:SER:C	1:F:318:ALA:H	2.20	0.43
1:F:495:LEU:CD2	1:F:521:LEU:HD23	2.48	0.43
1:A:124:LEU:HD23	1:A:124:LEU:C	2.39	0.43
1:A:432:SER:C	1:A:433:LEU:HD12	2.39	0.43
1:A:73:ILE:HG23	1:A:88:GLY:O	2.18	0.43
1:B:133:ASP:O	1:B:174:CYS:HA	2.18	0.43
1:B:237:VAL:HA	1:B:334:LYS:O	2.19	0.43
1:B:280:ALA:O	1:B:284:LEU:HD22	2.16	0.43
1:C:98:ILE:N	1:C:99:PRO:HD2	2.33	0.43
1:D:115:VAL:HG13	1:D:120:GLU:HB2	2.00	0.43
1:E:274:VAL:HG13	1:F:276:GLN:HG2	2.00	0.43
1:F:171:ALA:O	1:F:173:TRP:N	2.51	0.43
1:F:32:GLU:HA	1:F:64:LEU:HD11	2.00	0.43
1:B:125:SER:O	1:B:127:MET:N	2.51	0.43
3:B:542:IFP:H7A1	4:B:543:POP:O	2.18	0.43
1:C:144:LEU:CD1	1:C:144:LEU:H	2.13	0.43
1:C:402:THR:HG22	1:C:423:ALA:CB	2.49	0.43
1:D:281:ASN:CB	1:D:518:ILE:HD13	2.43	0.43
1:D:3:PHE:CD2	1:D:71:PRO:HG3	2.52	0.43
1:C:228:LEU:HA	1:C:228:LEU:HD12	1.84	0.43
1:C:399:ILE:HD11	1:C:421:PHE:CE2	2.53	0.43
1:D:15:VAL:HG22	1:D:43:GLN:HB3	2.00	0.43
1:F:110:VAL:CG1	1:F:111:ILE:N	2.82	0.43
1:F:124:LEU:HD23	1:F:125:SER:N	2.33	0.43
1:F:16:THR:CG2	1:F:17:ASP:N	2.80	0.43
1:F:271:THR:CA	1:F:313:ASN:HB3	2.43	0.43
1:A:140:LEU:HB3	1:A:141:PHE:CD2	2.53	0.43
1:A:296:GLN:HG3	1:A:322:MET:HA	1.99	0.43
1:C:183:HIS:HB3	1:C:184:PRO:CD	2.48	0.43
1:C:318:ALA:HA	1:C:319:PRO:HD3	1.84	0.43
1:C:59:LEU:CD2	1:C:84:ILE:HB	2.48	0.43
1:E:125:SER:C	1:E:127:MET:N	2.67	0.43
1:E:264:ARG:N	1:E:265:PRO:HD3	2.34	0.43
1:B:347:THR:OG1	1:B:350:ARG:HB2	2.18	0.43
1:B:479:GLN:HA	1:B:480:PRO:HD3	1.64	0.43
1:C:160:ILE:HD11	1:C:193:GLN:O	2.19	0.43
1:B:298:GLU:OE1	1:C:350:ARG:HD2	2.18	0.43
1:E:182:LEU:HA	1:E:186:ASN:HD21	1.83	0.43
1:E:98:ILE:H	1:E:99:PRO:HD2	1.80	0.43
1:F:8:PHE:CD2	1:F:110:VAL:HG21	2.45	0.43
1:F:335:ARG:CZ	1:F:336:PRO:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:MET:HE2	1:F:495:LEU:HD12	2.00	0.43
1:F:78:ILE:O	1:F:82:MET:HG3	2.18	0.43
1:B:74:ILE:HD12	1:B:81:ALA:HA	2.00	0.43
1:C:151:LYS:HB3	1:C:152:ALA:H	1.63	0.43
1:C:208:VAL:HG11	1:C:225:LEU:CD1	2.49	0.43
1:D:322:MET:HG3	1:D:323:LEU:N	2.33	0.43
1:E:335:ARG:HB3	1:E:336:PRO:HD3	2.00	0.43
1:E:368:GLY:O	1:E:415:CYS:HA	2.19	0.43
1:B:341:PRO:O	1:B:372:GLU:HG2	2.19	0.43
1:B:96:MET:O	1:B:97:PRO:C	2.55	0.43
1:B:98:ILE:HD13	1:B:98:ILE:HA	1.72	0.43
1:C:191:LEU:HD22	1:C:206:ILE:HD11	1.99	0.43
1:D:206:ILE:HB	1:D:229:ILE:HD11	2.00	0.43
1:D:78:ILE:O	1:D:82:MET:HG3	2.18	0.43
1:F:110:VAL:HG13	1:F:133:ASP:HB2	2.01	0.43
1:F:295:ILE:HD12	1:F:295:ILE:N	2.33	0.43
1:C:17:ASP:HB3	1:C:20:MET:HE2	2.01	0.43
1:C:348:GLU:OE1	1:C:348:GLU:HA	2.19	0.43
1:D:395:ASN:HA	1:D:398:LEU:HD12	1.99	0.43
1:E:31:VAL:O	1:E:31:VAL:HG12	2.19	0.43
1:A:65:CYS:HB3	1:A:70:VAL:O	2.19	0.42
1:A:78:ILE:CD1	1:A:104:LEU:HD12	2.49	0.42
1:B:228:LEU:N	1:B:228:LEU:HD12	2.34	0.42
1:C:101:ILE:O	1:C:105:VAL:CG2	2.66	0.42
1:C:17:ASP:CB	1:C:20:MET:HE1	2.48	0.42
1:C:451:GLU:HG2	1:C:452:ALA:N	2.34	0.42
1:D:187:ILE:HG23	1:D:206:ILE:HD12	2.00	0.42
1:A:16:THR:HB	1:A:44:ILE:HA	2.01	0.42
1:D:255:SER:O	1:D:259:ASN:ND2	2.52	0.42
1:E:253:ILE:O	1:E:257:ILE:HG13	2.18	0.42
1:E:344:TYR:C	1:E:346:ALA:H	2.22	0.42
1:F:266:LEU:HD23	1:F:305:ILE:HG21	2.00	0.42
1:A:140:LEU:HD23	1:A:182:LEU:HD11	2.01	0.42
1:A:192:TYR:CD1	1:A:234:TYR:CD2	3.01	0.42
1:A:241:LEU:O	1:A:428:GLU:HA	2.18	0.42
1:A:256:ILE:HG12	1:A:479:GLN:OE1	2.19	0.42
1:B:138:GLY:HA3	1:B:154:MET:HE2	2.01	0.42
1:B:305:ILE:HA	1:B:306:PRO:HD3	1.87	0.42
1:B:402:THR:OG1	1:B:415:CYS:HB2	2.20	0.42
1:C:10:TYR:O	1:C:205:GLY:HA3	2.19	0.42
1:C:402:THR:HG22	1:C:423:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:THR:C	1:C:439:GLY:H	2.21	0.42
1:C:16:THR:O	1:C:45:ARG:HB3	2.19	0.42
1:D:88:GLY:HA3	1:D:110:VAL:HG13	2.00	0.42
1:D:427:ILE:C	1:D:429:GLY:H	2.21	0.42
1:D:80:VAL:O	1:D:84:ILE:HG12	2.19	0.42
1:E:450:VAL:O	1:E:450:VAL:HG12	2.20	0.42
1:F:121:VAL:O	1:F:124:LEU:CD2	2.67	0.42
1:F:141:PHE:HB3	1:F:142:PRO:CD	2.49	0.42
1:F:479:GLN:HA	1:F:480:PRO:HD3	1.66	0.42
1:A:313:ASN:ND2	1:A:342:VAL:HG22	2.31	0.42
1:A:193:GLN:NE2	1:A:362:GLN:HE21	2.17	0.42
1:B:310:LEU:HD23	1:B:337:ILE:CG2	2.47	0.42
1:B:323:LEU:HD12	1:B:357:LEU:HD11	2.02	0.42
1:B:414:VAL:HG22	1:B:422:ILE:HG13	2.02	0.42
1:B:276:GLN:OE1	1:C:273:LYS:CB	2.67	0.42
1:E:101:ILE:O	1:E:105:VAL:CG2	2.59	0.42
1:E:270:ILE:HD12	1:E:310:LEU:HD11	2.01	0.42
1:A:139:THR:HG23	2:A:541:3NM:O1	2.19	0.42
1:A:314:THR:HG21	1:A:354:ASN:HD21	1.84	0.42
1:A:322:MET:HG3	1:A:323:LEU:N	2.34	0.42
1:B:333:VAL:O	1:B:334:LYS:HB2	2.20	0.42
1:B:45:ARG:NH2	4:B:543:POP:O1	2.40	0.42
1:C:176:THR:O	1:C:204:ASP:HB2	2.19	0.42
1:C:272:ASN:ND2	1:C:315:GLY:O	2.53	0.42
1:D:234:TYR:HB2	1:D:431:TYR:CE1	2.54	0.42
1:D:98:ILE:N	1:D:99:PRO:HD2	2.35	0.42
1:E:289:SER:HA	1:E:290:PRO:HD3	1.76	0.42
1:F:35:LEU:CD2	1:F:70:VAL:HG11	2.40	0.42
1:F:97:PRO:HG2	1:F:100:MET:HE3	2.01	0.42
1:A:358:LEU:HD23	1:A:363:PHE:CE1	2.53	0.42
1:A:253:ILE:CD1	1:A:494:MET:CE	2.95	0.42
1:A:534:ALA:H	1:A:535:PRO:HD3	1.84	0.42
1:C:115:VAL:HG13	1:C:120:GLU:CB	2.50	0.42
1:C:257:ILE:HA	1:C:260:THR:HG22	2.01	0.42
1:D:183:HIS:HB2	1:D:185:ASP:OD1	2.19	0.42
1:D:217:ASP:OD1	1:D:219:ALA:HB3	2.18	0.42
1:D:350:ARG:HD2	1:E:298:GLU:OE1	2.20	0.42
1:D:73:ILE:HA	1:D:88:GLY:O	2.18	0.42
1:E:117:PHE:N	1:E:117:PHE:CD2	2.85	0.42
1:E:39:VAL:HG12	1:E:41:LEU:H	1.85	0.42
1:E:534:ALA:N	1:E:535:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:ALA:HA	1:F:319:PRO:HD3	1.87	0.42
1:F:193:GLN:HE21	1:F:362:GLN:HE21	1.65	0.42
1:A:512:SER:HA	1:A:515:VAL:CG1	2.49	0.42
1:C:124:LEU:HD11	1:C:174:CYS:SG	2.60	0.42
1:C:335:ARG:HB3	1:C:336:PRO:CD	2.50	0.42
1:D:355:ASN:O	1:D:359:THR:HG23	2.20	0.42
1:E:15:VAL:HB	1:E:209:VAL:CG2	2.49	0.42
1:E:168:ARG:CG	1:E:168:ARG:O	2.68	0.42
1:E:16:THR:CG2	1:E:17:ASP:N	2.83	0.42
1:E:248:THR:HG23	1:E:487:HIS:ND1	2.35	0.42
1:F:123:GLU:O	1:F:127:MET:HG3	2.19	0.42
1:F:340:ASP:HA	1:F:341:PRO:HD3	1.76	0.42
1:F:59:LEU:HD21	1:F:84:ILE:CG2	2.49	0.42
1:A:336:PRO:HA	1:A:364:SER:OG	2.19	0.42
1:B:276:GLN:HG3	1:B:292:MET:HE2	2.01	0.42
1:C:406:ALA:HB2	1:C:413:ALA:HB3	2.01	0.42
1:C:495:LEU:HD11	1:C:525:THR:HG22	2.01	0.42
1:D:21:ILE:HA	1:D:22:PRO:HD3	1.81	0.42
1:C:77:ARG:NH2	1:D:77:ARG:HH12	2.17	0.42
1:E:144:LEU:HD12	1:E:144:LEU:N	2.34	0.42
1:E:175:ARG:HA	1:E:175:ARG:NE	2.34	0.42
1:F:112:GLY:HA3	1:F:134:TYR:CE2	2.55	0.42
1:F:124:LEU:HA	1:F:127:MET:HE3	1.99	0.42
1:A:102:ARG:HA	1:A:102:ARG:HD3	1.68	0.42
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.60	0.42
1:B:239:ILE:HG22	1:B:240:GLY:H	1.84	0.42
1:B:326:ALA:O	1:B:329:ALA:HB3	2.20	0.42
1:B:73:ILE:HG23	1:B:89:ILE:HA	2.01	0.42
1:C:270:ILE:HD12	1:C:310:LEU:HD11	2.02	0.42
1:D:314:THR:HG21	1:D:354:ASN:HD21	1.85	0.42
1:D:34:GLY:O	1:D:39:VAL:N	2.50	0.42
1:D:353:LEU:O	1:D:357:LEU:HD13	2.20	0.42
1:D:253:ILE:HD11	1:D:494:MET:HE2	2.02	0.42
1:E:163:LEU:HD22	1:E:201:ARG:CD	2.50	0.42
1:F:16:THR:HG23	1:F:17:ASP:N	2.34	0.42
1:F:228:LEU:N	1:F:228:LEU:HD12	2.35	0.42
1:F:533:TRP:HB3	1:F:535:PRO:HD2	2.01	0.42
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.83	0.42
1:B:192:TYR:CZ	1:B:410:LYS:HB3	2.54	0.42
1:B:437:THR:O	1:B:439:GLY:N	2.53	0.42
1:A:523:ARG:HD3	1:B:508:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LEU:HA	1:C:524:LEU:HD12	1.84	0.42
1:D:44:ILE:CD1	1:D:58:ALA:HA	2.50	0.42
1:E:179:ILE:HD12	3:E:542:IFP:C2A	2.50	0.42
1:F:28:TYR:CZ	1:F:64:LEU:HG	2.55	0.42
1:B:468:LEU:HG	1:B:472:ILE:HD11	2.02	0.41
1:C:322:MET:HG3	1:C:323:LEU:HD23	2.01	0.41
1:E:138:GLY:HA3	1:E:154:MET:CE	2.50	0.41
1:E:433:LEU:O	1:E:434:SER:CB	2.68	0.41
1:E:15:VAL:HG22	1:E:43:GLN:HB3	2.01	0.41
1:F:527:GLU:O	1:F:529:THR:N	2.53	0.41
1:A:89:ILE:HD11	1:A:101:ILE:HG23	2.00	0.41
1:B:28:TYR:CE1	1:B:64:LEU:CG	3.01	0.41
1:C:72:LEU:N	1:C:87:ASP:OD1	2.53	0.41
1:D:352:LEU:HA	1:D:352:LEU:HD22	1.72	0.41
1:E:416:THR:HA	1:E:420:ASP:OD1	2.21	0.41
1:A:70:VAL:HG23	1:A:71:PRO:HD2	2.02	0.41
1:B:37:ASN:HD22	1:B:219:ALA:HA	1.85	0.41
1:B:428:GLU:HG3	1:B:430:LYS:NZ	2.33	0.41
1:D:269:HIS:HB2	1:D:292:MET:CE	2.51	0.41
1:D:527:GLU:O	1:D:527:GLU:HG3	2.19	0.41
1:D:88:GLY:HA3	1:D:110:VAL:CG1	2.50	0.41
1:E:189:ARG:O	1:E:193:GLN:HG3	2.20	0.41
1:E:73:ILE:H	1:E:73:ILE:HD12	1.85	0.41
1:A:276:GLN:OE1	1:B:273:LYS:CB	2.69	0.41
1:A:501:LYS:O	1:A:504:SER:N	2.54	0.41
1:B:257:ILE:HG22	1:B:257:ILE:O	2.20	0.41
1:C:20:MET:HE3	1:C:213:ILE:HB	2.01	0.41
1:D:141:PHE:HB3	1:D:142:PRO:CD	2.51	0.41
1:D:253:ILE:HD11	1:D:494:MET:CE	2.50	0.41
1:D:479:GLN:HA	1:D:480:PRO:HD3	1.73	0.41
1:E:347:THR:HG21	1:F:298:GLU:CG	2.49	0.41
1:E:143:THR:HG21	2:E:541:3NM:H7	2.02	0.41
1:F:399:ILE:HG12	1:F:421:PHE:CD1	2.54	0.41
1:F:247:LEU:CD2	1:F:537:LEU:HG	2.49	0.41
1:A:226:ARG:HA	1:A:226:ARG:HD3	1.69	0.41
1:A:323:LEU:HD12	1:A:357:LEU:HD11	2.02	0.41
1:A:78:ILE:O	1:A:82:MET:HG3	2.20	0.41
1:B:78:ILE:HD12	1:B:101:ILE:HG23	2.03	0.41
1:C:73:ILE:HG22	1:C:74:ILE:N	2.36	0.41
1:D:247:LEU:HD23	1:D:247:LEU:HA	1.85	0.41
1:D:318:ALA:HA	1:D:319:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LEU:HA	1:F:59:LEU:HD23	1.75	0.41
1:F:98:ILE:HG21	1:F:132:VAL:HG22	2.02	0.41
1:B:98:ILE:N	1:B:99:PRO:HD2	2.36	0.41
1:C:192:TYR:CD1	1:C:234:TYR:HD2	2.38	0.41
1:C:313:ASN:O	1:C:314:THR:O	2.38	0.41
1:C:89:ILE:HD11	1:C:101:ILE:HG21	2.02	0.41
1:D:78:ILE:HG21	1:D:96:MET:HE1	2.01	0.41
1:E:175:ARG:HE	1:E:175:ARG:HA	1.85	0.41
1:A:350:ARG:O	1:A:351:LEU:C	2.57	0.41
1:B:351:LEU:O	1:B:351:LEU:HD12	2.20	0.41
1:C:319:PRO:HA	1:C:320:PRO:HD3	1.97	0.41
1:C:77:ARG:NH2	1:D:77:ARG:NH1	2.69	0.41
1:D:192:TYR:C	1:D:192:TYR:CD2	2.93	0.41
1:D:206:ILE:HB	1:D:229:ILE:CD1	2.50	0.41
1:D:468:LEU:O	1:D:472:ILE:HG13	2.21	0.41
1:D:96:MET:CE	1:D:101:ILE:HG12	2.51	0.41
1:E:275:HIS:N	1:E:275:HIS:CD2	2.89	0.41
1:F:171:ALA:C	1:F:173:TRP:H	2.24	0.41
1:A:499:ALA:HB1	1:A:520:ALA:HB3	2.02	0.41
1:A:8:PHE:HD1	1:A:71:PRO:HG2	1.86	0.41
1:A:98:ILE:HD11	1:A:113:TRP:CE2	2.55	0.41
1:B:265:PRO:O	1:B:288:SER:HB3	2.20	0.41
1:B:404:ILE:HA	1:B:442:VAL:HG13	2.01	0.41
1:C:342:VAL:HG23	1:C:343:GLY:N	2.33	0.41
1:D:347:THR:HG21	1:E:298:GLU:OE1	2.20	0.41
1:D:98:ILE:HD11	1:D:113:TRP:CD1	2.56	0.41
1:E:369:ASN:O	1:E:370:SER:C	2.59	0.41
1:F:98:ILE:HG21	1:F:132:VAL:CG2	2.51	0.41
1:F:272:ASN:HD22	1:F:272:ASN:HA	1.51	0.41
1:B:427:ILE:C	1:B:429:GLY:N	2.74	0.41
1:C:182:LEU:HD12	1:C:190:VAL:HG21	2.03	0.41
1:C:278:PHE:CE2	1:C:467:SER:OG	2.70	0.41
1:C:357:LEU:HA	1:C:360:PHE:CD1	2.56	0.41
1:D:266:LEU:HD11	1:D:291:ILE:HG13	2.01	0.41
1:A:495:LEU:HD22	1:A:521:LEU:HD22	2.02	0.41
1:B:189:ARG:HG3	1:B:193:GLN:NE2	2.36	0.41
1:B:196:SER:HB3	1:B:201:ARG:H	1.86	0.41
1:C:329:ALA:O	1:C:333:VAL:HG23	2.21	0.41
1:D:124:LEU:HD11	1:D:174:CYS:SG	2.61	0.41
1:E:249:THR:HG23	1:E:252:GLU:OE1	2.21	0.41
1:E:342:VAL:HG23	1:E:343:GLY:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:LEU:HD22	1:E:409:TYR:CD2	2.55	0.41
1:E:367:LYS:NZ	1:E:466:CYS:HA	2.35	0.41
1:F:117:PHE:HA	1:F:118:PRO:HD3	1.91	0.41
1:F:282:VAL:HG21	1:F:467:SER:OG	2.19	0.41
1:A:270:ILE:HD12	1:A:310:LEU:HD11	2.03	0.41
1:C:192:TYR:CZ	1:C:410:LYS:HB3	2.56	0.41
1:C:402:THR:O	1:C:403:LYS:C	2.60	0.41
1:E:167:GLU:C	1:E:169:ASN:N	2.74	0.41
1:E:402:THR:OG1	1:E:415:CYS:HB2	2.21	0.41
1:F:283:THR:CG2	1:F:288:SER:HB2	2.51	0.41
1:A:55:ILE:CG1	1:A:80:VAL:HG13	2.52	0.40
1:B:160:ILE:HD11	1:B:193:GLN:O	2.20	0.40
1:D:313:ASN:O	1:D:314:THR:C	2.60	0.40
1:E:299:VAL:HG21	1:E:326:ALA:CA	2.38	0.40
1:E:349:THR:HG21	1:F:297:SER:OG	2.21	0.40
1:F:66:HIS:HE1	1:F:87:ASP:OD1	2.04	0.40
1:B:167:GLU:C	1:B:169:ASN:N	2.72	0.40
1:C:75:ASN:ND2	1:C:76:ASP:OD1	2.54	0.40
1:D:21:ILE:HD11	1:D:27:LEU:CD1	2.50	0.40
1:D:437:THR:O	1:D:438:ASN:C	2.59	0.40
1:E:276:GLN:CG	1:E:292:MET:HE2	2.51	0.40
1:A:14:LEU:HB3	1:A:42:VAL:HG22	2.03	0.40
1:B:228:LEU:N	1:B:228:LEU:CD1	2.85	0.40
1:B:296:GLN:HG3	1:B:322:MET:HB2	2.03	0.40
1:B:70:VAL:HA	1:B:71:PRO:HD3	1.82	0.40
1:C:495:LEU:HD22	1:C:495:LEU:O	2.20	0.40
1:D:143:THR:HG23	1:D:143:THR:O	2.22	0.40
1:D:189:ARG:O	1:D:193:GLN:HG2	2.20	0.40
1:D:427:ILE:HG22	1:D:427:ILE:O	2.21	0.40
2:E:541:3NM:N	3:E:542:IFP:C7A	2.85	0.40
1:F:356:LEU:O	1:F:357:LEU:C	2.60	0.40
1:A:121:VAL:O	1:A:124:LEU:HB3	2.21	0.40
1:A:218:ALA:O	1:A:219:ALA:C	2.60	0.40
1:B:145:THR:O	1:B:145:THR:HG22	2.20	0.40
1:B:163:LEU:HA	1:B:163:LEU:HD23	1.89	0.40
1:B:165:ALA:O	1:B:169:ASN:HB2	2.21	0.40
1:B:189:ARG:HG3	1:B:193:GLN:HE21	1.86	0.40
1:B:344:TYR:CZ	1:B:376:LEU:HD23	2.57	0.40
1:B:192:TYR:HA	1:B:431:TYR:HB3	2.04	0.40
1:E:276:GLN:HG3	1:E:292:MET:HE2	2.03	0.40
1:E:269:HIS:HB2	1:E:292:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:LEU:HD13	1:F:312:LEU:HA	1.91	0.40
1:F:77:ARG:HE	1:F:80:VAL:CG2	2.35	0.40
1:A:192:TYR:C	1:A:192:TYR:CD2	2.92	0.40
1:A:192:TYR:CD2	1:A:192:TYR:O	2.75	0.40
1:A:529:THR:N	1:A:530:PRO:HD3	2.36	0.40
1:B:276:GLN:CG	1:B:292:MET:HG3	2.51	0.40
1:C:310:LEU:HD21	1:C:312:LEU:HD21	2.03	0.40
1:E:274:VAL:HG12	1:F:277:ASN:HA	2.04	0.40
1:E:339:PHE:HE1	1:E:357:LEU:HD23	1.85	0.40
1:A:94:ASP:O	1:E:52:LYS:HB2	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	493/540 (91%)	398 (81%)	78 (16%)	17 (3%)	3	23
1	B	493/540 (91%)	423 (86%)	49 (10%)	21 (4%)	2	19
1	C	493/540 (91%)	430 (87%)	42 (8%)	21 (4%)	2	19
1	D	493/540 (91%)	411 (83%)	61 (12%)	21 (4%)	2	19
1	E	489/540 (91%)	418 (86%)	49 (10%)	22 (4%)	2	17
1	F	493/540 (91%)	411 (83%)	70 (14%)	12 (2%)	6	32
All	All	2954/3240 (91%)	2491 (84%)	349 (12%)	114 (4%)	3	20

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	76	ASP

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Mol	Chain	Res	Type
1	A	247	LEU
1	A	317	VAL
1	B	20	MET
1	B	126	LYS
1	B	317	VAL
1	C	76	ASP
1	C	247	LEU
1	C	314	THR
1	C	438	ASN
1	C	481	SER
1	D	20	MET
1	D	76	ASP
1	D	138	GLY
1	D	247	LEU
1	D	314	THR
1	D	342	VAL
1	D	344	TYR
1	D	370	SER
1	D	438	ASN
1	D	528	ASN
1	E	20	MET
1	E	76	ASP
1	E	272	ASN
1	E	317	VAL
1	F	20	MET
1	F	76	ASP
1	F	126	LYS
1	F	247	LEU
1	F	272	ASN
1	F	317	VAL
1	F	438	ASN
1	A	138	GLY
1	A	168	ARG
1	A	438	ASN
1	A	441	SER
1	A	528	ASN
1	B	11	SER
1	B	138	GLY
1	B	247	LEU
1	B	370	SER
1	B	439	GLY
1	C	20	MET

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Mol	Chain	Res	Type
1	C	138	GLY
1	C	172	HIS
1	C	238	ASN
1	C	317	VAL
1	D	11	SER
1	D	343	GLY
1	E	126	LYS
1	E	138	GLY
1	E	247	LEU
1	E	342	VAL
1	E	343	GLY
1	E	344	TYR
1	F	172	HIS
1	A	152	ALA
1	A	345	SER
1	A	481	SER
1	B	76	ASP
1	B	172	HIS
1	B	272	ASN
1	B	315	GLY
1	B	481	SER
1	C	49	ALA
1	C	272	ASN
1	C	345	SER
1	C	370	SER
1	C	410	LYS
1	D	152	ALA
1	D	186	ASN
1	D	395	ASN
1	D	442	VAL
1	D	452	ALA
1	D	481	SER
1	E	345	SER
1	F	314	THR
1	F	410	LYS
1	B	344	TYR
1	C	170	ASN
1	C	495	LEU
1	D	217	ASP
1	E	6	GLU
1	E	170	ASN
1	E	438	ASN

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Mol	Chain	Res	Type
1	F	11	SER
1	F	276	GLN
1	A	272	ASN
1	A	314	THR
1	B	343	GLY
1	B	428	GLU
1	C	254	GLN
1	C	344	TYR
1	E	186	ASN
1	E	494	MET
1	E	495	LEU
1	E	535	PRO
1	A	170	ASN
1	B	186	ASN
1	B	238	ASN
1	B	438	ASN
1	C	105	VAL
1	E	370	SER
1	B	97	PRO
1	B	483	GLY
1	E	315	GLY
1	A	343	GLY
1	C	343	GLY
1	E	97	PRO
1	A	448	VAL
1	D	148	ASN
1	E	105	VAL
1	D	317	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/449 (90%)	361 (89%)	44 (11%)	6	25
1	B	405/449 (90%)	352 (87%)	53 (13%)	4	18
1	C	405/449 (90%)	346 (85%)	59 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	405/449 (90%)	358 (88%)	47 (12%)	5	23
1	E	403/449 (90%)	352 (87%)	51 (13%)	4	19
1	F	405/449 (90%)	352 (87%)	53 (13%)	4	18
All	All	2428/2694 (90%)	2121 (87%)	307 (13%)	4	20

All (307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	13	TYR
1	A	16	THR
1	A	54	PHE
1	A	64	LEU
1	A	70	VAL
1	A	78	ILE
1	A	94	ASP
1	A	98	ILE
1	A	105	VAL
1	A	113	TRP
1	A	117	PHE
1	A	139	THR
1	A	140	LEU
1	A	144	LEU
1	A	160	ILE
1	A	177	VAL
1	A	185	ASP
1	A	187	ILE
1	A	191	LEU
1	A	192	TYR
1	A	216	LEU
1	A	226	ARG
1	A	228	LEU
1	A	242	SER
1	A	260	THR
1	A	272	ASN
1	A	296	GLN
1	A	311	LEU
1	A	312	LEU
1	A	317	VAL
1	A	322	MET
1	A	328	ARG

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	337	ILE
1	A	352	LEU
1	A	362	GLN
1	A	374	LEU
1	A	437	THR
1	A	467	SER
1	A	481	SER
1	A	482	GLU
1	A	495	LEU
1	A	524	LEU
1	B	2	LYS
1	B	4	SER
1	B	13	TYR
1	B	51	THR
1	B	54	PHE
1	B	78	ILE
1	B	82	MET
1	B	93	GLN
1	B	104	LEU
1	B	105	VAL
1	B	113	TRP
1	B	124	LEU
1	B	140	LEU
1	B	144	LEU
1	B	182	LEU
1	B	187	ILE
1	B	191	LEU
1	B	197	SER
1	B	202	SER
1	B	221	SER
1	B	226	ARG
1	B	241	LEU
1	B	260	THR
1	B	266	LEU
1	B	272	ASN
1	B	275	HIS
1	B	284	LEU
1	B	291	ILE
1	B	292	MET
1	B	293	SER
1	B	296	GLN

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Mol	Chain	Res	Type
1	B	297	SER
1	B	302	LEU
1	B	312	LEU
1	B	322	MET
1	B	328	ARG
1	B	333	VAL
1	B	337	ILE
1	B	342	VAL
1	B	350	ARG
1	B	352	LEU
1	B	371	SER
1	B	372	GLU
1	B	399	ILE
1	B	418	GLU
1	B	428	GLU
1	B	443	GLU
1	B	481	SER
1	B	482	GLU
1	B	495	LEU
1	B	510	SER
1	B	515	VAL
1	B	517	LEU
1	C	2	LYS
1	C	11	SER
1	C	13	TYR
1	C	54	PHE
1	C	64	LEU
1	C	70	VAL
1	C	78	ILE
1	C	82	MET
1	C	89	ILE
1	C	105	VAL
1	C	113	TRP
1	C	124	LEU
1	C	144	LEU
1	C	161	ARG
1	C	182	LEU
1	C	185	ASP
1	C	191	LEU
1	C	193	GLN
1	C	195	VAL
1	C	207	CYS

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Mol	Chain	Res	Type
1	C	208	VAL
1	C	221	SER
1	C	226	ARG
1	C	228	LEU
1	C	241	LEU
1	C	249	THR
1	C	266	LEU
1	C	272	ASN
1	C	274	VAL
1	C	275	HIS
1	C	284	LEU
1	C	289	SER
1	C	291	ILE
1	C	293	SER
1	C	296	GLN
1	C	297	SER
1	C	302	LEU
1	C	311	LEU
1	C	312	LEU
1	C	322	MET
1	C	328	ARG
1	C	337	ILE
1	C	348	GLU
1	C	352	LEU
1	C	371	SER
1	C	374	LEU
1	C	399	ILE
1	C	404	ILE
1	C	443	GLU
1	C	466	CYS
1	C	467	SER
1	C	481	SER
1	C	482	GLU
1	C	495	LEU
1	C	510	SER
1	C	515	VAL
1	C	517	LEU
1	C	524	LEU
1	C	538	THR
1	D	2	LYS
1	D	13	TYR
1	D	16	THR

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Mol	Chain	Res	Type
1	D	54	PHE
1	D	64	LEU
1	D	75	ASN
1	D	76	ASP
1	D	77	ARG
1	D	78	ILE
1	D	124	LEU
1	D	139	THR
1	D	144	LEU
1	D	177	VAL
1	D	182	LEU
1	D	186	ASN
1	D	191	LEU
1	D	192	TYR
1	D	196	SER
1	D	216	LEU
1	D	241	LEU
1	D	250	THR
1	D	260	THR
1	D	272	ASN
1	D	284	LEU
1	D	291	ILE
1	D	293	SER
1	D	297	SER
1	D	302	LEU
1	D	312	LEU
1	D	313	ASN
1	D	314	THR
1	D	322	MET
1	D	328	ARG
1	D	335	ARG
1	D	348	GLU
1	D	350	ARG
1	D	352	LEU
1	D	362	GLN
1	D	372	GLU
1	D	374	LEU
1	D	416	THR
1	D	467	SER
1	D	482	GLU
1	D	495	LEU
1	D	504	SER

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Mol	Chain	Res	Type
1	D	519	ASP
1	D	524	LEU
1	E	4	SER
1	E	13	TYR
1	E	40	THR
1	E	54	PHE
1	E	63	GLU
1	E	64	LEU
1	E	77	ARG
1	E	78	ILE
1	E	94	ASP
1	E	101	ILE
1	E	113	TRP
1	E	134	TYR
1	E	143	THR
1	E	144	LEU
1	E	154	MET
1	E	156	THR
1	E	160	ILE
1	E	177	VAL
1	E	186	ASN
1	E	189	ARG
1	E	191	LEU
1	E	193	GLN
1	E	197	SER
1	E	226	ARG
1	E	241	LEU
1	E	249	THR
1	E	257	ILE
1	E	271	THR
1	E	284	LEU
1	E	289	SER
1	E	296	GLN
1	E	297	SER
1	E	311	LEU
1	E	312	LEU
1	E	313	ASN
1	E	322	MET
1	E	328	ARG
1	E	348	GLU
1	E	349	THR
1	E	352	LEU

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Mol	Chain	Res	Type
1	E	362	GLN
1	E	399	ILE
1	E	442	VAL
1	E	446	PRO
1	E	466	CYS
1	E	467	SER
1	E	495	LEU
1	E	504	SER
1	E	515	VAL
1	E	524	LEU
1	E	532	THR
1	F	2	LYS
1	F	13	TYR
1	F	16	THR
1	F	40	THR
1	F	54	PHE
1	F	61	ILE
1	F	64	LEU
1	F	70	VAL
1	F	76	ASP
1	F	78	ILE
1	F	82	MET
1	F	89	ILE
1	F	91	VAL
1	F	94	ASP
1	F	105	VAL
1	F	113	TRP
1	F	124	LEU
1	F	139	THR
1	F	144	LEU
1	F	161	ARG
1	F	187	ILE
1	F	191	LEU
1	F	226	ARG
1	F	241	LEU
1	F	272	ASN
1	F	274	VAL
1	F	276	GLN
1	F	284	LEU
1	F	289	SER
1	F	291	ILE
1	F	296	GLN

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Mol	Chain	Res	Type
1	F	297	SER
1	F	299	VAL
1	F	300	ASN
1	F	302	LEU
1	F	311	LEU
1	F	322	MET
1	F	328	ARG
1	F	333	VAL
1	F	342	VAL
1	F	357	LEU
1	F	362	GLN
1	F	374	LEU
1	F	408	LYS
1	F	415	CYS
1	F	418	GLU
1	F	466	CYS
1	F	482	GLU
1	F	495	LEU
1	F	514	GLN
1	F	524	LEU
1	F	532	THR
1	F	538	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	93	GLN
1	A	169	ASN
1	A	183	HIS
1	A	193	GLN
1	A	281	ASN
1	A	313	ASN
1	A	479	GLN
1	A	484	ASN
1	B	37	ASN
1	B	66	HIS
1	B	169	ASN
1	B	172	HIS
1	B	183	HIS
1	B	193	GLN
1	B	269	HIS

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Mol	Chain	Res	Type
1	B	272	ASN
1	B	281	ASN
1	B	484	ASN
1	C	43	GLN
1	C	75	ASN
1	C	93	GLN
1	C	169	ASN
1	C	193	GLN
1	C	272	ASN
1	C	355	ASN
1	C	484	ASN
1	D	75	ASN
1	D	93	GLN
1	D	169	ASN
1	D	186	ASN
1	D	193	GLN
1	D	259	ASN
1	D	272	ASN
1	D	275	HIS
1	D	276	GLN
1	D	281	ASN
1	D	313	ASN
1	D	355	ASN
1	D	484	ASN
1	E	43	GLN
1	E	66	HIS
1	E	93	GLN
1	E	186	ASN
1	E	275	HIS
1	E	281	ASN
1	E	313	ASN
1	E	355	ASN
1	E	362	GLN
1	E	484	ASN
1	F	43	GLN
1	F	66	HIS
1	F	93	GLN
1	F	169	ASN
1	F	193	GLN
1	F	259	ASN
1	F	272	ASN
1	F	313	ASN

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Mol	Chain	Res	Type
1	F	355	ASN
1	F	479	GLN
1	F	484	ASN
1	F	514	GLN

### 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 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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$
2	3NM	B	541	-	12,16,16	5.55	5 (41%)	8,23,23	1.84	1 (12%)
2	3NM	D	541	-	12,16,16	5.50	5 (41%)	8,23,23	1.62	1 (12%)
3	IFP	A	542	-	9,12,12	2.89	3 (33%)	12,18,18	2.86	6 (50%)
2	3NM	F	541	-	12,16,16	5.50	5 (41%)	8,23,23	3.28	1 (12%)
2	3NM	A	541	-	12,16,16	5.53	6 (50%)	8,23,23	2.05	1 (12%)
4	POP	E	543	5	6,8,8	0.57	0	13,13,13	1.26	1 (7%)
4	POP	C	543	5	6,8,8	0.60	0	13,13,13	1.27	2 (15%)
4	POP	A	543	5	6,8,8	0.54	0	13,13,13	1.41	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	POP	F	543	5	6,8,8	0.64	0	13,13,13	1.30	1 (7%)
3	IFP	D	542	-	9,12,12	2.95	3 (33%)	12,18,18	2.90	7 (58%)
3	IFP	F	542	-	9,12,12	2.82	3 (33%)	12,18,18	2.73	4 (33%)
3	IFP	E	542	-	9,12,12	3.14	3 (33%)	12,18,18	2.79	3 (25%)
3	IFP	B	542	-	9,12,12	3.07	3 (33%)	12,18,18	2.72	3 (25%)
2	3NM	E	541	-	12,16,16	5.59	5 (41%)	8,23,23	1.53	1 (12%)
4	POP	B	543	5	6,8,8	0.72	0	13,13,13	1.35	1 (7%)
3	IFP	C	542	-	9,12,12	3.01	3 (33%)	12,18,18	2.90	3 (25%)
4	POP	D	543	5	6,8,8	0.66	0	13,13,13	1.25	1 (7%)
2	3NM	C	541	-	12,16,16	5.58	5 (41%)	8,23,23	1.44	1 (12%)

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
2	3NM	B	541	-	-	5/6/11/11	0/1/1/1
2	3NM	D	541	-	-	5/6/11/11	0/1/1/1
3	IFP	A	542	-	-	0/6/19/19	0/1/1/1
2	3NM	F	541	-	-	4/6/11/11	0/1/1/1
2	3NM	A	541	-	-	2/6/11/11	0/1/1/1
4	POP	E	543	5	-	0/6/6/6	-
4	POP	C	543	5	-	3/6/6/6	-
4	POP	A	543	5	-	0/6/6/6	-
4	POP	F	543	5	-	1/6/6/6	-
3	IFP	D	542	-	-	0/6/19/19	0/1/1/1
3	IFP	F	542	-	-	0/6/19/19	0/1/1/1
3	IFP	E	542	-	-	0/6/19/19	0/1/1/1
3	IFP	B	542	-	-	0/6/19/19	0/1/1/1
2	3NM	E	541	-	-	3/6/11/11	0/1/1/1
4	POP	B	543	5	-	0/6/6/6	-
3	IFP	C	542	-	-	0/6/19/19	0/1/1/1
4	POP	D	543	5	-	0/6/6/6	-
2	3NM	C	541	-	-	2/6/11/11	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	541	3NM	C5-S	-12.91	1.50	1.74
2	D	541	3NM	C5-S	-12.90	1.50	1.74
2	B	541	3NM	C5-S	-12.87	1.50	1.74
2	C	541	3NM	C5-S	-12.65	1.50	1.74
2	A	541	3NM	C5-S	-12.48	1.50	1.74
2	F	541	3NM	C5-S	-12.30	1.51	1.74
2	C	541	3NM	C3-N	9.97	1.45	1.31
2	E	541	3NM	C3-N	9.68	1.45	1.31
2	A	541	3NM	C3-N	9.65	1.45	1.31
2	D	541	3NM	C3-N	9.53	1.45	1.31
2	F	541	3NM	C3-N	9.41	1.45	1.31
2	B	541	3NM	C3-N	9.23	1.44	1.31
2	E	541	3NM	C5-C2	8.13	1.58	1.42
2	C	541	3NM	C5-C2	8.00	1.58	1.42
2	B	541	3NM	C5-C2	7.96	1.58	1.42
2	D	541	3NM	C5-C2	7.96	1.58	1.42
2	A	541	3NM	C5-C2	7.89	1.58	1.42
2	F	541	3NM	C5-C2	7.81	1.58	1.42
2	F	541	3NM	C6-C5	-6.21	1.48	1.50
3	B	542	IFP	C7A-C5A	6.19	1.50	1.33
3	A	542	IFP	C7A-C5A	6.10	1.49	1.33
3	F	542	IFP	C7A-C5A	6.09	1.49	1.33
3	E	542	IFP	C7A-C5A	6.07	1.49	1.33
3	C	542	IFP	C7A-C5A	6.00	1.49	1.33
3	D	542	IFP	C7A-C5A	5.99	1.49	1.33
2	A	541	3NM	C6-C5	-5.73	1.48	1.50
2	B	541	3NM	C6-C5	-5.72	1.48	1.50
2	C	541	3NM	C6-C5	-5.57	1.48	1.50
2	E	541	3NM	C6-C5	-5.40	1.48	1.50
3	E	542	IFP	C2A-N3A	5.18	1.39	1.33
3	E	542	IFP	C6A-N1A	4.97	1.41	1.32
3	B	542	IFP	C2A-N3A	4.78	1.38	1.33
2	D	541	3NM	C6-C5	-4.77	1.48	1.50
3	C	542	IFP	C6A-N1A	4.73	1.41	1.32
3	B	542	IFP	C6A-N1A	4.71	1.40	1.32
3	C	542	IFP	C2A-N3A	4.70	1.38	1.33
3	D	542	IFP	C2A-N3A	4.70	1.38	1.33
3	D	542	IFP	C6A-N1A	4.40	1.40	1.32
3	A	542	IFP	C6A-N1A	4.34	1.40	1.32
3	F	542	IFP	C6A-N1A	4.32	1.40	1.32
3	A	542	IFP	C2A-N3A	4.22	1.38	1.33
3	F	542	IFP	C2A-N3A	3.76	1.37	1.33
2	B	541	3NM	C3-S	-3.28	1.69	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	541	3NM	C3-S	-3.25	1.69	1.73
2	F	541	3NM	C3-S	-3.23	1.69	1.73
2	D	541	3NM	C3-S	-3.19	1.69	1.73
2	E	541	3NM	C3-S	-3.10	1.69	1.73
2	C	541	3NM	C3-S	-2.89	1.69	1.73
2	A	541	3NM	O3-C7	-2.09	1.36	1.44

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	541	3NM	C6-C5-C2	-9.02	120.19	127.43
3	C	542	IFP	CM2-C2A-N1A	7.31	121.88	114.21
3	F	542	IFP	CM2-C2A-N1A	6.57	121.11	114.21
3	E	542	IFP	CM2-C2A-N1A	6.40	120.93	114.21
3	D	542	IFP	CM2-C2A-N3A	6.00	120.42	114.11
3	A	542	IFP	CM2-C2A-N3A	5.76	120.17	114.11
3	B	542	IFP	CM2-C2A-N1A	5.68	120.18	114.21
2	A	541	3NM	C6-C5-C2	-5.60	122.94	127.43
3	B	542	IFP	CM2-C2A-N3A	5.01	119.38	114.11
3	A	542	IFP	CM2-C2A-N1A	5.01	119.47	114.21
2	B	541	3NM	C6-C5-C2	-4.92	123.48	127.43
3	E	542	IFP	CM2-C2A-N3A	4.86	119.22	114.11
3	D	542	IFP	CM2-C2A-N1A	4.86	119.31	114.21
2	D	541	3NM	C6-C5-C2	-4.29	123.99	127.43
3	C	542	IFP	CM2-C2A-N3A	4.05	118.36	114.11
3	C	542	IFP	N1A-C2A-N3A	-4.04	119.73	128.21
3	E	542	IFP	N1A-C2A-N3A	-4.03	119.75	128.21
4	B	543	POP	P2-O-P1	-3.84	119.66	132.83
3	D	542	IFP	N1A-C2A-N3A	-3.82	120.19	128.21
4	E	543	POP	P2-O-P1	-3.77	119.88	132.83
3	F	542	IFP	CM2-C2A-N3A	3.76	118.06	114.11
2	E	541	3NM	C6-C5-C2	-3.74	124.43	127.43
3	A	542	IFP	N1A-C2A-N3A	-3.74	120.36	128.21
3	B	542	IFP	N1A-C2A-N3A	-3.71	120.41	128.21
3	F	542	IFP	N1A-C2A-N3A	-3.55	120.76	128.21
2	C	541	3NM	C6-C5-C2	-3.45	124.67	127.43
4	F	543	POP	P2-O-P1	-3.44	121.01	132.83
4	A	543	POP	P2-O-P1	-3.23	121.76	132.83
4	D	543	POP	P2-O-P1	-3.20	121.83	132.83
4	C	543	POP	P2-O-P1	-3.07	122.30	132.83
3	A	542	IFP	F1-CM2-C2A	-3.04	106.19	112.28
3	D	542	IFP	F3-CM2-C2A	-2.71	106.84	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	542	IFP	F2-CM2-C2A	-2.56	107.14	112.28
3	A	542	IFP	C7A-C5A-C6A	-2.42	118.32	121.94
3	D	542	IFP	F2-CM2-C2A	-2.38	107.50	112.28
3	A	542	IFP	C6A-N1A-C2A	2.23	120.09	115.63
3	D	542	IFP	C7A-C5A-C6A	-2.20	118.66	121.94
4	A	543	POP	O2-P1-O	2.19	112.00	104.64
4	C	543	POP	O2-P1-O	2.09	111.65	104.64
3	D	542	IFP	C6A-N1A-C2A	2.00	119.63	115.63

There are no chirality outliers.

All (25) torsion outliers are listed below:

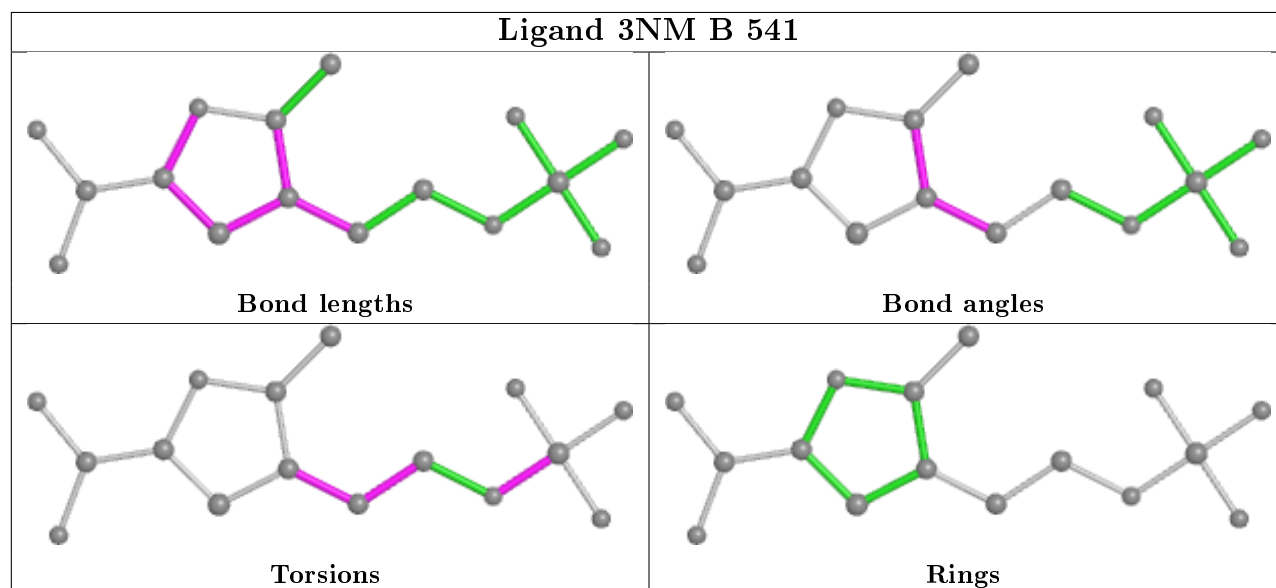
Mol	Chain	Res	Type	Atoms
2	A	541	3NM	C5-C6-C7-O3
4	F	543	POP	P1-O-P2-O5
2	C	541	3NM	C5-C6-C7-O3
2	B	541	3NM	C7-O3-P-O5
2	B	541	3NM	C7-O3-P-O6
2	B	541	3NM	C5-C6-C7-O3
4	C	543	POP	P1-O-P2-O6
2	D	541	3NM	C7-O3-P-O4
2	D	541	3NM	C7-O3-P-O5
2	D	541	3NM	C7-O3-P-O6
2	D	541	3NM	C5-C6-C7-O3
2	F	541	3NM	C7-O3-P-O5
2	F	541	3NM	C7-O3-P-O6
2	E	541	3NM	C5-C6-C7-O3
2	F	541	3NM	C7-O3-P-O4
2	E	541	3NM	C7-O3-P-O6
2	A	541	3NM	C2-C5-C6-C7
2	D	541	3NM	C2-C5-C6-C7
4	C	543	POP	P1-O-P2-O4
2	B	541	3NM	C7-O3-P-O4
4	C	543	POP	P1-O-P2-O5
2	C	541	3NM	C2-C5-C6-C7
2	B	541	3NM	C2-C5-C6-C7
2	F	541	3NM	C2-C5-C6-C7
2	E	541	3NM	C2-C5-C6-C7

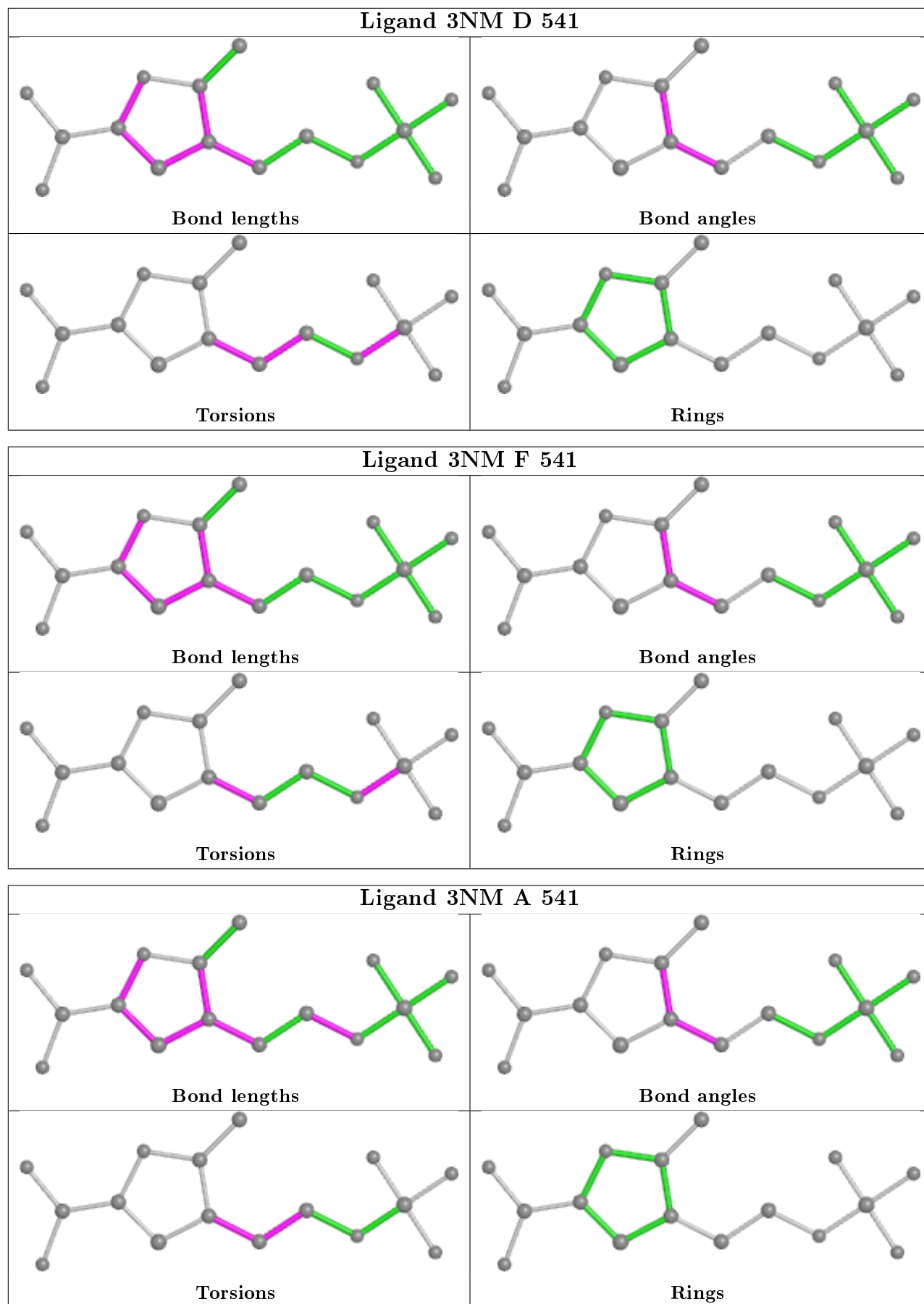
There are no ring outliers.

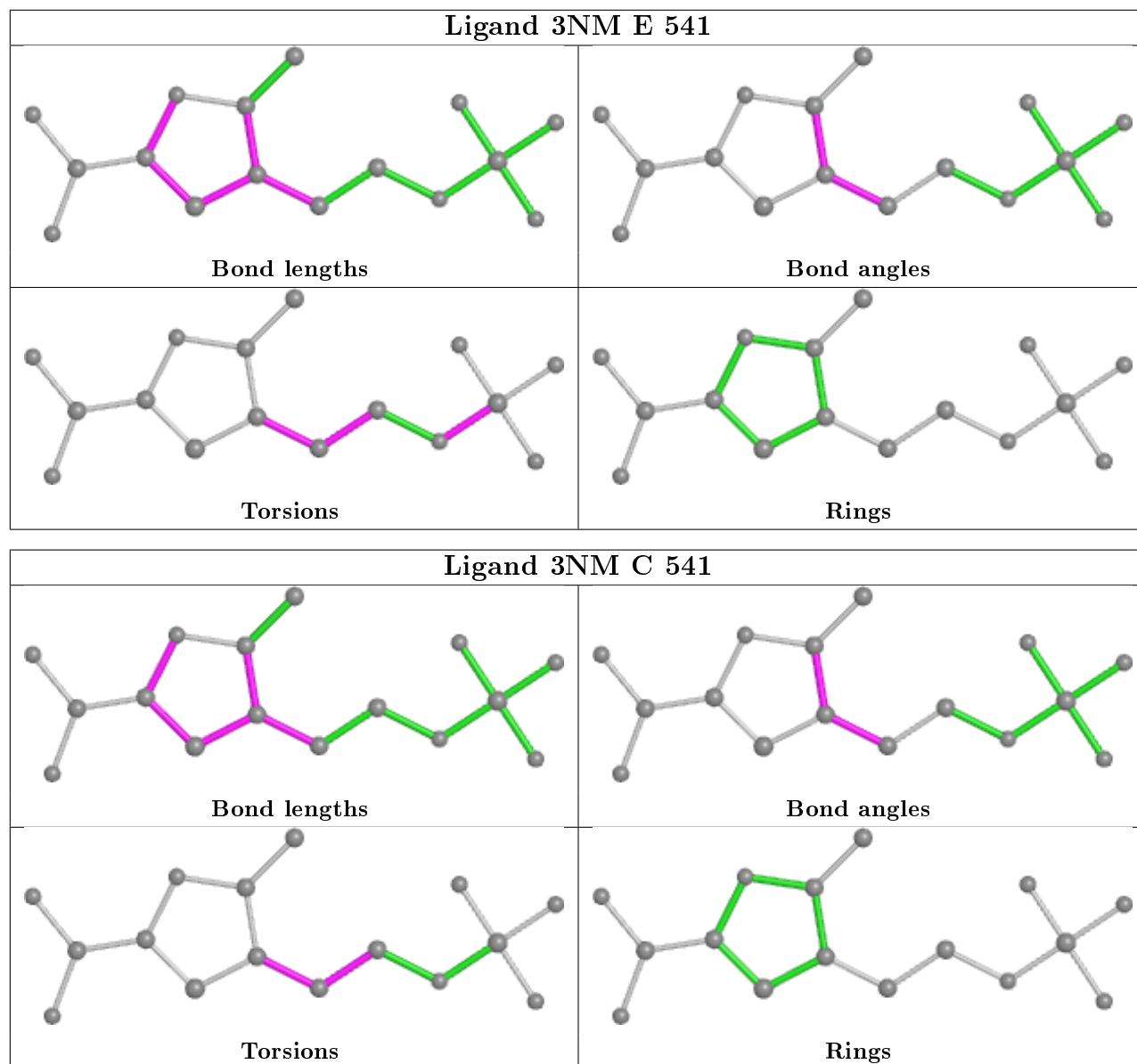
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	541	3NM	3	0
2	D	541	3NM	1	0
3	A	542	IFP	1	0
2	F	541	3NM	2	0
2	A	541	3NM	3	0
4	A	543	POP	1	0
3	E	542	IFP	2	0
3	B	542	IFP	1	0
2	E	541	3NM	2	0
4	B	543	POP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [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	507/540 (93%)	-0.41	3 (0%) 89 84	30, 79, 99, 120	0
1	B	507/540 (93%)	-0.44	0 100 100	41, 81, 103, 127	0
1	C	507/540 (93%)	-0.36	2 (0%) 92 89	41, 74, 96, 117	0
1	D	507/540 (93%)	-0.39	2 (0%) 92 89	39, 75, 99, 120	0
1	E	505/540 (93%)	-0.44	2 (0%) 92 89	42, 80, 101, 124	0
1	F	507/540 (93%)	-0.41	2 (0%) 92 89	42, 78, 100, 119	0
All	All	3040/3240 (93%)	-0.41	11 (0%) 92 89	30, 78, 101, 127	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	465	GLY	4.5
1	E	437	THR	2.9
1	A	465	GLY	2.7
1	F	275	HIS	2.4
1	C	277	ASN	2.4
1	C	281	ASN	2.3
1	D	277	ASN	2.3
1	A	394	SER	2.2
1	A	277	ASN	2.2
1	E	465	GLY	2.1
1	D	454	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

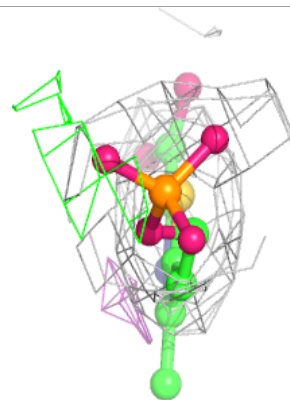
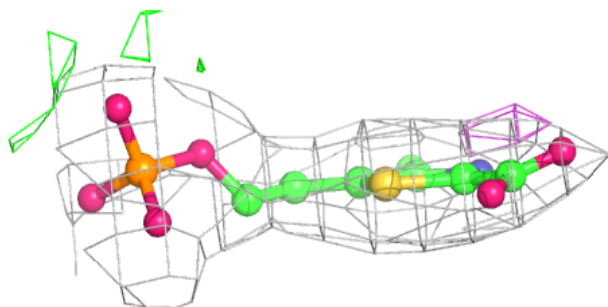
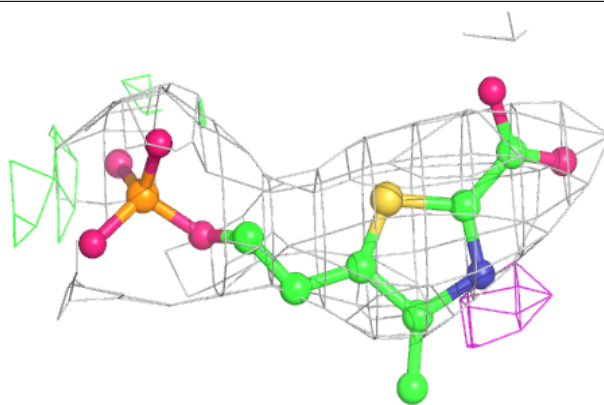
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	E	544	1/1	0.87	0.28	61,61,61,61	0
5	MG	B	544	1/1	0.90	0.31	56,56,56,56	0
5	MG	F	544	1/1	0.92	0.33	60,60,60,60	0
5	MG	D	544	1/1	0.92	0.27	61,61,61,61	0
2	3NM	B	541	16/16	0.94	0.21	76,78,85,88	0
5	MG	C	544	1/1	0.94	0.28	56,56,56,56	0
3	IFP	B	542	12/12	0.96	0.18	75,77,81,83	0
2	3NM	D	541	16/16	0.96	0.21	70,75,81,83	0
2	3NM	E	541	16/16	0.96	0.18	69,76,79,83	0
2	3NM	A	541	16/16	0.97	0.19	71,77,84,87	0
4	POP	E	543	9/9	0.97	0.19	64,79,88,90	0
4	POP	D	543	9/9	0.97	0.22	61,72,74,74	0
5	MG	A	544	1/1	0.97	0.32	66,66,66,66	0
4	POP	F	543	9/9	0.97	0.20	68,79,86,86	0
2	3NM	F	541	16/16	0.97	0.18	69,78,87,88	0
4	POP	A	543	9/9	0.97	0.19	64,80,89,91	0
4	POP	B	543	9/9	0.97	0.22	70,78,81,87	0
3	IFP	D	542	12/12	0.98	0.18	65,69,72,74	0
2	3NM	C	541	16/16	0.98	0.15	65,69,75,77	0
3	IFP	E	542	12/12	0.98	0.23	68,73,80,80	0
3	IFP	A	542	12/12	0.98	0.18	70,73,77,77	0
3	IFP	C	542	12/12	0.99	0.15	62,66,71,74	0
3	IFP	F	542	12/12	0.99	0.17	70,74,78,79	0
4	POP	C	543	9/9	0.99	0.17	62,72,80,82	0

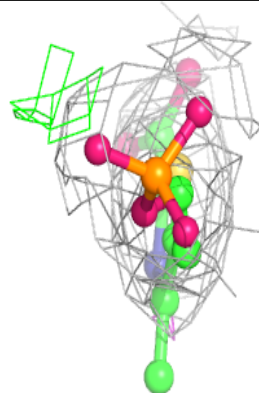
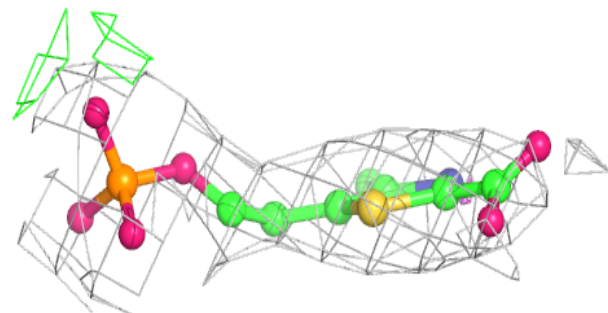
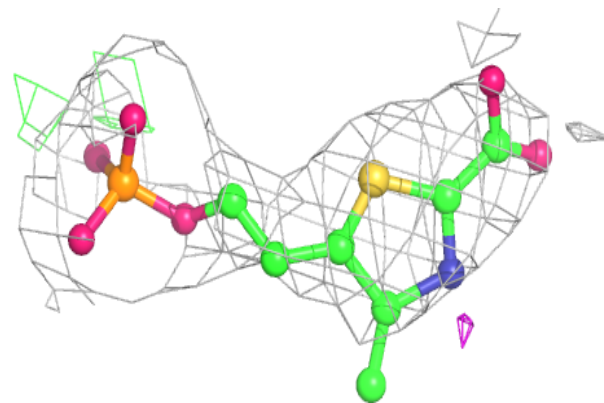
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 3NM B 541:**

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

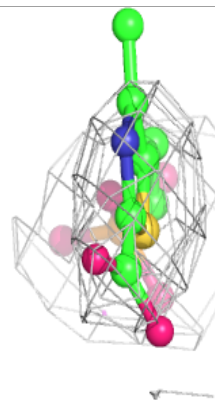
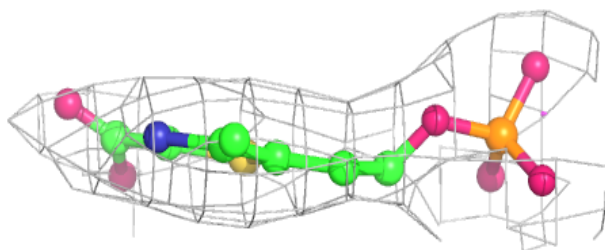
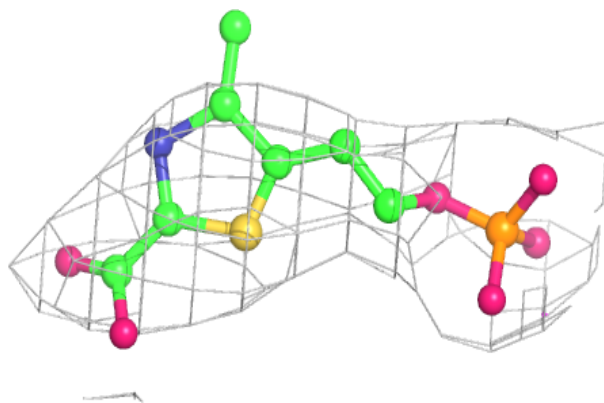
**Electron density around 3NM D 541:**

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

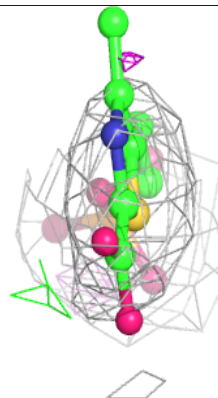
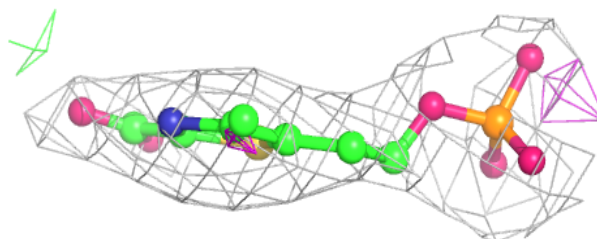
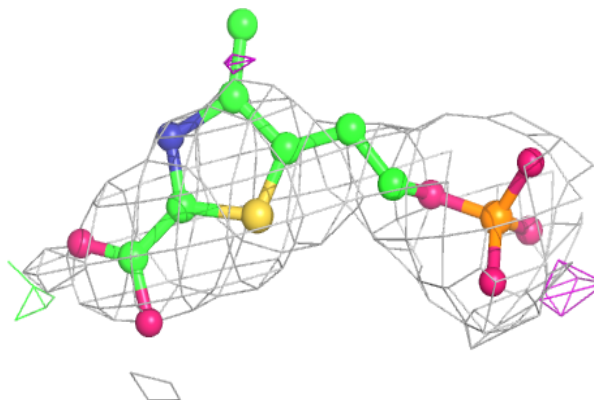


**Electron density around 3NM E 541:**

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

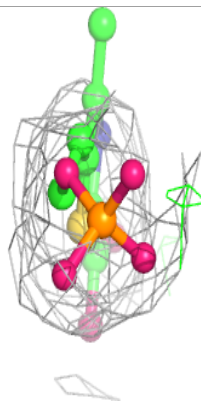
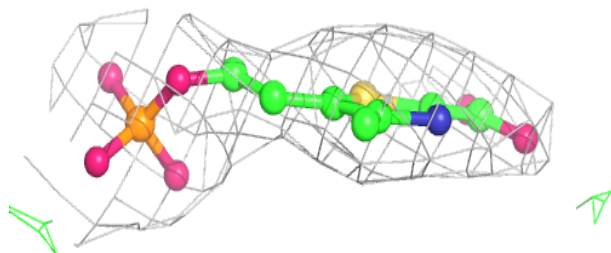
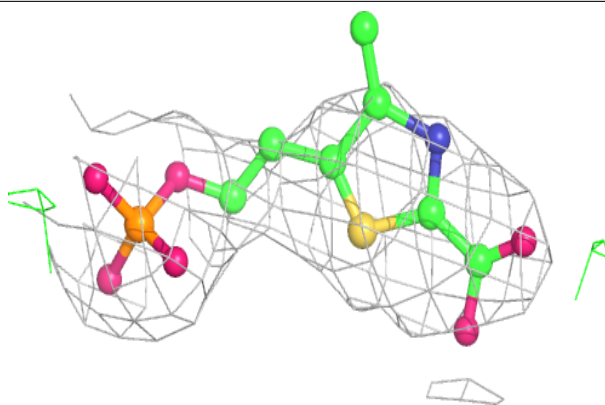
**Electron density around 3NM A 541:**

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

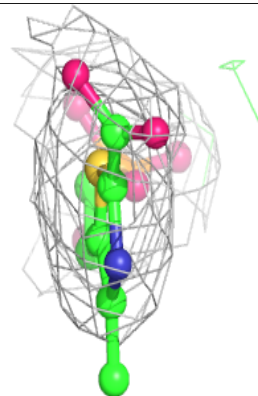
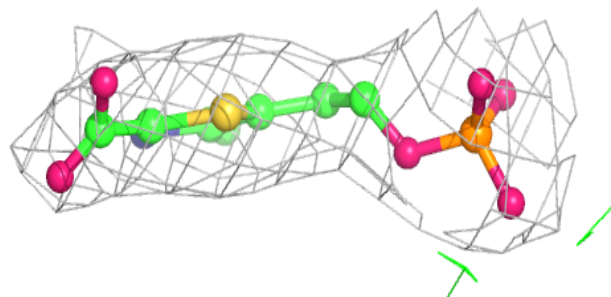
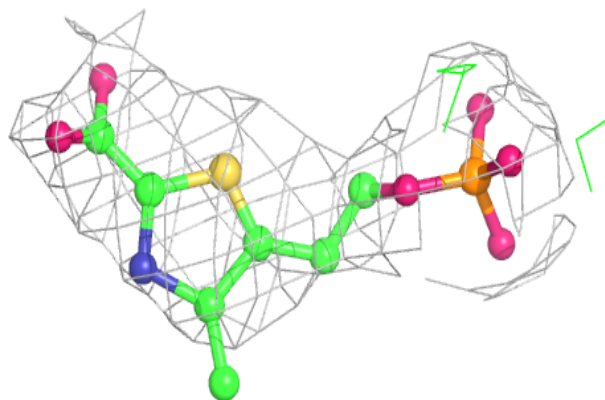


**Electron density around 3NM F 541:**

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

**Electron density around 3NM C 541:**

$2mF_o-DF_c$  (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.