



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:36 am BST

PDB ID : 3NM3  
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 : 3.10 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

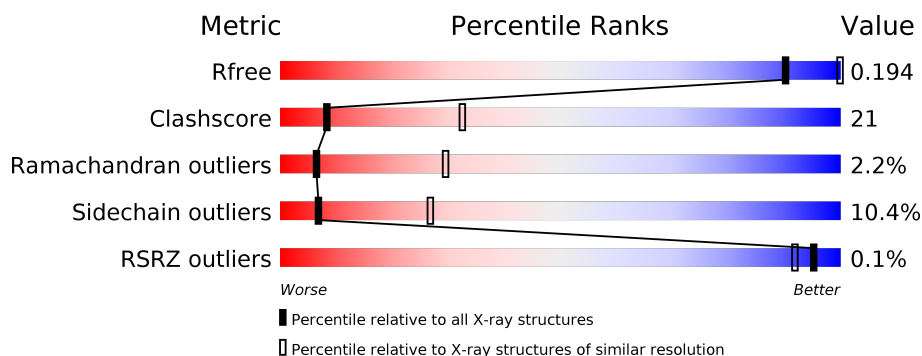
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	
1	B	540	
1	C	540	
1	D	540	
1	E	540	
1	F	540	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22991 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.

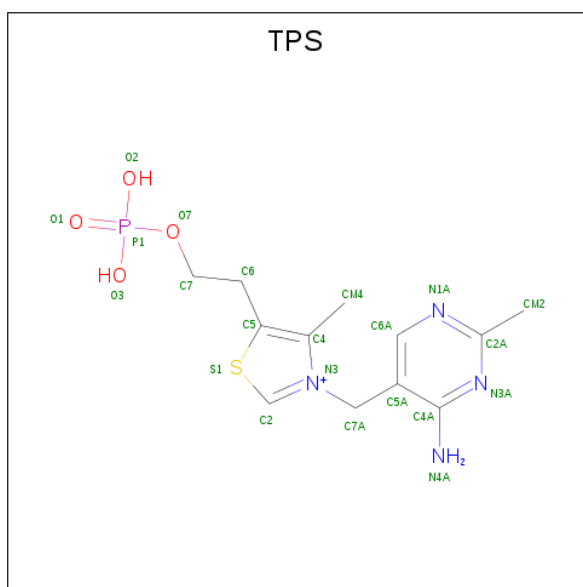
- Molecule 1 is a protein called Thiamine biosynthetic bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			3809	2408	643	736	22			
1	B	508	Total	C	N	O	S	0	0	0
			3799	2402	641	734	22			
1	C	510	Total	C	N	O	S	0	0	0
			3803	2403	642	736	22			
1	D	511	Total	C	N	O	S	0	0	0
			3812	2409	644	737	22			
1	E	507	Total	C	N	O	S	0	0	0
			3792	2397	640	733	22			
1	F	507	Total	C	N	O	S	0	0	0
			3784	2391	638	733	22			

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

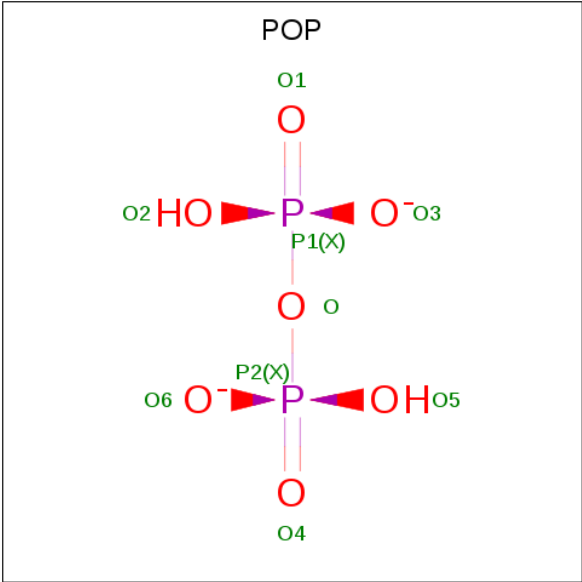
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMIN PHOSPHATE (three-letter code: TPS) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>4</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	B	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	C	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	D	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	E	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	F	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0

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

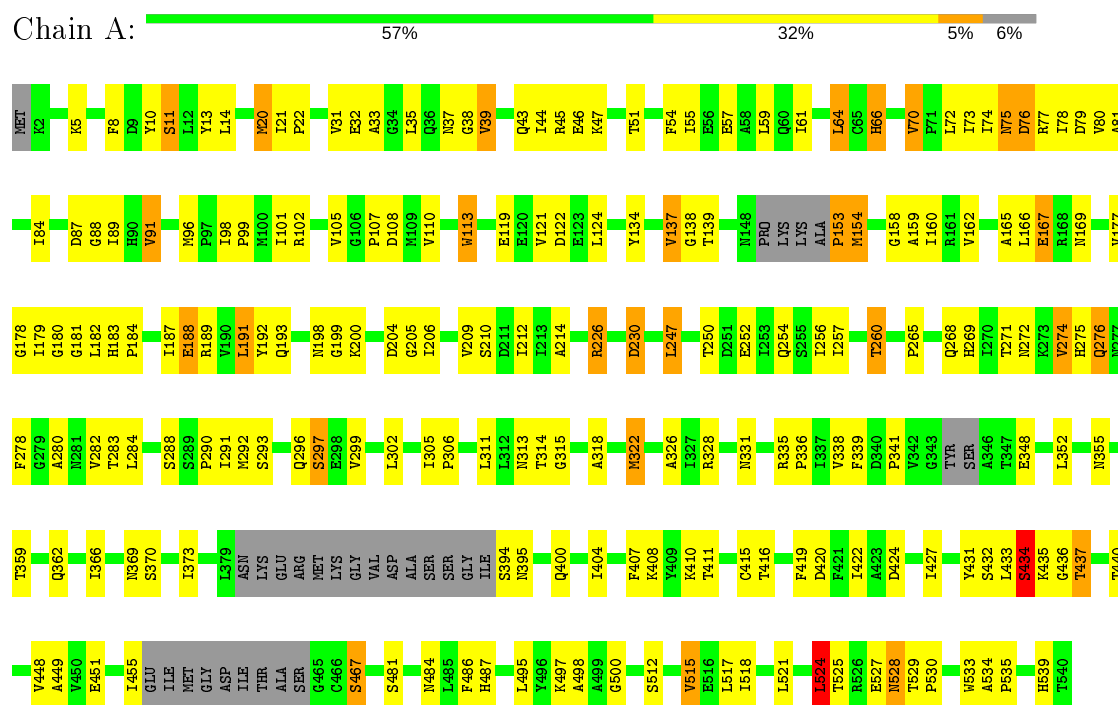


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		
4	C	1	Total	O	P	1	0
			9	7	2		
4	D	1	Total	O	P	0	0
			9	7	2		
4	E	1	Total	O	P	1	0
			9	7	2		
4	F	1	Total	O	P	0	0
			9	7	2		

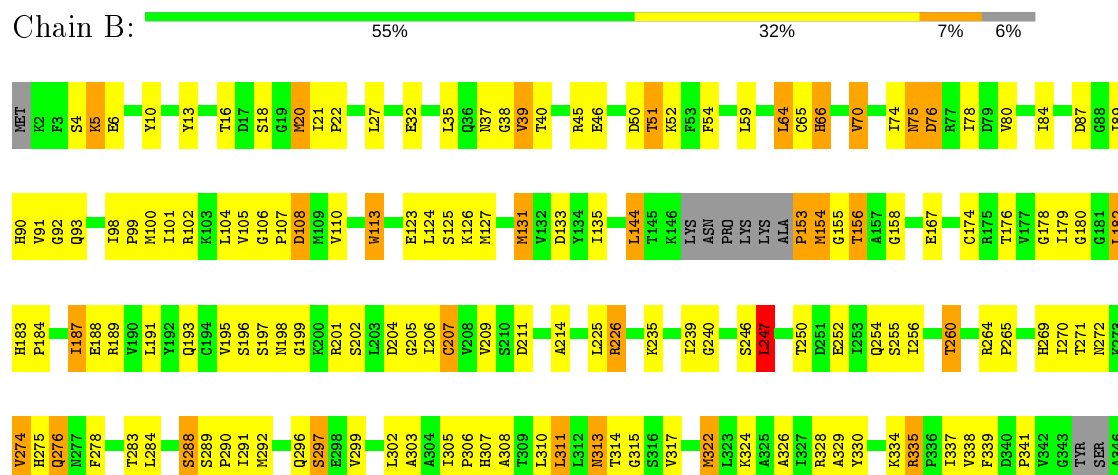
### 3 Residue-property plots

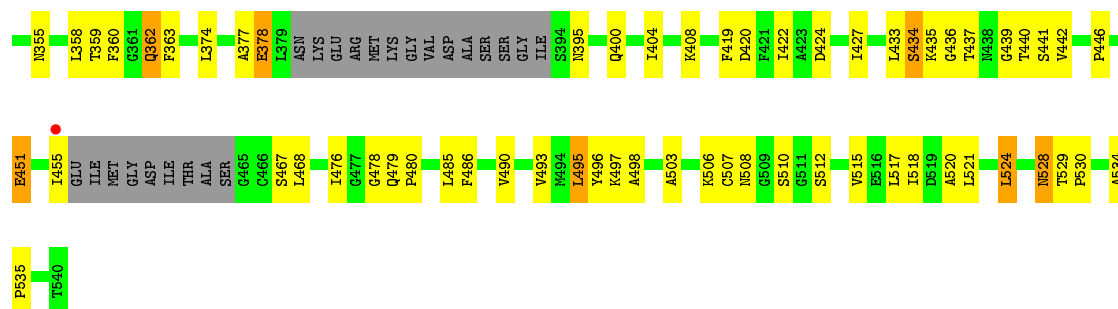
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



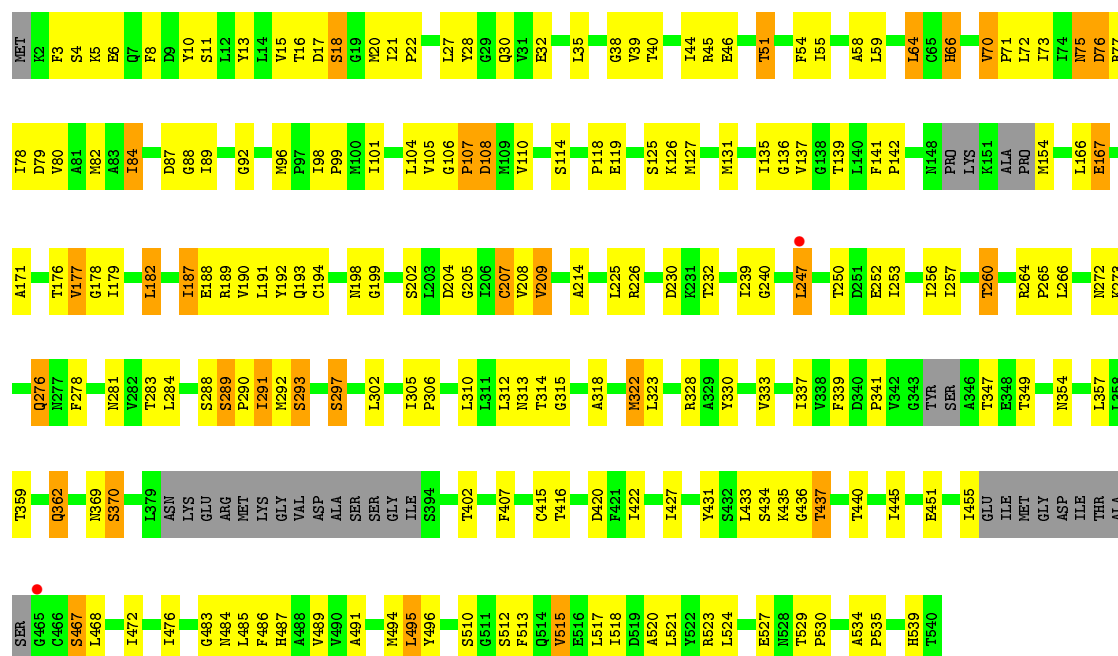
- Molecule 1: Thiamine biosynthetic bifunctional enzyme





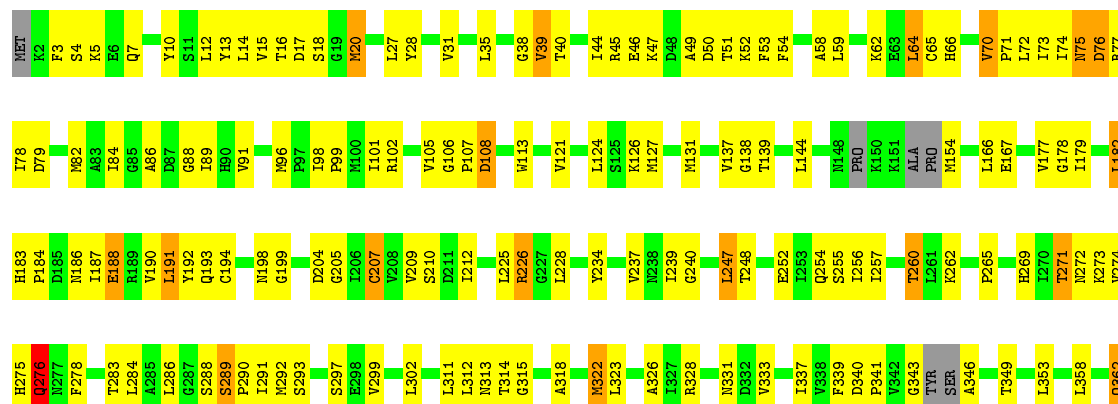
- Molecule 1: Thiamine biosynthetic bifunctional enzyme

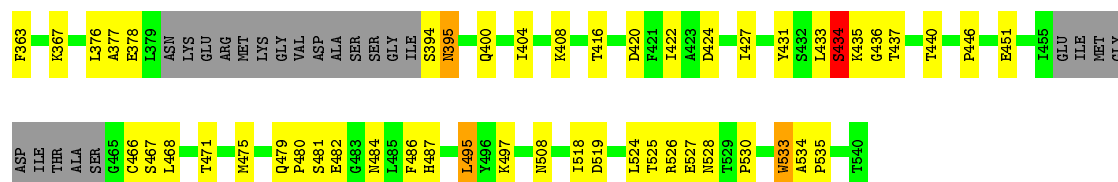
Chain C: 57% 31% 6% 6%



- Molecule 1: Thiamine biosynthetic bifunctional enzyme

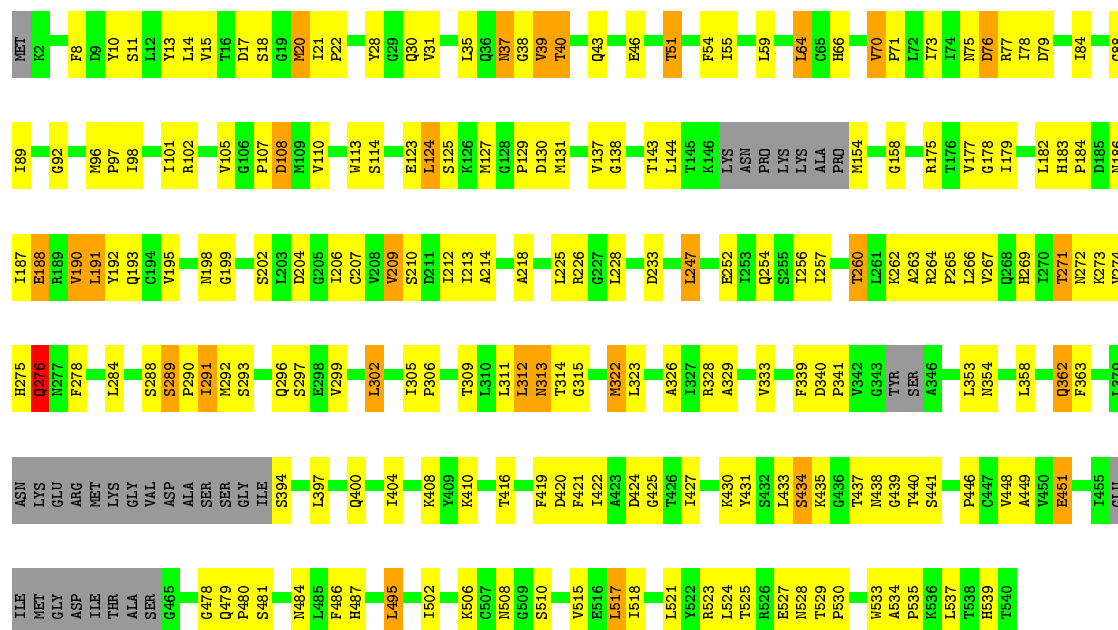
Chain D: 57% 34% 5%





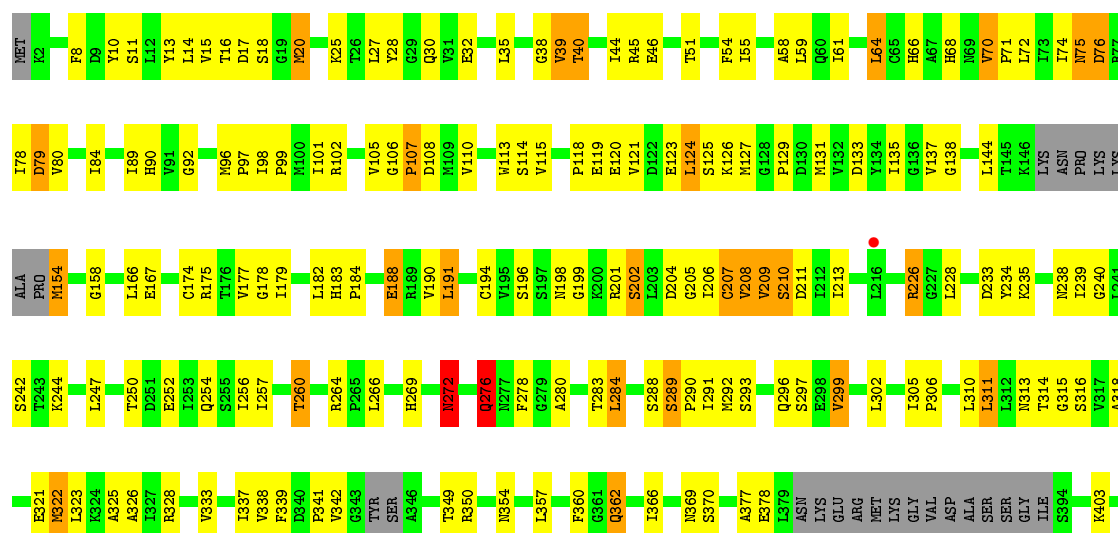
- Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain E: 56% 32% 5% 6%

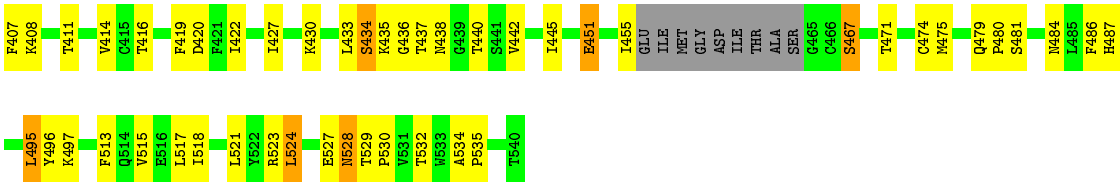


- Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain F: 53% 35% 6% 6%







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.19Å 154.60Å 148.65Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	46.00 – 3.10 47.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	80.6 (46.00-3.10) 59.4 (47.87-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.12Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, $R_{free}$	0.197 , 0.251 0.194 , 0.194	Depositor DCC
$R_{free}$ test set	2678 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 52.7	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	22991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.05% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPS, 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	0.37	0/3869	0.57	1/5246 (0.0%)
1	B	0.37	0/3859	0.57	1/5232 (0.0%)
1	C	0.37	0/3861	0.55	0/5235
1	D	0.38	0/3870	0.56	0/5246
1	E	0.37	0/3851	0.55	0/5221
1	F	0.36	0/3843	0.57	0/5213
All	All	0.37	0/23153	0.56	2/31393 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	PRO	CA-N-CD	-8.58	99.49	111.50
1	B	153	PRO	CA-N-CD	-8.57	99.51	111.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3809	0	3814	163	0
1	B	3799	0	3810	166	0
1	C	3803	0	3796	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3812	0	3809	156	0
1	E	3792	0	3802	162	0
1	F	3784	0	3780	173	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	22	0	16	4	0
3	B	22	0	16	3	0
3	C	22	0	16	0	0
3	D	22	0	16	1	0
3	E	22	0	16	4	0
3	F	22	0	16	4	0
4	A	9	0	0	2	0
4	B	9	0	0	1	0
4	C	9	0	0	2	0
4	D	9	0	0	1	0
4	E	9	0	0	0	0
4	F	9	0	0	1	0
All	All	22991	0	22907	962	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 21.

All (962) 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:F:209:VAL:HG11	1:F:213:ILE:HG12	1.27	1.13
1:A:167:GLU:HG2	1:A:198:ASN:HD21	1.14	1.12
1:F:208:VAL:HB	1:F:209:VAL:HA	1.30	1.08
1:C:266:LEU:HD11	1:C:291:ILE:HG13	1.43	1.01
1:B:78:ILE:HG13	1:B:89:ILE:HD12	1.45	0.96
1:F:266:LEU:HD11	1:F:291:ILE:HG13	1.50	0.94
1:F:167:GLU:HG2	1:F:198:ASN:HD21	1.31	0.94
1:F:44:ILE:HG13	1:F:72:LEU:HD11	1.54	0.90
1:D:167:GLU:HG2	1:D:198:ASN:HD21	1.37	0.90
1:A:265:PRO:HD2	1:A:288:SER:HB3	1.55	0.88
1:A:74:ILE:HD11	1:A:84:ILE:HD11	1.57	0.84
1:B:400:GLN:O	1:B:404:ILE:HG13	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:PHE:CE2	1:D:341:PRO:HG3	2.13	0.83
1:F:339:PHE:CE2	1:F:341:PRO:HG3	2.13	0.83
1:D:484:ASN:HD22	1:D:487:HIS:H	1.27	0.82
1:F:10:TYR:O	1:F:205:GLY:HA3	1.80	0.82
1:A:167:GLU:HG2	1:A:198:ASN:ND2	1.94	0.82
1:F:89:ILE:HD11	1:F:101:ILE:HG21	1.62	0.81
1:C:89:ILE:O	1:C:89:ILE:HG13	1.78	0.81
1:D:17:ASP:HB3	1:D:20:MET:HE2	1.61	0.80
1:A:44:ILE:HG13	1:A:72:LEU:HD11	1.63	0.80
1:E:339:PHE:CE2	1:E:341:PRO:HG3	2.16	0.80
1:C:199:GLY:O	1:C:437:THR:HG22	1.80	0.80
1:D:265:PRO:HD2	1:D:288:SER:HB3	1.65	0.79
1:F:254:GLN:HG3	1:F:528:ASN:HB3	1.65	0.79
1:D:286:LEU:HD11	1:D:471:THR:HG23	1.65	0.79
1:A:280:ALA:HB2	1:A:292:MET:HE3	1.63	0.78
1:A:59:LEU:HD21	1:A:84:ILE:HB	1.66	0.78
1:A:20:MET:HG2	1:A:214:ALA:HB2	1.63	0.78
1:B:339:PHE:CE2	1:B:341:PRO:HG3	2.18	0.78
1:A:101:ILE:O	1:A:105:VAL:HG22	1.84	0.78
1:B:74:ILE:HD11	1:B:84:ILE:HD11	1.64	0.78
1:C:35:LEU:HD22	1:C:70:VAL:HG11	1.66	0.77
1:C:265:PRO:HD2	1:C:288:SER:HB3	1.67	0.77
1:E:199:GLY:O	1:E:437:THR:HG22	1.85	0.77
1:E:358:LEU:HD23	1:E:363:PHE:HE1	1.49	0.77
1:E:89:ILE:HD11	1:E:101:ILE:HG21	1.65	0.76
1:D:137:VAL:HG22	1:D:178:GLY:HA2	1.66	0.76
1:D:484:ASN:ND2	1:D:487:HIS:H	1.84	0.76
1:E:59:LEU:HD21	1:E:84:ILE:HB	1.67	0.76
1:C:520:ALA:O	1:C:524:LEU:HB2	1.86	0.76
1:D:127:MET:HB3	1:D:131:MET:HG3	1.68	0.76
1:E:40:THR:HG21	1:E:226:ARG:HH21	1.51	0.75
1:F:208:VAL:HG23	1:F:209:VAL:HG22	1.66	0.75
1:E:299:VAL:HG11	1:E:326:ALA:HA	1.68	0.75
1:C:167:GLU:HG2	1:C:198:ASN:HD21	1.50	0.75
1:E:272:ASN:O	1:E:276:GLN:HG2	1.87	0.75
1:D:256:ILE:O	1:D:260:THR:HG22	1.87	0.74
1:D:127:MET:HE3	1:D:131:MET:HB3	1.68	0.74
1:B:254:GLN:HG3	1:B:528:ASN:HB3	1.69	0.73
1:F:101:ILE:O	1:F:105:VAL:HG22	1.87	0.73
1:F:137:VAL:HG22	1:F:177:VAL:O	1.88	0.73
1:B:179:ILE:HG12	1:B:180:GLY:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PRO:HB2	1:D:292:MET:HE2	1.70	0.73
1:B:265:PRO:HD2	1:B:288:SER:HB3	1.69	0.73
1:C:407:PHE:HE2	1:C:427:ILE:HD11	1.53	0.73
1:F:407:PHE:HE2	1:F:427:ILE:HD11	1.52	0.73
1:E:437:THR:O	1:E:439:GLY:N	2.22	0.73
1:D:35:LEU:HD22	1:D:70:VAL:HG11	1.70	0.72
1:D:44:ILE:HG13	1:D:72:LEU:HD11	1.71	0.72
1:B:101:ILE:O	1:B:105:VAL:HG22	1.90	0.72
1:B:270:ILE:HD12	1:B:310:LEU:HD11	1.69	0.72
1:F:190:VAL:O	1:F:194:CYS:HB2	1.90	0.71
1:B:269:HIS:CD2	1:B:311:LEU:HD12	2.26	0.70
1:E:43:GLN:HE22	3:E:2005:TPS:HM21	1.55	0.70
1:D:193:GLN:NE2	1:D:362:GLN:HE21	1.88	0.70
1:D:10:TYR:O	1:D:205:GLY:HA3	1.91	0.70
1:C:80:VAL:O	1:C:84:ILE:HG23	1.92	0.70
1:A:280:ALA:HB2	1:A:292:MET:CE	2.21	0.70
1:B:269:HIS:HD2	1:B:311:LEU:HD12	1.55	0.70
1:D:14:LEU:HD13	1:D:212:ILE:HD12	1.74	0.70
1:B:98:ILE:HD11	1:B:113:TRP:CD1	2.27	0.69
1:A:250:THR:HG23	1:A:530:PRO:HB2	1.74	0.69
1:A:91:VAL:HG11	1:A:101:ILE:HD13	1.75	0.69
1:A:420:ASP:OD2	1:A:497:LYS:HD3	1.92	0.69
1:A:254:GLN:HG3	1:A:528:ASN:HB3	1.74	0.69
1:A:373:ILE:HG13	1:A:415:CYS:HB2	1.73	0.69
1:B:154:MET:O	1:B:154:MET:HG3	1.91	0.69
1:B:272:ASN:O	1:B:276:GLN:HG2	1.92	0.69
1:B:20:MET:HG2	1:B:214:ALA:HB2	1.75	0.69
1:E:358:LEU:HD23	1:E:363:PHE:CE1	2.28	0.69
1:F:89:ILE:CD1	1:F:101:ILE:HG21	2.22	0.69
1:F:272:ASN:O	1:F:276:GLN:HG2	1.92	0.69
1:D:204:ASP:OD1	1:D:434:SER:HB3	1.92	0.69
1:A:78:ILE:O	1:A:81:ALA:HB3	1.93	0.69
1:F:422:ILE:HG22	1:F:486:PHE:HE1	1.58	0.69
1:C:187:ILE:HD12	1:C:225:LEU:HD22	1.75	0.68
1:E:265:PRO:HD2	1:E:288:SER:HB3	1.75	0.68
1:D:167:GLU:HG2	1:D:198:ASN:ND2	2.08	0.68
1:A:137:VAL:CG2	1:A:178:GLY:HA2	2.24	0.68
1:E:101:ILE:O	1:E:105:VAL:HG22	1.94	0.68
1:F:208:VAL:HB	1:F:209:VAL:CA	2.18	0.68
1:E:195:VAL:HG12	1:E:202:SER:HB3	1.76	0.68
1:B:260:THR:HA	1:B:478:GLY:HA3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ILE:HD11	1:D:101:ILE:HG21	1.76	0.67
1:B:437:THR:HG21	1:B:440:THR:O	1.95	0.67
1:A:268:GLN:OE1	1:A:302:LEU:HD23	1.95	0.67
1:F:534:ALA:N	1:F:535:PRO:HD2	2.10	0.67
1:E:78:ILE:HG13	1:E:89:ILE:HD12	1.75	0.67
1:E:73:ILE:HG23	1:E:88:GLY:C	2.14	0.67
1:A:534:ALA:N	1:A:535:PRO:HD2	2.10	0.67
1:B:311:LEU:HD23	1:B:338:VAL:HB	1.77	0.67
1:D:314:THR:HG23	1:D:353:LEU:HD23	1.76	0.66
1:E:534:ALA:N	1:E:535:PRO:HD2	2.10	0.66
1:A:154:MET:SD	1:A:158:GLY:HA3	2.35	0.66
1:A:137:VAL:HG23	1:A:178:GLY:HA2	1.76	0.66
1:C:416:THR:HA	1:C:420:ASP:OD1	1.95	0.66
1:F:182:LEU:HD23	1:F:206:ILE:HG23	1.78	0.66
1:C:407:PHE:CE2	1:C:427:ILE:HD11	2.31	0.66
1:A:89:ILE:HD11	1:A:101:ILE:HG21	1.75	0.66
1:E:508:ASN:HB3	1:F:523:ARG:NH1	2.11	0.66
1:C:17:ASP:HB3	1:C:20:MET:HE1	1.76	0.66
1:D:276:GLN:HE21	1:D:276:GLN:HA	1.59	0.65
1:B:40:THR:HG21	1:B:226:ARG:HH21	1.62	0.65
1:A:154:MET:HG3	1:A:158:GLY:HA3	1.79	0.65
1:D:254:GLN:HG3	1:D:528:ASN:HB3	1.77	0.65
1:F:233:ASP:OD1	1:F:430:LYS:HE2	1.97	0.65
1:A:252:GLU:O	1:A:256:ILE:HG12	1.97	0.65
1:B:89:ILE:HD11	1:B:101:ILE:CG2	2.27	0.65
1:C:467:SER:HB2	1:C:496:TYR:CE1	2.31	0.65
1:D:290:PRO:HB2	1:D:292:MET:CE	2.27	0.65
1:F:407:PHE:CE2	1:F:427:ILE:HD11	2.32	0.65
1:B:179:ILE:HG13	1:B:207:CYS:HB3	1.79	0.65
1:E:123:GLU:O	1:E:127:MET:HG3	1.96	0.65
1:E:15:VAL:HB	1:E:209:VAL:CG2	2.27	0.65
1:E:78:ILE:HD13	1:E:96:MET:HE2	1.79	0.65
1:F:314:THR:HG22	1:F:315:GLY:H	1.59	0.65
1:A:35:LEU:HD22	1:A:70:VAL:HG11	1.80	0.65
1:A:204:ASP:OD1	1:A:434:SER:HB3	1.96	0.64
1:F:35:LEU:CD2	1:F:70:VAL:HG11	2.27	0.64
1:B:256:ILE:O	1:B:260:THR:HG22	1.96	0.64
1:B:419:PHE:CE1	1:B:451:GLU:HG2	2.32	0.64
1:C:20:MET:HG2	1:C:214:ALA:HB2	1.79	0.64
1:C:422:ILE:HG22	1:C:486:PHE:HE1	1.61	0.64
1:C:272:ASN:O	1:C:276:GLN:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ILE:O	1:D:105:VAL:HG22	1.96	0.64
1:E:322:MET:HG3	1:E:323:LEU:N	2.11	0.64
1:A:296:GLN:HG3	1:A:322:MET:HB2	1.79	0.64
1:C:32:GLU:HB2	1:C:64:LEU:HD11	1.78	0.64
1:D:484:ASN:HD21	1:D:486:PHE:HB3	1.63	0.64
1:E:37:ASN:HD22	1:E:37:ASN:N	1.96	0.64
1:A:407:PHE:HE2	1:A:427:ILE:HD11	1.63	0.64
1:F:310:LEU:HD23	1:F:337:ILE:HG23	1.80	0.63
1:A:80:VAL:O	1:A:84:ILE:HG12	1.97	0.63
1:F:10:TYR:HE1	1:F:175:ARG:HG3	1.64	0.63
1:B:153:PRO:O	1:B:153:PRO:HD2	1.98	0.63
1:F:35:LEU:HD22	1:F:70:VAL:HG11	1.81	0.63
1:C:58:ALA:HB1	1:C:84:ILE:HD13	1.80	0.63
1:A:529:THR:N	1:A:530:PRO:HD3	2.14	0.63
1:B:211:ASP:OD2	1:B:225:LEU:HD11	1.99	0.63
1:C:15:VAL:HB	1:C:209:VAL:HG22	1.79	0.63
1:E:419:PHE:CE1	1:E:451:GLU:HG2	2.34	0.63
1:E:8:PHE:CE1	1:E:110:VAL:HG21	2.34	0.63
1:D:199:GLY:O	1:D:437:THR:HG22	1.99	0.62
1:F:78:ILE:HD12	1:F:78:ILE:N	2.13	0.62
1:E:78:ILE:HD12	1:E:78:ILE:N	2.14	0.62
1:F:455:ILE:O	1:F:455:ILE:HG22	1.99	0.62
1:C:318:ALA:HB1	1:C:322:MET:HG2	1.81	0.62
1:D:3:PHE:CD2	1:D:71:PRO:HG3	2.34	0.62
1:A:153:PRO:HD2	1:A:153:PRO:O	1.98	0.62
1:D:322:MET:HE3	1:D:326:ALA:HB2	1.81	0.62
1:F:202:SER:HB3	1:F:436:GLY:HA3	1.82	0.62
1:F:199:GLY:O	1:F:437:THR:HG22	1.98	0.62
1:F:256:ILE:O	1:F:260:THR:HG22	1.99	0.62
1:F:179:ILE:HG13	1:F:207:CYS:HB3	1.80	0.62
1:F:484:ASN:HD22	1:F:487:HIS:H	1.47	0.62
1:F:322:MET:HG3	1:F:323:LEU:N	2.14	0.62
1:B:156:THR:HG21	1:B:193:GLN:HG3	1.82	0.62
1:A:199:GLY:O	1:A:437:THR:HG22	2.00	0.62
1:B:269:HIS:HB2	1:B:292:MET:SD	2.40	0.62
1:D:77:ARG:HH12	1:E:77:ARG:HG2	1.63	0.62
1:F:28:TYR:CE1	1:F:64:LEU:HD12	2.35	0.62
1:B:38:GLY:O	1:B:39:VAL:C	2.37	0.61
1:C:484:ASN:HD22	1:C:487:HIS:H	1.47	0.61
1:E:15:VAL:HB	1:E:209:VAL:HG22	1.82	0.61
1:D:35:LEU:CD2	1:D:70:VAL:HG11	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ARG:HG2	1:E:264:ARG:O	2.00	0.61
1:C:190:VAL:O	1:C:194:CYS:HB2	2.01	0.61
1:E:437:THR:HG21	1:E:440:THR:O	2.00	0.61
1:A:14:LEU:HD13	1:A:212:ILE:HD12	1.80	0.61
1:C:78:ILE:HG12	1:C:96:MET:HE2	1.83	0.61
1:D:314:THR:CG2	1:D:353:LEU:HD23	2.31	0.61
1:D:38:GLY:O	1:D:39:VAL:C	2.39	0.61
1:A:181:GLY:O	1:A:183:HIS:HD2	1.84	0.61
1:C:78:ILE:HG22	1:C:82:MET:CE	2.31	0.61
1:F:269:HIS:HB2	1:F:292:MET:SD	2.41	0.61
1:B:420:ASP:OD2	1:B:497:LYS:HD3	2.00	0.60
1:E:78:ILE:HD12	1:E:78:ILE:H	1.66	0.60
1:C:18:SER:HB2	1:C:46:GLU:OE2	2.00	0.60
1:C:310:LEU:HD13	1:C:330:TYR:CE1	2.35	0.60
1:C:534:ALA:N	1:C:535:PRO:HD2	2.16	0.60
1:F:32:GLU:HB2	1:F:64:LEU:HD11	1.82	0.60
1:A:272:ASN:O	1:A:276:GLN:HG2	2.00	0.60
1:B:89:ILE:HD11	1:B:101:ILE:HG21	1.82	0.60
1:F:420:ASP:OD2	1:F:497:LYS:HD3	2.01	0.60
1:A:154:MET:CG	1:A:158:GLY:HA3	2.31	0.60
1:A:305:ILE:HG23	1:A:306:PRO:HD2	1.84	0.60
1:B:154:MET:HG3	1:B:158:GLY:HA3	1.83	0.60
1:F:416:THR:HA	1:F:420:ASP:OD1	2.02	0.60
1:A:437:THR:HG21	1:A:440:THR:O	2.01	0.60
1:A:265:PRO:O	1:A:288:SER:HB2	2.01	0.59
1:B:193:GLN:NE2	1:B:362:GLN:HE21	2.00	0.59
1:A:183:HIS:HB3	1:A:184:PRO:HD2	1.84	0.59
1:F:10:TYR:CE1	1:F:175:ARG:HG3	2.37	0.59
1:F:252:GLU:O	1:F:256:ILE:HG12	2.01	0.59
1:B:534:ALA:N	1:B:535:PRO:HD2	2.16	0.59
1:E:314:THR:HG22	1:E:315:GLY:N	2.16	0.59
1:F:283:THR:HB	1:F:290:PRO:HG3	1.85	0.59
1:A:89:ILE:HD11	1:A:101:ILE:CG2	2.33	0.59
1:E:193:GLN:NE2	1:E:362:GLN:HE21	2.01	0.59
1:D:193:GLN:HE21	1:D:362:GLN:HE21	1.51	0.59
1:E:523:ARG:O	1:E:527:GLU:HG2	2.03	0.59
1:A:495:LEU:HD22	1:A:521:LEU:CD2	2.32	0.59
1:B:91:VAL:HG11	1:B:101:ILE:HD13	1.83	0.59
1:B:308:ALA:O	1:B:335:ARG:HD3	2.03	0.59
1:F:28:TYR:CZ	1:F:64:LEU:HG	2.38	0.59
1:A:437:THR:HG23	1:A:440:THR:H	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ILE:N	1:B:422:ILE:HD12	2.18	0.58
1:F:209:VAL:CG1	1:F:213:ILE:H	2.16	0.58
1:A:198:ASN:OD1	1:A:200:LYS:HB2	2.02	0.58
1:D:254:GLN:HG3	1:D:528:ASN:HD22	1.68	0.58
1:A:269:HIS:HB2	1:A:292:MET:SD	2.44	0.58
1:A:495:LEU:HD22	1:A:521:LEU:HD23	1.85	0.58
1:B:252:GLU:O	1:B:256:ILE:HG12	2.03	0.58
1:E:311:LEU:HD22	1:E:312:LEU:H	1.67	0.58
1:A:98:ILE:HD11	1:A:113:TRP:CD1	2.39	0.58
1:C:179:ILE:HG13	1:C:207:CYS:HB3	1.86	0.58
1:D:400:GLN:O	1:D:404:ILE:HG13	2.04	0.58
1:C:136:GLY:HA2	1:C:177:VAL:HG23	1.86	0.58
1:D:358:LEU:HD23	1:D:363:PHE:HE1	1.68	0.58
1:F:154:MET:SD	1:F:158:GLY:HA3	2.43	0.58
1:F:208:VAL:CB	1:F:209:VAL:HA	2.12	0.58
1:E:252:GLU:O	1:E:256:ILE:HG12	2.03	0.58
1:F:257:ILE:HB	1:F:528:ASN:ND2	2.19	0.58
1:C:167:GLU:HG2	1:C:198:ASN:ND2	2.19	0.58
1:A:407:PHE:CE2	1:A:427:ILE:HD11	2.38	0.58
1:A:59:LEU:CD2	1:A:84:ILE:HB	2.32	0.58
1:C:78:ILE:HG12	1:C:96:MET:CE	2.34	0.58
1:D:16:THR:O	1:D:45:ARG:HB3	2.03	0.58
1:C:265:PRO:O	1:C:288:SER:HB2	2.04	0.57
1:E:528:ASN:C	1:E:530:PRO:HD3	2.23	0.57
1:B:5:LYS:HZ1	1:B:108:ASP:H	1.51	0.57
1:E:314:THR:HG23	1:E:353:LEU:HD23	1.85	0.57
1:B:91:VAL:HG11	1:B:101:ILE:CD1	2.35	0.57
1:C:78:ILE:N	1:C:78:ILE:HD12	2.20	0.57
1:D:528:ASN:C	1:D:530:PRO:HD3	2.24	0.57
4:F:4006:POP:O3	4:F:4006:POP:O6	2.20	0.57
1:B:299:VAL:HG11	1:B:326:ALA:HA	1.86	0.57
1:C:297:SER:HB2	1:D:349:THR:OG1	2.05	0.57
1:D:299:VAL:HG11	1:D:326:ALA:HA	1.86	0.57
1:F:414:VAL:HG22	1:F:422:ILE:HG13	1.86	0.57
1:E:40:THR:HG21	1:E:226:ARG:NH2	2.18	0.57
1:F:110:VAL:HA	1:F:133:ASP:OD2	2.04	0.57
1:B:377:ALA:O	1:B:378:GLU:HB2	2.04	0.57
1:C:127:MET:HB3	1:C:131:MET:HG3	1.84	0.57
1:F:8:PHE:CE1	1:F:110:VAL:HG21	2.40	0.57
1:B:305:ILE:HG23	1:B:306:PRO:HD2	1.87	0.57
1:B:424:ASP:HB2	1:B:486:PHE:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HG12	1:A:80:VAL:HG13	1.87	0.57
1:B:195:VAL:HG12	1:B:202:SER:HB3	1.86	0.57
1:C:101:ILE:O	1:C:105:VAL:HG22	2.05	0.57
1:D:394:SER:OG	1:D:395:ASN:N	2.38	0.57
1:E:233:ASP:OD1	1:E:430:LYS:HE3	2.05	0.57
1:B:271:THR:HB	1:B:313:ASN:HB2	1.87	0.56
1:E:278:PHE:CE1	1:E:518:ILE:HD11	2.40	0.56
1:B:424:ASP:HB3	1:B:446:PRO:HG2	1.86	0.56
1:A:283:THR:HB	1:A:290:PRO:HG3	1.86	0.56
1:B:100:MET:O	1:B:104:LEU:HG	2.04	0.56
1:B:427:ILE:HG22	1:B:427:ILE:O	2.05	0.56
1:E:17:ASP:HB3	1:E:20:MET:HE1	1.87	0.56
1:A:11:SER:HB3	1:A:226:ARG:NH2	2.21	0.56
1:C:125:SER:C	1:C:127:MET:H	2.08	0.56
1:C:28:TYR:CZ	1:C:64:LEU:HG	2.40	0.56
1:B:35:LEU:HD22	1:B:70:VAL:HG11	1.87	0.56
1:C:89:ILE:HD11	1:C:101:ILE:HG21	1.87	0.56
1:E:305:ILE:HG23	1:E:306:PRO:HD2	1.87	0.56
1:E:422:ILE:HG22	1:E:486:PHE:HE1	1.70	0.56
1:E:278:PHE:HE1	1:E:518:ILE:HD11	1.70	0.56
1:F:264:ARG:O	1:F:264:ARG:HG2	2.05	0.56
1:A:271:THR:HA	1:A:313:ASN:HB2	1.86	0.56
1:A:291:ILE:HG22	1:A:293:SER:H	1.70	0.56
1:A:419:PHE:CE1	1:A:451:GLU:HG2	2.41	0.56
1:B:176:THR:O	1:B:204:ASP:HB2	2.04	0.56
1:B:307:HIS:HA	1:B:335:ARG:NH1	2.21	0.56
1:B:296:GLN:HG2	1:B:322:MET:HB2	1.88	0.56
1:A:256:ILE:O	1:A:260:THR:HG22	2.05	0.56
1:A:265:PRO:HD2	1:A:288:SER:CB	2.34	0.56
1:A:32:GLU:HB2	1:A:64:LEU:HD11	1.87	0.56
1:B:18:SER:HB2	1:B:46:GLU:OE2	2.05	0.56
1:C:310:LEU:HD23	1:C:337:ILE:HG23	1.88	0.56
1:D:271:THR:HA	1:D:313:ASN:HB2	1.87	0.55
1:F:242:SER:HB2	1:F:244:LYS:HE2	1.88	0.55
1:B:199:GLY:O	1:B:437:THR:HG22	2.05	0.55
1:D:339:PHE:HE2	1:D:341:PRO:HG3	1.70	0.55
1:D:437:THR:HG21	1:D:440:THR:O	2.06	0.55
1:F:121:VAL:CG1	1:F:166:LEU:HD23	2.36	0.55
1:B:204:ASP:CG	1:B:434:SER:HB3	2.26	0.55
1:C:232:THR:HG22	1:C:431:TYR:O	2.06	0.55
1:C:59:LEU:HD21	1:C:84:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:529:THR:O	1:F:532:THR:HB	2.07	0.55
1:D:183:HIS:O	1:D:187:ILE:HG13	2.06	0.55
1:B:187:ILE:HD12	1:B:225:LEU:HD22	1.88	0.55
1:E:421:PHE:C	1:E:422:ILE:HD12	2.27	0.55
1:B:314:THR:HG22	1:B:315:GLY:N	2.22	0.55
1:B:264:ARG:HG2	1:B:264:ARG:O	2.07	0.55
1:C:98:ILE:N	1:C:99:PRO:HD2	2.22	0.55
1:D:137:VAL:CG2	1:D:178:GLY:HA2	2.35	0.55
1:B:187:ILE:HG23	1:B:206:ILE:HD13	1.87	0.55
1:C:40:THR:HG21	1:C:226:ARG:HH21	1.72	0.55
1:E:209:VAL:HB	3:E:2005:TPS:O7	2.07	0.55
1:E:254:GLN:HG3	1:E:528:ASN:HB3	1.89	0.55
1:A:66:HIS:HE1	1:A:87:ASP:OD1	1.90	0.54
1:E:14:LEU:HD13	1:E:212:ILE:HD12	1.89	0.54
1:F:257:ILE:HB	1:F:528:ASN:HD21	1.72	0.54
1:B:16:THR:HB	1:B:27:LEU:HD11	1.89	0.54
1:E:37:ASN:N	1:E:37:ASN:ND2	2.54	0.54
1:D:187:ILE:HD12	1:D:225:LEU:HD22	1.88	0.54
1:D:78:ILE:HG13	1:D:89:ILE:HD12	1.88	0.54
1:F:419:PHE:CE1	1:F:451:GLU:HG2	2.43	0.54
1:E:247:LEU:HD13	1:E:539:HIS:NE2	2.22	0.54
1:E:107:PRO:O	1:E:108:ASP:CB	2.56	0.54
1:F:495:LEU:HD22	1:F:521:LEU:HD23	1.90	0.54
1:A:47:LYS:NZ	4:A:4001:POP:O4	2.39	0.54
1:E:422:ILE:HD12	1:E:422:ILE:N	2.22	0.54
1:A:366:ILE:HD12	1:A:411:THR:HG21	1.90	0.54
1:D:337:ILE:HG21	1:D:363:PHE:CD2	2.43	0.54
1:E:154:MET:HG3	1:E:158:GLY:HA3	1.90	0.54
1:A:484:ASN:HD22	1:A:487:HIS:H	1.55	0.53
1:E:15:VAL:O	1:E:209:VAL:HG22	2.07	0.53
1:F:124:LEU:HD23	1:F:124:LEU:C	2.28	0.53
1:A:10:TYR:O	1:A:205:GLY:HA3	2.07	0.53
1:A:419:PHE:CD1	1:A:451:GLU:HG2	2.43	0.53
1:C:45:ARG:NH2	4:C:4003:POP:O5	2.38	0.53
1:C:3:PHE:CD2	1:C:71:PRO:HG3	2.43	0.53
1:E:187:ILE:CD1	1:E:225:LEU:HD22	2.38	0.53
1:E:339:PHE:HE2	1:E:341:PRO:HG3	1.72	0.53
1:B:189:ARG:O	1:B:193:GLN:HG2	2.08	0.53
1:D:107:PRO:O	1:D:108:ASP:CB	2.57	0.53
1:E:433:LEU:O	1:E:435:LYS:N	2.40	0.53
1:F:98:ILE:N	1:F:99:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ALA:HB1	1:D:322:MET:HG2	1.91	0.53
1:E:20:MET:HG2	1:E:214:ALA:HB2	1.90	0.53
1:E:400:GLN:O	1:E:404:ILE:HG13	2.08	0.53
1:E:495:LEU:HD11	1:E:525:THR:HG22	1.91	0.53
1:D:192:TYR:CD1	1:D:234:TYR:HD2	2.26	0.53
1:E:262:LYS:HG2	1:E:262:LYS:O	2.06	0.53
1:F:366:ILE:HG13	1:F:411:THR:HG21	1.90	0.53
1:E:527:GLU:HG3	1:E:527:GLU:O	2.07	0.53
1:D:248:THR:HG23	1:D:487:HIS:ND1	2.23	0.53
1:C:107:PRO:O	1:C:108:ASP:CB	2.56	0.53
1:C:35:LEU:CD2	1:C:70:VAL:HG11	2.37	0.53
1:D:102:ARG:NH1	1:D:107:PRO:HA	2.24	0.53
1:E:59:LEU:CD2	1:E:84:ILE:HB	2.37	0.53
1:C:127:MET:HE1	1:C:131:MET:HB3	1.91	0.53
1:C:523:ARG:NH1	1:D:508:ASN:HB3	2.22	0.53
1:D:433:LEU:O	1:D:435:LYS:N	2.40	0.53
1:E:484:ASN:HD22	1:E:487:HIS:H	1.56	0.53
1:F:16:THR:CG2	1:F:27:LEU:HD11	2.39	0.53
1:B:107:PRO:O	1:B:108:ASP:CB	2.57	0.52
1:C:189:ARG:O	1:C:193:GLN:HG2	2.09	0.52
1:B:125:SER:C	1:B:127:MET:H	2.12	0.52
1:D:252:GLU:O	1:D:256:ILE:HG12	2.08	0.52
1:A:311:LEU:HD23	1:A:338:VAL:HB	1.91	0.52
1:B:16:THR:O	1:B:45:ARG:HB3	2.08	0.52
1:C:139:THR:O	1:C:154:MET:HB3	2.10	0.52
1:E:266:LEU:CD1	1:E:291:ILE:HG13	2.40	0.52
1:E:78:ILE:CD1	1:E:78:ILE:H	2.22	0.52
1:F:283:THR:HG23	1:F:474:CYS:SG	2.50	0.52
1:F:339:PHE:HE2	1:F:341:PRO:HG3	1.70	0.52
1:B:32:GLU:HB2	1:B:64:LEU:HD11	1.90	0.52
1:D:98:ILE:N	1:D:99:PRO:HD2	2.25	0.52
1:F:278:PHE:CE1	1:F:518:ILE:HD11	2.45	0.52
1:F:28:TYR:CD1	1:F:64:LEU:HD12	2.44	0.52
1:A:179:ILE:HG12	1:A:180:GLY:N	2.25	0.52
1:C:264:ARG:HG2	1:C:264:ARG:O	2.10	0.52
1:D:272:ASN:O	1:D:276:GLN:HG2	2.10	0.52
1:E:187:ILE:HG23	1:E:206:ILE:CD1	2.40	0.52
1:B:183:HIS:HB3	1:B:184:PRO:HD2	1.92	0.52
1:B:512:SER:HA	1:B:515:VAL:HG12	1.91	0.52
1:D:275:HIS:O	1:D:276:GLN:C	2.49	0.52
1:D:420:ASP:OD2	1:D:497:LYS:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ILE:HG22	1:D:427:ILE:O	2.10	0.52
1:F:90:HIS:CE1	3:F:2006:TPS:C2A	2.92	0.52
1:A:75:ASN:HD22	1:A:76:ASP:HB3	1.75	0.52
1:C:495:LEU:HD22	1:C:521:LEU:HD23	1.91	0.52
1:F:78:ILE:CD1	1:F:78:ILE:H	2.23	0.52
1:B:5:LYS:NZ	1:B:108:ASP:H	2.07	0.51
1:E:43:GLN:NE2	3:E:2005:TPS:HM21	2.23	0.51
1:F:167:GLU:CG	1:F:198:ASN:HD21	2.14	0.51
1:F:433:LEU:O	1:F:435:LYS:N	2.42	0.51
1:A:484:ASN:ND2	1:A:487:HIS:H	2.09	0.51
1:B:40:THR:CG2	1:B:226:ARG:HH21	2.23	0.51
1:D:424:ASP:HB3	1:D:446:PRO:HG2	1.92	0.51
1:C:256:ILE:O	1:C:260:THR:HG22	2.10	0.51
1:A:96:MET:HG2	1:A:101:ILE:HG13	1.93	0.51
1:C:527:GLU:O	1:C:527:GLU:HG3	2.11	0.51
1:D:179:ILE:HG13	1:D:207:CYS:HB3	1.92	0.51
1:A:98:ILE:N	1:A:99:PRO:HD2	2.24	0.51
1:B:180:GLY:HA2	3:B:2002:TPS:H72	1.92	0.51
1:B:290:PRO:HB2	1:B:292:MET:HE2	1.92	0.51
1:C:266:LEU:HD11	1:C:291:ILE:CG1	2.29	0.51
1:C:78:ILE:HG22	1:C:82:MET:HE2	1.92	0.51
1:E:329:ALA:O	1:E:333:VAL:HG23	2.10	0.51
1:F:15:VAL:O	1:F:209:VAL:HG21	2.11	0.51
1:A:210:SER:HB3	3:A:2001:TPS:O2	2.11	0.51
1:B:337:ILE:HG21	1:B:363:PHE:CD2	2.46	0.51
1:D:534:ALA:N	1:D:535:PRO:HD2	2.26	0.51
1:E:276:GLN:HE21	1:E:276:GLN:HA	1.76	0.51
1:A:318:ALA:HB1	1:A:322:MET:HG2	1.93	0.51
1:C:20:MET:O	1:C:20:MET:HG2	2.11	0.51
1:F:123:GLU:O	1:F:127:MET:HG3	2.11	0.51
1:F:196:SER:HB2	1:F:201:ARG:HB3	1.93	0.51
1:F:90:HIS:CE1	3:F:2006:TPS:HM22	2.45	0.51
1:D:482:GLU:H	1:D:482:GLU:CD	2.13	0.51
1:A:274:VAL:HG13	1:E:292:MET:HG3	1.93	0.51
1:F:209:VAL:C	1:F:211:ASP:N	2.63	0.51
1:A:355:ASN:O	1:A:359:THR:HG23	2.11	0.51
1:E:517:LEU:HD23	1:E:517:LEU:O	2.11	0.51
1:E:260:THR:HA	1:E:478:GLY:HA3	1.93	0.51
1:F:78:ILE:CD1	1:F:78:ILE:N	2.73	0.51
1:C:35:LEU:HD12	1:C:64:LEU:HD22	1.93	0.50
1:D:102:ARG:HH11	1:D:107:PRO:HA	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:ILE:O	1:E:260:THR:HG22	2.12	0.50
1:F:305:ILE:HG23	1:F:306:PRO:HD2	1.91	0.50
1:A:424:ASP:HB2	1:A:486:PHE:CD1	2.46	0.50
1:B:187:ILE:HG23	1:B:206:ILE:CD1	2.41	0.50
1:C:202:SER:OG	1:C:436:GLY:HA3	2.11	0.50
1:E:77:ARG:HB3	1:E:79:ASP:OD1	2.11	0.50
1:A:247:LEU:HD13	1:A:539:HIS:NE2	2.26	0.50
1:A:209:VAL:CG1	3:A:2001:TPS:O7	2.60	0.50
1:A:31:VAL:O	1:A:35:LEU:HG	2.12	0.50
1:C:137:VAL:HG22	1:C:177:VAL:O	2.10	0.50
1:F:135:ILE:O	1:F:135:ILE:HG13	2.10	0.50
1:A:121:VAL:HG13	1:A:166:LEU:HD23	1.94	0.50
3:A:2001:TPS:HM43	3:A:2001:TPS:N4A	2.26	0.50
1:A:282:VAL:HG21	1:A:467:SER:HB3	1.92	0.50
1:B:337:ILE:CG2	1:B:363:PHE:HD2	2.24	0.50
1:E:137:VAL:HG22	1:E:177:VAL:O	2.11	0.50
1:E:264:ARG:CG	1:E:264:ARG:O	2.60	0.50
1:F:17:ASP:HB3	1:F:20:MET:HE1	1.94	0.50
1:F:20:MET:O	1:F:20:MET:HG2	2.11	0.50
1:A:299:VAL:HG11	1:A:326:ALA:HA	1.94	0.50
1:A:89:ILE:O	1:A:89:ILE:HG13	2.11	0.50
1:B:124:LEU:HA	1:B:127:MET:HE2	1.94	0.50
1:C:16:THR:O	1:C:45:ARG:HB3	2.11	0.50
3:D:2004:TPS:N4A	3:D:2004:TPS:HM43	2.27	0.50
1:D:15:VAL:O	1:D:209:VAL:HG22	2.11	0.50
1:E:495:LEU:HD22	1:E:521:LEU:CD2	2.41	0.50
1:F:137:VAL:CG2	1:F:178:GLY:HA2	2.42	0.50
1:A:77:ARG:NH1	1:C:77:ARG:NH1	2.60	0.50
1:B:358:LEU:HD23	1:B:363:PHE:CE1	2.47	0.50
1:E:341:PRO:HB3	1:E:354:ASN:OD1	2.12	0.50
1:B:59:LEU:HD21	1:B:84:ILE:HB	1.93	0.49
1:E:137:VAL:CG2	1:E:178:GLY:HA2	2.42	0.49
1:C:333:VAL:HG12	1:C:333:VAL:O	2.12	0.49
1:F:513:PHE:CD2	1:F:513:PHE:C	2.84	0.49
1:C:291:ILE:HG22	1:C:293:SER:H	1.76	0.49
1:C:44:ILE:HG13	1:C:72:LEU:HD11	1.94	0.49
1:D:44:ILE:CD1	1:D:58:ALA:HA	2.43	0.49
1:E:183:HIS:HB3	1:E:184:PRO:HD2	1.93	0.49
1:A:416:THR:HG22	1:A:420:ASP:OD1	2.12	0.49
1:E:17:ASP:HB3	1:E:20:MET:CE	2.41	0.49
1:E:31:VAL:O	1:E:31:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:HIS:HE1	1:B:87:ASP:OD1	1.94	0.49
1:C:468:LEU:O	1:C:472:ILE:HG13	2.12	0.49
1:C:322:MET:HG3	1:C:323:LEU:N	2.28	0.49
1:D:183:HIS:HB3	1:D:184:PRO:CD	2.43	0.49
1:C:135:ILE:HG13	1:C:176:THR:HG22	1.95	0.49
1:C:467:SER:HB2	1:C:496:TYR:HE1	1.78	0.49
1:C:75:ASN:ND2	1:C:76:ASP:OD2	2.46	0.49
1:E:296:GLN:HG3	1:E:322:MET:HB2	1.94	0.49
1:F:102:ARG:NH1	1:F:107:PRO:HA	2.28	0.49
1:A:257:ILE:HD11	1:A:533:TRP:HH2	1.77	0.49
1:A:534:ALA:N	1:A:535:PRO:CD	2.75	0.49
1:B:193:GLN:HE21	1:B:362:GLN:HE21	1.59	0.49
1:E:314:THR:HG22	1:E:315:GLY:H	1.78	0.49
1:E:75:ASN:ND2	1:E:76:ASP:HB3	2.28	0.49
1:F:299:VAL:HG11	1:F:326:ALA:HA	1.95	0.49
1:C:192:TYR:HA	1:C:431:TYR:HB3	1.95	0.49
1:E:18:SER:HB2	1:E:46:GLU:OE2	2.13	0.49
1:A:91:VAL:HG11	1:A:101:ILE:CD1	2.42	0.49
1:E:437:THR:HG23	1:E:440:THR:N	2.28	0.49
1:F:314:THR:HG22	1:F:315:GLY:N	2.28	0.49
1:C:529:THR:N	1:C:530:PRO:HD3	2.27	0.48
1:A:314:THR:HG22	1:A:315:GLY:N	2.29	0.48
1:E:495:LEU:HD11	1:E:525:THR:CG2	2.43	0.48
1:F:167:GLU:HG2	1:F:198:ASN:ND2	2.13	0.48
1:F:61:ILE:O	1:F:61:ILE:CG2	2.61	0.48
1:E:416:THR:HA	1:E:420:ASP:OD1	2.12	0.48
1:F:280:ALA:HB2	1:F:292:MET:CE	2.43	0.48
1:B:154:MET:SD	1:B:158:GLY:HA3	2.53	0.48
1:B:90:HIS:CE1	3:B:2002:TPS:C2A	2.96	0.48
1:C:433:LEU:O	1:C:435:LYS:N	2.44	0.48
1:D:273:LYS:HA	1:D:276:GLN:CG	2.44	0.48
1:A:137:VAL:HG22	1:A:177:VAL:O	2.13	0.48
1:A:495:LEU:HD11	1:A:525:THR:CG2	2.43	0.48
1:C:305:ILE:HG23	1:C:306:PRO:HD2	1.96	0.48
1:C:78:ILE:N	1:C:78:ILE:CD1	2.76	0.48
1:D:422:ILE:N	1:D:422:ILE:HD12	2.28	0.48
1:D:533:TRP:C	1:D:535:PRO:HD2	2.33	0.48
1:E:502:ILE:O	1:E:506:LYS:HG3	2.13	0.48
1:B:314:THR:HG22	1:B:315:GLY:H	1.78	0.48
1:C:427:ILE:O	1:C:427:ILE:HG22	2.13	0.48
1:C:92:GLY:HA2	1:C:114:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:CG	1:A:434:SER:HB3	2.33	0.48
1:C:283:THR:HB	1:C:290:PRO:HG3	1.96	0.48
1:D:137:VAL:HG23	1:D:137:VAL:O	2.12	0.48
1:D:262:LYS:HG2	1:D:262:LYS:O	2.13	0.48
1:E:275:HIS:O	1:E:276:GLN:C	2.51	0.48
1:E:78:ILE:HD13	1:E:96:MET:CE	2.42	0.48
1:E:257:ILE:HA	1:E:260:THR:CG2	2.43	0.48
1:F:437:THR:HG23	1:F:438:ASN:N	2.29	0.48
1:A:121:VAL:CG1	1:A:166:LEU:HD23	2.44	0.48
1:D:18:SER:HB2	1:D:46:GLU:OE2	2.13	0.48
1:E:78:ILE:CD1	1:E:96:MET:HE2	2.42	0.48
1:F:276:GLN:HE21	1:F:276:GLN:HA	1.78	0.48
1:F:377:ALA:O	1:F:378:GLU:HB2	2.14	0.48
1:A:160:ILE:HD11	1:A:193:GLN:O	2.14	0.47
1:B:339:PHE:CD2	1:B:341:PRO:HG3	2.48	0.47
1:B:204:ASP:OD1	1:B:434:SER:HB3	2.13	0.47
1:D:15:VAL:HB	1:D:209:VAL:CG2	2.44	0.47
1:E:186:ASN:O	1:E:190:VAL:HG23	2.14	0.47
1:E:271:THR:HA	1:E:313:ASN:HB2	1.96	0.47
1:A:33:ALA:O	1:A:37:ASN:ND2	2.46	0.47
1:D:254:GLN:O	1:D:528:ASN:ND2	2.48	0.47
1:D:495:LEU:HD11	1:D:525:THR:CG2	2.44	0.47
1:D:78:ILE:H	1:D:78:ILE:HD12	1.79	0.47
3:E:2005:TPS:N4A	3:E:2005:TPS:HM43	2.29	0.47
1:F:90:HIS:CE1	3:F:2006:TPS:CM2	2.97	0.47
1:F:239:ILE:HG22	1:F:240:GLY:N	2.30	0.47
1:A:38:GLY:O	1:A:39:VAL:C	2.51	0.47
1:A:77:ARG:HH11	1:C:77:ARG:NH1	2.12	0.47
1:D:322:MET:HG3	1:D:323:LEU:N	2.29	0.47
1:E:192:TYR:CZ	1:E:410:LYS:HB3	2.49	0.47
1:B:124:LEU:C	1:B:124:LEU:HD23	2.35	0.47
1:B:296:GLN:CG	1:B:322:MET:HB2	2.44	0.47
1:C:51:THR:O	1:C:55:ILE:HG13	2.14	0.47
1:D:50:ASP:C	1:D:52:LYS:H	2.17	0.47
1:E:127:MET:HB3	1:E:131:MET:HG3	1.96	0.47
1:A:43:GLN:HA	1:A:73:ILE:O	2.14	0.47
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.79	0.47
1:A:8:PHE:CZ	1:A:110:VAL:HG21	2.50	0.47
1:B:40:THR:HG21	1:B:226:ARG:NH2	2.29	0.47
1:C:21:ILE:HD11	1:C:27:LEU:HD13	1.95	0.47
1:C:30:GLN:OE1	1:C:30:GLN:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:PHE:CE2	1:C:341:PRO:HG3	2.49	0.47
1:E:20:MET:HE3	1:E:213:ILE:HB	1.95	0.47
1:F:183:HIS:ND1	1:F:211:ASP:OD1	2.47	0.47
1:F:435:LYS:N	1:F:436:GLY:HA2	2.29	0.47
1:C:485:LEU:O	1:C:489:VAL:HG23	2.15	0.47
1:E:269:HIS:HB2	1:E:292:MET:SD	2.55	0.47
1:C:127:MET:CE	1:C:131:MET:HB3	2.43	0.47
1:C:402:THR:OG1	1:C:415:CYS:HB2	2.15	0.47
1:D:367:LYS:HD2	1:D:468:LEU:HD23	1.95	0.47
1:F:318:ALA:HB1	1:F:322:MET:HG2	1.97	0.47
1:F:350:ARG:O	1:F:354:ASN:ND2	2.47	0.47
1:F:89:ILE:HG13	1:F:89:ILE:O	2.15	0.47
1:A:400:GLN:O	1:A:404:ILE:HG13	2.15	0.47
3:B:2002:TPS:N4A	3:B:2002:TPS:HM43	2.30	0.47
1:B:486:PHE:O	1:B:490:VAL:HG23	2.15	0.47
1:D:339:PHE:CD2	1:D:341:PRO:HG3	2.50	0.47
1:F:102:ARG:HH11	1:F:107:PRO:HA	1.80	0.47
1:F:16:THR:HG22	1:F:27:LEU:HD11	1.97	0.47
1:F:35:LEU:CD1	1:F:64:LEU:HD22	2.45	0.47
1:A:107:PRO:O	1:A:108:ASP:CB	2.63	0.47
1:A:189:ARG:O	1:A:193:GLN:HG2	2.15	0.47
1:A:512:SER:HA	1:A:515:VAL:CG1	2.45	0.47
1:A:533:TRP:HB3	1:A:535:PRO:HD2	1.95	0.47
1:C:58:ALA:HB1	1:C:84:ILE:CD1	2.45	0.47
1:D:311:LEU:HD13	1:D:312:LEU:N	2.30	0.47
1:F:18:SER:HB2	1:F:46:GLU:OE2	2.15	0.47
1:F:204:ASP:CG	1:F:434:SER:HB3	2.36	0.47
1:A:32:GLU:HG3	1:A:64:LEU:HD21	1.97	0.47
1:B:355:ASN:O	1:B:359:THR:HG23	2.14	0.47
1:B:515:VAL:O	1:B:515:VAL:HG22	2.15	0.47
1:B:75:ASN:HD22	1:B:76:ASP:HB3	1.80	0.47
1:E:75:ASN:HD22	1:E:76:ASP:HB3	1.80	0.47
1:A:498:ALA:HB2	1:A:535:PRO:HG3	1.97	0.46
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.71	0.46
1:E:78:ILE:HG13	1:E:89:ILE:CD1	2.41	0.46
1:C:264:ARG:O	1:C:264:ARG:CG	2.64	0.46
1:F:28:TYR:OH	1:F:64:LEU:HG	2.15	0.46
1:A:11:SER:CB	1:A:226:ARG:NH2	2.78	0.46
1:A:529:THR:N	1:A:530:PRO:CD	2.77	0.46
1:B:125:SER:C	1:B:127:MET:N	2.68	0.46
1:B:479:GLN:HA	1:B:480:PRO:HD3	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:HD11	1:B:493:VAL:HG22	1.96	0.46
1:B:528:ASN:C	1:B:530:PRO:HD3	2.35	0.46
1:B:80:VAL:O	1:B:84:ILE:HG12	2.15	0.46
1:E:226:ARG:HA	1:E:226:ARG:HD3	1.74	0.46
1:E:38:GLY:O	1:E:39:VAL:C	2.53	0.46
1:F:107:PRO:O	1:F:108:ASP:CB	2.62	0.46
1:A:274:VAL:HG23	1:A:275:HIS:CE1	2.51	0.46
1:B:271:THR:CB	1:B:313:ASN:HB2	2.44	0.46
1:B:274:VAL:HG11	1:D:292:MET:HE3	1.97	0.46
1:B:92:GLY:HA3	4:B:4002:POP:O3	2.14	0.46
1:B:98:ILE:N	1:B:99:PRO:HD2	2.31	0.46
1:D:182:LEU:HA	1:D:182:LEU:HD12	1.80	0.46
1:D:78:ILE:N	1:D:78:ILE:HD12	2.30	0.46
1:D:4:SER:N	1:D:7:GLN:OE1	2.48	0.46
1:E:35:LEU:HD22	1:E:70:VAL:HG11	1.97	0.46
1:F:121:VAL:HG13	1:F:166:LEU:HD23	1.96	0.46
1:F:74:ILE:HD11	1:F:84:ILE:HD11	1.98	0.46
1:A:153:PRO:CD	1:A:153:PRO:O	2.64	0.46
1:E:30:GLN:NE2	1:E:218:ALA:HB2	2.31	0.46
1:E:424:ASP:HB3	1:E:446:PRO:HG2	1.96	0.46
1:F:78:ILE:HG12	1:F:96:MET:CE	2.46	0.46
1:B:433:LEU:O	1:B:435:LYS:N	2.49	0.46
1:C:491:ALA:O	1:C:494:MET:HB2	2.16	0.46
1:A:45:ARG:HG3	1:A:75:ASN:OD1	2.16	0.46
1:B:290:PRO:HB2	1:B:292:MET:CE	2.45	0.46
1:B:78:ILE:CG1	1:B:89:ILE:HD12	2.32	0.46
1:C:191:LEU:HD12	1:C:191:LEU:HA	1.80	0.46
1:C:435:LYS:N	1:C:436:GLY:HA2	2.31	0.46
1:E:273:LYS:HA	1:E:276:GLN:HG3	1.97	0.46
1:E:311:LEU:HD22	1:E:312:LEU:N	2.31	0.46
1:A:278:PHE:CE1	1:A:518:ILE:HD11	2.51	0.46
1:B:179:ILE:CG1	1:B:180:GLY:N	2.77	0.46
1:D:239:ILE:HG22	1:D:240:GLY:H	1.81	0.46
1:D:289:SER:HA	1:D:290:PRO:HD3	1.71	0.46
1:F:92:GLY:HA2	1:F:114:SER:HB2	1.97	0.46
1:F:278:PHE:HE1	1:F:518:ILE:HD11	1.81	0.46
1:B:21:ILE:HA	1:B:22:PRO:HD3	1.82	0.45
1:C:252:GLU:O	1:C:256:ILE:HG12	2.17	0.45
1:D:237:VAL:HG22	1:D:239:ILE:HG13	1.99	0.45
1:D:75:ASN:HA	1:D:76:ASP:HA	1.53	0.45
1:D:98:ILE:HD11	1:D:113:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ILE:HG22	1:B:455:ILE:O	2.16	0.45
1:C:193:GLN:NE2	1:C:362:GLN:HE21	2.15	0.45
1:E:534:ALA:N	1:E:535:PRO:CD	2.78	0.45
1:C:78:ILE:HG22	1:C:82:MET:HE1	1.99	0.45
1:C:89:ILE:HD11	1:C:101:ILE:CG2	2.46	0.45
1:E:28:TYR:CZ	1:E:64:LEU:HG	2.52	0.45
1:E:302:LEU:HA	1:E:302:LEU:HD12	1.68	0.45
1:F:422:ILE:CG2	1:F:486:PHE:HE1	2.26	0.45
1:B:247:LEU:HD12	1:B:247:LEU:HA	1.66	0.45
1:C:10:TYR:O	1:C:205:GLY:HA3	2.17	0.45
1:E:124:LEU:HD23	1:E:124:LEU:C	2.36	0.45
1:E:266:LEU:HD11	1:E:291:ILE:HG13	1.98	0.45
1:F:45:ARG:NE	3:F:2006:TPS:HM42	2.31	0.45
1:B:167:GLU:HG2	1:B:198:ASN:ND2	2.31	0.45
1:B:235:LYS:O	1:B:334:LYS:HD3	2.16	0.45
1:B:310:LEU:HB3	1:B:337:ILE:HG12	1.98	0.45
1:B:75:ASN:ND2	1:B:76:ASP:HB3	2.32	0.45
1:E:89:ILE:HD11	1:E:101:ILE:CG2	2.41	0.45
1:F:17:ASP:HB3	1:F:20:MET:CE	2.47	0.45
1:B:437:THR:O	1:B:439:GLY:N	2.40	0.45
1:B:476:ILE:HD13	1:B:485:LEU:HD11	1.99	0.45
1:C:178:GLY:O	1:C:207:CYS:HB2	2.17	0.45
1:C:208:VAL:HG11	1:C:225:LEU:HD11	1.98	0.45
1:F:124:LEU:O	1:F:124:LEU:HD23	2.16	0.45
1:A:432:SER:OG	1:A:436:GLY:O	2.35	0.45
1:B:337:ILE:HG21	1:B:363:PHE:HD2	1.82	0.45
1:C:289:SER:HA	1:C:290:PRO:HD3	1.59	0.45
1:C:75:ASN:HA	1:C:76:ASP:HA	1.75	0.45
1:F:183:HIS:HB3	1:F:184:PRO:HD2	1.99	0.45
1:F:55:ILE:HG12	1:F:80:VAL:HG13	1.97	0.45
1:A:296:GLN:CG	1:A:322:MET:HB2	2.45	0.45
1:B:153:PRO:O	1:B:153:PRO:CD	2.64	0.45
1:D:49:ALA:HB1	1:D:53:PHE:HD2	1.81	0.45
1:A:124:LEU:HD23	1:A:124:LEU:C	2.37	0.45
1:A:422:ILE:N	1:A:422:ILE:HD12	2.31	0.45
1:C:141:PHE:HB3	1:C:142:PRO:CD	2.47	0.45
1:C:253:ILE:O	1:C:257:ILE:HG13	2.16	0.45
1:C:534:ALA:N	1:C:535:PRO:CD	2.80	0.45
1:D:77:ARG:HH22	1:E:77:ARG:HA	1.81	0.45
1:F:191:LEU:HD12	1:F:191:LEU:HA	1.80	0.45
1:F:284:LEU:HA	1:F:284:LEU:HD12	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:PRO:O	1:F:101:ILE:HG13	2.16	0.45
1:A:98:ILE:HD11	1:A:113:TRP:NE1	2.32	0.45
1:A:119:GLU:O	1:A:122:ASP:HB2	2.17	0.45
1:C:513:PHE:CD2	1:C:513:PHE:C	2.90	0.45
1:C:58:ALA:CB	1:C:84:ILE:HD13	2.47	0.45
1:D:533:TRP:CD1	1:D:533:TRP:N	2.82	0.45
1:F:75:ASN:HA	1:F:76:ASP:HA	1.52	0.45
1:A:79:ASP:C	1:A:81:ALA:N	2.69	0.44
1:B:246:SER:O	1:B:247:LEU:C	2.56	0.44
1:C:3:PHE:CG	1:C:71:PRO:HG3	2.52	0.44
1:D:278:PHE:CE1	1:D:518:ILE:HD11	2.52	0.44
1:D:77:ARG:NH2	1:D:79:ASP:OD2	2.50	0.44
1:A:154:MET:SD	1:A:158:GLY:CA	3.05	0.44
1:A:8:PHE:CE1	1:A:110:VAL:HG21	2.52	0.44
1:B:196:SER:HB2	1:B:201:ARG:HB3	1.98	0.44
1:B:324:LYS:HA	1:B:360:PHE:CD1	2.51	0.44
1:C:66:HIS:HE1	1:C:87:ASP:OD1	2.00	0.44
1:C:73:ILE:HG23	1:C:88:GLY:C	2.37	0.44
1:D:27:LEU:O	1:D:31:VAL:HG23	2.16	0.44
1:F:527:GLU:O	1:F:529:THR:N	2.49	0.44
1:B:278:PHE:CE1	1:B:518:ILE:HD11	2.52	0.44
1:C:276:GLN:HE22	1:C:292:MET:HB3	1.82	0.44
1:E:192:TYR:HA	1:E:431:TYR:HB3	1.99	0.44
1:A:407:PHE:O	1:A:410:LYS:NZ	2.41	0.44
1:B:435:LYS:N	1:B:436:GLY:HA2	2.31	0.44
1:D:47:LYS:HZ1	4:D:4004:POP:P2	2.41	0.44
1:D:278:PHE:HE1	1:D:518:ILE:HD11	1.81	0.44
1:F:15:VAL:O	1:F:209:VAL:CG2	2.64	0.44
1:F:495:LEU:HD22	1:F:521:LEU:CD2	2.47	0.44
1:F:527:GLU:HG3	1:F:527:GLU:O	2.17	0.44
1:F:75:ASN:HB2	1:F:90:HIS:HB3	2.00	0.44
1:B:144:LEU:HA	1:B:144:LEU:HD13	1.78	0.44
1:D:377:ALA:O	1:D:378:GLU:HB2	2.18	0.44
1:D:74:ILE:HD12	1:D:86:ALA:HB2	1.99	0.44
1:E:78:ILE:CD1	1:E:78:ILE:N	2.79	0.44
1:F:234:TYR:HE2	1:F:362:GLN:HG3	1.81	0.44
1:F:291:ILE:HG22	1:F:293:SER:H	1.83	0.44
1:F:467:SER:HB2	1:F:496:TYR:CE1	2.52	0.44
1:B:123:GLU:O	1:B:127:MET:HG3	2.18	0.44
1:B:498:ALA:HB2	1:B:535:PRO:HG3	2.00	0.44
1:C:17:ASP:HB3	1:C:20:MET:CE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:VAL:HG12	1:D:31:VAL:O	2.18	0.44
1:D:50:ASP:O	1:D:52:LYS:N	2.51	0.44
1:D:73:ILE:HA	1:D:88:GLY:O	2.17	0.44
1:F:235:LYS:NZ	1:F:238:ASN:HA	2.33	0.44
1:A:187:ILE:HG23	1:A:206:ILE:CD1	2.47	0.44
1:B:178:GLY:O	1:B:207:CYS:HB2	2.17	0.44
1:C:17:ASP:CB	1:C:20:MET:HE1	2.46	0.44
1:C:314:THR:HG22	1:C:315:GLY:H	1.83	0.44
1:D:62:LYS:HB2	1:D:72:LEU:HD22	2.00	0.44
1:D:78:ILE:HG22	1:D:82:MET:HE2	1.98	0.44
1:E:125:SER:C	1:E:127:MET:H	2.21	0.44
1:E:340:ASP:C	1:E:340:ASP:OD2	2.56	0.44
1:A:188:GLU:HG2	1:A:188:GLU:H	1.52	0.44
1:A:73:ILE:HA	1:A:88:GLY:O	2.17	0.44
1:A:74:ILE:HD11	1:A:84:ILE:CD1	2.39	0.44
1:C:166:LEU:HA	1:C:166:LEU:HD23	1.70	0.44
1:C:226:ARG:O	1:C:230:ASP:OD2	2.34	0.44
1:E:533:TRP:C	1:E:535:PRO:HD2	2.37	0.44
1:F:133:ASP:O	1:F:174:CYS:HA	2.17	0.44
1:F:208:VAL:CG2	1:F:209:VAL:HG22	2.41	0.44
1:F:289:SER:HA	1:F:290:PRO:HD3	1.78	0.44
1:A:230:ASP:N	1:A:230:ASP:OD2	2.51	0.44
1:C:21:ILE:HA	1:C:22:PRO:HD3	1.88	0.44
1:C:472:ILE:O	1:C:476:ILE:HG13	2.18	0.44
1:B:278:PHE:HE1	1:B:518:ILE:HD11	1.83	0.43
1:C:166:LEU:HD22	1:C:171:ALA:HB3	1.99	0.43
1:C:182:LEU:HD12	1:C:182:LEU:HA	1.81	0.43
1:C:40:THR:CG2	1:C:226:ARG:HH21	2.31	0.43
1:C:79:ASP:HA	1:C:82:MET:CE	2.47	0.43
1:D:12:LEU:HD23	1:D:39:VAL:H	1.82	0.43
1:D:495:LEU:HD11	1:D:525:THR:HG21	1.99	0.43
1:E:40:THR:CG2	1:E:226:ARG:HH21	2.25	0.43
1:E:314:THR:CG2	1:E:315:GLY:N	2.81	0.43
1:F:322:MET:O	1:F:325:ALA:HB3	2.18	0.43
1:A:47:LYS:NZ	4:A:4001:POP:P2	2.91	0.43
1:A:46:GLU:HA	1:A:46:GLU:OE1	2.17	0.43
1:A:533:TRP:C	1:A:535:PRO:HD2	2.38	0.43
1:B:154:MET:CG	1:B:158:GLY:HA3	2.48	0.43
1:D:275:HIS:CD2	1:D:466:CYS:HB2	2.53	0.43
1:E:394:SER:HB3	1:E:397:LEU:HB3	2.00	0.43
1:E:419:PHE:CD1	1:E:451:GLU:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:ILE:HG13	1:E:84:ILE:O	2.17	0.43
1:A:339:PHE:CE2	1:A:341:PRO:HG3	2.53	0.43
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.75	0.43
1:B:20:MET:CE	1:B:209:VAL:HG12	2.48	0.43
1:D:247:LEU:HD12	1:D:247:LEU:HA	1.72	0.43
1:F:118:PRO:HD2	1:F:119:GLU:OE1	2.18	0.43
1:A:159:ALA:O	1:A:162:VAL:HB	2.18	0.43
1:A:78:ILE:HG13	1:A:89:ILE:HD12	1.99	0.43
1:B:529:THR:N	1:B:530:PRO:HD3	2.33	0.43
1:B:59:LEU:CD2	1:B:84:ILE:HB	2.49	0.43
1:C:239:ILE:HG22	1:C:240:GLY:N	2.32	0.43
1:C:278:PHE:HE2	1:C:467:SER:HG	1.61	0.43
1:D:188:GLU:H	1:D:188:GLU:HG2	1.47	0.43
1:D:191:LEU:HD12	1:D:191:LEU:HA	1.84	0.43
1:B:10:TYR:O	1:B:205:GLY:HA3	2.18	0.43
1:B:467:SER:HB2	1:B:496:TYR:CE1	2.53	0.43
1:C:416:THR:HG21	1:C:468:LEU:HD23	2.00	0.43
1:D:257:ILE:HA	1:D:260:THR:HG23	2.00	0.43
1:E:479:GLN:HA	1:E:480:PRO:HD3	1.66	0.43
1:A:297:SER:HB2	1:F:349:THR:OG1	2.18	0.43
1:B:437:THR:HG23	1:B:440:THR:N	2.34	0.43
1:C:104:LEU:HD23	1:C:104:LEU:N	2.32	0.43
1:C:266:LEU:CD1	1:C:291:ILE:HG13	2.30	0.43
1:D:435:LYS:N	1:D:436:GLY:HA2	2.34	0.43
1:E:289:SER:HA	1:E:290:PRO:HD3	1.74	0.43
1:F:226:ARG:HD3	1:F:226:ARG:HA	1.69	0.43
1:D:256:ILE:HG23	1:D:479:GLN:OE1	2.19	0.43
1:D:526:ARG:HA	1:D:526:ARG:HD2	1.84	0.43
1:E:70:VAL:HA	1:E:71:PRO:HD3	1.88	0.43
1:F:188:GLU:H	1:F:188:GLU:HG2	1.48	0.43
1:A:181:GLY:N	3:A:2001:TPS:O1	2.50	0.43
1:C:118:PRO:HD2	1:C:119:GLU:OE1	2.18	0.43
1:C:484:ASN:HD21	1:C:486:PHE:HB3	1.84	0.43
1:D:475:MET:O	1:D:479:GLN:HG2	2.19	0.43
1:F:528:ASN:C	1:F:530:PRO:HD3	2.39	0.43
1:A:20:MET:CG	1:A:214:ALA:HB2	2.42	0.43
1:B:274:VAL:HG13	1:D:292:MET:HG3	2.01	0.43
1:B:303:ALA:HB2	1:B:330:TYR:CE1	2.54	0.43
1:C:38:GLY:O	1:C:39:VAL:C	2.57	0.43
1:D:422:ILE:HG22	1:D:486:PHE:HE1	1.84	0.43
1:E:188:GLU:H	1:E:188:GLU:HG2	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ALA:HB2	1:F:292:MET:HE2	2.01	0.43
1:B:182:LEU:HA	1:B:182:LEU:HD12	1.88	0.43
1:B:250:THR:HG23	1:B:530:PRO:HB2	2.01	0.43
1:B:283:THR:HG22	1:B:288:SER:O	2.19	0.43
1:B:520:ALA:O	1:B:524:LEU:HB2	2.18	0.43
1:C:135:ILE:CG1	1:C:176:THR:HG22	2.49	0.43
1:D:139:THR:O	1:D:154:MET:HB3	2.18	0.43
1:D:333:VAL:HG12	1:D:333:VAL:O	2.19	0.43
1:D:59:LEU:CD2	1:D:84:ILE:HB	2.49	0.43
1:E:21:ILE:HA	1:E:22:PRO:HD3	1.90	0.43
1:E:73:ILE:HG23	1:E:88:GLY:O	2.19	0.43
1:F:357:LEU:HD23	1:F:360:PHE:CE1	2.54	0.43
1:F:369:ASN:O	1:F:370:SER:C	2.58	0.43
1:A:183:HIS:HB3	1:A:184:PRO:CD	2.48	0.42
1:C:512:SER:HA	1:C:515:VAL:CG1	2.49	0.42
1:F:40:THR:HG21	1:F:226:ARG:HH21	1.84	0.42
1:A:533:TRP:CD1	1:A:533:TRP:N	2.87	0.42
1:B:495:LEU:HD22	1:B:521:LEU:HD23	2.02	0.42
1:B:495:LEU:HD22	1:B:521:LEU:CD2	2.49	0.42
1:D:226:ARG:HD3	1:D:226:ARG:HA	1.69	0.42
1:A:498:ALA:C	1:A:500:GLY:H	2.22	0.42
1:B:239:ILE:HG22	1:B:240:GLY:N	2.34	0.42
1:D:209:VAL:HG12	1:D:210:SER:N	2.34	0.42
1:D:73:ILE:HG23	1:D:88:GLY:O	2.19	0.42
1:F:407:PHE:CD1	1:F:442:VAL:HG23	2.54	0.42
1:A:75:ASN:ND2	1:A:76:ASP:HB3	2.34	0.42
1:C:8:PHE:CZ	1:C:110:VAL:HG21	2.55	0.42
1:E:137:VAL:HG23	1:E:178:GLY:HA2	2.01	0.42
1:F:430:LYS:HA	1:F:430:LYS:HD3	1.87	0.42
1:F:534:ALA:N	1:F:535:PRO:CD	2.80	0.42
1:F:68:HIS:O	1:F:70:VAL:HG12	2.19	0.42
1:F:44:ILE:CG1	1:F:72:LEU:HD11	2.37	0.42
1:D:121:VAL:HG13	1:D:166:LEU:HD23	1.99	0.42
1:E:191:LEU:HD13	1:E:206:ILE:HD11	2.00	0.42
1:F:209:VAL:HG12	1:F:210:SER:N	2.34	0.42
1:A:102:ARG:HA	1:A:102:ARG:HD3	1.77	0.42
1:A:192:TYR:HA	1:A:431:TYR:HB3	2.01	0.42
1:E:179:ILE:HD12	1:E:207:CYS:SG	2.59	0.42
1:F:129:PRO:C	1:F:131:MET:H	2.23	0.42
1:F:59:LEU:CD2	1:F:84:ILE:HB	2.48	0.42
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:VAL:HG22	1:B:317:VAL:O	2.20	0.42
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.60	0.42
1:F:137:VAL:HG23	1:F:178:GLY:HA2	2.00	0.42
1:F:79:ASP:OD1	1:F:79:ASP:N	2.51	0.42
1:C:70:VAL:HA	1:C:71:PRO:HD3	1.87	0.42
1:D:239:ILE:HG22	1:D:240:GLY:N	2.35	0.42
1:F:38:GLY:O	1:F:39:VAL:C	2.57	0.42
1:A:369:ASN:O	1:A:370:SER:C	2.59	0.42
1:C:59:LEU:CD2	1:C:84:ILE:HB	2.49	0.42
1:D:121:VAL:CG1	1:D:166:LEU:HD23	2.49	0.42
1:E:422:ILE:HG22	1:E:486:PHE:CE1	2.54	0.42
1:E:204:ASP:OD1	1:E:434:SER:HB3	2.20	0.42
1:E:508:ASN:HB3	1:F:523:ARG:HH12	1.81	0.42
1:F:125:SER:C	1:F:127:MET:H	2.23	0.42
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.82	0.42
1:A:331:ASN:HA	1:A:331:ASN:HD22	1.59	0.42
1:A:433:LEU:O	1:A:435:LYS:N	2.53	0.42
1:B:297:SER:HB2	1:C:349:THR:OG1	2.20	0.42
1:B:271:THR:HA	1:B:313:ASN:HB2	2.02	0.42
1:C:45:ARG:NE	4:C:4003:POP:O5	2.48	0.42
1:C:524:LEU:HA	1:C:524:LEU:HD12	1.84	0.42
1:D:190:VAL:O	1:D:194:CYS:HB2	2.20	0.42
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.89	0.42
1:F:278:PHE:HE2	1:F:467:SER:HG	1.63	0.42
1:F:314:THR:C	1:F:316:SER:H	2.23	0.42
1:A:75:ASN:HA	1:A:76:ASP:HA	1.66	0.41
1:A:98:ILE:HA	1:A:101:ILE:HD12	2.01	0.41
1:D:70:VAL:HA	1:D:71:PRO:HD3	1.88	0.41
1:B:437:THR:HG23	1:B:440:THR:H	1.85	0.41
1:D:137:VAL:HG22	1:D:177:VAL:O	2.20	0.41
1:D:73:ILE:HG23	1:D:88:GLY:C	2.40	0.41
1:E:102:ARG:NE	1:E:130:ASP:O	2.54	0.41
1:F:209:VAL:C	1:F:211:ASP:H	2.22	0.41
1:F:25:LYS:HD3	1:F:30:GLN:NE2	2.35	0.41
1:A:165:ALA:O	1:A:169:ASN:HB2	2.20	0.41
1:B:506:LYS:HE3	1:B:506:LYS:HB3	1.81	0.41
1:D:192:TYR:HA	1:D:431:TYR:HB3	2.03	0.41
1:D:260:THR:HG21	1:D:475:MET:SD	2.60	0.41
1:E:209:VAL:HG12	1:E:210:SER:N	2.36	0.41
1:E:263:ALA:O	1:E:264:ARG:C	2.58	0.41
1:F:471:THR:O	1:F:475:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ALA:O	1:B:507:CYS:HB3	2.20	0.41
1:C:281:ASN:HB3	1:C:518:ILE:HD13	2.01	0.41
1:E:10:TYR:HE1	1:E:175:ARG:HG3	1.85	0.41
1:E:51:THR:O	1:E:55:ILE:HG13	2.20	0.41
1:E:529:THR:N	1:E:530:PRO:HD3	2.34	0.41
1:F:524:LEU:HA	1:F:524:LEU:HD12	1.91	0.41
1:D:16:THR:HB	1:D:27:LEU:HD11	2.02	0.41
1:A:448:VAL:HG23	1:A:449:ALA:N	2.35	0.41
1:B:102:ARG:HD3	1:B:102:ARG:HA	1.82	0.41
1:B:508:ASN:HB2	1:D:519:ASP:OD2	2.21	0.41
1:C:226:ARG:HD3	1:C:226:ARG:HA	1.75	0.41
1:D:273:LYS:HA	1:D:276:GLN:HG3	2.02	0.41
1:D:78:ILE:HG12	1:D:96:MET:CE	2.51	0.41
1:E:267:VAL:HA	1:E:309:THR:O	2.21	0.41
1:E:75:ASN:HA	1:E:76:ASP:HA	1.77	0.41
1:A:394:SER:OG	1:A:395:ASN:N	2.54	0.41
1:D:283:THR:HG22	1:D:288:SER:O	2.20	0.41
1:D:479:GLN:HA	1:D:480:PRO:HD3	1.67	0.41
1:E:198:ASN:HA	1:E:441:SER:HB2	2.02	0.41
1:F:14:LEU:HD12	1:F:209:VAL:HG22	2.03	0.41
1:F:15:VAL:H	1:F:209:VAL:CG2	2.34	0.41
1:F:479:GLN:HA	1:F:480:PRO:HD3	1.65	0.41
1:F:44:ILE:HD12	1:F:58:ALA:HA	2.01	0.41
1:A:271:THR:OG1	1:A:272:ASN:N	2.54	0.41
1:A:527:GLU:O	1:A:529:THR:N	2.53	0.41
1:A:57:GLU:HG2	1:A:57:GLU:O	2.21	0.41
1:B:135:ILE:HG23	1:B:174:CYS:SG	2.61	0.41
1:B:197:SER:O	1:B:442:VAL:HG23	2.21	0.41
1:C:314:THR:HG21	1:C:354:ASN:ND2	2.35	0.41
1:C:357:LEU:C	1:C:359:THR:H	2.24	0.41
1:C:495:LEU:HD22	1:C:521:LEU:CD2	2.50	0.41
1:D:341:PRO:HG2	1:D:376:LEU:HD11	2.03	0.41
1:E:425:GLY:O	1:E:427:ILE:HG13	2.20	0.41
1:E:59:LEU:HA	1:E:59:LEU:HD23	1.84	0.41
1:E:98:ILE:HD13	1:E:101:ILE:HD12	2.02	0.41
1:A:373:ILE:HA	1:A:373:ILE:HD13	1.84	0.41
1:B:127:MET:HB3	1:B:131:MET:HG3	2.02	0.41
1:F:407:PHE:HE2	1:F:427:ILE:CD1	2.29	0.41
1:F:78:ILE:H	1:F:78:ILE:HD12	1.80	0.41
1:B:358:LEU:HD23	1:B:363:PHE:HE1	1.86	0.41
1:C:273:LYS:HA	1:C:276:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:THR:HG21	1:C:440:THR:O	2.20	0.41
1:C:455:ILE:HG22	1:C:455:ILE:O	2.20	0.41
1:C:4:SER:O	1:C:6:GLU:N	2.54	0.41
1:D:322:MET:CE	1:D:326:ALA:HB2	2.49	0.41
1:D:38:GLY:O	1:D:40:THR:N	2.54	0.41
1:E:422:ILE:CD1	1:E:422:ILE:N	2.83	0.41
1:A:335:ARG:HB3	1:A:336:PRO:CD	2.50	0.41
1:B:110:VAL:HA	1:B:133:ASP:OD2	2.21	0.41
1:D:416:THR:HA	1:D:420:ASP:OD1	2.21	0.41
1:D:28:TYR:CZ	1:D:64:LEU:HG	2.55	0.41
1:F:403:LYS:HD3	1:F:445:ILE:HG13	2.02	0.41
1:B:124:LEU:O	1:B:124:LEU:HD23	2.21	0.40
1:B:167:GLU:HG2	1:B:198:ASN:HD21	1.85	0.40
1:B:4:SER:O	1:B:6:GLU:N	2.54	0.40
1:B:50:ASP:O	1:B:52:LYS:N	2.54	0.40
1:B:65:CYS:HB3	1:B:70:VAL:O	2.21	0.40
1:D:343:GLY:HA2	1:D:346:ALA:HB2	2.03	0.40
1:C:523:ARG:HH11	1:D:508:ASN:HB3	1.86	0.40
1:E:495:LEU:HD22	1:E:521:LEU:HD23	2.02	0.40
1:F:115:VAL:HG13	1:F:120:GLU:HB2	2.03	0.40
1:F:333:VAL:O	1:F:333:VAL:HG12	2.21	0.40
1:A:278:PHE:HE1	1:A:518:ILE:HD11	1.86	0.40
1:A:55:ILE:HG23	1:A:84:ILE:CG2	2.51	0.40
1:D:314:THR:HG22	1:D:315:GLY:N	2.37	0.40
1:D:340:ASP:HA	1:D:341:PRO:HD3	1.88	0.40
1:E:339:PHE:CD2	1:E:341:PRO:HG3	2.54	0.40
1:C:369:ASN:O	1:C:370:SER:C	2.58	0.40
1:C:247:LEU:HD13	1:C:539:HIS:NE2	2.36	0.40
1:D:269:HIS:HB2	1:D:292:MET:SD	2.62	0.40
1:E:129:PRO:C	1:E:131:MET:H	2.24	0.40
1:E:198:ASN:C	1:E:198:ASN:OD1	2.59	0.40
1:E:96:MET:HA	1:E:97:PRO:HD3	1.92	0.40
1:A:435:LYS:N	1:A:436:GLY:HA2	2.35	0.40
1:A:455:ILE:HG22	1:A:455:ILE:O	2.21	0.40
1:B:274:VAL:HG23	1:B:275:HIS:CE1	2.55	0.40
1:B:50:ASP:C	1:B:52:LYS:H	2.24	0.40
1:B:75:ASN:HA	1:B:76:ASP:HA	1.68	0.40
1:D:331:ASN:HD22	1:D:331:ASN:HA	1.64	0.40
1:D:437:THR:HG23	1:D:440:THR:H	1.86	0.40
1:E:291:ILE:HG22	1:E:293:SER:H	1.86	0.40
1:E:40:THR:H	1:E:40:THR:HG23	1.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:ALA:O	1:E:537:LEU:HD12	2.22	0.40
1:E:92:GLY:HA2	1:E:114:SER:HB2	2.03	0.40
1:A:265:PRO:CD	1:A:288:SER:HB3	2.38	0.40
1:B:265:PRO:CD	1:B:288:SER:HB3	2.45	0.40
1:B:299:VAL:HG12	1:B:329:ALA:CB	2.52	0.40
1:C:204:ASP:OD1	1:C:434:SER:HB3	2.21	0.40
1:F:311:LEU:HD23	1:F:338:VAL:HB	2.02	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	500/540 (93%)	438 (88%)	53 (11%)	9 (2%)	8	34
1	B	498/540 (92%)	446 (90%)	39 (8%)	13 (3%)	5	26
1	C	499/540 (92%)	446 (89%)	44 (9%)	9 (2%)	8	34
1	D	499/540 (92%)	448 (90%)	41 (8%)	10 (2%)	7	31
1	E	497/540 (92%)	440 (88%)	47 (10%)	10 (2%)	7	31
1	F	497/540 (92%)	427 (86%)	55 (11%)	15 (3%)	4	23
All	All	2990/3240 (92%)	2645 (88%)	279 (9%)	66 (2%)	6	29

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	138	GLY
1	B	20	MET
1	B	434	SER
1	D	39	VAL

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Mol	Chain	Res	Type
1	E	11	SER
1	E	434	SER
1	E	438	ASN
1	F	138	GLY
1	F	210	SER
1	A	434	SER
1	A	528	ASN
1	B	39	VAL
1	B	108	ASP
1	B	155	GLY
1	C	5	LYS
1	C	370	SER
1	D	20	MET
1	D	434	SER
1	E	138	GLY
1	F	11	SER
1	F	20	MET
1	F	106	GLY
1	F	208	VAL
1	F	528	ASN
1	A	5	LYS
1	B	5	LYS
1	B	106	GLY
1	B	247	LEU
1	B	528	ASN
1	C	11	SER
1	C	108	ASP
1	C	126	LYS
1	D	5	LYS
1	D	108	ASP
1	D	276	GLN
1	E	20	MET
1	F	39	VAL
1	F	107	PRO
1	F	276	GLN
1	F	434	SER
1	A	20	MET
1	A	276	GLN
1	B	51	THR
1	B	131	MET
1	B	378	GLU
1	C	106	GLY

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Mol	Chain	Res	Type
1	D	186	ASN
1	E	39	VAL
1	E	108	ASP
1	F	209	VAL
1	F	272	ASN
1	A	524	LEU
1	B	126	LYS
1	C	107	PRO
1	C	483	GLY
1	D	126	LYS
1	E	276	GLN
1	F	126	LYS
1	A	39	VAL
1	D	106	GLY
1	D	138	GLY
1	E	209	VAL
1	E	190	VAL
1	F	71	PRO
1	C	209	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	413/449 (92%)	374 (91%)	39 (9%)	8	32
1	B	413/449 (92%)	368 (89%)	45 (11%)	6	25
1	C	411/449 (92%)	371 (90%)	40 (10%)	8	30
1	D	412/449 (92%)	369 (90%)	43 (10%)	7	27
1	E	412/449 (92%)	371 (90%)	41 (10%)	7	28
1	F	410/449 (91%)	362 (88%)	48 (12%)	5	22
All	All	2471/2694 (92%)	2215 (90%)	256 (10%)	7	27

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	TYR
1	A	51	THR
1	A	54	PHE
1	A	61	ILE
1	A	64	LEU
1	A	66	HIS
1	A	70	VAL
1	A	75	ASN
1	A	76	ASP
1	A	91	VAL
1	A	113	TRP
1	A	134	TYR
1	A	137	VAL
1	A	139	THR
1	A	154	MET
1	A	167	GLU
1	A	182	LEU
1	A	188	GLU
1	A	191	LEU
1	A	226	ARG
1	A	230	ASP
1	A	247	LEU
1	A	260	THR
1	A	274	VAL
1	A	284	LEU
1	A	297	SER
1	A	322	MET
1	A	328	ARG
1	A	348	GLU
1	A	352	LEU
1	A	362	GLN
1	A	408	LYS
1	A	434	SER
1	A	437	THR
1	A	467	SER
1	A	481	SER
1	A	515	VAL
1	A	517	LEU
1	A	524	LEU
1	B	13	TYR
1	B	37	ASN
1	B	51	THR
1	B	54	PHE

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Mol	Chain	Res	Type
1	B	64	LEU
1	B	66	HIS
1	B	70	VAL
1	B	75	ASN
1	B	76	ASP
1	B	93	GLN
1	B	113	TRP
1	B	144	LEU
1	B	154	MET
1	B	156	THR
1	B	182	LEU
1	B	187	ILE
1	B	188	GLU
1	B	191	LEU
1	B	207	CYS
1	B	226	ARG
1	B	247	LEU
1	B	255	SER
1	B	260	THR
1	B	274	VAL
1	B	276	GLN
1	B	284	LEU
1	B	288	SER
1	B	289	SER
1	B	291	ILE
1	B	297	SER
1	B	302	LEU
1	B	311	LEU
1	B	313	ASN
1	B	322	MET
1	B	328	ARG
1	B	335	ARG
1	B	362	GLN
1	B	395	ASN
1	B	408	LYS
1	B	441	SER
1	B	451	GLU
1	B	495	LEU
1	B	510	SER
1	B	517	LEU
1	B	524	LEU
1	C	13	TYR

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Mol	Chain	Res	Type
1	C	18	SER
1	C	51	THR
1	C	54	PHE
1	C	64	LEU
1	C	66	HIS
1	C	70	VAL
1	C	75	ASN
1	C	76	ASP
1	C	84	ILE
1	C	167	GLU
1	C	177	VAL
1	C	182	LEU
1	C	187	ILE
1	C	188	GLU
1	C	207	CYS
1	C	247	LEU
1	C	250	THR
1	C	260	THR
1	C	276	GLN
1	C	284	LEU
1	C	289	SER
1	C	291	ILE
1	C	293	SER
1	C	297	SER
1	C	302	LEU
1	C	312	LEU
1	C	313	ASN
1	C	322	MET
1	C	328	ARG
1	C	347	THR
1	C	362	GLN
1	C	437	THR
1	C	445	ILE
1	C	451	GLU
1	C	467	SER
1	C	495	LEU
1	C	510	SER
1	C	515	VAL
1	C	517	LEU
1	D	13	TYR
1	D	51	THR
1	D	54	PHE

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Mol	Chain	Res	Type
1	D	64	LEU
1	D	65	CYS
1	D	66	HIS
1	D	70	VAL
1	D	75	ASN
1	D	76	ASP
1	D	91	VAL
1	D	124	LEU
1	D	144	LEU
1	D	182	LEU
1	D	188	GLU
1	D	191	LEU
1	D	207	CYS
1	D	226	ARG
1	D	228	LEU
1	D	247	LEU
1	D	255	SER
1	D	260	THR
1	D	271	THR
1	D	274	VAL
1	D	276	GLN
1	D	284	LEU
1	D	289	SER
1	D	291	ILE
1	D	293	SER
1	D	297	SER
1	D	302	LEU
1	D	322	MET
1	D	328	ARG
1	D	362	GLN
1	D	395	ASN
1	D	408	LYS
1	D	434	SER
1	D	451	GLU
1	D	467	SER
1	D	481	SER
1	D	495	LEU
1	D	524	LEU
1	D	527	GLU
1	D	533	TRP
1	E	13	TYR
1	E	37	ASN

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Mol	Chain	Res	Type
1	E	40	THR
1	E	51	THR
1	E	54	PHE
1	E	64	LEU
1	E	66	HIS
1	E	70	VAL
1	E	76	ASP
1	E	113	TRP
1	E	124	LEU
1	E	143	THR
1	E	144	LEU
1	E	182	LEU
1	E	188	GLU
1	E	191	LEU
1	E	228	LEU
1	E	247	LEU
1	E	260	THR
1	E	271	THR
1	E	274	VAL
1	E	276	GLN
1	E	284	LEU
1	E	289	SER
1	E	291	ILE
1	E	297	SER
1	E	302	LEU
1	E	312	LEU
1	E	313	ASN
1	E	322	MET
1	E	328	ARG
1	E	362	GLN
1	E	408	LYS
1	E	448	VAL
1	E	451	GLU
1	E	481	SER
1	E	495	LEU
1	E	510	SER
1	E	515	VAL
1	E	517	LEU
1	E	524	LEU
1	F	13	TYR
1	F	40	THR
1	F	51	THR

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Mol	Chain	Res	Type
1	F	54	PHE
1	F	64	LEU
1	F	66	HIS
1	F	70	VAL
1	F	75	ASN
1	F	76	ASP
1	F	79	ASP
1	F	113	TRP
1	F	124	LEU
1	F	144	LEU
1	F	154	MET
1	F	188	GLU
1	F	191	LEU
1	F	202	SER
1	F	207	CYS
1	F	226	ARG
1	F	228	LEU
1	F	247	LEU
1	F	250	THR
1	F	260	THR
1	F	272	ASN
1	F	276	GLN
1	F	284	LEU
1	F	288	SER
1	F	289	SER
1	F	296	GLN
1	F	297	SER
1	F	299	VAL
1	F	302	LEU
1	F	311	LEU
1	F	313	ASN
1	F	321	GLU
1	F	322	MET
1	F	328	ARG
1	F	342	VAL
1	F	362	GLN
1	F	408	LYS
1	F	440	THR
1	F	451	GLU
1	F	467	SER
1	F	481	SER
1	F	495	LEU

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Mol	Chain	Res	Type
1	F	515	VAL
1	F	517	LEU
1	F	524	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) 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	259	ASN
1	A	272	ASN
1	A	275	HIS
1	A	276	GLN
1	A	281	ASN
1	A	313	ASN
1	A	355	ASN
1	A	362	GLN
1	A	484	ASN
1	A	514	GLN
1	B	37	ASN
1	B	66	HIS
1	B	75	ASN
1	B	93	GLN
1	B	193	GLN
1	B	272	ASN
1	B	275	HIS
1	B	276	GLN
1	B	281	ASN
1	B	313	ASN
1	B	355	ASN
1	B	484	ASN
1	B	514	GLN
1	C	66	HIS
1	C	93	GLN
1	C	193	GLN
1	C	272	ASN
1	C	275	HIS
1	C	276	GLN
1	C	281	ASN
1	C	313	ASN

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Mol	Chain	Res	Type
1	C	355	ASN
1	C	479	GLN
1	C	484	ASN
1	C	514	GLN
1	D	37	ASN
1	D	66	HIS
1	D	93	GLN
1	D	193	GLN
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	D	528	ASN
1	E	37	ASN
1	E	43	GLN
1	E	66	HIS
1	E	93	GLN
1	E	193	GLN
1	E	272	ASN
1	E	275	HIS
1	E	276	GLN
1	E	281	ASN
1	E	313	ASN
1	E	355	ASN
1	E	484	ASN
1	F	93	GLN
1	F	193	GLN
1	F	272	ASN
1	F	275	HIS
1	F	276	GLN
1	F	281	ASN
1	F	313	ASN
1	F	355	ASN
1	F	484	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\# Z  > 2$
4	POP	B	4002	2	6,8,8	0.62	0	13,13,13	1.58	2 (15%)
4	POP	F	4006	2	6,8,8	0.61	0	13,13,13	1.88	4 (30%)
3	TPS	B	2002	-	20,23,23	6.06	11 (55%)	25,33,33	1.63	5 (20%)
4	POP	C	4003	2	6,8,8	0.69	0	13,13,13	1.69	1 (7%)
3	TPS	E	2005	-	20,23,23	6.33	12 (60%)	25,33,33	1.99	7 (28%)
3	TPS	C	2003	-	20,23,23	6.79	12 (60%)	25,33,33	2.20	11 (44%)
4	POP	D	4004	2	6,8,8	0.75	0	13,13,13	1.51	2 (15%)
4	POP	E	4005	2	6,8,8	0.79	0	13,13,13	1.49	2 (15%)
3	TPS	D	2004	-	20,23,23	6.52	10 (50%)	25,33,33	2.16	9 (36%)
4	POP	A	4001	2	6,8,8	0.53	0	13,13,13	1.64	2 (15%)
3	TPS	F	2006	-	20,23,23	6.56	11 (55%)	25,33,33	2.01	8 (32%)
3	TPS	A	2001	-	20,23,23	6.43	11 (55%)	25,33,33	2.19	11 (44%)

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
4	POP	B	4002	2	-	3/6/6/6	-
4	POP	F	4006	2	-	4/6/6/6	-
3	TPS	B	2002	-	-	3/10/11/11	0/2/2/2
4	POP	C	4003	2	-	1/6/6/6	-
3	TPS	E	2005	-	-	5/10/11/11	0/2/2/2
3	TPS	C	2003	-	-	2/10/11/11	0/2/2/2
4	POP	D	4004	2	-	0/6/6/6	-
4	POP	E	4005	2	-	2/6/6/6	-
3	TPS	D	2004	-	-	3/10/11/11	0/2/2/2
4	POP	A	4001	2	-	2/6/6/6	-
3	TPS	F	2006	-	-	7/10/11/11	0/2/2/2
3	TPS	A	2001	-	-	5/10/11/11	0/2/2/2

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2003	TPS	C4-N3	26.19	1.62	1.39
3	F	2006	TPS	C4-N3	24.04	1.60	1.39
3	D	2004	TPS	C4-N3	23.50	1.60	1.39
3	A	2001	TPS	C4-N3	23.27	1.59	1.39
3	E	2005	TPS	C4-N3	23.00	1.59	1.39
3	B	2002	TPS	C4-N3	21.94	1.58	1.39
3	D	2004	TPS	C6-C5	9.34	1.55	1.50
3	A	2001	TPS	C6-C5	8.63	1.54	1.50
3	E	2005	TPS	C6-C5	7.80	1.54	1.50
3	F	2006	TPS	C6-C5	7.79	1.54	1.50
3	F	2006	TPS	C2-N3	7.77	1.52	1.36
3	C	2003	TPS	C2-N3	7.74	1.52	1.36
3	B	2002	TPS	C2-N3	7.71	1.52	1.36
3	D	2004	TPS	C2-N3	7.71	1.52	1.36
3	A	2001	TPS	C2-N3	7.71	1.52	1.36
3	E	2005	TPS	C2-N3	7.49	1.51	1.36
3	F	2006	TPS	C6A-N1A	7.04	1.49	1.34
3	B	2002	TPS	C6-C5	6.95	1.54	1.50
3	C	2003	TPS	C6A-N1A	6.75	1.48	1.34
3	E	2005	TPS	C6A-N1A	6.71	1.48	1.34
3	B	2002	TPS	C6A-N1A	6.56	1.48	1.34
3	A	2001	TPS	C6A-N1A	6.54	1.48	1.34
3	D	2004	TPS	C6A-N1A	6.14	1.47	1.34
3	F	2006	TPS	C4A-N3A	5.91	1.43	1.35
3	C	2003	TPS	C4A-N3A	5.53	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	TPS	C4A-N3A	5.49	1.42	1.35
3	D	2004	TPS	C4A-N3A	5.43	1.42	1.35
3	B	2002	TPS	C4A-N3A	5.25	1.42	1.35
3	E	2005	TPS	C4A-N3A	5.22	1.42	1.35
3	C	2003	TPS	C6-C5	4.98	1.53	1.50
3	F	2006	TPS	C4A-N4A	4.96	1.46	1.34
3	D	2004	TPS	C4A-N4A	4.82	1.46	1.34
3	C	2003	TPS	C4A-N4A	4.74	1.46	1.34
3	E	2005	TPS	C4A-N4A	4.70	1.45	1.34
3	B	2002	TPS	C4A-N4A	4.61	1.45	1.34
3	A	2001	TPS	C4A-N4A	4.58	1.45	1.34
3	E	2005	TPS	P1-O1	4.55	1.65	1.50
3	D	2004	TPS	P1-O1	4.20	1.64	1.50
3	B	2002	TPS	P1-O1	3.88	1.63	1.50
3	A	2001	TPS	P1-O1	3.70	1.62	1.50
3	C	2003	TPS	P1-O1	3.58	1.62	1.50
3	F	2006	TPS	P1-O1	3.55	1.62	1.50
3	D	2004	TPS	C6A-C5A	-2.88	1.31	1.37
3	F	2006	TPS	C2A-N3A	2.88	1.39	1.34
3	A	2001	TPS	C7A-N3	-2.88	1.43	1.48
3	A	2001	TPS	C6A-C5A	-2.86	1.31	1.37
3	E	2005	TPS	P1-O2	2.84	1.65	1.54
3	F	2006	TPS	P1-O3	-2.81	1.44	1.54
3	D	2004	TPS	P1-O2	2.80	1.65	1.54
3	B	2002	TPS	C6A-C5A	-2.71	1.32	1.37
3	C	2003	TPS	C2A-N3A	2.61	1.38	1.34
3	E	2005	TPS	C6A-C5A	-2.58	1.32	1.37
3	B	2002	TPS	P1-O3	-2.57	1.44	1.54
3	C	2003	TPS	C6A-C5A	-2.56	1.32	1.37
3	A	2001	TPS	P1-O3	-2.50	1.45	1.54
3	C	2003	TPS	P1-O3	-2.47	1.45	1.54
3	C	2003	TPS	P1-O2	2.40	1.64	1.54
3	D	2004	TPS	C2A-N3A	2.39	1.38	1.34
3	E	2005	TPS	C2A-N3A	2.39	1.38	1.34
3	A	2001	TPS	C2A-N3A	2.28	1.38	1.34
3	B	2002	TPS	C7A-N3	-2.27	1.44	1.48
3	F	2006	TPS	C6A-C5A	-2.26	1.33	1.37
3	B	2002	TPS	P1-O2	2.18	1.63	1.54
3	E	2005	TPS	P1-O7	2.10	1.67	1.60
3	F	2006	TPS	P1-O2	2.05	1.62	1.54
3	E	2005	TPS	C7A-N3	-2.03	1.44	1.48
3	C	2003	TPS	P1-O7	2.02	1.66	1.60

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	TPS	C6-C5-C4	-5.33	123.16	127.43
4	C	4003	POP	P2-O-P1	-5.16	115.12	132.83
3	D	2004	TPS	C6-C5-C4	-4.92	123.48	127.43
4	A	4001	POP	P2-O-P1	-4.72	116.62	132.83
3	D	2004	TPS	C6A-C5A-C4A	4.56	121.93	115.72
4	E	4005	POP	P2-O-P1	-4.52	117.32	132.83
4	F	4006	POP	P2-O-P1	-4.51	117.34	132.83
4	B	4002	POP	P2-O-P1	-4.46	117.54	132.83
3	E	2005	TPS	C6-C5-C4	-4.25	124.02	127.43
4	D	4004	POP	P2-O-P1	-4.20	118.40	132.83
3	D	2004	TPS	C5A-C7A-N3	-4.06	106.52	113.28
3	E	2005	TPS	C6A-C5A-C4A	4.04	121.22	115.72
3	A	2001	TPS	C6A-C5A-C4A	3.96	121.11	115.72
3	C	2003	TPS	C6A-C5A-C4A	3.91	121.04	115.72
3	F	2006	TPS	C6A-C5A-C4A	3.83	120.93	115.72
3	B	2002	TPS	C6A-C5A-C4A	3.78	120.87	115.72
3	C	2003	TPS	O3-P1-O7	3.70	116.57	106.73
3	F	2006	TPS	N4A-C4A-N3A	3.69	122.25	117.03
3	F	2006	TPS	O3-P1-O7	3.63	116.39	106.73
3	C	2003	TPS	N4A-C4A-N3A	3.59	122.11	117.03
3	C	2003	TPS	CM4-C4-N3	3.50	126.99	122.53
3	E	2005	TPS	CM2-C2A-N1A	3.48	120.97	117.14
3	B	2002	TPS	CM2-C2A-N1A	3.42	120.90	117.14
3	A	2001	TPS	CM2-C2A-N1A	3.37	120.85	117.14
3	C	2003	TPS	C5A-C7A-N3	-3.26	107.86	113.28
3	E	2005	TPS	C5A-C7A-N3	-3.25	107.86	113.28
4	F	4006	POP	O5-P2-O	3.25	115.52	104.64
3	F	2006	TPS	N1A-C2A-N3A	-3.20	120.04	125.54
3	A	2001	TPS	CM4-C4-C5	-3.17	120.68	127.60
3	D	2004	TPS	C5A-C6A-N1A	-3.03	118.77	123.82
3	A	2001	TPS	C5A-C6A-N1A	-2.98	118.86	123.82
3	A	2001	TPS	C5A-C7A-N3	-2.90	108.45	113.28
3	C	2003	TPS	N1A-C2A-N3A	-2.88	120.59	125.54
3	B	2002	TPS	C5A-C6A-N1A	-2.87	119.04	123.82
4	D	4004	POP	O2-P1-O	2.60	113.37	104.64
3	C	2003	TPS	CM2-C2A-N1A	2.60	119.99	117.14
3	A	2001	TPS	N4A-C4A-N3A	2.59	120.69	117.03
3	C	2003	TPS	C5A-C6A-N1A	-2.53	119.61	123.82
3	E	2005	TPS	C5A-C6A-N1A	-2.52	119.62	123.82
3	E	2005	TPS	N4A-C4A-N3A	2.48	120.54	117.03
3	D	2004	TPS	N4A-C4A-N3A	2.46	120.50	117.03
3	C	2003	TPS	C5A-C4A-N4A	-2.44	118.73	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	TPS	O3-P1-O7	2.39	113.09	106.73
3	F	2006	TPS	CM2-C2A-N1A	2.38	119.75	117.14
3	E	2005	TPS	N1A-C2A-N3A	-2.38	121.45	125.54
3	A	2001	TPS	C6A-N1A-C2A	2.37	120.00	115.96
3	A	2001	TPS	N1A-C2A-N3A	-2.37	121.46	125.54
3	D	2004	TPS	C6A-N1A-C2A	2.35	119.95	115.96
3	B	2002	TPS	N1A-C2A-N3A	-2.31	121.57	125.54
3	D	2004	TPS	N1A-C2A-N3A	-2.30	121.59	125.54
3	A	2001	TPS	C5A-C4A-N4A	-2.29	118.94	122.19
3	B	2002	TPS	C6A-N1A-C2A	2.25	119.79	115.96
3	C	2003	TPS	CM4-C4-C5	-2.23	122.72	127.60
4	A	4001	POP	O5-P2-O	2.22	112.07	104.64
4	E	4005	POP	O2-P1-O	2.21	112.03	104.64
4	F	4006	POP	O3-P1-O	2.19	111.98	104.64
3	C	2003	TPS	C6A-N1A-C2A	2.19	119.68	115.96
3	F	2006	TPS	C2A-N3A-C4A	2.12	121.39	118.08
4	F	4006	POP	O2-P1-O	2.10	111.68	104.64
3	D	2004	TPS	C7A-C5A-C6A	-2.10	116.68	120.69
3	F	2006	TPS	CM4-C4-C5	-2.05	123.12	127.60
3	F	2006	TPS	C5A-C4A-N3A	-2.04	118.05	121.24
4	B	4002	POP	O2-P1-O	2.02	111.41	104.64
3	D	2004	TPS	CM2-C2A-N1A	2.01	119.35	117.14

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4002	POP	P1-O-P2-O5
4	B	4002	POP	P1-O-P2-O6
4	F	4006	POP	P2-O-P1-O3
4	F	4006	POP	P1-O-P2-O5
4	F	4006	POP	P1-O-P2-O6
3	B	2002	TPS	C5-C6-C7-O7
3	B	2002	TPS	C6A-C5A-C7A-N3
3	E	2005	TPS	C7-O7-P1-O1
3	E	2005	TPS	C7-O7-P1-O2
3	E	2005	TPS	C7-O7-P1-O3
3	E	2005	TPS	C6A-C5A-C7A-N3
3	C	2003	TPS	C7-O7-P1-O2
3	C	2003	TPS	C6A-C5A-C7A-N3
4	E	4005	POP	P1-O-P2-O5
4	E	4005	POP	P1-O-P2-O6

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Mol	Chain	Res	Type	Atoms
4	A	4001	POP	P2-O-P1-O2
3	D	2004	TPS	C7-O7-P1-O2
3	D	2004	TPS	C6A-C5A-C7A-N3
3	A	2001	TPS	C5A-C7A-N3-C4
3	A	2001	TPS	C4-C5-C6-C7
3	A	2001	TPS	C6A-C5A-C7A-N3
3	F	2006	TPS	C4-C5-C6-C7
3	F	2006	TPS	C5-C6-C7-O7
3	F	2006	TPS	C7-O7-P1-O1
3	F	2006	TPS	C7-O7-P1-O2
3	F	2006	TPS	C7-O7-P1-O3
3	F	2006	TPS	C6A-C5A-C7A-N3
3	B	2002	TPS	C4A-C5A-C7A-N3
3	E	2005	TPS	C4A-C5A-C7A-N3
3	D	2004	TPS	C4A-C5A-C7A-N3
3	A	2001	TPS	C4A-C5A-C7A-N3
3	F	2006	TPS	C4A-C5A-C7A-N3
4	C	4003	POP	P1-O-P2-O6
4	F	4006	POP	P2-O-P1-O1
3	A	2001	TPS	C7-O7-P1-O2
4	B	4002	POP	P2-O-P1-O1
4	A	4001	POP	P2-O-P1-O1

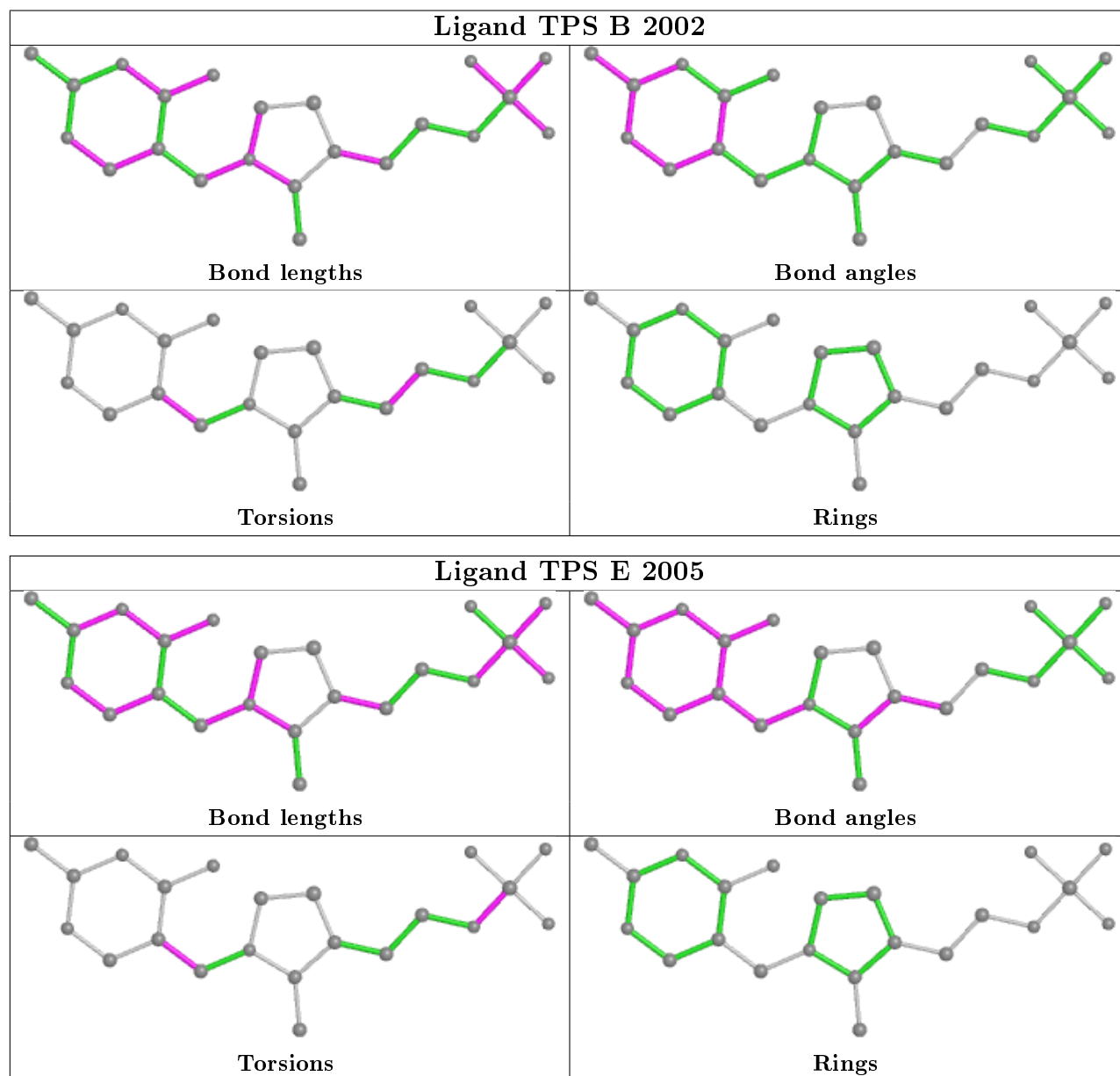
There are no ring outliers.

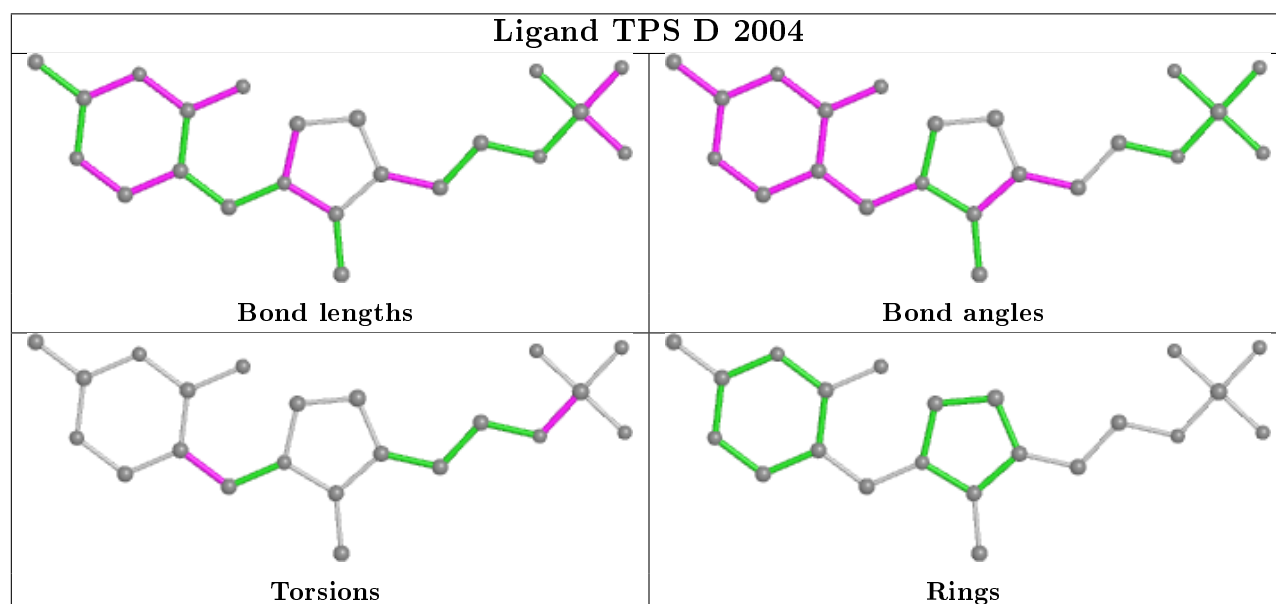
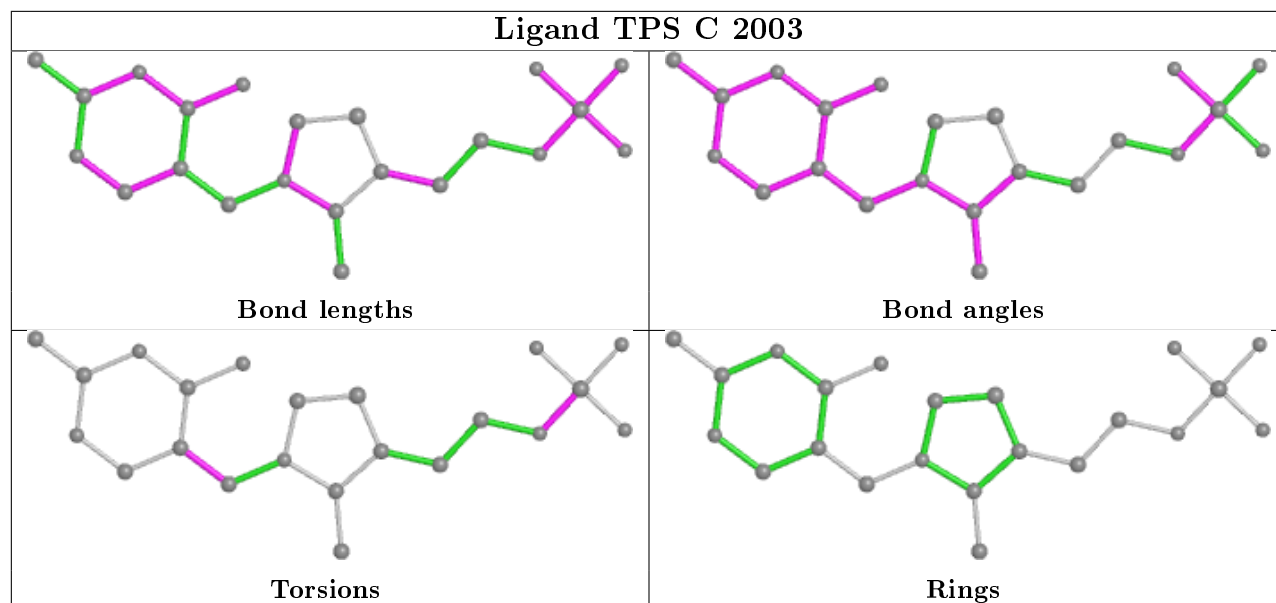
10 monomers are involved in 23 short contacts:

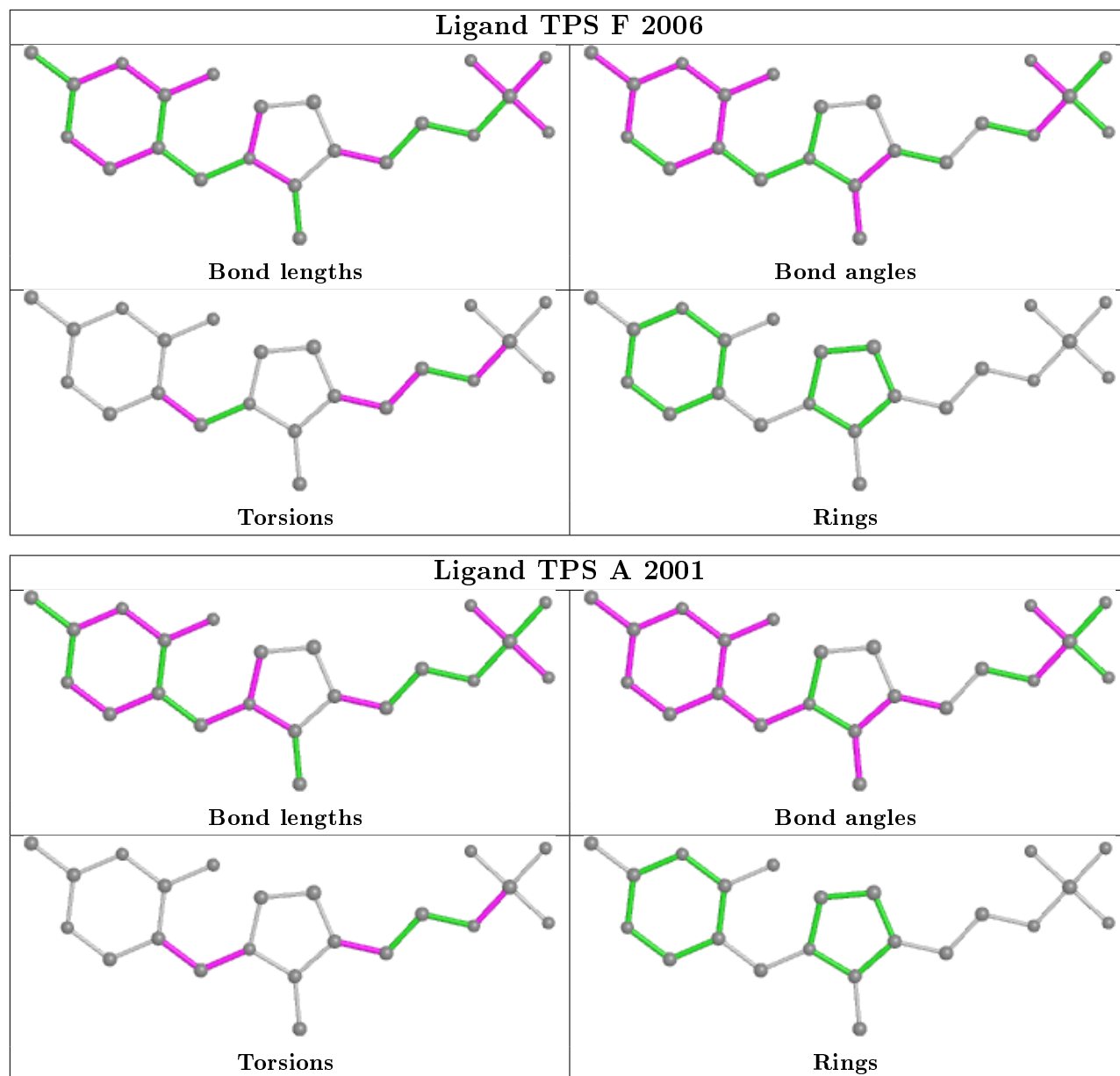
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4002	POP	1	0
4	F	4006	POP	1	0
3	B	2002	TPS	3	0
4	C	4003	POP	2	0
3	E	2005	TPS	4	0
4	D	4004	POP	1	0
3	D	2004	TPS	1	0
4	A	4001	POP	2	0
3	F	2006	TPS	4	0
3	A	2001	TPS	4	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	510/540 (94%)	-0.51	0 <span>100</span> <span>100</span>	26, 86, 109, 133	0
1	B	508/540 (94%)	-0.57	1 (0%) <span>95</span> <span>90</span>	26, 80, 103, 129	0
1	C	510/540 (94%)	-0.42	2 (0%) <span>92</span> <span>84</span>	42, 87, 113, 135	0
1	D	511/540 (94%)	-0.56	0 <span>100</span> <span>100</span>	40, 79, 107, 134	0
1	E	507/540 (93%)	-0.52	0 <span>100</span> <span>100</span>	40, 80, 105, 129	0
1	F	507/540 (93%)	-0.42	1 (0%) <span>95</span> <span>90</span>	43, 87, 113, 131	0
All	All	3053/3240 (94%)	-0.50	4 (0%) <span>95</span> <span>92</span>	26, 83, 109, 135	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	GLY	2.7
1	B	455	ILE	2.2
1	F	216	LEU	2.1
1	C	247	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



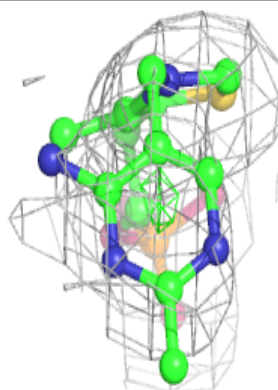
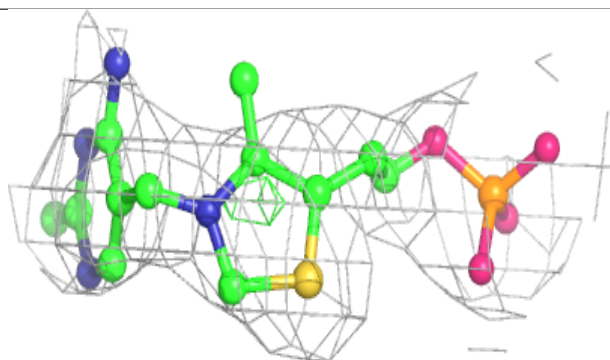
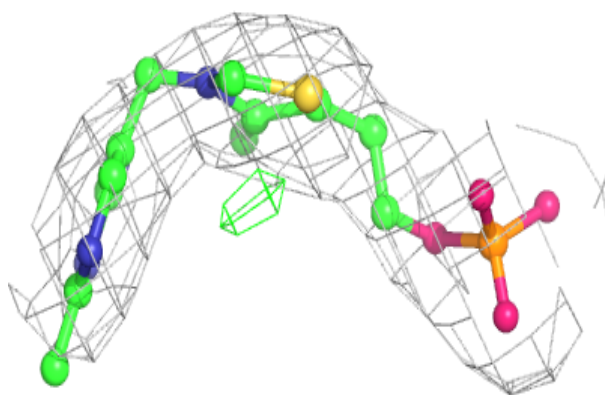
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	3002	1/1	0.91	0.28	61,61,61,61	0
3	TPS	E	2005	22/22	0.97	0.19	54,60,66,68	8
2	MG	D	3004	1/1	0.97	0.23	61,61,61,61	0
3	TPS	C	2003	22/22	0.97	0.21	66,73,76,79	7
4	POP	D	4004	9/9	0.97	0.17	53,60,65,68	5
2	MG	A	3001	1/1	0.97	0.15	70,70,70,70	0
2	MG	F	3006	1/1	0.97	0.28	63,63,63,63	0
4	POP	B	4002	9/9	0.97	0.20	48,57,67,70	2
3	TPS	F	2006	22/22	0.97	0.19	68,73,77,83	8
4	POP	E	4005	9/9	0.98	0.15	57,61,63,64	6
4	POP	F	4006	9/9	0.98	0.16	55,63,69,69	4
2	MG	C	3003	1/1	0.98	0.28	55,55,55,55	0
2	MG	E	3005	1/1	0.98	0.21	48,48,48,48	0
4	POP	A	4001	9/9	0.98	0.17	56,67,80,80	3
3	TPS	D	2004	22/22	0.98	0.19	57,63,69,74	6
3	TPS	B	2002	22/22	0.98	0.18	55,62,70,73	8
3	TPS	A	2001	22/22	0.98	0.18	60,69,76,77	7
4	POP	C	4003	9/9	0.98	0.22	55,68,75,82	3

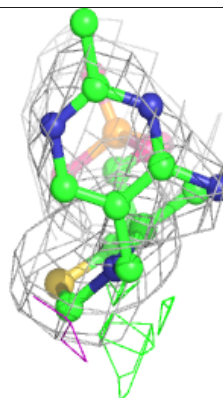
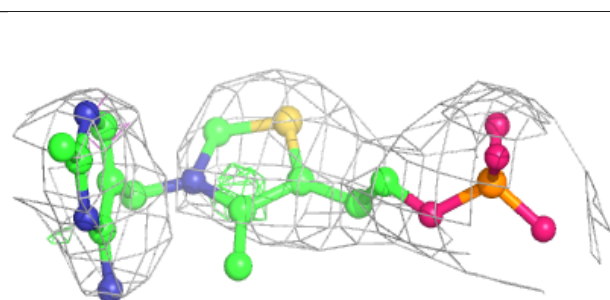
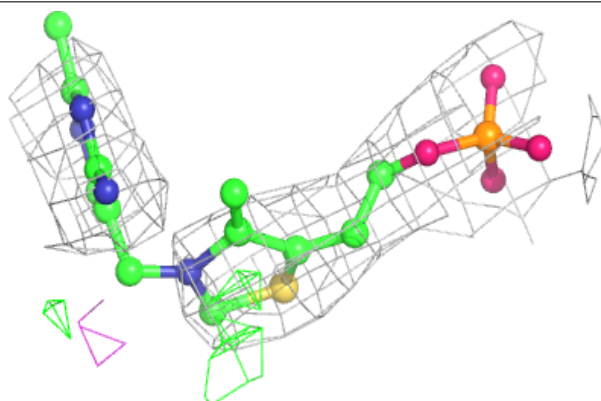
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPS E 2005:**

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

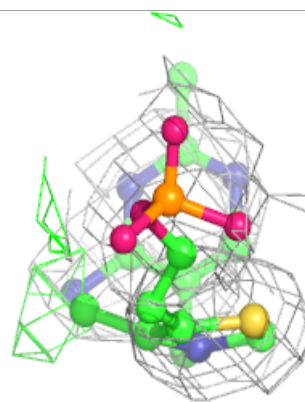
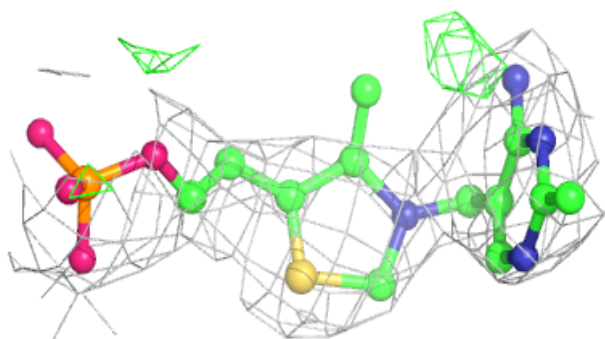
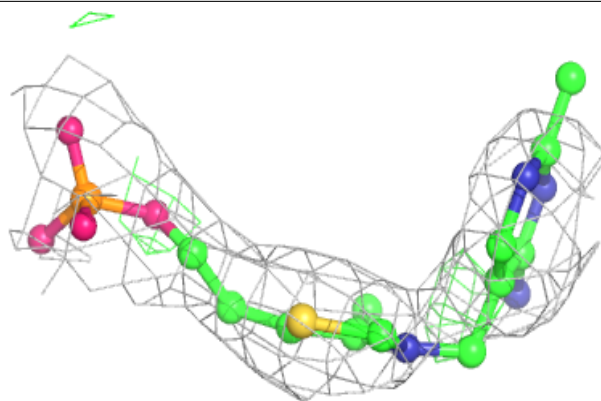
**Electron density around TPS C 2003:**

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

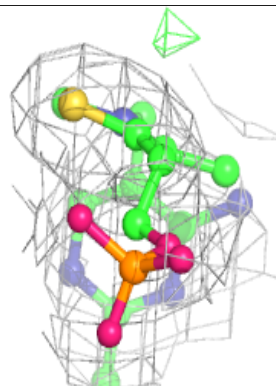
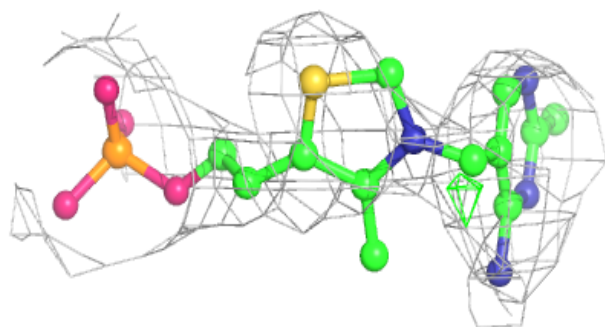
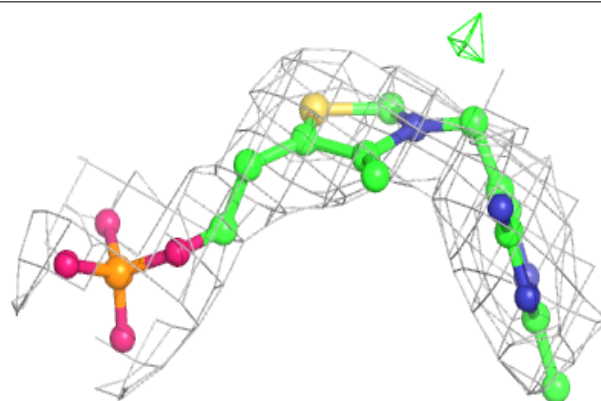


**Electron density around TPS F 2006:**

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

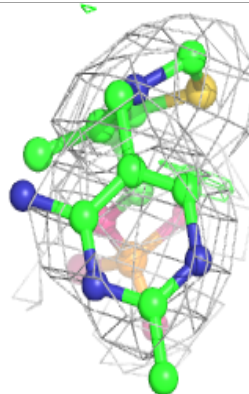
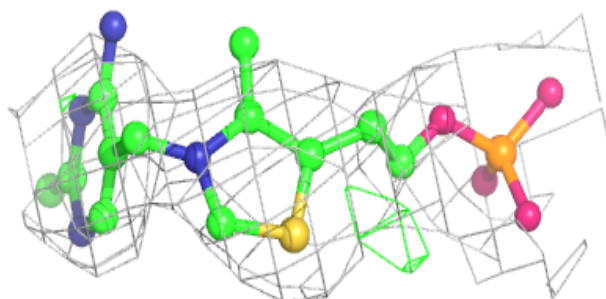
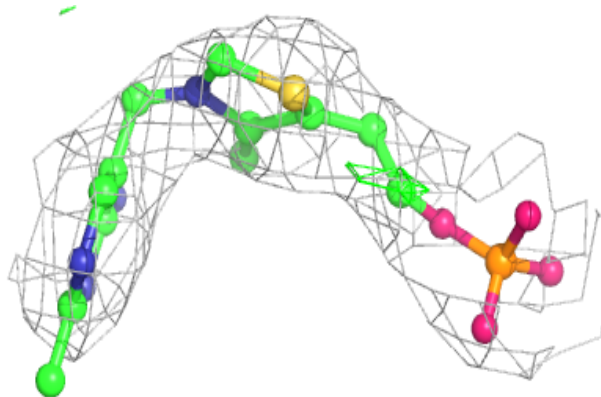
**Electron density around TPS D 2004:**

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

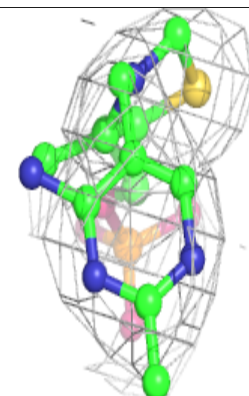
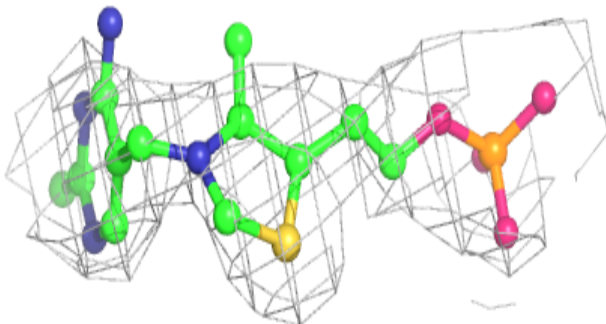
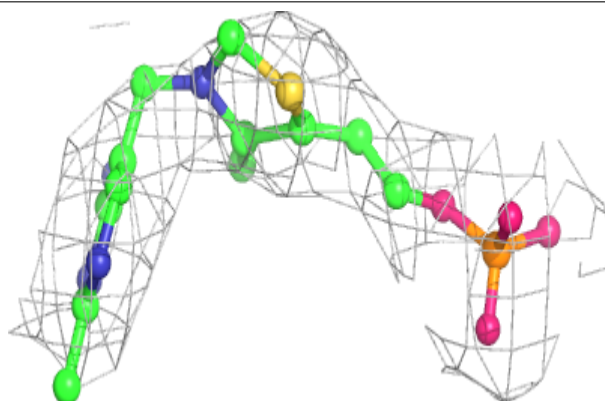


**Electron density around TPS B 2002:**

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

**Electron density around TPS A 2001:**

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



## 6.5 Other polymers

There are no such residues in this entry.