



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 PM UTC

PDB ID : 3NM3 / pdb_00003nm3
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

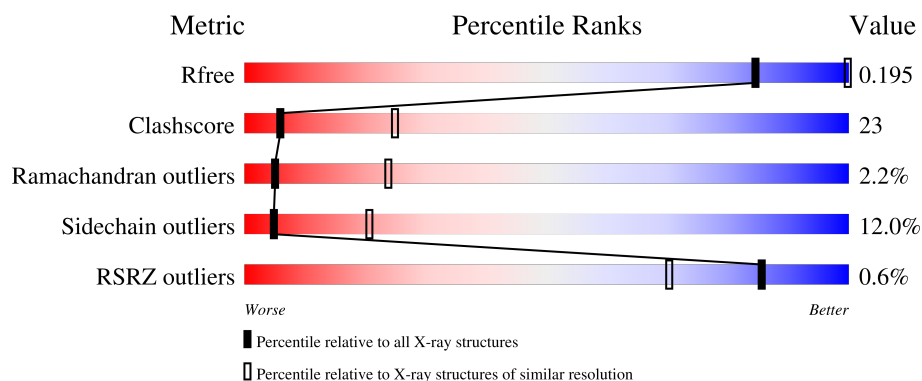
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	54% 34% 6% 6%
1	B	540	52% 35% 7% 6%
1	C	540	54% 34% 6% 6%
1	D	540	55% 34% 5% 5%
1	E	540	54% 33% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	540	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TPS	A	2001	-	X	-	-
3	TPS	C	2003	-	X	-	-
3	TPS	D	2004	-	X	-	-
3	TPS	E	2005	-	X	-	-
3	TPS	F	2006	-	X	-	-

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.

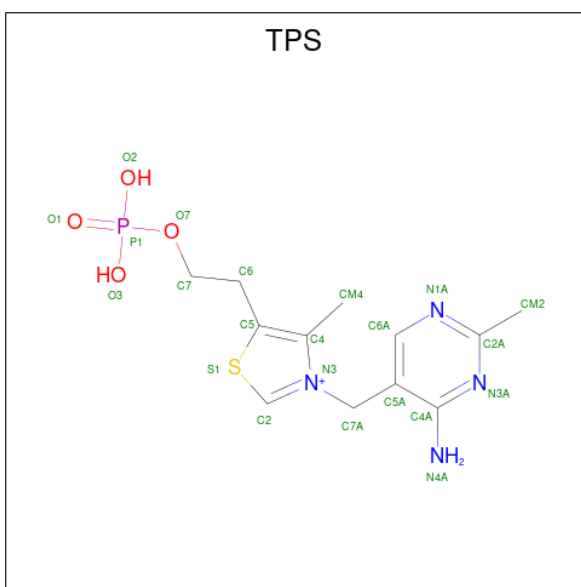
- Molecule 1 is a protein called Thiamine biosynthetic bifunctional enzyme.

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 (CCD ID: MG) (formula: Mg).

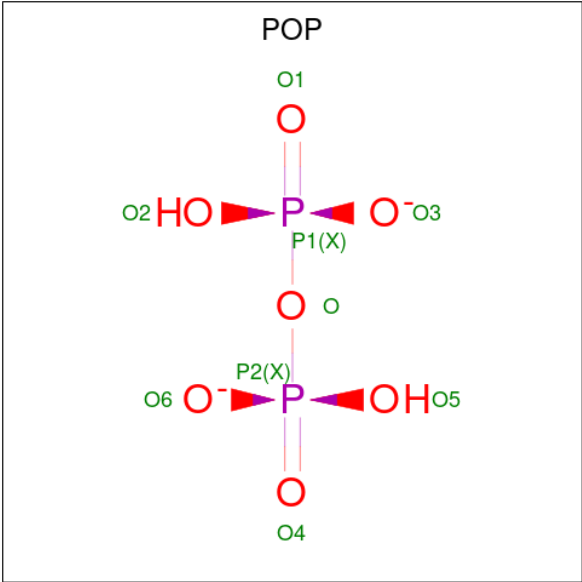
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMIN PHOSPHATE (CCD ID: TPS) (formula: C₁₂H₁₈N₄O₄PS).



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- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).

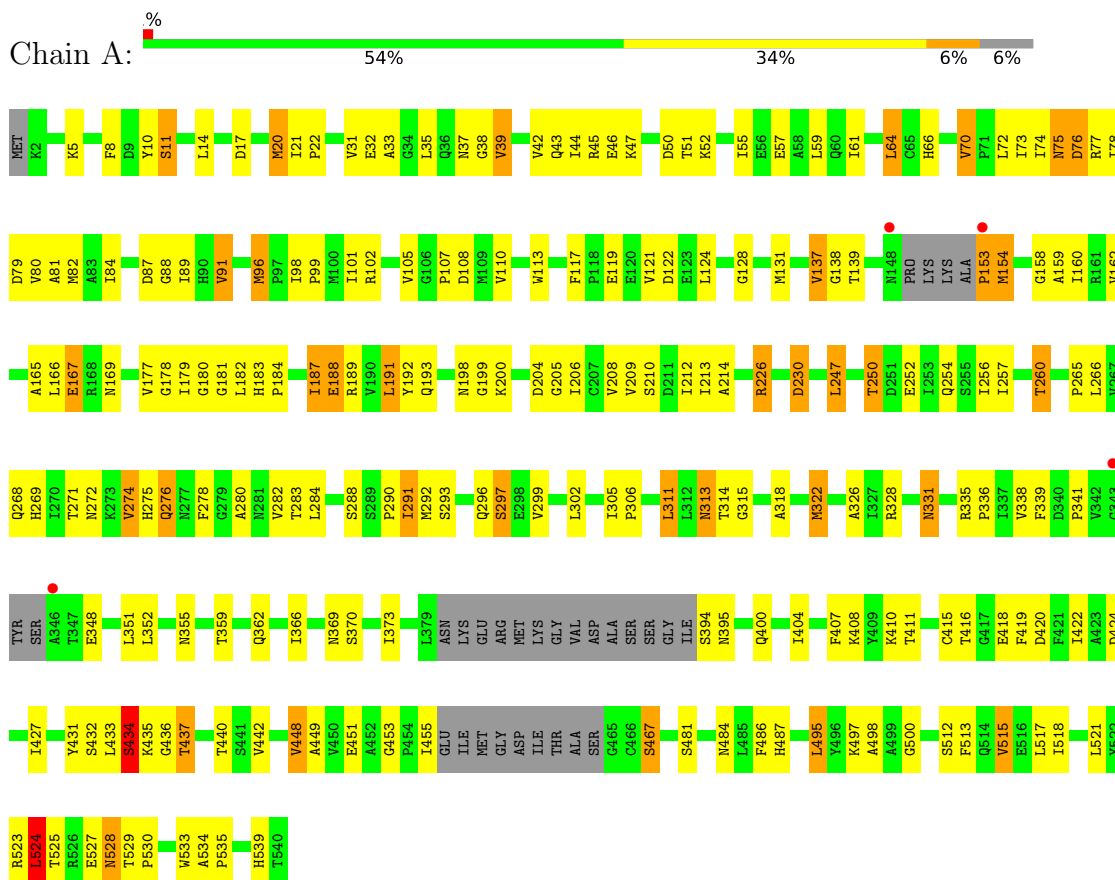


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		
4	C	1	Total	O	P	1	0
			9	7	2		
4	D	1	Total	O	P	0	0
			9	7	2		
4	E	1	Total	O	P	1	0
			9	7	2		
4	F	1	Total	O	P	0	0
			9	7	2		

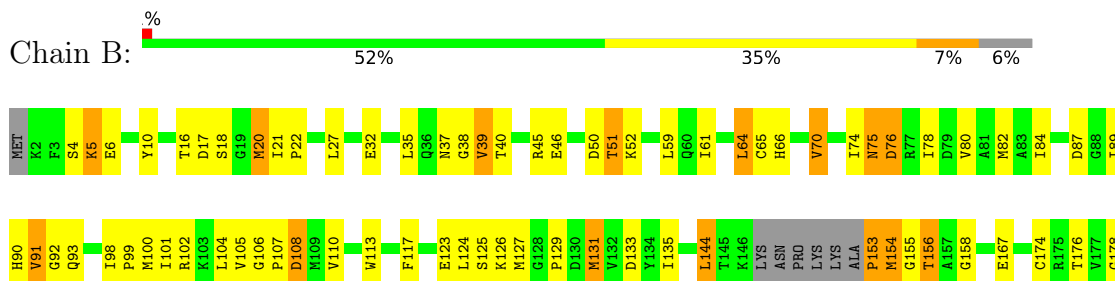
3 Residue-property plots [i](#)

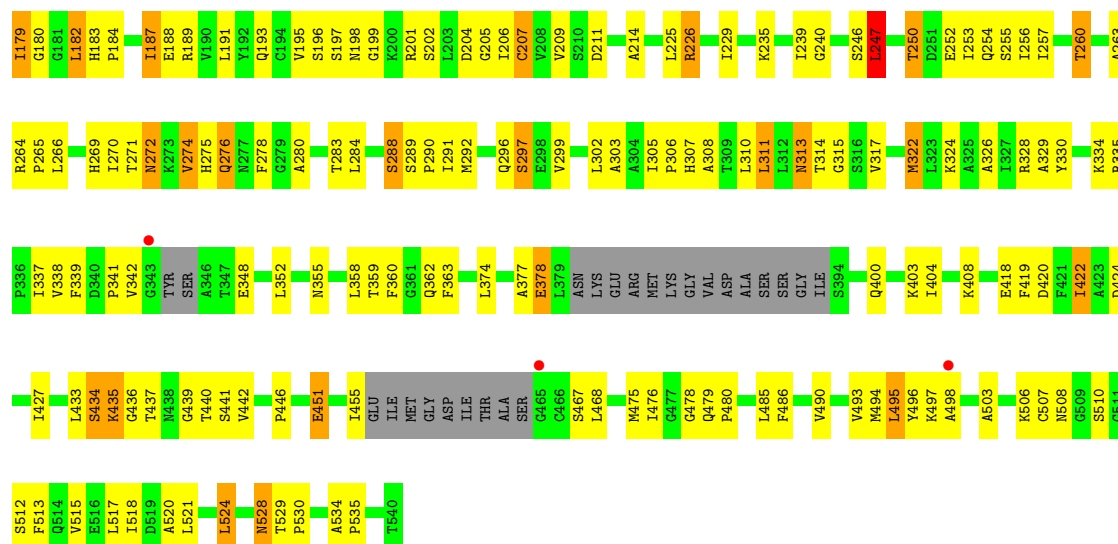
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Thiamine biosynthetic bifunctional enzyme

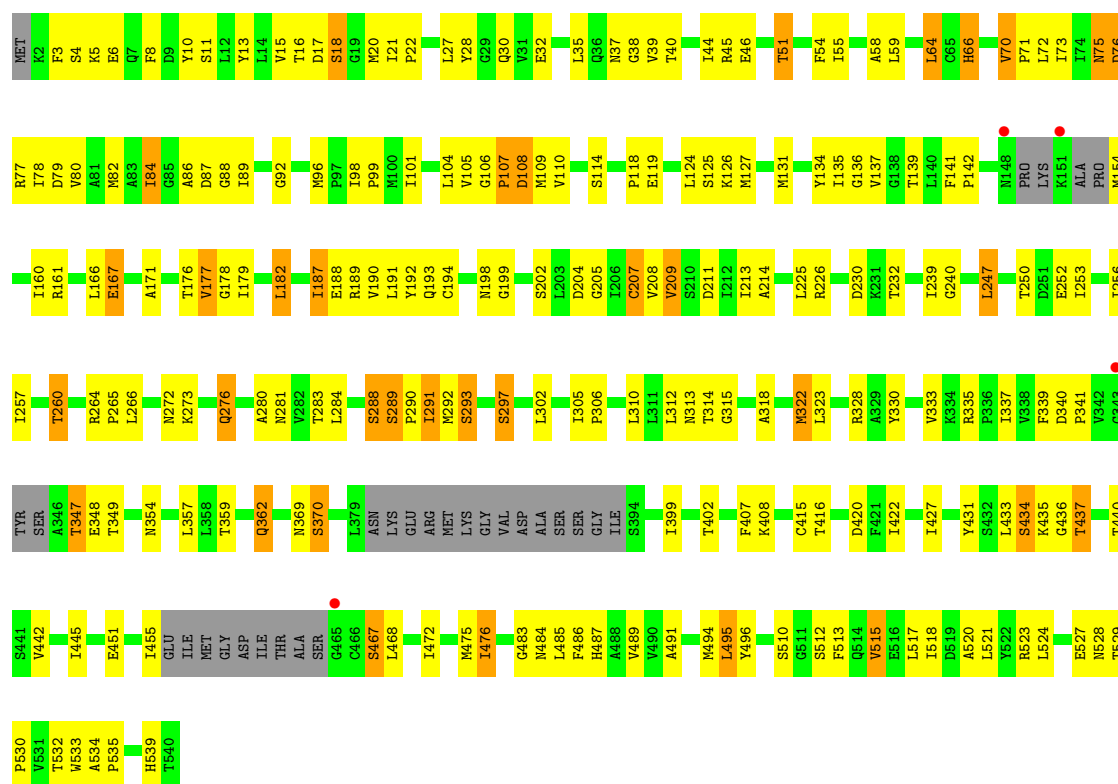


• Molecule 1: Thiamine biosynthetic bifunctional enzyme

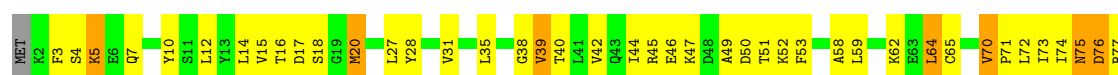


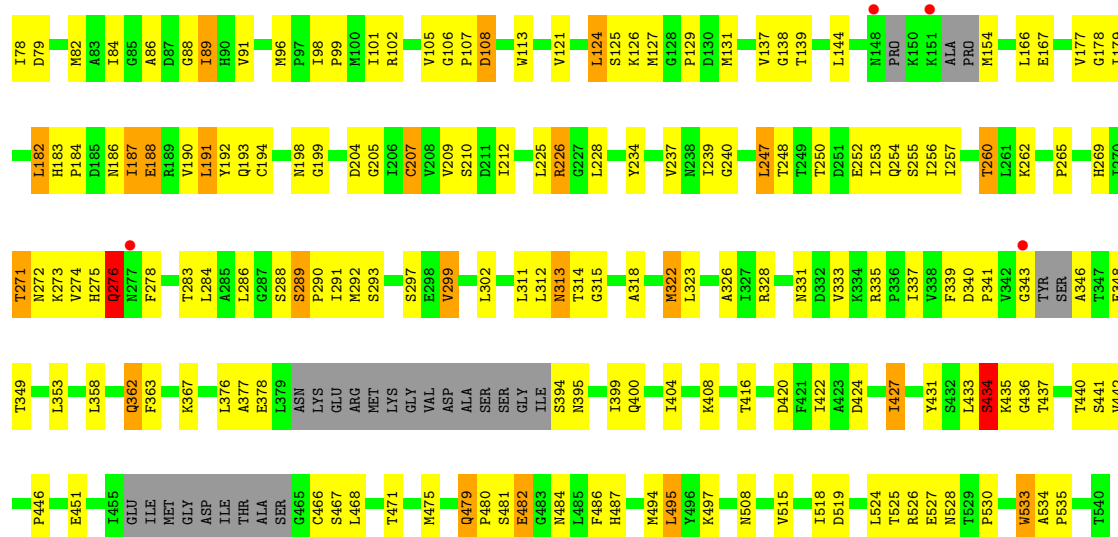


• Molecule 1: Thiamine biosynthetic bifunctional enzyme



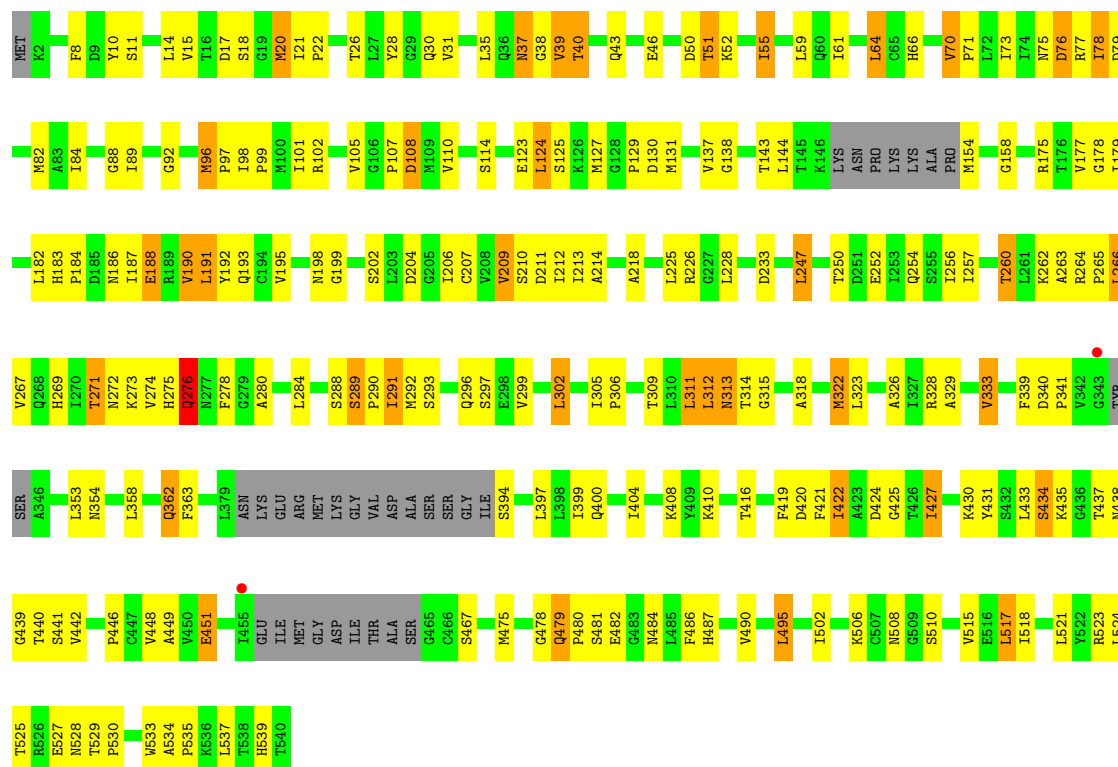
• Molecule 1: Thiamine biosynthetic bifunctional enzyme





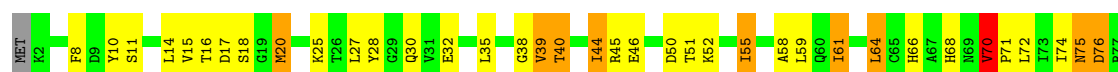
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

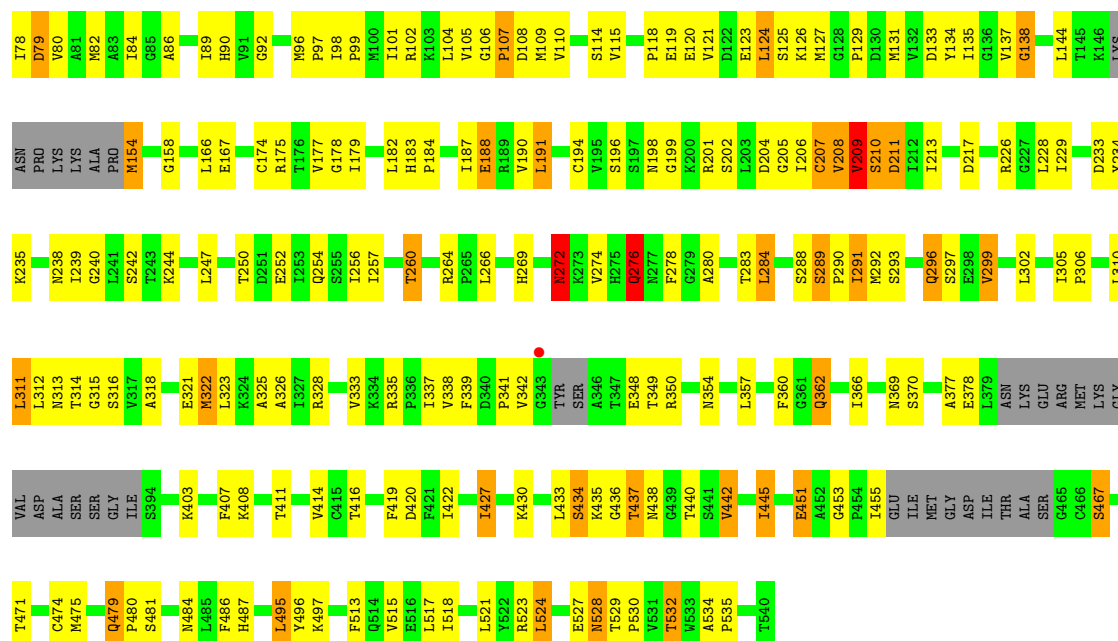
Chain E: 54% 33% 7% 6%



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain F: 51% 35% 8% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.19Å 154.60Å 148.65Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	46.00 – 3.10 46.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	80.6 (46.00-3.10) 59.4 (46.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.251 0.195 , 0.195	Depositor DCC
R_{free} test set	2678 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/3869	0.91	11/5246 (0.2%)
1	B	0.50	0/3859	0.89	7/5232 (0.1%)
1	C	0.48	0/3861	0.88	5/5235 (0.1%)
1	D	0.50	0/3870	0.90	5/5246 (0.1%)
1	E	0.49	0/3851	0.89	6/5221 (0.1%)
1	F	0.48	0/3843	0.92	10/5213 (0.2%)
All	All	0.49	0/23153	0.90	44/31393 (0.1%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	PRO	CA-N-CD	-8.93	99.49	112.00
1	B	153	PRO	CA-N-CD	-8.92	99.51	112.00
1	B	435	LYS	N-CA-C	7.78	119.45	110.97
1	E	318	ALA	CA-C-N	7.31	124.92	119.66
1	E	318	ALA	C-N-CA	7.31	124.92	119.66
1	E	479	GLN	CA-C-N	6.94	127.11	120.31
1	E	479	GLN	C-N-CA	6.94	127.11	120.31
1	A	96	MET	CA-C-N	6.43	126.44	119.89
1	A	96	MET	C-N-CA	6.43	126.44	119.89
1	C	533	TRP	N-CA-C	6.39	118.96	110.53
1	B	229	ILE	N-CA-C	6.29	117.08	110.72
1	D	335	ARG	CA-C-N	6.15	126.36	119.90
1	D	335	ARG	C-N-CA	6.15	126.36	119.90
1	F	335	ARG	CA-C-N	6.11	125.87	119.76
1	F	335	ARG	C-N-CA	6.11	125.87	119.76
1	D	479	GLN	CA-C-N	5.97	127.30	119.84
1	D	479	GLN	C-N-CA	5.97	127.30	119.84
1	C	476	ILE	CB-CA-C	-5.81	104.29	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	96	MET	CA-C-N	5.71	125.72	119.90
1	E	96	MET	C-N-CA	5.71	125.72	119.90
1	D	42	VAL	N-CA-C	5.63	116.11	107.77
1	B	418	GLU	N-CA-C	-5.60	105.18	111.28
1	F	211	ASP	N-CA-C	-5.54	107.53	114.56
1	F	479	GLN	CA-C-N	5.52	126.74	119.84
1	F	479	GLN	C-N-CA	5.52	126.74	119.84
1	A	117	PHE	CA-C-N	5.49	124.68	118.97
1	A	117	PHE	C-N-CA	5.49	124.68	118.97
1	A	128	GLY	CA-C-N	5.46	125.93	120.14
1	A	128	GLY	C-N-CA	5.46	125.93	120.14
1	F	296	GLN	N-CA-C	5.45	117.22	111.28
1	A	42	VAL	N-CA-C	5.43	115.94	108.12
1	A	453	GLY	CA-C-N	5.33	125.25	119.76
1	A	453	GLY	C-N-CA	5.33	125.25	119.76
1	F	229	ILE	N-CA-C	5.31	116.09	110.72
1	F	70	VAL	N-CA-C	5.29	113.66	107.89
1	F	453	GLY	CA-C-N	5.21	124.97	119.76
1	F	453	GLY	C-N-CA	5.21	124.97	119.76
1	C	335	ARG	CA-C-N	5.20	125.60	119.99
1	C	335	ARG	C-N-CA	5.20	125.60	119.99
1	A	418	GLU	N-CA-C	-5.08	105.75	111.28
1	C	532	THR	N-CA-C	5.07	117.70	111.82
1	B	117	PHE	CA-C-N	5.04	126.14	119.84
1	B	117	PHE	C-N-CA	5.04	126.14	119.84
1	B	179	ILE	N-CA-C	5.01	114.86	107.75

There are no chirality outliers.

There are no planarity outliers.

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	3809	0	3814	181	0
1	B	3799	0	3810	181	0
1	C	3803	0	3796	172	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3812	0	3809	177	0
1	E	3792	0	3802	174	0
1	F	3784	0	3780	184	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	3	0
3	F	22	0	16	3	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	1052	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 23.

All (1052) 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:167:GLU:HG2	1:F:198:ASN:HD21	1.31	0.94
1:F:266:LEU:HD11	1:F:291:ILE:HG13	1.50	0.94
1:C:78:ILE:HG22	1:C:82:MET:HE2	1.53	0.90
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:E:17:ASP:HB3	1:E:20:MET:HE2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:HE1	1:B:209:VAL:HG12	1.56	0.85
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
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:C:89:ILE:HG13	1:C:89:ILE:O	1.78	0.81
1:F:89:ILE:HD11	1:F:101:ILE:HG21	1.62	0.81
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:F:17:ASP:HB3	1:F:20:MET:HE2	1.63	0.80
1:C:17:ASP:HB3	1:C:20:MET:HE2	1.62	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: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:C:127:MET:HE3	1:C:131:MET:HB3	1.67	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:F:257:ILE:HG12	1:F:475:MET:HE1	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ALA:HB2	1:A:292:MET:HE3	1.67	0.74
1:D:78:ILE:HG22	1:D:82:MET:HE2	1.69	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: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:B:179:ILE:HG12	1:B:180:GLY:N	2.03	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:86:ALA:O	1:F:109:MET:HE2	1.88	0.72
1:E:73:ILE:HG23	1:E:88:GLY:C	2.14	0.71
1:F:190:VAL:O	1:F:194:CYS:HB2	1.90	0.71
1:B:322:MET:HE3	1:B:322:MET:O	1.90	0.71
1:A:280:ALA:HB2	1:A:292:MET:CE	2.21	0.71
1:A:78:ILE:HG22	1:A:82:MET:HE2	1.72	0.71
1:B:269:HIS:CD2	1:B:311:LEU:HD12	2.26	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:B:269:HIS:HD2	1:B:311:LEU:HD12	1.55	0.70
1:A:82:MET:HE1	1:C:82:MET:HE1	1.73	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:91:VAL:HG11	1:A:101:ILE:HD13	1.75	0.69
1:A:250:THR:HG23	1:A:530:PRO:HB2	1.74	0.69
1:A:254:GLN:HG3	1:A:528:ASN:HB3	1.74	0.69
1:A:420:ASP:OD2	1:A:497:LYS:HD3	1.92	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:D:127:MET:HE3	1:D:131:MET:HB3	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:257:ILE:HG12	1:C:475:MET:HE1	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:B:17:ASP:HB3	1:B:20:MET:HE2	1.74	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:43:GLN:HE22	3:E:2005:TPS:HM23	1.59	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
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: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:137:VAL:HG23	1:A:178:GLY:HA2	1.76	0.66
1:A:154:MET:SD	1:A:158:GLY:HA3	2.35	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:B:38:GLY:O	1:B:39:VAL:C	2.37	0.66
1:C:407:PHE:CE2	1:C:427:ILE:HD11	2.31	0.66
1:A:20:MET:HE1	1:A:209:VAL:HG22	1.77	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:D:38:GLY:O	1:D:39:VAL:C	2.39	0.65
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:17:ASP:HB3	1:A:20:MET:HE2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:VAL:HB	1:E:209:VAL:CG2	2.27	0.65
1:E:123:GLU:O	1:E:127:MET:HG3	1.96	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
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:A:96:MET:HE3	1:A:101:ILE:HG12	1.79	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:B:82:MET:HE1	1:F:82:MET:HE1	1.80	0.63
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:HD2	1:B:153:PRO:O	1.98	0.63
1:D:82:MET:HE1	1:E:82:MET:HE1	1.81	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:C:280:ALA:HB2	1:C:292:MET:HE3	1.81	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:N	1:F:78:ILE:HD12	2.13	0.62
1:E:78:ILE:HD12	1:E:78:ILE:N	2.14	0.62
1:F:455:ILE:HG22	1:F:455:ILE:O	1.99	0.62
1:C:318:ALA:HB1	1:C:322:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:199:GLY:O	1:F:437:THR:HG22	1.98	0.62
1:F:202:SER:HB3	1:F:436:GLY:HA3	1.82	0.62
1:E:528:ASN:C	1:E:530:PRO:HD3	2.23	0.62
1:F:256:ILE:O	1:F:260:THR:HG22	1.99	0.62
1:D:528:ASN:C	1:D:530:PRO:HD3	2.24	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:C:78:ILE:HG12	1:C:96:MET:HE3	1.81	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:C:86:ALA:O	1:C:109:MET:HE2	1.98	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:C:125:SER:C	1:C:127:MET:H	2.08	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:A:322:MET:O	1:A:322:MET:HE3	2.00	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:C:20:MET:HE1	1:C:209:VAL:HG12	1.81	0.61
1:D:35:LEU:CD2	1:D:70:VAL:HG11	2.31	0.61
1:E:264:ARG:O	1:E:264:ARG:HG2	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:D:17:ASP:HB3	1:D:20:MET:HE2	1.83	0.61
1:D:314:THR:CG2	1:D:353:LEU:HD23	2.31	0.61
1:B:257:ILE:HG12	1:B:475:MET:HE1	1.82	0.61
1:A:79:ASP:HB2	1:C:96:MET:HE1	1.83	0.61
1:A:181:GLY:O	1:A:183:HIS:HD2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:204:ASP:CG	1:B:434:SER:HB3	2.26	0.60
1:C:127:MET:HE3	1:C:131:MET:CB	2.32	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:E:99:PRO:HA	1:E:131:MET:HE1	1.83	0.59
1:E:421:PHE:C	1:E:422:ILE:HD12	2.27	0.59
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:D:290:PRO:HB2	1:D:292:MET:HE2	1.82	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:B:5:LYS:HZ1	1:B:108:ASP:H	1.50	0.59
1:A:89:ILE:HD11	1:A:101:ILE:CG2	2.33	0.59
1:B:290:PRO:HB2	1:B:292:MET:HE2	1.85	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:F:124:LEU:C	1:F:124:LEU:HD23	2.28	0.59
1:A:437:THR:HG23	1:A:440:THR:H	1.66	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:LEU:CD2	1:A:84:ILE:HB	2.32	0.58
1:A:407:PHE:CE2	1:A:427:ILE:HD11	2.38	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:E:280:ALA:HB2	1:E:292:MET:HE3	1.86	0.58
1:F:20:MET:HE3	1:F:213:ILE:HB	1.84	0.58
1:A:20:MET:HE3	1:A:213:ILE:HB	1.85	0.57
1:C:265:PRO:O	1:C:288:SER:HB2	2.04	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
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:125:SER:C	1:B:127:MET:H	2.12	0.57
1:B:424:ASP:HB2	1:B:486:PHE:CD1	2.40	0.57
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:20:MET:HE1	1:E:209:VAL:HG12	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:SER:HB3	1:A:226:ARG:NH2	2.21	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:C:28:TYR:CZ	1:C:64:LEU:HG	2.40	0.56
1:D:275:HIS:O	1:D:276:GLN:C	2.49	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:278:PHE:HE1	1:E:518:ILE:HD11	1.70	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: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:99:PRO:HA	1:B:131:MET:HE1	1.87	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:D:482:GLU:CD	1:D:482:GLU:H	2.13	0.55
1:F:209:VAL:C	1:F:211:ASP:N	2.63	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: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
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:20:MET:HE3	1:E:213:ILE:HB	1.89	0.55
1:A:292:MET:HE3	1:F:274:VAL:HG11	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:280:ALA:HB2	1:B:292:MET:HE3	1.90	0.54
1:E:37:ASN:N	1:E:37:ASN:ND2	2.54	0.54
1:D:78:ILE:HG13	1:D:89:ILE:HD12	1.88	0.54
1:D:187:ILE:HD12	1:D:225:LEU:HD22	1.88	0.54
1:F:419:PHE:CE1	1:F:451:GLU:HG2	2.43	0.54
1:F:513:PHE:CD2	1:F:513:PHE:C	2.84	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:256:ILE:HG22	1:D:475:MET:HE3	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: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:3:PHE:CD2	1:C:71:PRO:HG3	2.43	0.53
1:C:45:ARG:NH2	4:C:4003:POP:O5	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:TYR:CD1	1:D:234:TYR:HD2	2.26	0.53
1:F:366:ILE:HG13	1:F:411:THR:HG21	1.90	0.53
1:C:78:ILE:HG22	1:C:82:MET:CE	2.31	0.53
1:E:262:LYS:HG2	1:E:262:LYS:O	2.06	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:D:533:TRP:C	1:D:535:PRO:HD2	2.33	0.53
1:C:35:LEU:CD2	1:C:70:VAL:HG11	2.37	0.53
1:C:107:PRO:O	1:C:108:ASP:CB	2.56	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:523:ARG:NH1	1:D:508:ASN:HB3	2.22	0.53
1:E:275:HIS:O	1:E:276:GLN:C	2.51	0.53
1:A:204:ASP:CG	1:A:434:SER:HB3	2.33	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:D:252:GLU:O	1:D:256:ILE:HG12	2.08	0.52
1:A:38:GLY:O	1:A:39:VAL:C	2.51	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:78:ILE:H	1:E:78:ILE:CD1	2.22	0.52
1:E:266:LEU:CD1	1:E:291:ILE:HG13	2.40	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:B:124:LEU:C	1:B:124:LEU:HD23	2.35	0.52
1:D:98:ILE:N	1:D:99:PRO:HD2	2.25	0.52
1:D:253:ILE:HD11	1:D:494:MET:HE2	1.91	0.52
1:F:28:TYR:CD1	1:F:64:LEU:HD12	2.44	0.52
1:F:278:PHE:CE1	1:F:518:ILE:HD11	2.45	0.52
1:C:264:ARG:O	1:C:264:ARG:HG2	2.10	0.52
1:D:50:ASP:C	1:D:52:LYS:H	2.17	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:A:179:ILE:HG12	1:A:180:GLY:N	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ASP:OD2	1:D:497:LYS:HD3	2.10	0.52
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: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:B:253:ILE:HD11	1:B:494:MET:HE2	1.92	0.51
1:D:424:ASP:HB3	1:D:446:PRO:HG2	1.92	0.51
1:F:204:ASP:CG	1:F:434:SER:HB3	2.36	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:D:179:ILE:HG13	1:D:207:CYS:HB3	1.92	0.51
1:D:322:MET:HE3	1:D:322:MET:O	2.10	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:C:79:ASP:HA	1:C:82:MET:HE3	1.91	0.51
1:C:266:LEU:HD11	1:C:291:ILE:CG1	2.29	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:38:GLY:O	1:E:39:VAL:C	2.53	0.51
1:E:276:GLN:HA	1:E:276:GLN:HE21	1.76	0.51
1:F:99:PRO:HA	1:F:131:MET:HE1	1.92	0.51
1:A:318:ALA:HB1	1:A:322:MET:HG2	1.93	0.51
1:C:20:MET:HG2	1:C:20:MET:O	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:A:274:VAL:HG13	1:E:292:MET:HG3	1.93	0.51
1:B:528:ASN:C	1:B:530:PRO:HD3	2.35	0.51
1:A:355:ASN:O	1:A:359:THR:HG23	2.11	0.51
1:E:517:LEU:O	1:E:517:LEU:HD23	2.11	0.51
1:B:125:SER:C	1:B:127:MET:N	2.68	0.51
1:E:260:THR:HA	1:E:478:GLY:HA3	1.93	0.51
1:F:78:ILE:N	1:F:78:ILE:CD1	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:31:VAL:O	1:A:35:LEU:HG	2.12	0.50
1:A:209:VAL:CG1	3:A:2001:TPS:O7	2.60	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
1:A:282:VAL:HG21	1:A:467:SER:HB3	1.92	0.50
3:A:2001:TPS:HM43	3:A:2001:TPS:N4A	2.26	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:O	1:E:264:ARG:CG	2.60	0.50
1:F:20:MET:O	1:F:20:MET:HG2	2.11	0.50
1:A:89:ILE:O	1:A:89:ILE:HG13	2.11	0.50
1:A:299:VAL:HG11	1:A:326:ALA:HA	1.94	0.50
1:E:124:LEU:C	1:E:124:LEU:HD23	2.36	0.50
1:C:16:THR:O	1:C:45:ARG:HB3	2.11	0.50
1:C:527:GLU:HG3	1:C:527:GLU:O	2.11	0.50
1:D:15:VAL:O	1:D:209:VAL:HG22	2.11	0.50
3:D:2004:TPS:HM43	3:D:2004:TPS:N4A	2.27	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:F:138:GLY:HA3	1:F:154:MET:HE2	1.94	0.49
1:C:333:VAL:HG12	1:C:333:VAL:O	2.12	0.49
1:C:44:ILE:HG13	1:C:72:LEU:HD11	1.94	0.49
1:C:291:ILE:HG22	1:C:293:SER:H	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:PHE:C	1:C:513:PHE:CD2	2.90	0.49
1:E:31:VAL:HG12	1:E:31:VAL:O	2.12	0.49
1:B:66:HIS:HE1	1:B:87:ASP:OD1	1.94	0.49
1:B:246:SER:O	1:B:247:LEU:C	2.56	0.49
1:C:468:LEU:O	1:C:472:ILE:HG13	2.12	0.49
1:E:154:MET:HE3	1:E:158:GLY:O	2.12	0.49
1:A:79:ASP:C	1:A:81:ALA:N	2.69	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:75:ASN:ND2	1:C:76:ASP:OD2	2.46	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: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:75:ASN:ND2	1:E:76:ASP:HB3	2.28	0.49
1:E:314:THR:HG22	1:E:315:GLY:H	1.78	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:A:124:LEU:C	1:A:124:LEU:HD23	2.37	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:73:ILE:HG23	1:C:88:GLY:C	2.37	0.48
1:C:529:THR:N	1:C:530:PRO:HD3	2.27	0.48
1:E:78:ILE:HD13	1:E:96:MET:CE	2.42	0.48
1:E:340:ASP:OD2	1:E:340:ASP:C	2.56	0.48
1:E:533:TRP:C	1:E:535:PRO:HD2	2.37	0.48
1:A:314:THR:HG22	1:A:315:GLY:N	2.29	0.48
1:E:125:SER:C	1:E:127:MET:H	2.21	0.48
1:E:495:LEU:HD11	1:E:525:THR:CG2	2.43	0.48
1:F:61:ILE:O	1:F:61:ILE:CG2	2.61	0.48
1:F:167:GLU:HG2	1:F:198:ASN:ND2	2.13	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:90:HIS:CE1	3:B:2002:TPS:C2A	2.96	0.48
1:B:154:MET:SD	1:B:158:GLY:HA3	2.53	0.48
1:C:433:LEU:O	1:C:435:LYS:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:533:TRP:C	1:A:535:PRO:HD2	2.38	0.48
1:C:78:ILE:N	1:C:78:ILE:CD1	2.76	0.48
1:C:305:ILE:HG23	1:C:306:PRO:HD2	1.96	0.48
1:D:422:ILE:HD12	1:D:422:ILE:N	2.28	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:92:GLY:HA2	1:C:114:SER:HB2	1.95	0.48
1:C:427:ILE:O	1:C:427:ILE:HG22	2.13	0.48
1:C:283:THR:HB	1:C:290:PRO:HG3	1.96	0.48
1:D:99:PRO:HA	1:D:131:MET:HE1	1.95	0.48
1:D:137:VAL:HG23	1:D:137:VAL:O	2.12	0.48
1:D:262:LYS:O	1:D:262:LYS:HG2	2.13	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:C:256:ILE:HG22	1:C:475:MET:HE3	1.96	0.48
1:D:18:SER:HB2	1:D:46:GLU:OE2	2.13	0.48
1:F:276:GLN:HA	1:F:276:GLN:HE21	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:204:ASP:OD1	1:B:434:SER:HB3	2.13	0.47
1:B:339:PHE:CD2	1:B:341:PRO:HG3	2.48	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:F:528:ASN:C	1:F:530:PRO:HD3	2.39	0.47
1:A:33:ALA:O	1:A:37:ASN:ND2	2.46	0.47
1:C:38:GLY:O	1:C:39:VAL:C	2.57	0.47
1:D:78:ILE:H	1:D:78:ILE:HD12	1.79	0.47
1:D:79:ASP:HB2	1:E:96:MET:HE1	1.96	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
3:E:2005:TPS:HM43	3:E:2005:TPS:N4A	2.29	0.47
1:F:90:HIS:CE1	3:F:2006:TPS:CM2	2.97	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:F:369:ASN:O	1:F:370:SER:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ILE:HG22	1:F:240:GLY:N	2.30	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:E:127:MET:HB3	1:E:131:MET:HG3	1.96	0.47
1:A:8:PHE:CZ	1:A:110:VAL:HG21	2.50	0.47
1:A:43:GLN:HA	1:A:73:ILE:O	2.14	0.47
1:A:77:ARG:HH11	1:A:77:ARG:HG2	1.79	0.47
1:A:498:ALA:C	1:A:500:GLY:H	2.22	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:HA	1:C:30:GLN:OE1	2.15	0.47
1:C:339:PHE:CE2	1:C:341:PRO:HG3	2.49	0.47
1:D:256:ILE:CG2	1:D:475:MET:HE3	2.44	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:B:274:VAL:HG11	1:D:292:MET:HE3	1.97	0.47
1:C:402:THR:OG1	1:C:415:CYS:HB2	2.15	0.47
1:C:485:LEU:O	1:C:489:VAL:HG23	2.15	0.47
1:D:367:LYS:HD2	1:D:468:LEU:HD23	1.95	0.47
1:D:433:LEU:C	1:D:435:LYS:H	2.23	0.47
1:E:269:HIS:HB2	1:E:292:MET:SD	2.55	0.47
1:F:209:VAL:C	1:F:211:ASP:H	2.22	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:A:400:GLN:O	1:A:404:ILE:HG13	2.15	0.47
1:B:486:PHE:O	1:B:490:VAL:HG23	2.15	0.47
3:B:2002:TPS:N4A	3:B:2002:TPS:HM43	2.30	0.47
1:D:339:PHE:CD2	1:D:341:PRO:HG3	2.50	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:F:102:ARG:HH11	1:F:107:PRO:HA	1.80	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:129:PRO:C	1:F:131:MET:H	2.23	0.47
1:A:32:GLU:HG3	1:A:64:LEU:HD21	1.97	0.47
1:B:75:ASN:HD22	1:B:76:ASP:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:75:ASN:HD22	1:E:76:ASP:HB3	1.80	0.47
1:A:369:ASN:O	1:A:370:SER:C	2.59	0.46
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:D:253:ILE:CD1	1:D:494:MET:HE2	2.45	0.46
1:E:78:ILE:HG13	1:E:89:ILE:CD1	2.41	0.46
1:F:125:SER:C	1:F:127:MET:H	2.23	0.46
1:C:264:ARG:O	1:C:264:ARG:CG	2.64	0.46
1:D:322:MET:HE3	1:D:326:ALA:HB2	1.97	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:80:VAL:O	1:B:84:ILE:HG12	2.15	0.46
1:B:468:LEU:HD11	1:B:493:VAL:HG22	1.96	0.46
1:B:479:GLN:HA	1:B:480:PRO:HD3	1.71	0.46
1:D:73:ILE:HG23	1:D:88:GLY:C	2.40	0.46
1:E:226:ARG:HA	1:E:226:ARG:HD3	1.74	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: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:B:271:THR:CB	1:B:313:ASN:HB2	2.44	0.46
1:D:4:SER:N	1:D:7:GLN:OE1	2.48	0.46
1:D:78:ILE:HD12	1:D:78:ILE:N	2.30	0.46
1:D:182:LEU:HD12	1:D:182:LEU:HA	1.80	0.46
1:E:35:LEU:HD22	1:E:70:VAL:HG11	1.97	0.46
1:F:74:ILE:HD11	1:F:84:ILE:HD11	1.98	0.46
1:F:121:VAL:HG13	1:F:166:LEU:HD23	1.96	0.46
1:A:153:PRO:O	1:A:153:PRO:CD	2.64	0.46
1:E:30:GLN:NE2	1:E:218:ALA:HB2	2.31	0.46
1:E:263:ALA:O	1:E:264:ARG:C	2.58	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:F:89:ILE:O	1:F:89:ILE:HG13	2.15	0.46
1:B:433:LEU:O	1:B:435:LYS:N	2.49	0.46
1:F:38:GLY:O	1:F:39:VAL:C	2.57	0.46
1:A:407:PHE:O	1:A:410:LYS:NZ	2.41	0.46
1:C:127:MET:CE	1:C:131:MET:HB3	2.43	0.46
1:C:491:ALA:O	1:C:494:MET:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ILE:HG22	1:F:82:MET:HE2	1.98	0.46
1:A:45:ARG:HG3	1:A:75:ASN:OD1	2.16	0.46
1:B:78:ILE:CG1	1:B:89:ILE:HD12	2.32	0.46
1:B:290:PRO:HB2	1:B:292:MET:CE	2.45	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:F:314:THR:C	1:F:316:SER:H	2.23	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:C:357:LEU:C	1:C:359:THR:H	2.24	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: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
1:D:237:VAL:HG22	1:D:239:ILE:HG13	1.99	0.45
1:B:455:ILE:O	1:B:455:ILE:HG22	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: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:78:ILE:HG12	1:E:96:MET:HE3	1.98	0.45
1:E:302:LEU:HD12	1:E:302:LEU:HA	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:C:125:SER:C	1:C:127:MET:N	2.74	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:75:ASN:ND2	1:B:76:ASP:HB3	2.32	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:E:89:ILE:HD11	1:E:101:ILE:CG2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:369:ASN:O	1:C:370:SER:C	2.58	0.45
1:A:432:SER:OG	1:A:436:GLY:O	2.35	0.45
1:B:50:ASP:C	1:B:52:LYS:H	2.24	0.45
1:B:337:ILE:HG21	1:B:363:PHE:HD2	1.82	0.45
1:C:75:ASN:HA	1:C:76:ASP:HA	1.75	0.45
1:C:289:SER:HA	1:C:290:PRO:HD3	1.59	0.45
1:E:198:ASN:C	1:E:198:ASN:OD1	2.59	0.45
1:F:55:ILE:HG12	1:F:80:VAL:HG13	1.97	0.45
1:F:183:HIS:HB3	1:F:184:PRO:HD2	1.99	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:422:ILE:HD12	1:A:422:ILE:N	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:50:ASP:C	1:F:52:LYS:H	2.25	0.45
1:F:97:PRO:O	1:F:101:ILE:HG13	2.16	0.45
1:F:191:LEU:HD12	1:F:191:LEU:HA	1.80	0.45
1:F:284:LEU:HD12	1:F:284:LEU:HA	1.73	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:A:513:PHE:CD2	1:A:513:PHE:C	2.93	0.45
1:C:58:ALA:CB	1:C:84:ILE:HD13	2.47	0.45
1:D:533:TRP:N	1:D:533:TRP:CD1	2.82	0.45
1:F:75:ASN:HA	1:F:76:ASP:HA	1.52	0.45
1:C:3:PHE:CG	1:C:71:PRO:HG3	2.52	0.44
1:D:77:ARG:NH2	1:D:79:ASP:OD2	2.50	0.44
1:D:278:PHE:CE1	1:D:518:ILE:HD11	2.52	0.44
1:E:20:MET:HE1	1:E:209:VAL:CG1	2.47	0.44
1:E:129:PRO:C	1:E:131:MET:H	2.24	0.44
1:A:8:PHE:CE1	1:A:110:VAL:HG21	2.52	0.44
1:A:154:MET:SD	1:A:158:GLY:CA	3.05	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:124:LEU:HD23	1:C:124:LEU:C	2.43	0.44
1:D:27:LEU:O	1:D:31:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ASP:C	1:D:52:LYS:N	2.76	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:D:311:LEU:HD13	1:D:311:LEU:C	2.42	0.44
1:E:192:TYR:HA	1:E:431:TYR:HB3	1.99	0.44
1:A:79:ASP:C	1:A:81:ALA:H	2.25	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:75:ASN:HB2	1:F:90:HIS:HB3	2.00	0.44
1:F:495:LEU:HD22	1:F:521:LEU:CD2	2.47	0.44
1:F:527:GLU:O	1:F:527:GLU:HG3	2.17	0.44
1:B:144:LEU:HD13	1:B:144:LEU:HA	1.78	0.44
1:D:74:ILE:HD12	1:D:86:ALA:HB2	1.99	0.44
1:D:377:ALA:O	1:D:378:GLU:HB2	2.18	0.44
1:E:78:ILE:N	1:E:78:ILE:CD1	2.79	0.44
1:F:124:LEU:HD23	1:F:124:LEU:O	2.16	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:D:31:VAL:O	1:D:31:VAL:HG12	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: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:82:MET:CE	1:E:82:MET:HE1	2.47	0.44
1:E:433:LEU:C	1:E:435:LYS:H	2.26	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:A:188:GLU:H	1:A:188:GLU:HG2	1.52	0.44
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.70	0.44
1:C:226:ARG:O	1:C:230:ASP:OD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:SER:HA	1:F:290:PRO:HD3	1.78	0.44
1:A:230:ASP:OD2	1:A:230:ASP:N	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:D:124:LEU:C	1:D:124:LEU:HD23	2.42	0.44
1:B:278:PHE:HE1	1:B:518:ILE:HD11	1.83	0.43
1:C:40:THR:CG2	1:C:226:ARG:HH21	2.31	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: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:46:GLU:OE1	1:A:46:GLU:HA	2.17	0.43
1:A:47:LYS:NZ	4:A:4001:POP:P2	2.91	0.43
1:B:154:MET:CG	1:B:158:GLY:HA3	2.48	0.43
1:C:209:VAL:C	1:C:211:ASP:H	2.26	0.43
1:D:275:HIS:CD2	1:D:466:CYS:HB2	2.53	0.43
1:E:84:ILE:O	1:E:84:ILE:HG13	2.17	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
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:C:79:ASP:HA	1:C:82:MET:CE	2.47	0.43
1:C:256:ILE:CG2	1:C:475:MET:HE3	2.49	0.43
1:D:247:LEU:HA	1:D:247:LEU:HD12	1.72	0.43
1:F:118:PRO:HD2	1:F:119:GLU:OE1	2.18	0.43
1:A:78:ILE:HG13	1:A:89:ILE:HD12	1.99	0.43
1:A:154:MET:SD	1:A:158:GLY:C	3.02	0.43
1:A:159:ALA:O	1:A:162:VAL:HB	2.18	0.43
1:B:59:LEU:CD2	1:B:84:ILE:HB	2.49	0.43
1:B:529:THR:N	1:B:530:PRO:HD3	2.33	0.43
1:C:239:ILE:HG22	1:C:240:GLY:N	2.32	0.43
1:C:290:PRO:HB2	1:C:292:MET:HE2	2.00	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:E:209:VAL:C	1:E:211:ASP:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ASN:C	1:C:530:PRO:HD3	2.44	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:N	1:C:104:LEU:HD23	2.32	0.43
1:C:266:LEU:CD1	1:C:291:ILE:HG13	2.30	0.43
1:D:322:MET:CE	1:D:326:ALA:HB2	2.49	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:HA	1:F:226:ARG:HD3	1.69	0.43
1:D:256:ILE:HG23	1:D:479:GLN:OE1	2.19	0.43
1:D:526:ARG:HD2	1:D:526:ARG:HA	1.84	0.43
1:E:70:VAL:HA	1:E:71:PRO:HD3	1.88	0.43
1:E:154:MET:HE3	1:E:158:GLY:C	2.44	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:125:SER:C	1:D:127:MET:H	2.26	0.43
1:D:340:ASP:OD2	1:D:340:ASP:C	2.62	0.43
1:D:475:MET:O	1:D:479:GLN:HG2	2.19	0.43
1:A:20:MET:CG	1:A:214:ALA:HB2	2.42	0.43
1:A:73:ILE:HG23	1:A:88:GLY:C	2.44	0.43
1:B:256:ILE:HG22	1:B:475:MET:HE3	2.01	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:20:MET:HE3	1:C:213:ILE:HB	2.00	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
1:A:523:ARG:O	1:A:524:LEU:C	2.62	0.43
1:B:182:LEU:HD12	1:B:182:LEU:HA	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:59:LEU:CD2	1:D:84:ILE:HB	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:LEU:HD23	1:F:360:PHE:CE1	2.54	0.43
1:A:183:HIS:HB3	1:A:184:PRO:CD	2.48	0.42
1:B:256:ILE:CG2	1:B:475:MET:HE3	2.49	0.42
1:C:512:SER:HA	1:C:515:VAL:CG1	2.49	0.42
1:D:441:SER:O	1:D:442:VAL:C	2.62	0.42
1:F:40:THR:HG21	1:F:226:ARG:HH21	1.84	0.42
1:F:530:PRO:C	1:F:532:THR:N	2.75	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:HA	1:D:226:ARG:HD3	1.69	0.42
1:B:239:ILE:HG22	1:B:240:GLY:N	2.34	0.42
1:D:73:ILE:HG23	1:D:88:GLY:O	2.19	0.42
1:D:209:VAL:HG12	1:D:210:SER:N	2.34	0.42
1:F:78:ILE:HG12	1:F:96:MET:HE3	2.00	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:B:124:LEU:HA	1:B:127:MET:HE2	2.01	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:44:ILE:CG1	1:F:72:LEU:HD11	2.37	0.42
1:F:68:HIS:O	1:F:70:VAL:HG12	2.19	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: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:59:LEU:CD2	1:F:84:ILE:HB	2.48	0.42
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.74	0.42
1:B:263:ALA:O	1:B:264:ARG:C	2.61	0.42
1:B:269:HIS:ND1	1:B:292:MET:HE1	2.35	0.42
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.60	0.42
1:D:129:PRO:C	1:D:131:MET:H	2.28	0.42
1:F:79:ASP:OD1	1:F:79:ASP:N	2.51	0.42
1:F:137:VAL:HG23	1:F:178:GLY:HA2	2.00	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:D:434:SER:O	1:D:435:LYS:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:CD2	1:C:84:ILE:HB	2.49	0.42
1:C:82:MET:HE3	1:C:82:MET:HB2	1.88	0.42
1:D:121:VAL:CG1	1:D:166:LEU:HD23	2.49	0.42
1:E:204:ASP:OD1	1:E:434:SER:HB3	2.20	0.42
1:E:422:ILE:HG22	1:E:486:PHE:CE1	2.54	0.42
1:E:508:ASN:HB3	1:F:523:ARG:HH12	1.81	0.42
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.82	0.42
1:A:331:ASN:HD22	1:A:331:ASN:HA	1.59	0.42
1:A:433:LEU:O	1:A:435:LYS:N	2.53	0.42
1:B:271:THR:HA	1:B:313:ASN:HB2	2.02	0.42
1:B:297:SER:HB2	1:C:349:THR:OG1	2.20	0.42
1:C:45:ARG:NE	4:C:4003:POP:O5	2.48	0.42
1:C:524:LEU:HD12	1:C:524:LEU:HA	1.84	0.42
1:D:78:ILE:HD13	1:D:96:MET:HE2	2.02	0.42
1:D:190:VAL:O	1:D:194:CYS:HB2	2.20	0.42
1:D:204:ASP:CG	1:D:434:SER:HB3	2.45	0.42
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.89	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:A:99:PRO:HA	1:A:131:MET:HE1	2.02	0.41
1:B:129:PRO:C	1:B:131:MET:H	2.28	0.41
1:B:437:THR:HG23	1:B:440:THR:H	1.85	0.41
1:B:437:THR:C	1:B:439:GLY:H	2.25	0.41
1:D:137:VAL:HG22	1:D:177:VAL:O	2.20	0.41
1:E:102:ARG:NE	1:E:130:ASP:O	2.54	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:HB3	1:B:506:LYS:HE3	1.81	0.41
1:C:204:ASP:CG	1:C:434:SER:HB3	2.45	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:F:471:THR:O	1:F:475:MET:HG2	2.20	0.41
1:B:437:THR:C	1:B:439:GLY:N	2.79	0.41
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:HD12	1:F:524:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:PHE:C	1:C:54:PHE:CD1	2.98	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:78:ILE:HG12	1:D:96:MET:CE	2.51	0.41
1:D:273:LYS:HA	1:D:276:GLN:HG3	2.02	0.41
1:E:75:ASN:HA	1:E:76:ASP:HA	1.77	0.41
1:E:267:VAL:HA	1:E:309:THR:O	2.21	0.41
1:F:50:ASP:C	1:F:52:LYS:N	2.78	0.41
1:A:394:SER:OG	1:A:395:ASN:N	2.54	0.41
1:D:4:SER:O	1:D:5:LYS:C	2.62	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:44:ILE:HD12	1:F:58:ALA:HA	2.01	0.41
1:F:134:TYR:CD1	1:F:134:TYR:C	2.99	0.41
1:F:479:GLN:HA	1:F:480:PRO:HD3	1.65	0.41
1:A:57:GLU:O	1:A:57:GLU:HG2	2.21	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: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:13:TYR:OH	1:C:134:TYR:OH	2.36	0.41
1:C:314:THR:HG21	1:C:354:ASN:ND2	2.35	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:59:LEU:HD23	1:E:59:LEU:HA	1.84	0.41
1:E:98:ILE:HD13	1:E:101:ILE:HD12	2.02	0.41
1:E:425:GLY:O	1:E:427:ILE:HG13	2.20	0.41
1:A:373:ILE:HD13	1:A:373:ILE:HA	1.84	0.41
1:A:498:ALA:C	1:A:500:GLY:N	2.79	0.41
1:B:127:MET:HB3	1:B:131:MET:HG3	2.02	0.41
1:B:358:LEU:HD23	1:B:363:PHE:HE1	1.86	0.41
1:C:4:SER:O	1:C:6:GLU:N	2.54	0.41
1:C:273:LYS:HA	1:C:276:GLN:HG3	2.03	0.41
1:C:437:THR:HG21	1:C:440:THR:O	2.20	0.41
1:C:455:ILE:O	1:C:455:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLY:O	1:D:40:THR:N	2.54	0.41
1:E:50:ASP:C	1:E:52:LYS:H	2.29	0.41
1:E:257:ILE:HG13	1:E:475:MET:HE1	2.02	0.41
1:E:422:ILE:N	1:E:422:ILE:CD1	2.83	0.41
1:F:78:ILE:HD12	1:F:78:ILE:H	1.80	0.41
1:F:217:ASP:OD1	1:F:217:ASP:C	2.63	0.41
1:F:407:PHE:HE2	1:F:427:ILE:CD1	2.29	0.41
1:F:530:PRO:C	1:F:532:THR:H	2.28	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:C:340:ASP:OD2	1:C:340:ASP:C	2.64	0.41
1:D:28:TYR:CZ	1:D:64:LEU:HG	2.55	0.41
1:D:416:THR:HA	1:D:420:ASP:OD1	2.21	0.41
1:F:403:LYS:HD3	1:F:445:ILE:HG13	2.02	0.41
1:A:50:ASP:C	1:A:52:LYS:H	2.28	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:B:124:LEU:HD23	1:B:124:LEU:O	2.21	0.40
1:B:167:GLU:HG2	1:B:198:ASN:HD21	1.85	0.40
1:C:523:ARG:HH11	1:D:508:ASN:HB3	1.86	0.40
1:D:343:GLY:HA2	1:D:346:ALA:HB2	2.03	0.40
1:E:78:ILE:HD13	1:E:96:MET:HE3	2.02	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:55:ILE:HG23	1:A:84:ILE:CG2	2.51	0.40
1:A:278:PHE:HE1	1:A:518:ILE:HD11	1.86	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:B:317:VAL:O	1:B:317:VAL:HG22	2.20	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:96:MET:HA	1:E:97:PRO:HD3	1.92	0.40
1:A:290:PRO:HB2	1:A:292:MET:HE2	2.03	0.40
1:A:435:LYS:N	1:A:436:GLY:HA2	2.35	0.40
1:A:455:ILE:O	1:A:455:ILE:HG22	2.21	0.40
1:B:75:ASN:HA	1:B:76:ASP:HA	1.68	0.40
1:B:274:VAL:HG23	1:B:275:HIS:CE1	2.55	0.40
1:C:160:ILE:O	1:C:161:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ASN:OD1	1:C:198:ASN:C	2.64	0.40
1:C:347:THR:O	1:C:348:GLU:C	2.64	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:40:THR:H	1:E:40:THR:HG23	1.58	0.40
1:E:92:GLY:HA2	1:E:114:SER:HB2	2.03	0.40
1:E:291:ILE:HG22	1:E:293:SER:H	1.86	0.40
1:E:437:THR:C	1:E:439:GLY:N	2.79	0.40
1:E:449:ALA:O	1:E:537:LEU:HD12	2.22	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:B:513:PHE:CD2	1:B:513:PHE:C	2.99	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%)	6	28
1	B	498/540 (92%)	446 (90%)	39 (8%)	13 (3%)	4	21
1	C	499/540 (92%)	446 (89%)	44 (9%)	9 (2%)	6	28
1	D	499/540 (92%)	448 (90%)	41 (8%)	10 (2%)	6	25
1	E	497/540 (92%)	440 (88%)	47 (10%)	10 (2%)	6	25
1	F	497/540 (92%)	427 (86%)	55 (11%)	15 (3%)	3	19
All	All	2990/3240 (92%)	2645 (88%)	279 (9%)	66 (2%)	5	24

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
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

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Mol	Chain	Res	Type
1	B	51	THR
1	B	131	MET
1	B	378	GLU
1	C	106	GLY
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%)	367 (89%)	46 (11%)	6	24
1	B	413/449 (92%)	365 (88%)	48 (12%)	5	22
1	C	411/449 (92%)	367 (89%)	44 (11%)	6	25
1	D	412/449 (92%)	363 (88%)	49 (12%)	5	21
1	E	412/449 (92%)	359 (87%)	53 (13%)	4	18
1	F	410/449 (91%)	353 (86%)	57 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2471/2694 (92%)	2174 (88%)	297 (12%)	5 21

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	61	ILE
1	A	64	LEU
1	A	70	VAL
1	A	75	ASN
1	A	76	ASP
1	A	91	VAL
1	A	137	VAL
1	A	139	THR
1	A	154	MET
1	A	167	GLU
1	A	182	LEU
1	A	187	ILE
1	A	188	GLU
1	A	191	LEU
1	A	208	VAL
1	A	226	ARG
1	A	230	ASP
1	A	247	LEU
1	A	250	THR
1	A	260	THR
1	A	266	LEU
1	A	274	VAL
1	A	284	LEU
1	A	291	ILE
1	A	297	SER
1	A	311	LEU
1	A	313	ASN
1	A	322	MET
1	A	328	ARG
1	A	331	ASN
1	A	348	GLU
1	A	351	LEU
1	A	352	LEU
1	A	362	GLN
1	A	408	LYS
1	A	434	SER

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Mol	Chain	Res	Type
1	A	437	THR
1	A	442	VAL
1	A	448	VAL
1	A	467	SER
1	A	481	SER
1	A	495	LEU
1	A	515	VAL
1	A	517	LEU
1	A	524	LEU
1	B	37	ASN
1	B	51	THR
1	B	61	ILE
1	B	64	LEU
1	B	70	VAL
1	B	75	ASN
1	B	76	ASP
1	B	91	VAL
1	B	93	GLN
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	250	THR
1	B	255	SER
1	B	260	THR
1	B	266	LEU
1	B	272	ASN
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

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Mol	Chain	Res	Type
1	B	313	ASN
1	B	322	MET
1	B	328	ARG
1	B	342	VAL
1	B	348	GLU
1	B	352	LEU
1	B	403	LYS
1	B	408	LYS
1	B	422	ILE
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	18	SER
1	C	37	ASN
1	C	51	THR
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	288	SER
1	C	289	SER
1	C	291	ILE
1	C	293	SER
1	C	297	SER
1	C	302	LEU
1	C	312	LEU

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Mol	Chain	Res	Type
1	C	313	ASN
1	C	322	MET
1	C	328	ARG
1	C	347	THR
1	C	362	GLN
1	C	399	ILE
1	C	408	LYS
1	C	434	SER
1	C	437	THR
1	C	442	VAL
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	51	THR
1	D	64	LEU
1	D	65	CYS
1	D	70	VAL
1	D	75	ASN
1	D	76	ASP
1	D	89	ILE
1	D	91	VAL
1	D	124	LEU
1	D	144	LEU
1	D	182	LEU
1	D	187	ILE
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	250	THR
1	D	255	SER
1	D	260	THR
1	D	271	THR
1	D	274	VAL
1	D	276	GLN
1	D	284	LEU

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Mol	Chain	Res	Type
1	D	289	SER
1	D	291	ILE
1	D	293	SER
1	D	297	SER
1	D	299	VAL
1	D	302	LEU
1	D	313	ASN
1	D	322	MET
1	D	328	ARG
1	D	348	GLU
1	D	362	GLN
1	D	399	ILE
1	D	408	LYS
1	D	427	ILE
1	D	434	SER
1	D	451	GLU
1	D	467	SER
1	D	481	SER
1	D	482	GLU
1	D	495	LEU
1	D	515	VAL
1	D	524	LEU
1	D	527	GLU
1	D	533	TRP
1	E	26	THR
1	E	37	ASN
1	E	40	THR
1	E	51	THR
1	E	55	ILE
1	E	61	ILE
1	E	64	LEU
1	E	66	HIS
1	E	70	VAL
1	E	76	ASP
1	E	78	ILE
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

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Mol	Chain	Res	Type
1	E	247	LEU
1	E	250	THR
1	E	260	THR
1	E	266	LEU
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	311	LEU
1	E	312	LEU
1	E	313	ASN
1	E	322	MET
1	E	328	ARG
1	E	333	VAL
1	E	362	GLN
1	E	399	ILE
1	E	408	LYS
1	E	422	ILE
1	E	427	ILE
1	E	442	VAL
1	E	448	VAL
1	E	451	GLU
1	E	467	SER
1	E	481	SER
1	E	482	GLU
1	E	490	VAL
1	E	495	LEU
1	E	510	SER
1	E	515	VAL
1	E	517	LEU
1	E	524	LEU
1	F	40	THR
1	F	44	ILE
1	F	51	THR
1	F	55	ILE
1	F	61	ILE
1	F	64	LEU
1	F	66	HIS

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Mol	Chain	Res	Type
1	F	70	VAL
1	F	75	ASN
1	F	76	ASP
1	F	79	ASP
1	F	104	LEU
1	F	124	LEU
1	F	144	LEU
1	F	154	MET
1	F	187	ILE
1	F	188	GLU
1	F	191	LEU
1	F	207	CYS
1	F	209	VAL
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	291	ILE
1	F	296	GLN
1	F	297	SER
1	F	299	VAL
1	F	302	LEU
1	F	311	LEU
1	F	312	LEU
1	F	313	ASN
1	F	321	GLU
1	F	322	MET
1	F	328	ARG
1	F	342	VAL
1	F	348	GLU
1	F	362	GLN
1	F	408	LYS
1	F	427	ILE
1	F	437	THR
1	F	440	THR
1	F	442	VAL
1	F	445	ILE

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Mol	Chain	Res	Type
1	F	451	GLU
1	F	467	SER
1	F	481	SER
1	F	495	LEU
1	F	515	VAL
1	F	517	LEU
1	F	524	LEU
1	F	532	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	69	ASN
1	A	93	GLN
1	A	183	HIS
1	A	245	ASN
1	A	259	ASN
1	A	275	HIS
1	A	281	ASN
1	A	313	ASN
1	A	355	ASN
1	A	362	GLN
1	A	484	ASN
1	B	37	ASN
1	B	66	HIS
1	B	75	ASN
1	B	93	GLN
1	B	169	ASN
1	B	272	ASN
1	B	275	HIS
1	B	281	ASN
1	B	313	ASN
1	B	355	ASN
1	B	362	GLN
1	B	484	ASN
1	C	37	ASN
1	C	66	HIS
1	C	69	ASN
1	C	93	GLN
1	C	169	ASN
1	C	193	GLN

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Mol	Chain	Res	Type
1	C	245	ASN
1	C	275	HIS
1	C	276	GLN
1	C	281	ASN
1	C	313	ASN
1	C	355	ASN
1	C	362	GLN
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	169	ASN
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	514	GLN
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	362	GLN
1	E	484	ASN
1	E	514	GLN
1	F	66	HIS
1	F	93	GLN
1	F	169	ASN
1	F	193	GLN

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Mol	Chain	Res	Type
1	F	269	HIS
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	362	GLN
1	F	484	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
3	TPS	F	2006	-	23,23,23	4.66	14 (60%)	33,33,33	3.73	15 (45%)
3	TPS	B	2002	-	23,23,23	4.48	12 (52%)	33,33,33	3.01	10 (30%)
4	POP	A	4001	2	6,8,8	0.55	0	12,13,13	1.03	1 (8%)
4	POP	B	4002	2	6,8,8	0.64	0	12,13,13	1.03	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POP	C	4003	2	6,8,8	0.72	0	12,13,13	0.93	0
3	TPS	E	2005	-	23,23,23	4.61	13 (56%)	33,33,33	3.68	11 (33%)
3	TPS	D	2004	-	23,23,23	4.62	13 (56%)	33,33,33	3.84	12 (36%)
4	POP	F	4006	2	6,8,8	0.62	0	12,13,13	1.47	3 (25%)
4	POP	E	4005	2	6,8,8	0.82	0	12,13,13	0.85	1 (8%)
3	TPS	A	2001	-	23,23,23	4.58	14 (60%)	33,33,33	2.68	16 (48%)
4	POP	D	4004	2	6,8,8	0.77	0	12,13,13	1.01	1 (8%)
3	TPS	C	2003	-	23,23,23	4.69	14 (60%)	33,33,33	3.77	14 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPS	F	2006	-	-	7/11/11/11	0/2/2/2
3	TPS	B	2002	-	-	3/11/11/11	0/2/2/2
4	POP	A	4001	2	-	2/6/6/6	-
4	POP	B	4002	2	-	3/6/6/6	-
4	POP	C	4003	2	-	1/6/6/6	-
3	TPS	E	2005	-	-	6/11/11/11	0/2/2/2
3	TPS	D	2004	-	-	3/11/11/11	0/2/2/2
4	POP	F	4006	2	-	4/6/6/6	-
4	POP	E	4005	2	-	2/6/6/6	-
3	TPS	A	2001	-	-	4/11/11/11	0/2/2/2
4	POP	D	4004	2	-	0/6/6/6	-
3	TPS	C	2003	-	-	3/11/11/11	0/2/2/2

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2004	TPS	C5-C4	11.89	1.60	1.35
3	E	2005	TPS	C5-C4	11.76	1.60	1.35
3	A	2001	TPS	C5-C4	11.63	1.59	1.35
3	B	2002	TPS	C5-C4	11.50	1.59	1.35
3	F	2006	TPS	C5-C4	11.49	1.59	1.35
3	C	2003	TPS	C5-C4	11.35	1.59	1.35
3	C	2003	TPS	C4-N3	10.98	1.62	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2006	TPS	C4-N3	10.08	1.60	1.39
3	D	2004	TPS	C4-N3	9.85	1.60	1.39
3	A	2001	TPS	C4-N3	9.75	1.59	1.39
3	E	2005	TPS	C4-N3	9.64	1.59	1.39
3	B	2002	TPS	C4-N3	9.19	1.58	1.39
3	F	2006	TPS	C2-N3	8.15	1.52	1.32
3	C	2003	TPS	C2-N3	8.13	1.52	1.32
3	B	2002	TPS	C2-N3	8.10	1.52	1.32
3	D	2004	TPS	C2-N3	8.10	1.52	1.32
3	A	2001	TPS	C2-N3	8.10	1.52	1.32
3	E	2005	TPS	C2-N3	7.91	1.51	1.32
3	F	2006	TPS	C6A-N1A	7.28	1.49	1.34
3	C	2003	TPS	C6A-N1A	6.98	1.48	1.34
3	E	2005	TPS	C6A-N1A	6.94	1.48	1.34
3	B	2002	TPS	C6A-N1A	6.79	1.48	1.34
3	A	2001	TPS	C6A-N1A	6.76	1.48	1.34
3	D	2004	TPS	C6A-N1A	6.35	1.47	1.34
3	F	2006	TPS	C4A-N3A	6.34	1.43	1.35
3	C	2003	TPS	C4A-N3A	5.93	1.42	1.35
3	A	2001	TPS	C4A-N3A	5.88	1.42	1.35
3	D	2004	TPS	C4A-N3A	5.82	1.42	1.35
3	B	2002	TPS	C4A-N3A	5.63	1.42	1.35
3	E	2005	TPS	C4A-N3A	5.60	1.42	1.35
3	F	2006	TPS	C4A-N4A	4.84	1.46	1.34
3	E	2005	TPS	P1-O1	4.75	1.65	1.50
3	D	2004	TPS	C4A-N4A	4.70	1.46	1.34
3	C	2003	TPS	C4A-N4A	4.63	1.46	1.34
3	E	2005	TPS	C4A-N4A	4.59	1.45	1.34
3	B	2002	TPS	C4A-N4A	4.50	1.45	1.34
3	A	2001	TPS	C4A-N4A	4.47	1.45	1.34
3	D	2004	TPS	P1-O1	4.38	1.64	1.50
3	C	2003	TPS	C5-S1	-4.06	1.62	1.72
3	B	2002	TPS	P1-O1	4.05	1.63	1.50
3	A	2001	TPS	P1-O1	3.86	1.62	1.50
3	E	2005	TPS	C5-S1	-3.76	1.62	1.72
3	C	2003	TPS	P1-O1	3.74	1.62	1.50
3	F	2006	TPS	P1-O1	3.71	1.62	1.50
3	F	2006	TPS	C5-S1	-3.71	1.63	1.72
3	A	2001	TPS	C2-S1	3.68	1.80	1.69
3	D	2004	TPS	C5-S1	-3.47	1.63	1.72
3	B	2002	TPS	C5-S1	-3.40	1.63	1.72
3	E	2005	TPS	C2-S1	3.38	1.79	1.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2004	TPS	C2-S1	3.37	1.79	1.69
3	B	2002	TPS	C2-S1	3.23	1.79	1.69
3	F	2006	TPS	C2-S1	3.12	1.78	1.69
3	C	2003	TPS	C2-S1	3.11	1.78	1.69
3	D	2004	TPS	C6A-C5A	-3.07	1.31	1.37
3	A	2001	TPS	C5-S1	-3.05	1.64	1.72
3	A	2001	TPS	C6A-C5A	-3.05	1.31	1.37
3	F	2006	TPS	C2A-N3A	2.97	1.39	1.34
3	E	2005	TPS	P1-O2	2.96	1.65	1.54
3	D	2004	TPS	P1-O2	2.91	1.65	1.54
3	F	2006	TPS	P1-O3	-2.90	1.44	1.54
3	B	2002	TPS	C6A-C5A	-2.89	1.32	1.37
3	E	2005	TPS	C6A-C5A	-2.75	1.32	1.37
3	C	2003	TPS	C6A-C5A	-2.73	1.32	1.37
3	C	2003	TPS	C2A-N3A	2.69	1.38	1.34
3	B	2002	TPS	P1-O3	-2.66	1.44	1.54
3	A	2001	TPS	P1-O3	-2.58	1.45	1.54
3	C	2003	TPS	P1-O3	-2.55	1.45	1.54
3	C	2003	TPS	P1-O2	2.50	1.64	1.54
3	D	2004	TPS	C2A-N3A	2.46	1.38	1.34
3	E	2005	TPS	C2A-N3A	2.46	1.38	1.34
3	F	2006	TPS	C6A-C5A	-2.42	1.33	1.37
3	A	2001	TPS	C7A-N3	-2.41	1.43	1.48
3	A	2001	TPS	C2A-N3A	2.35	1.38	1.34
3	B	2002	TPS	P1-O2	2.27	1.63	1.54
3	F	2006	TPS	P1-O2	2.14	1.62	1.54
3	E	2005	TPS	P1-O7	2.11	1.67	1.60
3	F	2006	TPS	C7A-C5A	2.09	1.55	1.51
3	A	2001	TPS	P1-O2	2.05	1.62	1.54
3	C	2003	TPS	P1-O7	2.03	1.66	1.60
3	D	2004	TPS	C6-C5	2.02	1.55	1.50

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2004	TPS	C2-S1-C5	18.55	103.50	91.22
3	F	2006	TPS	C2-S1-C5	17.76	102.98	91.22
3	E	2005	TPS	C2-S1-C5	17.71	102.95	91.22
3	C	2003	TPS	C2-S1-C5	17.33	102.69	91.22
3	B	2002	TPS	C2-S1-C5	13.45	100.12	91.22
3	A	2001	TPS	C2-S1-C5	8.74	97.01	91.22
3	A	2001	TPS	S1-C2-N3	-5.42	105.44	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2004	TPS	C6A-C5A-C4A	5.19	121.93	115.55
3	C	2003	TPS	S1-C2-N3	-4.77	106.26	112.30
3	E	2005	TPS	C6A-C5A-C4A	4.62	121.22	115.55
3	B	2002	TPS	S1-C2-N3	-4.61	106.46	112.30
3	D	2004	TPS	S1-C2-N3	-4.60	106.47	112.30
3	A	2001	TPS	C6A-C5A-C4A	4.52	121.11	115.55
3	C	2003	TPS	C6A-C5A-C4A	4.46	121.04	115.55
3	F	2006	TPS	C6A-C5A-C4A	4.38	120.93	115.55
3	B	2002	TPS	C6A-C5A-C4A	4.33	120.87	115.55
3	E	2005	TPS	S1-C2-N3	-4.17	107.02	112.30
3	E	2005	TPS	C2-N3-C4	-4.01	108.64	114.06
3	F	2006	TPS	N4A-C4A-N3A	3.87	122.25	117.03
3	C	2003	TPS	O3-P1-O7	3.80	116.57	106.67
3	C	2003	TPS	N4A-C4A-N3A	3.77	122.11	117.03
3	F	2006	TPS	S1-C2-N3	-3.74	107.56	112.30
3	F	2006	TPS	O3-P1-O7	3.73	116.39	106.67
3	E	2005	TPS	CM2-C2A-N1A	3.54	120.97	117.20
3	B	2002	TPS	CM2-C2A-N1A	3.47	120.90	117.20
3	A	2001	TPS	CM2-C2A-N1A	3.43	120.85	117.20
3	F	2006	TPS	N1A-C2A-N3A	-3.30	120.04	125.53
3	B	2002	TPS	C2-N3-C4	-3.26	109.65	114.06
4	F	4006	POP	O5-P2-O	3.25	115.52	104.64
3	F	2006	TPS	C2-N3-C4	-3.19	109.75	114.06
3	D	2004	TPS	C5A-C6A-N1A	-3.11	118.77	123.83
3	A	2001	TPS	C5A-C6A-N1A	-3.06	118.86	123.83
3	A	2001	TPS	C2-N3-C4	-3.05	109.93	114.06
3	A	2001	TPS	C6-C5-S1	3.03	128.00	120.90
3	D	2004	TPS	C5A-C7A-N3	-2.99	106.52	112.97
3	C	2003	TPS	N1A-C2A-N3A	-2.97	120.59	125.53
3	B	2002	TPS	C5A-C6A-N1A	-2.95	119.04	123.83
3	D	2004	TPS	C2-N3-C4	-2.81	110.27	114.06
3	C	2003	TPS	CM4-C4-N3	2.78	126.99	120.57
3	C	2003	TPS	C2-N3-C4	-2.77	110.32	114.06
3	A	2001	TPS	CM4-C4-C5	-2.76	120.68	127.75
3	A	2001	TPS	N4A-C4A-N3A	2.71	120.69	117.03
3	C	2003	TPS	CM2-C2A-N1A	2.62	119.99	117.20
3	E	2005	TPS	N4A-C4A-N3A	2.61	120.54	117.03
4	D	4004	POP	O2-P1-O	2.60	113.37	104.64
3	E	2005	TPS	C4-C5-S1	-2.60	106.50	110.56
3	C	2003	TPS	C5A-C6A-N1A	-2.60	119.61	123.83
3	E	2005	TPS	C5A-C6A-N1A	-2.59	119.62	123.83
3	D	2004	TPS	N4A-C4A-N3A	2.58	120.50	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	TPS	C5-C4-N3	-2.55	107.03	111.67
3	C	2003	TPS	C5A-C4A-N4A	-2.53	118.73	122.14
3	B	2002	TPS	C4-C5-S1	-2.46	106.72	110.56
3	A	2001	TPS	O3-P1-O7	2.46	113.09	106.67
3	E	2005	TPS	N1A-C2A-N3A	-2.45	121.45	125.53
3	A	2001	TPS	N1A-C2A-N3A	-2.45	121.46	125.53
3	D	2004	TPS	C6-C5-S1	2.41	126.53	120.90
3	F	2006	TPS	CM2-C2A-N1A	2.40	119.75	117.20
3	A	2001	TPS	C6A-N1A-C2A	2.39	120.00	116.07
3	B	2002	TPS	N1A-C2A-N3A	-2.38	121.57	125.53
3	A	2001	TPS	C5A-C4A-N4A	-2.38	118.94	122.14
3	C	2003	TPS	C5A-C7A-N3	-2.37	107.86	112.97
3	E	2005	TPS	C5A-C7A-N3	-2.37	107.86	112.97
3	D	2004	TPS	N1A-C2A-N3A	-2.37	121.59	125.53
3	D	2004	TPS	C6A-N1A-C2A	2.36	119.95	116.07
3	A	2001	TPS	C7A-C5A-C4A	-2.30	118.18	122.36
3	B	2002	TPS	C6A-N1A-C2A	2.27	119.79	116.07
3	F	2006	TPS	C5A-C4A-N3A	-2.23	118.05	121.31
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
3	C	2003	TPS	C6A-N1A-C2A	2.20	119.68	116.07
4	F	4006	POP	O3-P1-O	2.19	111.98	104.64
3	F	2006	TPS	C2A-N3A-C4A	2.14	121.39	118.10
3	D	2004	TPS	C7A-C5A-C6A	-2.13	116.68	120.69
3	C	2003	TPS	C7A-C5A-C4A	-2.13	118.49	122.36
4	F	4006	POP	O2-P1-O	2.10	111.68	104.64
3	A	2001	TPS	C5A-C7A-N3	-2.10	108.45	112.97
3	F	2006	TPS	CM2-C2A-N3A	2.05	120.20	117.13
3	F	2006	TPS	C5A-C6A-N1A	-2.05	120.50	123.83
3	F	2006	TPS	O7-C7-C6	2.04	116.84	108.63
3	F	2006	TPS	O3-P1-O1	-2.04	102.88	110.83
3	B	2002	TPS	C6-C5-S1	2.04	125.67	120.90
3	F	2006	TPS	C7A-C5A-C4A	-2.02	118.68	122.36
4	B	4002	POP	O2-P1-O	2.02	111.41	104.64
3	D	2004	TPS	CM2-C2A-N1A	2.02	119.35	117.20
3	E	2005	TPS	O3-P1-O7	2.01	111.91	106.67

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	TPS	C6A-C5A-C7A-N3

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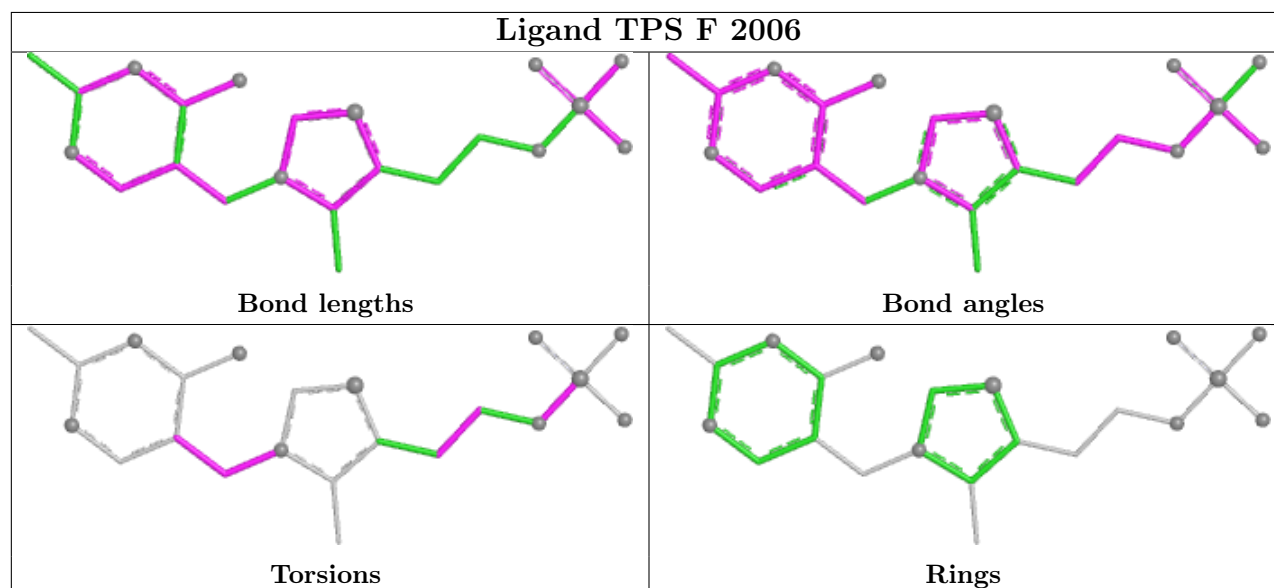
Mol	Chain	Res	Type	Atoms
3	B	2002	TPS	C6A-C5A-C7A-N3
3	C	2003	TPS	C7-O7-P1-O2
3	D	2004	TPS	C7-O7-P1-O2
3	E	2005	TPS	C7-O7-P1-O1
3	E	2005	TPS	C7-O7-P1-O2
3	E	2005	TPS	C7-O7-P1-O3
3	F	2006	TPS	C7-O7-P1-O1
3	F	2006	TPS	C7-O7-P1-O2
3	F	2006	TPS	C7-O7-P1-O3
3	F	2006	TPS	C4A-C5A-C7A-N3
4	A	4001	POP	P2-O-P1-O2
4	B	4002	POP	P1-O-P2-O5
4	B	4002	POP	P1-O-P2-O6
4	E	4005	POP	P1-O-P2-O5
4	E	4005	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	A	2001	TPS	C5A-C7A-N3-C4
3	C	2003	TPS	C6A-C5A-C7A-N3
3	D	2004	TPS	C6A-C5A-C7A-N3
3	E	2005	TPS	C6A-C5A-C7A-N3
3	F	2006	TPS	C6A-C5A-C7A-N3
3	A	2001	TPS	C4A-C5A-C7A-N3
3	B	2002	TPS	C4A-C5A-C7A-N3
3	F	2006	TPS	C5A-C7A-N3-C2
4	C	4003	POP	P1-O-P2-O6
3	B	2002	TPS	C5-C6-C7-O7
3	F	2006	TPS	C5-C6-C7-O7
3	D	2004	TPS	C4A-C5A-C7A-N3
3	E	2005	TPS	C4A-C5A-C7A-N3
4	F	4006	POP	P2-O-P1-O1
3	A	2001	TPS	C7-O7-P1-O2
4	A	4001	POP	P2-O-P1-O1
4	B	4002	POP	P2-O-P1-O1
3	C	2003	TPS	C5-C6-C7-O7
3	E	2005	TPS	C5A-C7A-N3-C2

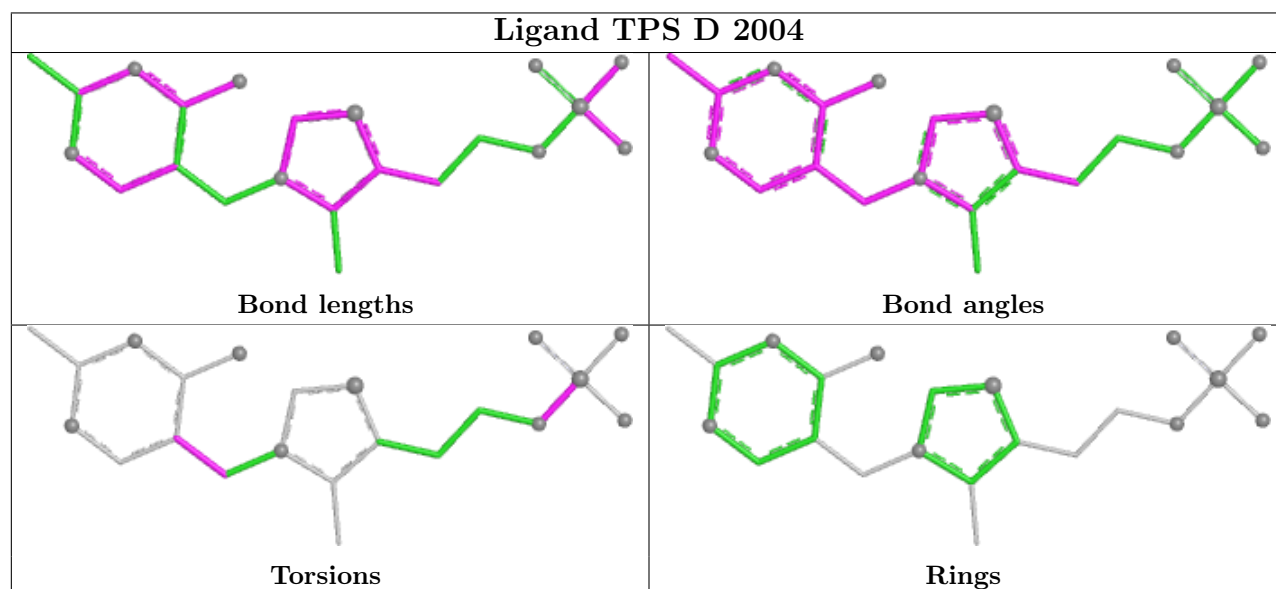
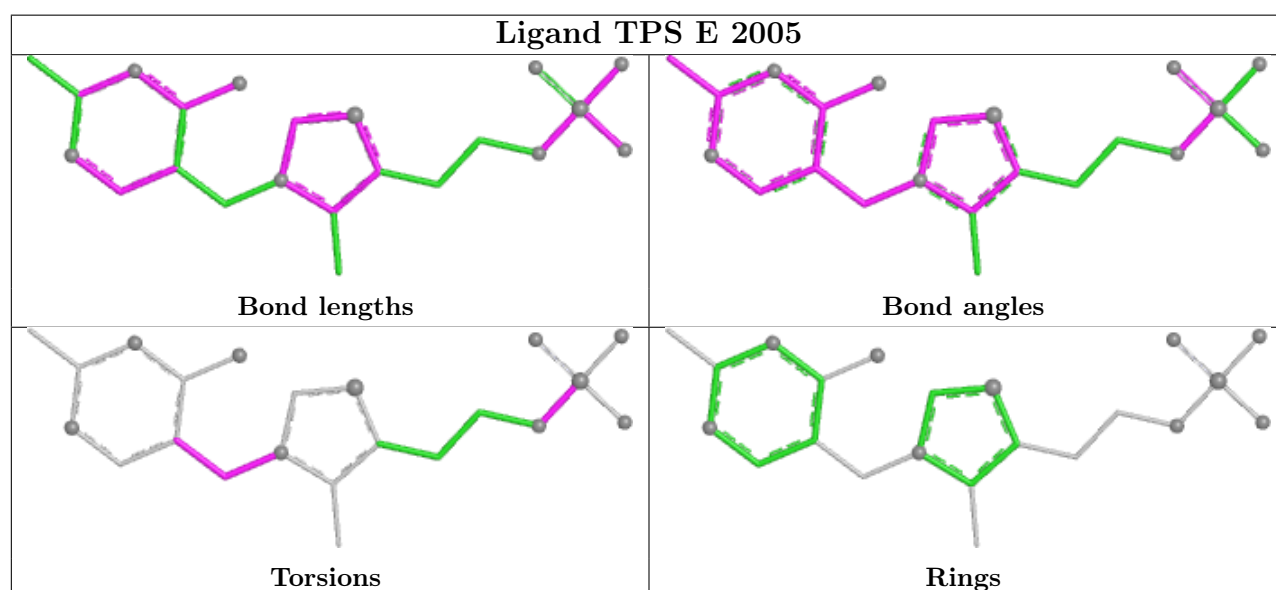
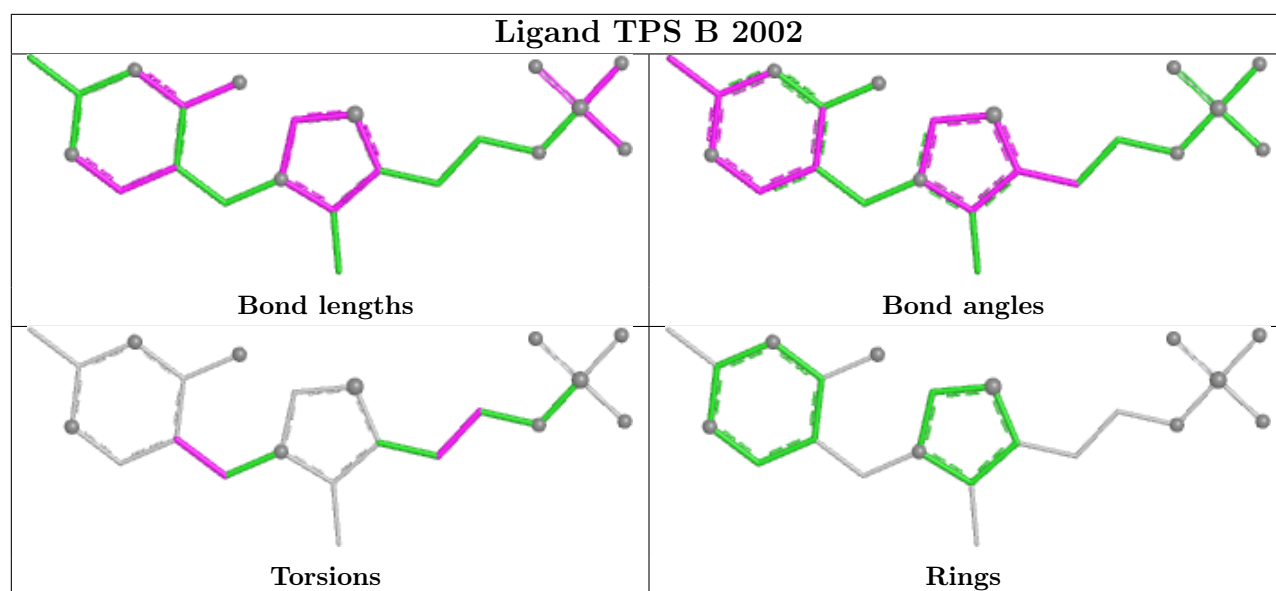
There are no ring outliers.

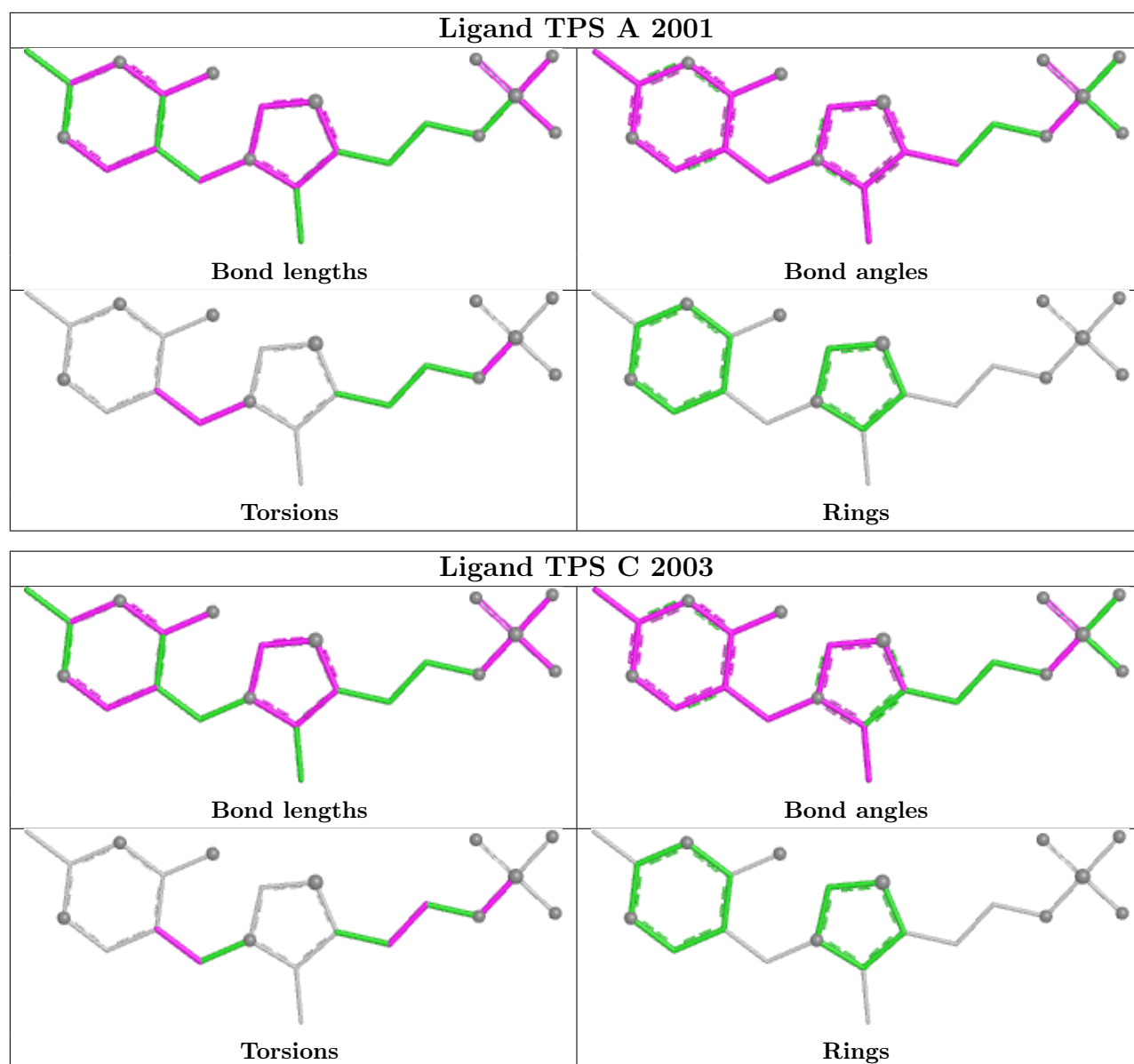
10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2006	TPS	3	0
3	B	2002	TPS	3	0
4	A	4001	POP	2	0
4	B	4002	POP	1	0
4	C	4003	POP	2	0
3	E	2005	TPS	3	0
3	D	2004	TPS	1	0
4	F	4006	POP	1	0
3	A	2001	TPS	4	0
4	D	4004	POP	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	510/540 (94%)	-0.39	4 (0%)	82 65	26, 86, 109, 133	0
1	B	508/540 (94%)	-0.50	3 (0%)	85 70	26, 80, 103, 129	0
1	C	510/540 (94%)	-0.49	4 (0%)	82 65	42, 87, 113, 135	0
1	D	511/540 (94%)	-0.51	4 (0%)	82 65	40, 79, 107, 134	0
1	E	507/540 (93%)	-0.52	2 (0%)	88 76	40, 80, 105, 129	0
1	F	507/540 (93%)	-0.48	1 (0%)	91 83	43, 87, 113, 131	0
All	All	3053/3240 (94%)	-0.48	18 (0%)	85 70	26, 83, 109, 135	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	GLY	6.8
1	C	343	GLY	6.6
1	E	343	GLY	5.9
1	B	343	GLY	5.6
1	D	343	GLY	5.0
1	F	343	GLY	4.8
1	C	148	ASN	3.7
1	D	277	ASN	3.2
1	A	346	ALA	2.8
1	A	148	ASN	2.8
1	D	151	LYS	2.7
1	E	455	ILE	2.5
1	B	465	GLY	2.5
1	B	498	ALA	2.5
1	C	465	GLY	2.5
1	D	148	ASN	2.4
1	C	151	LYS	2.3
1	A	153	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

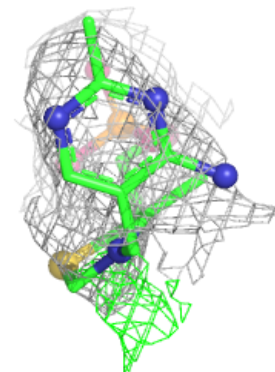
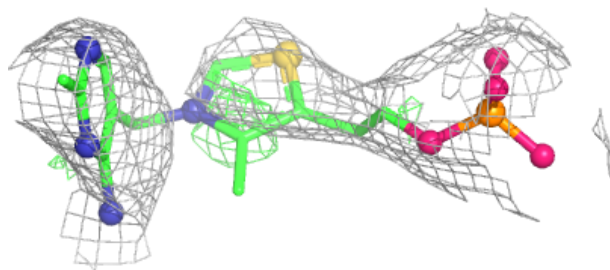
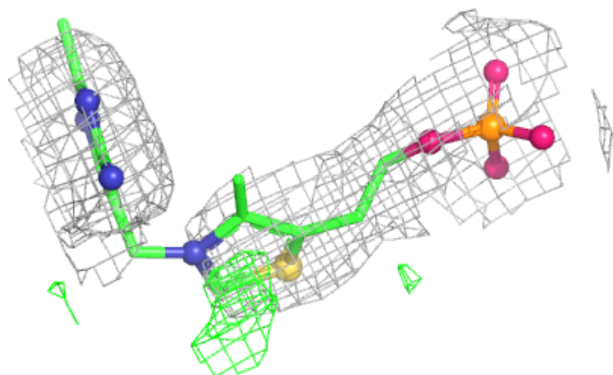
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	F	3006	1/1	0.82	0.16	63,63,63,63	0
2	MG	D	3004	1/1	0.86	0.17	61,61,61,61	0
2	MG	C	3003	1/1	0.91	0.15	55,55,55,55	0
2	MG	B	3002	1/1	0.93	0.15	61,61,61,61	0
2	MG	E	3005	1/1	0.94	0.12	48,48,48,48	0
4	POP	B	4002	9/9	0.95	0.10	48,57,67,70	2
3	TPS	C	2003	22/22	0.96	0.11	66,73,76,79	7
3	TPS	F	2006	22/22	0.97	0.09	68,73,77,83	8
4	POP	A	4001	9/9	0.97	0.07	56,67,80,80	3
3	TPS	E	2005	22/22	0.97	0.08	54,60,66,68	8
4	POP	C	4003	9/9	0.97	0.09	55,68,75,82	3
4	POP	E	4005	9/9	0.97	0.07	57,61,63,64	6
4	POP	F	4006	9/9	0.97	0.05	55,63,69,69	4
3	TPS	D	2004	22/22	0.98	0.06	57,63,69,74	6
3	TPS	A	2001	22/22	0.98	0.07	60,69,76,77	7
4	POP	D	4004	9/9	0.98	0.07	53,60,65,68	5
3	TPS	B	2002	22/22	0.98	0.08	55,62,70,73	8
2	MG	A	3001	1/1	0.98	0.06	70,70,70,70	0

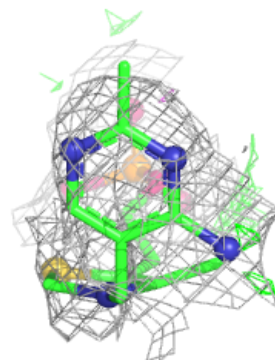
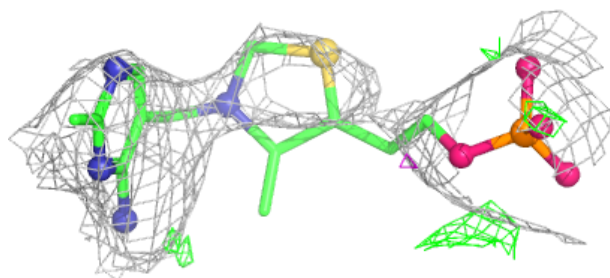
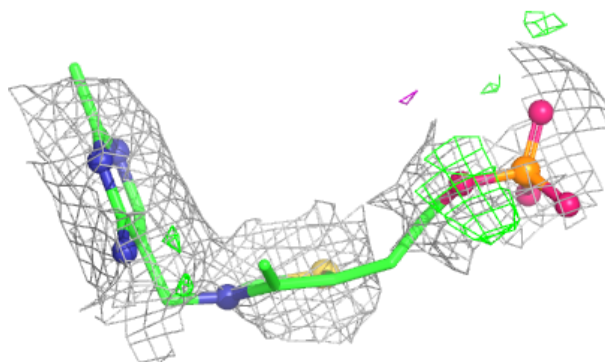
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

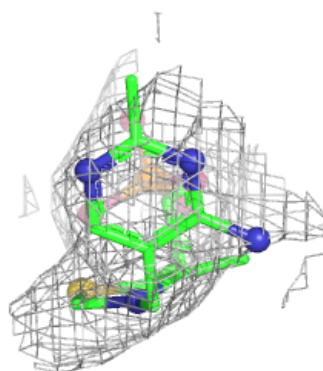
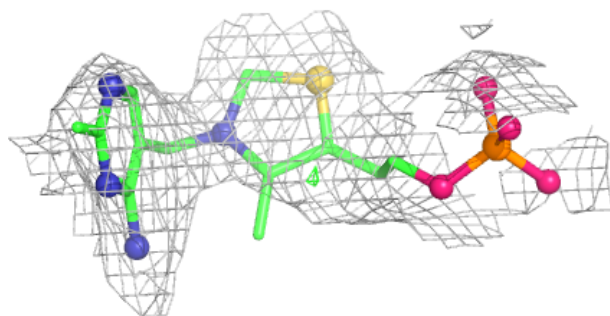
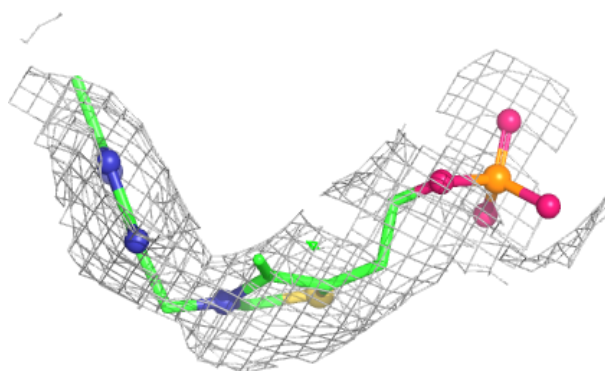
**Electron density around TPS F 2006:**

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

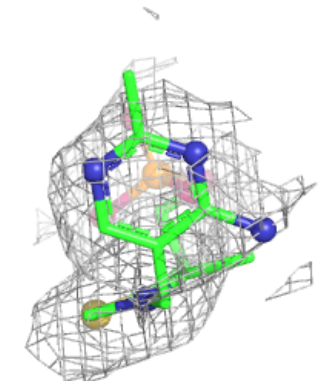
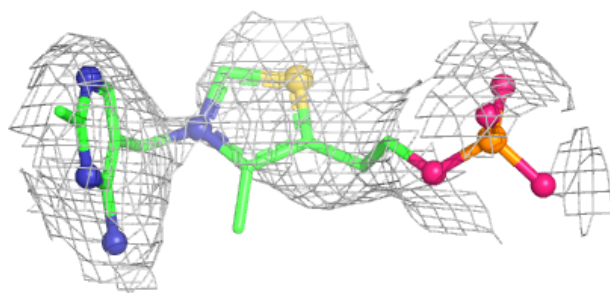
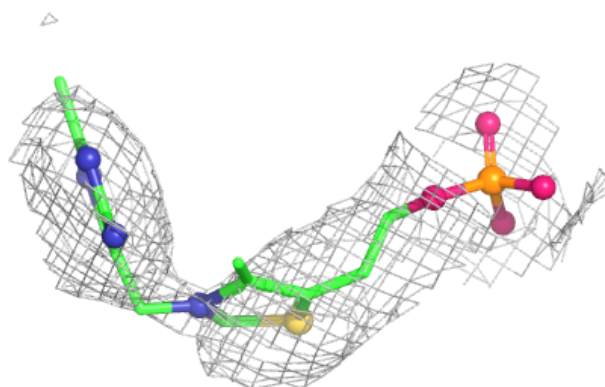


Electron density around TPS E 2005:

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

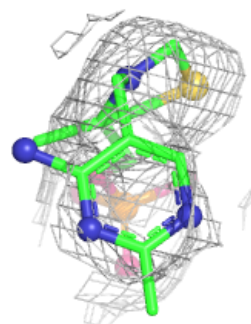
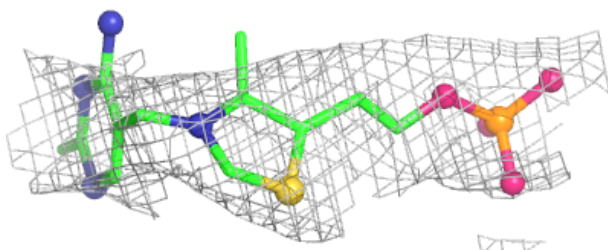
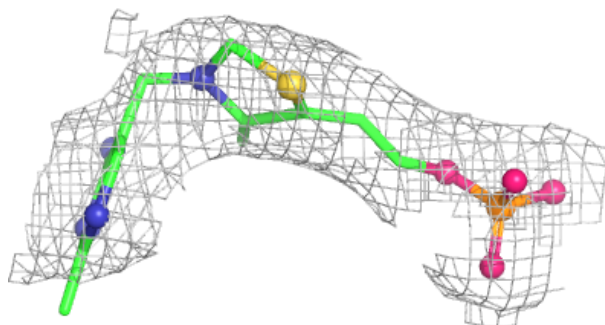
**Electron density around TPS D 2004:**

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

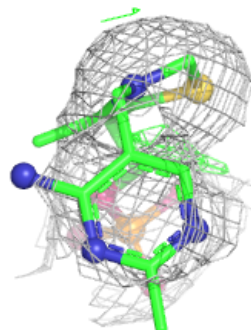
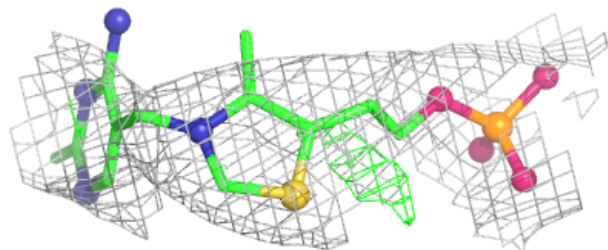
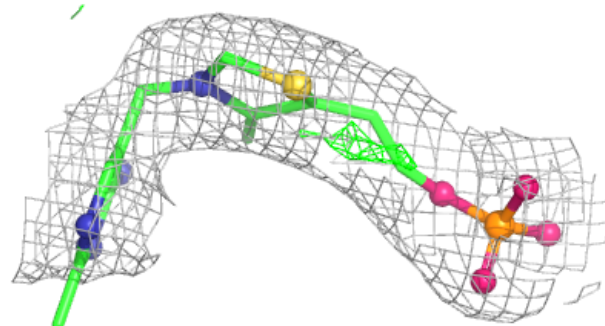


Electron density around TPS A 2001:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.