



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:07 AM UTC

PDB ID : 7C8I / pdb_00007c8i
Title : Ambient temperature structure of Bifidobacgterium longum phosphoketolase with thiamine diphosphate and phosphoenol pyruvate
Authors : Nakata, K.; Kashiwagi, T.; Nango, E.; Miyano, H.; Mizukoshi, T.; Iwata, S.
Deposited on : 2020-06-01
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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:

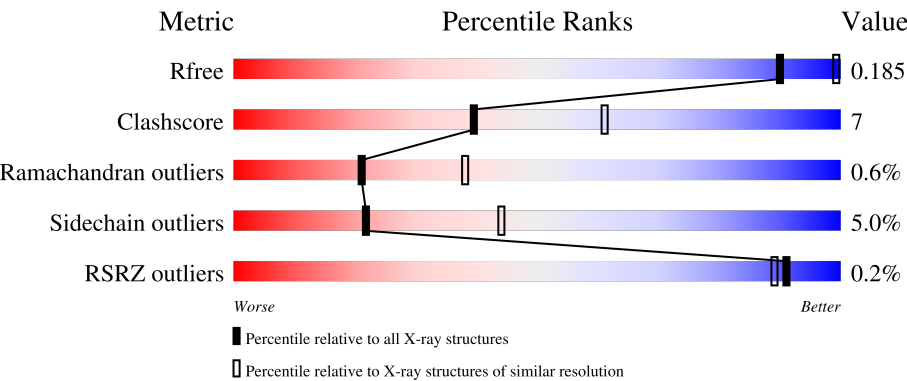
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	831	85%11%..
1	B	831	85%12%..
1	C	831	72%21%..
1	D	831	% 69%24%..
1	E	831	77%18%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	831	 78% 18% . .
1	G	831	 81% 15% . .
1	H	831	 83% 13% . .

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
2	PEP	A	901	-	-	X	-
2	PEP	B	901	-	-	X	-
2	PEP	H	901	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52775 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 Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	1	0
			6436	4085	1098	1234	19			
1	B	811	Total	C	N	O	S	0	1	0
			6458	4099	1103	1237	19			
1	C	806	Total	C	N	O	S	0	0	0
			6411	4071	1093	1228	19			
1	D	807	Total	C	N	O	S	0	0	0
			6418	4075	1094	1230	19			
1	E	809	Total	C	N	O	S	0	0	0
			6435	4085	1097	1234	19			
1	F	809	Total	C	N	O	S	0	0	0
			6435	4085	1097	1234	19			
1	G	807	Total	C	N	O	S	0	1	0
			6428	4081	1097	1231	19			
1	H	808	Total	C	N	O	S	0	1	0
			6436	4085	1098	1234	19			

There are 48 discrepancies between the modelled and reference sequences:

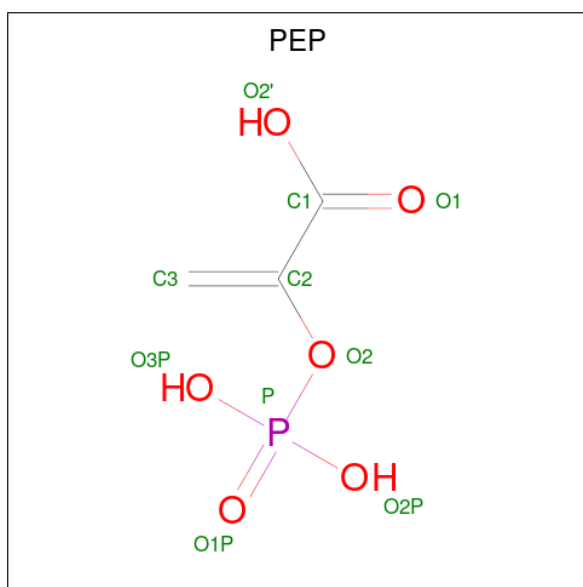
Chain	Residue	Modelled	Actual	Comment	Reference
A	826	HIS	-	expression tag	UNP Q6R2Q7
A	827	HIS	-	expression tag	UNP Q6R2Q7
A	828	HIS	-	expression tag	UNP Q6R2Q7
A	829	HIS	-	expression tag	UNP Q6R2Q7
A	830	HIS	-	expression tag	UNP Q6R2Q7
A	831	HIS	-	expression tag	UNP Q6R2Q7
B	826	HIS	-	expression tag	UNP Q6R2Q7
B	827	HIS	-	expression tag	UNP Q6R2Q7
B	828	HIS	-	expression tag	UNP Q6R2Q7
B	829	HIS	-	expression tag	UNP Q6R2Q7
B	830	HIS	-	expression tag	UNP Q6R2Q7
B	831	HIS	-	expression tag	UNP Q6R2Q7
C	826	HIS	-	expression tag	UNP Q6R2Q7

Continued on next page...

Continued from previous page...

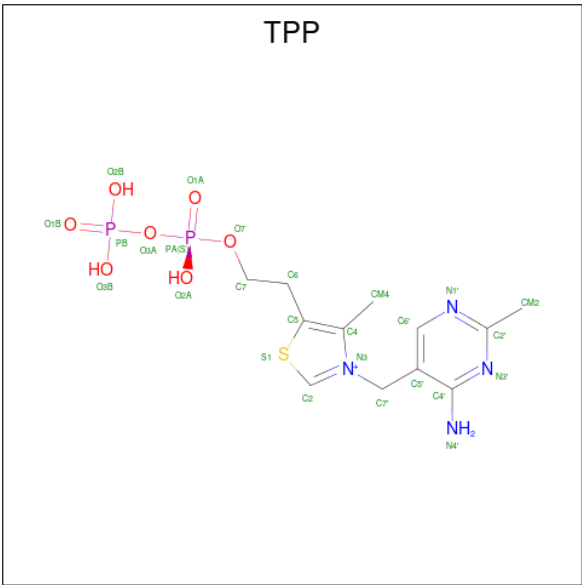
Chain	Residue	Modelled	Actual	Comment	Reference
C	827	HIS	-	expression tag	UNP Q6R2Q7
C	828	HIS	-	expression tag	UNP Q6R2Q7
C	829	HIS	-	expression tag	UNP Q6R2Q7
C	830	HIS	-	expression tag	UNP Q6R2Q7
C	831	HIS	-	expression tag	UNP Q6R2Q7
D	826	HIS	-	expression tag	UNP Q6R2Q7
D	827	HIS	-	expression tag	UNP Q6R2Q7
D	828	HIS	-	expression tag	UNP Q6R2Q7
D	829	HIS	-	expression tag	UNP Q6R2Q7
D	830	HIS	-	expression tag	UNP Q6R2Q7
D	831	HIS	-	expression tag	UNP Q6R2Q7
E	826	HIS	-	expression tag	UNP Q6R2Q7
E	827	HIS	-	expression tag	UNP Q6R2Q7
E	828	HIS	-	expression tag	UNP Q6R2Q7
E	829	HIS	-	expression tag	UNP Q6R2Q7
E	830	HIS	-	expression tag	UNP Q6R2Q7
E	831	HIS	-	expression tag	UNP Q6R2Q7
F	826	HIS	-	expression tag	UNP Q6R2Q7
F	827	HIS	-	expression tag	UNP Q6R2Q7
F	828	HIS	-	expression tag	UNP Q6R2Q7
F	829	HIS	-	expression tag	UNP Q6R2Q7
F	830	HIS	-	expression tag	UNP Q6R2Q7
F	831	HIS	-	expression tag	UNP Q6R2Q7
G	826	HIS	-	expression tag	UNP Q6R2Q7
G	827	HIS	-	expression tag	UNP Q6R2Q7
G	828	HIS	-	expression tag	UNP Q6R2Q7
G	829	HIS	-	expression tag	UNP Q6R2Q7
G	830	HIS	-	expression tag	UNP Q6R2Q7
G	831	HIS	-	expression tag	UNP Q6R2Q7
H	826	HIS	-	expression tag	UNP Q6R2Q7
H	827	HIS	-	expression tag	UNP Q6R2Q7
H	828	HIS	-	expression tag	UNP Q6R2Q7
H	829	HIS	-	expression tag	UNP Q6R2Q7
H	830	HIS	-	expression tag	UNP Q6R2Q7
H	831	HIS	-	expression tag	UNP Q6R2Q7

- Molecule 2 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	G	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	H	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0
4	G	1	Total 1	Ca 1	0	0
4	H	1	Total 1	Ca 1	0	0

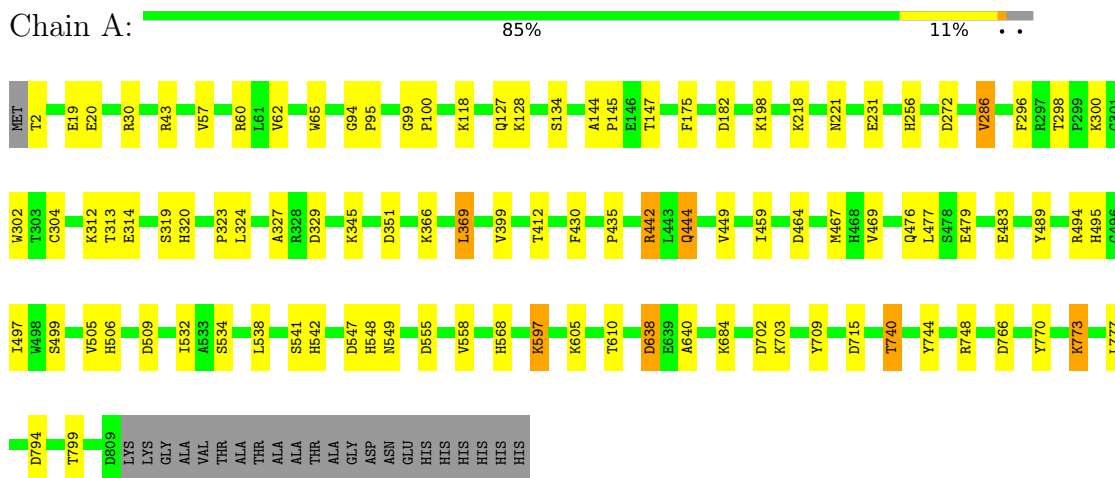
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	208	Total 208	O 208	0	0
5	B	225	Total 225	O 225	0	0
5	C	55	Total 55	O 55	0	0
5	D	53	Total 53	O 53	0	0
5	E	107	Total 107	O 107	0	0
5	F	92	Total 92	O 92	0	0
5	G	153	Total 153	O 153	0	0
5	H	129	Total 129	O 129	0	0

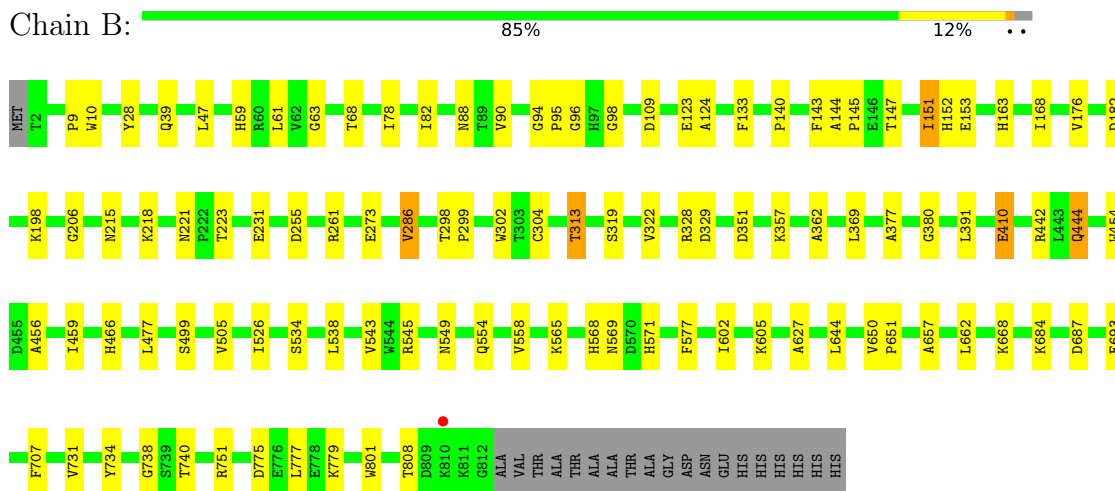
3 Residue-property plots

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: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

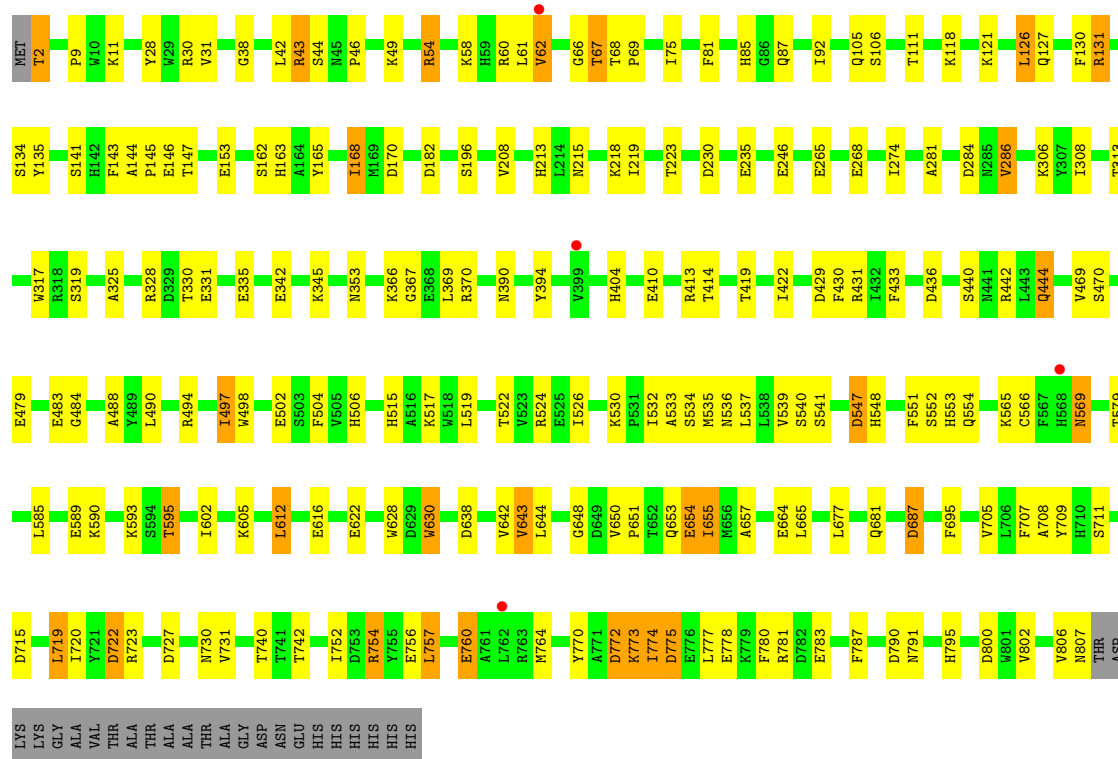


- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

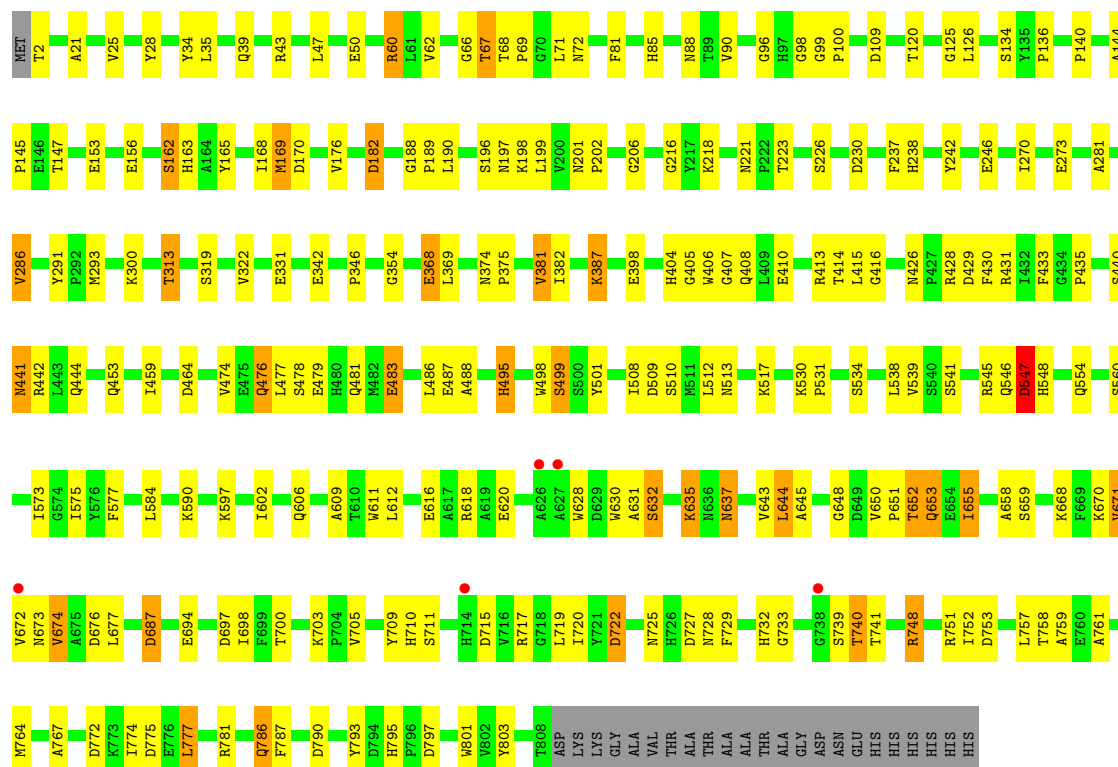


- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



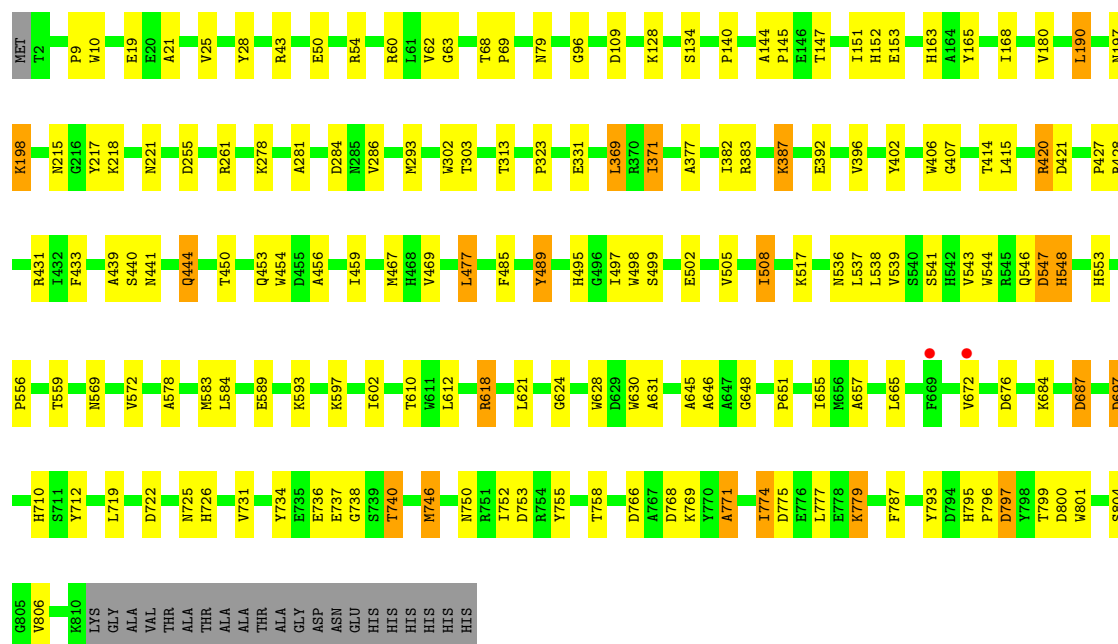


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



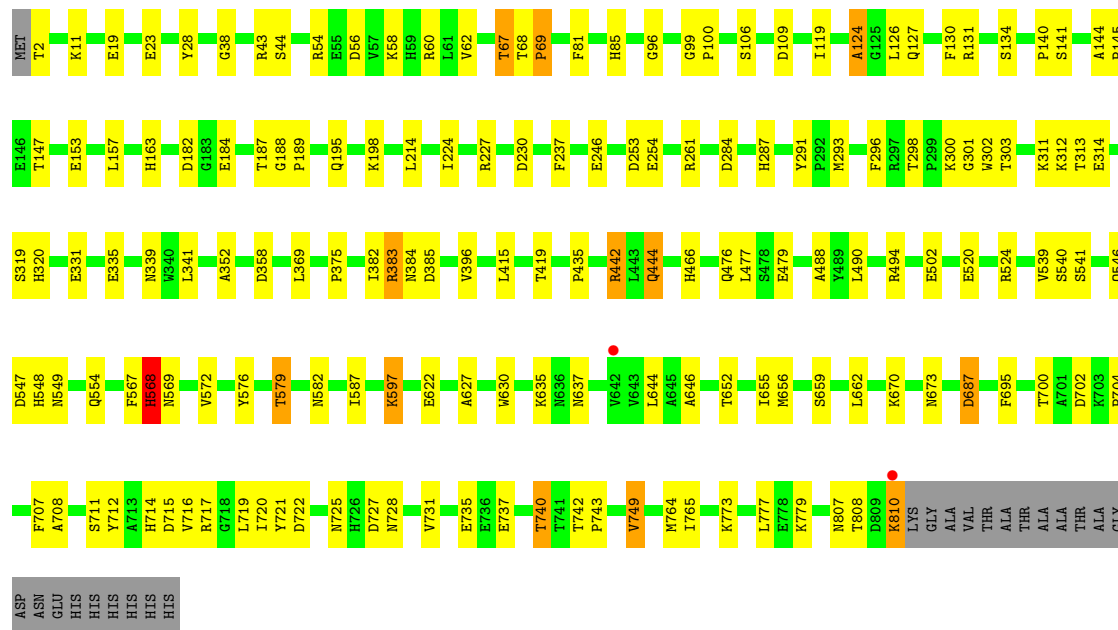
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain E:  77% 18% . .



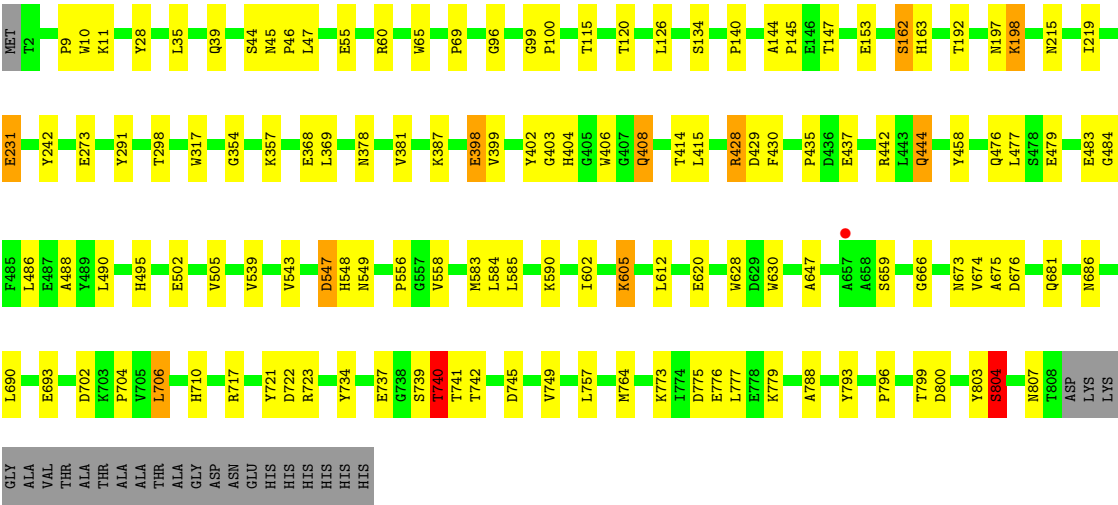
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain F:  78% 18% . .

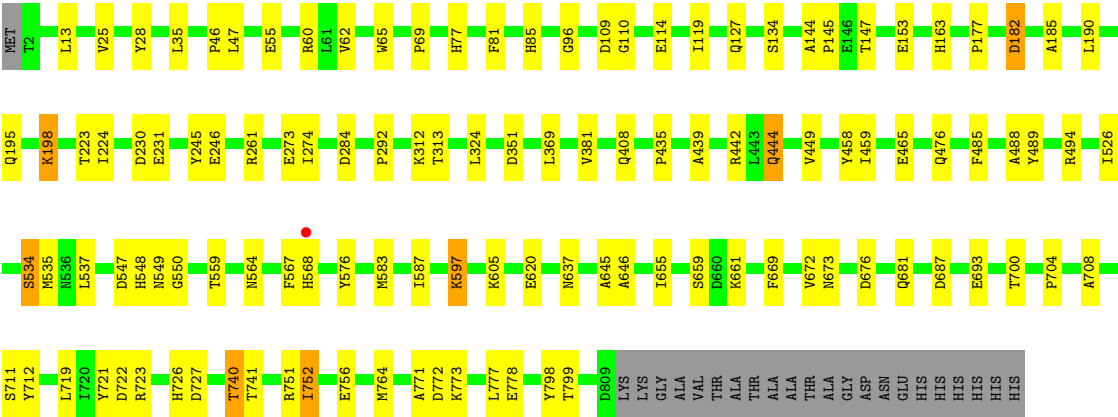
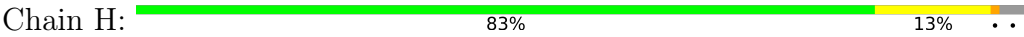


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

Chain G:  81% 15% . .



● Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.30Å 184.94Å 163.13Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	48.10 – 2.50 48.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.10-2.50) 99.9 (48.10-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.166 , 0.226 0.184 , 0.185	Depositor DCC
R_{free} test set	14632 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52775	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: TPP, PEP, CA

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	1.09	5/6614 (0.1%)	1.45	16/8996 (0.2%)
1	B	1.07	3/6636 (0.0%)	1.43	15/9023 (0.2%)
1	C	1.11	1/6588 (0.0%)	1.50	21/8960 (0.2%)
1	D	1.10	0/6595	1.50	23/8970 (0.3%)
1	E	1.10	4/6612 (0.1%)	1.47	13/8992 (0.1%)
1	F	1.08	2/6612 (0.0%)	1.49	15/8992 (0.2%)
1	G	1.09	0/6606	1.45	11/8985 (0.1%)
1	H	1.09	3/6614 (0.0%)	1.49	16/8996 (0.2%)
All	All	1.09	18/52877 (0.0%)	1.47	130/71914 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	ASP	C-O	5.82	1.30	1.24
1	C	345	LYS	N-CA	5.65	1.50	1.46
1	H	177	PRO	C-O	-5.59	1.17	1.23
1	B	466	HIS	CE1-NE2	5.50	1.38	1.32
1	F	627	ALA	C-O	5.42	1.30	1.23
1	E	495	HIS	CE1-NE2	5.37	1.38	1.32
1	E	553	HIS	CE1-NE2	5.37	1.38	1.32
1	A	320	HIS	CE1-NE2	5.35	1.38	1.32
1	A	256	HIS	CE1-NE2	5.35	1.38	1.32
1	F	466	HIS	CE1-NE2	5.34	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	GLY	C-O	5.30	1.27	1.23
1	A	497	ILE	C-O	5.29	1.29	1.23
1	B	534	SER	C-O	5.26	1.30	1.23
1	A	449	VAL	N-CA	5.14	1.50	1.46
1	B	322	VAL	N-CA	5.10	1.49	1.45
1	H	449	VAL	N-CA	5.10	1.50	1.46
1	E	217	TYR	C-O	5.05	1.30	1.23
1	H	312	LYS	C-O	5.04	1.29	1.23

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	740	THR	CB-CA-C	8.01	123.60	110.78
1	A	638	ASP	CA-CB-CG	7.68	120.28	112.60
1	B	98	GLY	CA-C-N	7.29	126.45	121.13
1	B	98	GLY	C-N-CA	7.29	126.45	121.13
1	H	109	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	329	ASP	CA-CB-CG	6.87	119.47	112.60
1	E	740	THR	CB-CA-C	6.83	120.50	110.26
1	B	124	ALA	CA-C-N	6.77	127.46	119.94
1	B	124	ALA	C-N-CA	6.77	127.46	119.94
1	H	798	TYR	CA-C-N	6.72	129.17	120.44
1	H	798	TYR	C-N-CA	6.72	129.17	120.44
1	B	109	ASP	CA-CB-CG	6.60	119.20	112.60
1	G	740	THR	CB-CA-C	6.59	121.11	110.29
1	D	441	ASN	N-CA-C	-6.58	105.13	112.57
1	H	740	THR	CB-CA-C	6.41	121.38	110.81
1	F	687	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	63	GLY	CA-C-O	-6.26	117.03	122.16
1	D	687	ASP	CA-CB-CG	6.24	118.84	112.60
1	H	182	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	483	GLU	CA-C-N	6.20	126.99	119.99
1	A	483	GLU	C-N-CA	6.20	126.99	119.99
1	A	740	THR	CB-CA-C	6.19	120.69	110.78
1	B	329	ASP	CA-CB-CG	6.09	118.69	112.60
1	C	42	LEU	CA-C-N	6.08	128.92	120.29
1	C	42	LEU	C-N-CA	6.08	128.92	120.29
1	E	687	ASP	CA-CB-CG	6.00	118.60	112.60
1	G	115	THR	CA-CB-OG1	-5.89	100.77	109.60
1	H	687	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	476	GLN	CA-C-O	-5.87	114.99	121.33
1	D	464	ASP	CA-CB-CG	5.87	118.47	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	702	ASP	CA-CB-CG	5.82	118.42	112.60
1	H	231	GLU	CB-CG-CD	5.79	122.44	112.60
1	C	483	GLU	CA-C-N	5.70	126.30	119.98
1	C	483	GLU	C-N-CA	5.70	126.30	119.98
1	D	637	ASN	CA-C-N	5.67	127.88	120.28
1	D	637	ASN	C-N-CA	5.67	127.88	120.28
1	B	68	THR	CA-CB-OG1	-5.67	101.09	109.60
1	G	547	ASP	N-CA-C	-5.66	105.48	112.90
1	C	367	GLY	CA-C-N	5.66	128.42	120.28
1	C	367	GLY	C-N-CA	5.66	128.42	120.28
1	H	485	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	627	ALA	CA-C-O	-5.64	115.41	121.56
1	B	151	ILE	N-CA-C	-5.64	107.25	112.43
1	D	547	ASP	CA-C-N	5.63	128.29	120.29
1	D	547	ASP	C-N-CA	5.63	128.29	120.29
1	B	738	GLY	CA-C-O	-5.57	117.59	122.16
1	C	772	ASP	CA-CB-CG	5.56	118.16	112.60
1	D	483	GLU	CA-C-N	5.55	126.11	119.94
1	D	483	GLU	C-N-CA	5.55	126.11	119.94
1	H	550	GLY	CA-C-N	5.55	127.99	120.44
1	H	550	GLY	C-N-CA	5.55	127.99	120.44
1	D	182	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	368	GLU	CA-C-N	5.50	127.66	120.28
1	D	368	GLU	C-N-CA	5.50	127.66	120.28
1	F	419	THR	CA-CB-OG1	-5.50	101.35	109.60
1	E	797	ASP	CA-C-N	5.46	127.87	120.44
1	E	797	ASP	C-N-CA	5.46	127.87	120.44
1	C	218	LYS	CB-CA-C	5.43	121.23	110.42
1	H	458	TYR	CA-C-O	-5.41	114.97	120.71
1	E	489	TYR	N-CA-C	-5.40	105.30	111.07
1	B	357	LYS	CA-C-N	5.39	127.76	120.38
1	B	357	LYS	C-N-CA	5.39	127.76	120.38
1	A	324	LEU	CA-C-N	5.38	127.49	120.28
1	A	324	LEU	C-N-CA	5.38	127.49	120.28
1	G	483	GLU	CA-C-N	5.37	125.90	119.94
1	G	483	GLU	C-N-CA	5.37	125.90	119.94
1	D	697	ASP	CA-C-N	5.37	127.27	120.72
1	D	697	ASP	C-N-CA	5.37	127.27	120.72
1	F	415	LEU	CA-C-N	5.37	125.90	119.94
1	F	415	LEU	C-N-CA	5.37	125.90	119.94
1	A	128	LYS	CA-C-N	5.34	127.38	120.44
1	A	128	LYS	C-N-CA	5.34	127.38	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	551	PHE	CA-C-N	5.34	127.69	120.38
1	C	551	PHE	C-N-CA	5.34	127.69	120.38
1	E	109	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	67	THR	CA-C-N	5.32	126.38	119.78
1	D	67	THR	C-N-CA	5.32	126.38	119.78
1	D	109	ASP	CA-CB-CG	5.32	117.92	112.60
1	F	124	ALA	CA-C-N	5.29	126.76	120.14
1	F	124	ALA	C-N-CA	5.29	126.76	120.14
1	C	760	GLU	N-CA-C	-5.27	106.91	113.55
1	C	648	GLY	CA-C-N	5.26	127.59	120.38
1	C	648	GLY	C-N-CA	5.26	127.59	120.38
1	E	215	ASN	N-CA-C	-5.26	106.54	113.17
1	H	559	THR	CA-C-N	5.26	127.76	120.29
1	H	559	THR	C-N-CA	5.26	127.76	120.29
1	A	412	THR	CA-CB-OG1	-5.25	101.72	109.60
1	F	352	ALA	CA-C-N	5.25	128.05	120.38
1	F	352	ALA	C-N-CA	5.25	128.05	120.38
1	G	458	TYR	CB-CA-C	5.23	118.15	109.53
1	B	261	ARG	N-CA-C	-5.22	105.50	111.14
1	B	380	GLY	CA-C-O	-5.22	115.69	120.80
1	C	2	THR	CA-C-N	5.18	127.60	120.39
1	C	2	THR	C-N-CA	5.18	127.60	120.39
1	C	695	PHE	CA-C-N	5.18	127.22	120.28
1	C	695	PHE	C-N-CA	5.18	127.22	120.28
1	F	69	PRO	CA-C-N	5.18	125.84	119.99
1	F	69	PRO	C-N-CA	5.18	125.84	119.99
1	G	399	VAL	N-CA-C	-5.17	107.78	112.12
1	F	568	HIS	CA-CB-CG	5.16	118.96	113.80
1	C	595	THR	CA-CB-OG1	-5.14	101.89	109.60
1	C	67	THR	CA-C-N	5.13	126.14	119.78
1	C	67	THR	C-N-CA	5.13	126.14	119.78
1	A	182	ASP	N-CA-C	-5.13	106.18	112.90
1	A	231	GLU	CB-CG-CD	5.12	121.31	112.60
1	F	765	ILE	N-CA-C	-5.12	106.80	111.67
1	D	590	LYS	CA-C-N	5.12	127.45	120.54
1	D	590	LYS	C-N-CA	5.12	127.45	120.54
1	G	403	GLY	CA-C-N	5.12	128.11	120.95
1	G	403	GLY	C-N-CA	5.12	128.11	120.95
1	F	579	THR	CB-CA-C	5.11	120.81	110.38
1	E	559	THR	CB-CA-C	5.11	118.97	110.90
1	H	261	ARG	CA-C-N	5.08	127.39	120.54
1	H	261	ARG	C-N-CA	5.08	127.39	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	291	TYR	CB-CA-C	5.07	116.71	109.26
1	H	722	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	542	HIS	CA-C-N	5.04	127.11	120.60
1	A	542	HIS	C-N-CA	5.04	127.11	120.60
1	D	767	ALA	CA-C-N	5.04	126.99	120.44
1	D	767	ALA	C-N-CA	5.04	126.99	120.44
1	G	231	GLU	N-CA-C	-5.04	105.87	111.36
1	D	476	GLN	N-CA-C	-5.03	101.42	109.07
1	E	485	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	182	ASP	CA-CB-CG	5.03	117.63	112.60
1	E	128	LYS	CA-C-N	5.03	126.98	120.44
1	E	128	LYS	C-N-CA	5.03	126.98	120.44
1	A	175	PHE	CA-C-O	-5.02	114.94	120.36
1	E	583	MET	CA-C-N	5.01	127.24	120.38
1	E	583	MET	C-N-CA	5.01	127.24	120.38
1	C	131	ARG	CA-C-O	-5.00	115.57	120.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	597	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6436	0	6118	50	0
1	B	6458	0	6147	59	0
1	C	6411	0	6101	114	0
1	D	6418	0	6108	138	0
1	E	6435	0	6125	106	0
1	F	6435	0	6125	96	0
1	G	6428	0	6114	82	0
1	H	6436	0	6118	65	0
2	A	10	0	2	4	0
2	B	10	0	2	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	2	2	0
2	D	10	0	2	1	0
2	E	10	0	2	2	0
2	F	10	0	2	2	0
2	G	10	0	2	3	0
2	H	10	0	2	4	0
3	A	26	0	16	2	0
3	B	26	0	16	3	0
3	C	26	0	16	4	0
3	D	26	0	16	4	0
3	E	26	0	16	3	0
3	F	26	0	16	4	0
3	G	26	0	16	2	0
3	H	26	0	16	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	208	0	0	4	0
5	B	225	0	0	3	0
5	C	55	0	0	1	0
5	D	53	0	0	2	0
5	E	107	0	0	1	0
5	F	92	0	0	1	0
5	G	153	0	0	1	0
5	H	129	0	0	2	0
All	All	52775	0	49100	679	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 7.

All (679) 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)
3:H:902:TPP:H2	3:H:902:TPP:HN42	1.25	0.97
1:G:442:ARG:HA	1:G:444:GLN:HE22	1.28	0.96
1:D:67:THR:OG1	3:D:902:TPP:O2B	1.84	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:ARG:HA	1:F:444:GLN:HE22	1.31	0.95
1:B:569:ASN:HD21	1:B:687:ASP:H	1.12	0.92
1:F:737:GLU:HB3	1:F:749:VAL:HG13	1.51	0.91
1:F:444:GLN:H	1:F:444:GLN:HE21	1.20	0.90
1:B:444:GLN:HE21	1:B:444:GLN:H	0.95	0.90
3:H:902:TPP:HN42	3:H:902:TPP:C2	1.84	0.90
1:B:442:ARG:HA	1:B:444:GLN:HE22	1.41	0.86
1:A:442:ARG:HA	1:A:444:GLN:HE22	1.40	0.86
1:F:67:THR:OG1	3:F:902:TPP:O2B	1.93	0.85
1:C:517:LYS:NZ	1:D:554:GLN:O	2.08	0.84
1:A:740:THR:CG2	1:B:140:PRO:HA	2.12	0.79
2:C:901:PEP:H32	2:C:901:PEP:O1P	1.84	0.77
1:E:738:GLY:HA3	1:E:746:MET:HE1	1.65	0.77
1:C:756:GLU:HB2	1:C:781:ARG:HE	1.48	0.77
1:B:444:GLN:HE21	1:B:444:GLN:N	1.77	0.76
1:F:579:THR:HG21	1:F:673:ASN:HD21	1.50	0.75
1:E:441:ASN:HD22	1:E:499:SER:HB2	1.51	0.74
1:G:740:THR:CG2	1:H:134:SER:HA	2.18	0.73
1:B:444:GLN:H	1:B:444:GLN:NE2	1.78	0.73
1:G:740:THR:HG21	1:H:134:SER:HA	1.68	0.73
1:F:569:ASN:HD21	1:F:687:ASP:HB3	1.53	0.73
1:F:58:LYS:NZ	1:F:131:ARG:O	2.22	0.72
1:G:404:HIS:CD2	1:G:630:TRP:CE3	2.76	0.72
1:C:67:THR:HB	3:C:902:TPP:O2B	1.87	0.72
1:B:569:ASN:ND2	1:B:687:ASP:H	1.89	0.71
1:D:440:SER:OG	2:D:901:PEP:O2P	2.09	0.70
1:E:543:VAL:HG21	1:E:734:TYR:CD1	2.26	0.70
1:D:720:ILE:O	1:D:720:ILE:HD12	1.92	0.70
1:G:799:THR:HG22	1:G:800:ASP:OD1	1.92	0.70
1:C:612:LEU:HD21	1:C:628:TRP:CZ2	2.27	0.69
1:E:197:ASN:OD1	1:E:198:LYS:HE3	1.91	0.69
1:D:441:ASN:ND2	1:D:499:SER:OG	2.23	0.69
1:D:797:ASP:O	1:D:801:TRP:HB2	1.93	0.69
1:C:146:GLU:OE2	1:C:526:ILE:HD11	1.94	0.68
1:H:704:PRO:HB2	1:H:764:MET:HE2	1.74	0.68
1:C:43:ARG:HH12	1:C:131:ARG:CZ	2.06	0.68
1:A:740:THR:HG21	1:B:140:PRO:HA	1.74	0.68
2:H:901:PEP:H32	2:H:901:PEP:O1P	1.93	0.67
1:E:134:SER:HA	1:F:740:THR:HG23	1.76	0.66
1:H:568[A]:HIS:CD2	1:H:568[A]:HIS:O	2.48	0.66
3:H:902:TPP:C2	3:H:902:TPP:N4'	2.57	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:442:ARG:CA	1:G:444:GLN:HE22	2.05	0.66
3:D:902:TPP:HN42	3:D:902:TPP:H2	1.60	0.66
1:C:756:GLU:HB2	1:C:781:ARG:NE	2.11	0.66
1:B:144:ALA:HB1	1:B:145:PRO:HD2	1.76	0.65
1:E:140:PRO:HA	1:F:740:THR:CG2	2.26	0.65
1:E:740:THR:CG2	1:F:134:SER:HA	2.25	0.65
1:G:197:ASN:OD1	1:G:198:LYS:HE3	1.95	0.65
1:G:444:GLN:H	1:G:444:GLN:NE2	1.95	0.65
1:D:620:GLU:OE1	1:D:673:ASN:ND2	2.25	0.65
1:G:444:GLN:H	1:G:444:GLN:HE21	1.45	0.65
1:D:430:PHE:HA	1:D:495:HIS:O	1.97	0.65
2:E:901:PEP:O2P	2:E:901:PEP:C3	2.41	0.65
1:E:612:LEU:HD11	1:E:628:TRP:CZ2	2.31	0.65
1:G:140:PRO:HA	1:H:740:THR:CG2	2.26	0.65
1:E:740:THR:HG21	1:F:134:SER:HA	1.79	0.64
1:F:737:GLU:HB3	1:F:749:VAL:CG1	2.27	0.64
1:D:410:GLU:OE1	1:D:413:ARG:NE	2.26	0.63
1:F:442:ARG:HA	1:F:444:GLN:NE2	2.11	0.63
1:F:637:ASN:ND2	1:F:700:THR:HG22	2.12	0.63
1:C:740:THR:CG2	1:D:140:PRO:HA	2.29	0.63
1:C:787:PHE:CD1	1:C:791:ASN:ND2	2.67	0.63
1:A:506:HIS:HA	1:A:509:ASP:OD1	1.99	0.63
1:C:506:HIS:CD2	1:D:513:ASN:ND2	2.66	0.63
1:D:541:SER:O	1:D:546:GLN:NE2	2.32	0.63
1:D:202:PRO:HB2	1:D:281:ALA:HB2	1.79	0.63
1:G:741:THR:OG1	1:G:742:THR:N	2.32	0.63
1:E:517:LYS:NZ	1:F:554:GLN:O	2.25	0.63
1:D:674:VAL:HG12	1:D:676:ASP:O	1.98	0.62
1:H:144:ALA:HB1	1:H:145:PRO:HD2	1.81	0.62
1:A:57:VAL:HG11	1:A:327:ALA:HB3	1.80	0.62
1:F:44:SER:HA	1:F:127:GLN:OE1	1.98	0.62
1:H:198:LYS:HE2	5:H:1072:HOH:O	1.99	0.62
1:E:766:ASP:CG	1:E:769:LYS:HB3	2.25	0.62
1:A:444:GLN:H	1:A:444:GLN:NE2	1.98	0.61
1:G:428:ARG:HG2	1:G:428:ARG:HH11	1.65	0.61
1:D:404:HIS:O	1:D:803:TYR:HD2	1.84	0.61
1:G:612:LEU:HD21	1:G:628:TRP:CZ2	2.36	0.61
1:F:96:GLY:HA3	1:F:153:GLU:O	2.00	0.60
1:C:780:PHE:O	1:C:783:GLU:N	2.33	0.60
1:G:408:GLN:HE21	1:G:408:GLN:HA	1.66	0.60
1:G:788:ALA:HA	1:G:793:TYR:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:902:TPP:C2	3:F:902:TPP:HN42	2.14	0.60
1:D:650:VAL:N	1:D:651:PRO:HD2	2.17	0.60
1:E:140:PRO:HA	1:F:740:THR:HG22	1.82	0.60
1:C:394:TYR:HB2	1:C:585:LEU:HD21	1.82	0.60
1:B:410:GLU:HB3	1:B:605:LYS:O	2.01	0.59
1:E:547:ASP:CG	1:F:60:ARG:HH22	2.09	0.59
1:G:620:GLU:OE1	1:G:673:ASN:ND2	2.30	0.59
1:H:182:ASP:CG	1:H:223:THR:HG21	2.28	0.59
1:G:681:GLN:OE1	1:G:686:ASN:HB2	2.01	0.59
1:C:502:GLU:HA	1:C:539:VAL:HG13	1.84	0.59
1:E:396:VAL:HG11	1:E:610:THR:HG21	1.84	0.59
2:A:901:PEP:O2P	2:A:901:PEP:H32	2.03	0.59
1:C:43:ARG:HH12	1:C:131:ARG:NH1	1.99	0.59
1:G:435:PRO:HA	1:G:476:GLN:O	2.03	0.58
1:F:19:GLU:OE1	1:F:261:ARG:NH1	2.34	0.58
1:D:67:THR:HG22	1:D:71:LEU:HG	1.86	0.58
1:D:68:THR:N	1:D:69:PRO:HD2	2.19	0.58
1:D:547:ASP:O	1:D:740:THR:HA	2.04	0.58
1:B:96:GLY:HA3	1:B:153:GLU:O	2.03	0.58
1:F:157:LEU:HB3	1:F:184:GLU:HG3	1.86	0.58
1:E:477:LEU:HD22	3:F:902:TPP:HM42	1.86	0.58
1:B:545:ARG:HD3	5:B:1091:HOH:O	2.02	0.58
3:F:902:TPP:HN42	3:F:902:TPP:H2	1.68	0.58
1:D:162:SER:OG	5:D:1001:HOH:O	2.16	0.57
1:A:489:TYR:CE2	1:A:494:ARG:HB3	2.39	0.57
3:E:902:TPP:HN42	3:E:902:TPP:C2	2.17	0.57
1:E:415:LEU:HD23	1:E:538:LEU:HD22	1.85	0.57
1:E:740:THR:CG2	1:F:140:PRO:HA	2.34	0.57
1:A:770:TYR:O	1:A:773:LYS:N	2.37	0.57
1:A:444:GLN:H	1:A:444:GLN:HE21	1.51	0.57
1:C:654:GLU:OE2	1:C:654:GLU:HA	2.04	0.57
3:C:902:TPP:H2	3:C:902:TPP:HN42	1.69	0.57
1:C:143:PHE:O	1:C:153:GLU:HA	2.05	0.57
1:C:740:THR:HG21	1:D:140:PRO:HA	1.87	0.57
1:E:543:VAL:CG2	1:E:734:TYR:CD1	2.87	0.56
1:F:230:ASP:OD1	1:F:246:GLU:OE2	2.22	0.56
1:D:163:HIS:HA	1:D:488:ALA:HB2	1.86	0.56
2:A:901:PEP:H32	5:A:1096:HOH:O	2.04	0.56
1:E:796:PRO:O	1:E:800:ASP:HB2	2.05	0.56
1:F:106:SER:HA	1:F:109:ASP:OD1	2.06	0.56
1:F:124:ALA:O	1:F:127:GLN:HB3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:PRO:HA	1:H:740:THR:HG21	1.85	0.56
1:H:245:TYR:OH	1:H:273:GLU:OE1	2.13	0.56
1:B:549:ASN:HD21	2:B:901:PEP:C3	2.18	0.56
1:C:730:ASN:ND2	1:C:760:GLU:OE1	2.39	0.56
1:D:81:PHE:CD1	1:D:85:HIS:CD2	2.93	0.56
1:E:441:ASN:ND2	1:E:499:SER:HB2	2.18	0.56
1:G:543:VAL:HG21	1:G:734:TYR:CD1	2.40	0.56
1:H:195:GLN:OE1	1:H:198:LYS:NZ	2.38	0.56
1:C:2:THR:N	1:C:429:ASP:OD1	2.39	0.56
1:D:612:LEU:HD21	1:D:628:TRP:CZ2	2.40	0.56
1:A:218:LYS:HE2	1:A:221:ASN:HB2	1.88	0.56
1:D:199:LEU:O	1:D:453:GLN:HG2	2.06	0.56
1:H:568[A]:HIS:O	1:H:568[A]:HIS:HD2	1.89	0.56
1:A:640:ALA:O	1:A:703:LYS:CD	2.55	0.56
1:D:787:PHE:CE2	1:D:795:HIS:HA	2.41	0.55
1:A:144:ALA:HB1	1:A:145:PRO:HD2	1.88	0.55
1:A:740:THR:HG22	1:B:140:PRO:HA	1.88	0.55
1:C:569:ASN:OD1	1:C:687:ASP:CG	2.49	0.55
1:F:435:PRO:HA	1:F:476:GLN:O	2.06	0.55
1:H:620:GLU:OE1	1:H:673:ASN:ND2	2.40	0.55
1:D:62:VAL:HG12	1:D:134:SER:HB3	1.89	0.55
1:D:218:LYS:O	1:D:300:LYS:NZ	2.40	0.55
1:D:645:ALA:HA	1:D:672:VAL:O	2.06	0.55
1:D:655:ILE:HD12	1:D:757:LEU:HD13	1.87	0.55
1:B:143:PHE:O	1:B:153:GLU:HA	2.07	0.55
1:C:709:TYR:CE2	1:C:711:SER:HB3	2.42	0.55
1:E:737:GLU:OE2	1:F:568:HIS:ND1	2.40	0.55
1:D:170:ASP:OD2	1:D:431:ARG:NE	2.25	0.55
1:E:738:GLY:CA	1:E:746:MET:HE1	2.35	0.55
1:G:47:LEU:HD11	1:G:354:GLY:HA2	1.89	0.55
1:D:453:GLN:HB3	1:D:474:VAL:HG22	1.89	0.54
1:C:165:TYR:CD2	1:C:196:SER:HB2	2.42	0.54
1:C:547:ASP:OD2	1:D:60:ARG:NH2	2.40	0.54
1:D:165:TYR:CD2	1:D:196:SER:HB2	2.43	0.54
1:E:21:ALA:O	1:E:25:VAL:HG23	2.08	0.54
1:G:408:GLN:HA	1:G:408:GLN:NE2	2.21	0.54
1:C:410:GLU:OE1	1:C:413:ARG:NE	2.37	0.54
1:G:378:ASN:O	1:G:381:VAL:HG22	2.06	0.54
1:C:182:ASP:CG	1:C:223:THR:HG21	2.33	0.54
1:D:709:TYR:N	1:D:732:HIS:O	2.35	0.54
1:G:65:TRP:O	1:G:69:PRO:HD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:547:ASP:OD2	1:H:60:ARG:NH2	2.37	0.54
3:C:902:TPP:N1'	1:D:479:GLU:OE2	2.41	0.54
1:E:454:TRP:CG	1:E:467:MET:HE3	2.43	0.54
1:H:576:TYR:HB3	1:H:587:ILE:HD13	1.90	0.54
1:D:169:MET:HE2	1:D:474:VAL:HG21	1.90	0.54
1:G:737:GLU:CG	1:H:568[B]:HIS:CE1	2.91	0.54
1:E:766:ASP:HB3	1:E:769:LYS:HB3	1.90	0.53
5:A:1130:HOH:O	2:B:901:PEP:C2	2.56	0.53
1:D:21:ALA:O	1:D:25:VAL:HG23	2.09	0.53
1:C:168:ILE:HD13	1:C:208:VAL:HG23	1.91	0.53
1:C:787:PHE:CE1	1:C:791:ASN:ND2	2.77	0.53
1:D:655:ILE:O	1:D:658:ALA:HB3	2.07	0.53
3:E:902:TPP:HN42	3:E:902:TPP:H2	1.72	0.53
1:A:444:GLN:HE21	1:A:444:GLN:N	2.05	0.53
1:A:505:VAL:HG11	1:A:558:VAL:HG21	1.90	0.53
1:A:549:ASN:HD21	2:A:901:PEP:C3	2.21	0.53
1:A:568[A]:HIS:CD2	1:A:568[A]:HIS:O	2.62	0.53
1:G:134:SER:HA	1:H:740:THR:CG2	2.38	0.53
1:G:408:GLN:HE21	1:G:408:GLN:CA	2.21	0.53
1:C:522:THR:HA	1:C:526:ILE:HD12	1.90	0.53
1:D:709:TYR:O	1:D:733:GLY:HA2	2.08	0.53
1:B:568[A]:HIS:O	1:B:568[A]:HIS:CD2	2.62	0.53
1:C:106:SER:HG	1:C:111:THR:HG1	1.54	0.53
1:E:420:ARG:HG3	1:E:421:ASP:N	2.19	0.53
1:D:218:LYS:HE2	1:D:221:ASN:HB2	1.91	0.53
1:D:407:GLY:O	1:D:408:GLN:NE2	2.37	0.53
1:E:736:GLU:OE1	1:F:520:GLU:OE2	2.27	0.53
1:E:497:ILE:HA	1:E:536:ASN:O	2.08	0.53
1:G:737:GLU:HG2	1:H:568[B]:HIS:CE1	2.44	0.53
1:F:646:ALA:HA	1:F:708:ALA:O	2.08	0.52
1:B:59:HIS:CE1	1:B:328:ARG:CZ	2.92	0.52
1:A:312:LYS:HE3	1:A:314:GLU:O	2.10	0.52
1:H:646:ALA:HB2	1:H:655:ILE:HG13	1.91	0.52
3:B:902:TPP:H2	3:B:902:TPP:HN42	1.74	0.52
1:F:442:ARG:CA	1:F:444:GLN:HE22	2.15	0.52
1:C:286:VAL:HA	1:C:469:VAL:HG11	1.92	0.52
1:F:313:THR:O	1:F:319:SER:HB3	2.09	0.52
1:C:740:THR:CG2	1:D:134:SER:HA	2.40	0.52
1:C:61:LEU:HD12	1:C:325:ALA:O	2.10	0.52
1:G:404:HIS:CD2	1:G:630:TRP:CD2	2.97	0.52
1:E:569:ASN:HB3	1:E:687:ASP:OD1	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:VAL:HG21	1:B:734:TYR:CD1	2.45	0.52
1:E:180:VAL:HG11	1:E:190:LEU:HD11	1.92	0.52
1:E:433:PHE:O	1:E:498:TRP:HA	2.09	0.52
1:G:140:PRO:HA	1:H:740:THR:HG22	1.91	0.52
1:G:796:PRO:HA	1:G:799:THR:HB	1.91	0.52
1:C:62:VAL:HG12	1:C:134:SER:HB3	1.92	0.51
3:G:902:TPP:H2	5:H:1058:HOH:O	2.08	0.51
5:A:1130:HOH:O	2:B:901:PEP:C1	2.58	0.51
1:B:215:ASN:HA	1:B:298:THR:O	2.10	0.51
1:B:168:ILE:HD12	1:B:206:GLY:O	2.11	0.51
1:C:163:HIS:HA	1:C:488:ALA:HB2	1.90	0.51
1:E:630:TRP:CZ3	1:E:631:ALA:HB2	2.46	0.51
1:E:676:ASP:OD1	1:E:676:ASP:C	2.53	0.51
1:G:549:ASN:HD21	2:G:901:PEP:C3	2.24	0.51
1:C:134:SER:OG	1:C:141:SER:HB3	2.11	0.51
1:C:708:ALA:HB1	1:C:752:ILE:HD11	1.93	0.51
1:C:654:GLU:OE2	1:C:654:GLU:CA	2.58	0.51
1:E:454:TRP:CE2	1:E:456:ALA:HB3	2.46	0.51
1:B:505:VAL:HG11	1:B:558:VAL:HG21	1.93	0.51
1:E:726:HIS:CE1	1:F:727:ASP:OD2	2.64	0.51
1:G:602:ILE:HG21	1:G:710:HIS:CD2	2.46	0.51
1:C:162:SER:HB3	1:C:484:GLY:HA3	1.92	0.51
1:E:140:PRO:HA	1:F:740:THR:HG21	1.92	0.51
1:E:544:TRP:HZ3	1:E:750:ASN:HD22	1.59	0.51
1:E:797:ASP:O	1:E:801:TRP:HB2	2.10	0.51
1:D:190:LEU:HD13	1:D:190:LEU:O	2.11	0.51
1:E:152:HIS:ND1	1:E:163:HIS:ND1	2.48	0.51
1:D:190:LEU:HD13	1:D:190:LEU:C	2.36	0.50
1:F:28:TYR:CD1	1:F:28:TYR:C	2.89	0.50
1:F:707:PHE:HB3	1:F:731:VAL:HG22	1.93	0.50
1:D:677:LEU:HG	1:D:677:LEU:O	2.11	0.50
1:E:396:VAL:CG1	1:E:610:THR:HG21	2.40	0.50
1:F:300:LYS:HE2	1:F:320:HIS:HA	1.92	0.50
1:F:572:VAL:O	1:F:597:LYS:HA	2.12	0.50
1:F:807:ASN:ND2	1:F:810:LYS:HB2	2.26	0.50
1:C:436:ASP:OD2	1:D:218:LYS:HB3	2.11	0.50
1:A:479:GLU:OE2	3:B:902:TPP:N1'	2.45	0.50
1:A:549:ASN:HD21	2:A:901:PEP:H31	1.76	0.50
1:D:99:GLY:N	1:D:100:PRO:HD2	2.26	0.50
1:D:602:ILE:HG21	1:D:710:HIS:CD2	2.45	0.50
1:G:612:LEU:HD21	1:G:628:TRP:CE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:901:PEP:O1P	2:H:901:PEP:C3	2.59	0.50
2:C:901:PEP:O1P	2:C:901:PEP:C3	2.55	0.50
1:G:740:THR:HG23	1:H:134:SER:HA	1.93	0.50
1:F:375:PRO:HB2	1:F:382:ILE:HD11	1.92	0.50
1:H:25:VAL:HG11	1:H:77:HIS:CE1	2.47	0.50
1:D:748:ARG:O	1:D:751:ARG:N	2.40	0.50
1:E:502:GLU:HG3	1:E:539:VAL:CG1	2.42	0.50
1:D:270:ILE:O	1:D:273:GLU:HB3	2.12	0.50
1:E:439:ALA:HA	1:E:444:GLN:HE21	1.76	0.50
1:E:541:SER:O	1:E:546:GLN:NE2	2.39	0.50
1:B:499:SER:HA	1:B:538:LEU:O	2.12	0.49
1:B:304:CYS:SG	1:B:313:THR:HG22	2.52	0.49
3:B:902:TPP:HN42	3:B:902:TPP:C2	2.24	0.49
1:C:740:THR:HG22	1:D:140:PRO:HA	1.94	0.49
1:F:284:ASP:CG	1:F:287:HIS:HD1	2.20	0.49
1:G:505:VAL:HG11	1:G:558:VAL:HG21	1.94	0.49
1:H:435:PRO:HA	1:H:476:GLN:O	2.13	0.49
1:C:540:SER:O	1:C:541:SER:C	2.56	0.49
1:C:687:ASP:C	1:C:687:ASP:OD1	2.55	0.49
1:D:709:TYR:CE2	1:D:711:SER:HB3	2.47	0.49
1:E:740:THR:HG21	1:F:140:PRO:HA	1.93	0.49
1:E:796:PRO:HA	1:E:799:THR:OG1	2.11	0.49
1:G:605:LYS:NZ	2:G:901:PEP:O2P	2.38	0.49
1:C:43:ARG:NH1	1:C:131:ARG:CZ	2.73	0.49
1:E:439:ALA:HA	1:E:444:GLN:NE2	2.27	0.49
1:C:442:ARG:HA	1:C:444:GLN:NE2	2.27	0.49
1:D:573:ILE:HG22	1:D:575:ILE:HD12	1.94	0.49
1:F:144:ALA:HB1	1:F:145:PRO:HD2	1.94	0.49
1:F:549:ASN:HD21	2:F:901:PEP:C3	2.26	0.49
1:D:415:LEU:HD23	1:D:538:LEU:HD22	1.94	0.49
1:D:478:SER:HB3	1:D:481:GLN:HB2	1.95	0.49
1:E:165:TYR:O	1:E:168:ILE:HG13	2.12	0.49
1:A:640:ALA:O	1:A:703:LYS:HD2	2.11	0.49
1:B:47:LEU:HD12	1:B:123:GLU:HG3	1.95	0.49
1:B:299:PRO:HA	5:B:1080:HOH:O	2.13	0.49
1:C:106:SER:OG	1:C:111:THR:OG1	2.27	0.49
1:D:144:ALA:HB1	1:D:145:PRO:HD2	1.94	0.49
1:E:602:ILE:HG21	1:E:710:HIS:CD2	2.48	0.49
1:F:546:GLN:OE1	1:F:549:ASN:HB2	2.11	0.49
1:C:665:LEU:HD11	1:C:773:LYS:HE3	1.95	0.49
1:E:281:ALA:HA	1:E:284:ASP:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:756:GLU:OE1	1:H:778:GLU:OE2	2.31	0.49
1:E:779:LYS:HE3	1:E:779:LYS:O	2.12	0.48
1:G:162:SER:HB2	1:G:484:GLY:HA3	1.94	0.48
1:G:134:SER:HA	1:H:740:THR:HG23	1.95	0.48
1:B:569:ASN:HD21	1:B:687:ASP:N	1.95	0.48
1:G:162:SER:CB	1:G:484:GLY:HA3	2.43	0.48
1:C:554:GLN:O	1:D:517:LYS:NZ	2.22	0.48
3:D:902:TPP:HN42	3:D:902:TPP:C2	2.26	0.48
1:A:541:SER:OG	1:A:605:LYS:HE2	2.14	0.48
1:B:94:GLY:N	1:B:95:PRO:CD	2.76	0.48
1:F:383:ARG:NH1	1:F:385:ASP:OD1	2.43	0.48
1:C:490:LEU:HD23	1:C:494:ARG:O	2.12	0.48
1:D:635:LYS:HA	1:D:635:LYS:HD3	1.72	0.48
1:H:583:MET:O	1:H:587:ILE:HG13	2.13	0.48
1:E:50:GLU:HB3	5:E:1062:HOH:O	2.14	0.48
1:F:637:ASN:HD22	1:F:700:THR:HG22	1.76	0.48
1:H:62:VAL:HG12	1:H:134:SER:HB3	1.96	0.48
1:H:230:ASP:OD1	1:H:246:GLU:OE2	2.32	0.48
1:C:774:ILE:HG22	1:C:775:ASP:N	2.28	0.47
3:C:902:TPP:HN42	3:C:902:TPP:C2	2.27	0.47
2:G:901:PEP:C3	2:G:901:PEP:O2P	2.62	0.47
1:B:313:THR:O	1:B:319:SER:HB3	2.15	0.47
1:B:568[B]:HIS:N	1:B:568[B]:HIS:CD2	2.82	0.47
1:C:506:HIS:CD2	1:D:513:ASN:HD22	2.32	0.47
1:D:404:HIS:HE1	1:D:616:GLU:OE1	1.97	0.47
1:E:134:SER:HA	1:F:740:THR:CG2	2.42	0.47
1:E:541:SER:C	1:E:546:GLN:HE21	2.23	0.47
1:F:704:PRO:HB2	1:F:764:MET:HE3	1.96	0.47
1:F:725:ASN:OD1	1:F:728:ASN:HB2	2.14	0.47
2:B:901:PEP:O2P	2:B:901:PEP:H32	2.15	0.47
1:D:28:TYR:CD1	1:D:28:TYR:C	2.91	0.47
1:F:253:ASP:O	1:F:254:GLU:C	2.57	0.47
1:F:711:SER:OG	1:F:712:TYR:N	2.47	0.47
1:F:714:HIS:O	1:F:715:ASP:C	2.57	0.47
1:G:486:LEU:O	1:G:490:LEU:HG	2.14	0.47
1:A:442:ARG:CA	1:A:444:GLN:HE22	2.21	0.47
1:D:408:GLN:NE2	1:D:408:GLN:HA	2.29	0.47
1:G:442:ARG:C	1:G:444:GLN:NE2	2.72	0.47
1:G:717:ARG:HD3	1:H:721:TYR:CD2	2.49	0.47
1:C:657:ALA:HB1	1:C:754:ARG:HD3	1.96	0.47
1:E:645:ALA:HA	1:E:672:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:657:ALA:HA	1:E:801:TRP:CZ2	2.50	0.47
1:F:195:GLN:OE1	1:F:198:LYS:NZ	2.48	0.47
1:D:182:ASP:CG	1:D:223:THR:HG21	2.38	0.47
1:D:534:SER:HB3	1:D:597:LYS:O	2.15	0.47
1:G:163:HIS:HA	1:G:488:ALA:HB2	1.96	0.47
3:H:902:TPP:H2	3:H:902:TPP:N4'	2.09	0.47
1:A:548:HIS:HD1	1:A:548:HIS:H	1.63	0.47
1:C:787:PHE:CE2	1:C:795:HIS:HA	2.50	0.47
1:E:79:ASN:OD1	1:E:371:ILE:HD12	2.15	0.47
1:G:215:ASN:HA	1:G:298:THR:O	2.13	0.47
1:G:739:SER:OG	1:G:740:THR:N	2.48	0.47
1:H:96:GLY:HA3	1:H:153:GLU:O	2.14	0.47
1:B:59:HIS:CE1	1:B:328:ARG:NH1	2.83	0.47
1:C:68:THR:N	1:C:69:PRO:HD2	2.30	0.47
1:E:726:HIS:NE2	1:F:727:ASP:OD2	2.48	0.47
1:H:439:ALA:HA	1:H:444:GLN:HE21	1.79	0.47
1:D:313:THR:O	1:D:319:SER:HB3	2.15	0.47
1:F:567:PHE:O	1:F:569:ASN:N	2.47	0.47
1:G:242:TYR:HA	1:G:291:TYR:O	2.15	0.47
1:B:362:ALA:HB3	5:B:1176:HOH:O	2.14	0.47
1:C:60:ARG:NH2	1:D:547:ASP:OD2	2.48	0.47
1:D:98:GLY:C	1:D:100:PRO:HD2	2.39	0.47
1:H:711:SER:OG	1:H:712:TYR:N	2.47	0.47
1:E:646:ALA:HB2	1:E:655:ILE:HG13	1.97	0.46
1:G:690:LEU:O	1:G:723:ARG:NH2	2.42	0.46
1:F:296:PHE:CZ	1:F:298:THR:HG21	2.50	0.46
1:H:46:PRO:HD3	1:H:127:GLN:HG3	1.96	0.46
1:H:163:HIS:HA	1:H:488:ALA:HB2	1.96	0.46
1:D:96:GLY:HA3	1:D:153:GLU:O	2.15	0.46
1:F:187:THR:HB	1:F:189:PRO:HD2	1.96	0.46
1:G:745:ASP:O	1:G:749:VAL:HG22	2.14	0.46
1:H:549:ASN:HD21	2:H:901:PEP:C3	2.28	0.46
1:D:715:ASP:O	1:D:719:LEU:HD12	2.16	0.46
1:E:630:TRP:CE3	1:E:631:ALA:HB2	2.51	0.46
1:F:38:GLY:HA3	1:F:130:PHE:CE2	2.51	0.46
1:F:44:SER:OG	1:F:56:ASP:HA	2.15	0.46
1:B:454:TRP:CE2	1:B:456:ALA:HB3	2.50	0.46
1:C:170:ASP:OD2	1:C:431:ARG:NE	2.29	0.46
1:C:182:ASP:OD2	1:C:223:THR:OG1	2.22	0.46
1:E:9:PRO:HB2	1:E:10:TRP:CD1	2.50	0.46
1:G:35:LEU:O	1:G:39:GLN:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLY:HA3	1:C:130:PHE:CE2	2.51	0.46
1:C:535:MET:HE1	1:C:537:LEU:HB2	1.96	0.46
1:D:381:VAL:O	1:D:381:VAL:CG2	2.63	0.46
1:G:502:GLU:HG3	1:G:539:VAL:CG1	2.45	0.46
1:D:35:LEU:O	1:D:39:GLN:HG3	2.15	0.46
1:E:766:ASP:CB	1:E:769:LYS:HB3	2.46	0.46
1:G:803:TYR:O	1:G:804:SER:C	2.58	0.46
1:F:68:THR:N	1:F:69:PRO:HD2	2.31	0.46
1:G:99:GLY:N	1:G:100:PRO:CD	2.79	0.46
1:B:182:ASP:CG	1:B:223:THR:HG21	2.41	0.46
1:A:313:THR:O	1:A:319:SER:HB3	2.16	0.46
1:A:597:LYS:HE2	5:A:1201:HOH:O	2.16	0.46
1:B:707:PHE:O	1:B:731:VAL:HA	2.15	0.46
1:C:756:GLU:OE1	1:C:778:GLU:OE2	2.34	0.46
1:D:230:ASP:OD1	1:D:246:GLU:OE2	2.34	0.46
1:G:647:ALA:HB2	1:G:674:VAL:HB	1.98	0.46
1:G:704:PRO:CB	1:G:764:MET:HE2	2.46	0.45
1:G:737:GLU:HG3	1:H:568[B]:HIS:CE1	2.51	0.45
1:H:676:ASP:C	1:H:676:ASP:OD1	2.58	0.45
1:A:99:GLY:N	1:A:100:PRO:CD	2.79	0.45
1:A:555:ASP:OD2	1:B:565:LYS:NZ	2.48	0.45
1:A:30:ARG:HH21	1:A:345:LYS:HB2	1.81	0.45
1:B:569:ASN:HD22	1:B:571:HIS:CE1	2.34	0.45
1:C:28:TYR:C	1:C:28:TYR:CD1	2.94	0.45
1:D:720:ILE:O	1:D:720:ILE:CD1	2.63	0.45
1:E:28:TYR:CD1	1:E:28:TYR:C	2.94	0.45
1:F:43:ARG:O	1:F:127:GLN:NE2	2.49	0.45
1:A:351:ASP:C	1:A:351:ASP:OD1	2.59	0.45
1:C:75:ILE:HG21	1:C:105:GLN:HG3	1.98	0.45
1:A:709:TYR:CE2	1:A:715:ASP:HB2	2.51	0.45
1:C:85:HIS:HE2	1:C:268:GLU:CD	2.23	0.45
1:C:54:ARG:HD3	1:C:328:ARG:O	2.16	0.45
1:G:548:HIS:CD2	1:G:548:HIS:H	2.34	0.45
3:E:902:TPP:N1'	1:F:479:GLU:OE2	2.50	0.45
1:F:644:LEU:HD11	1:F:662:LEU:HD12	1.99	0.45
1:F:717:ARG:NH2	1:F:731:VAL:O	2.50	0.45
1:A:464:ASP:HA	1:A:467:MET:HE2	1.99	0.45
1:B:218:LYS:HE2	1:B:221:ASN:HB2	1.98	0.45
1:B:549:ASN:HD21	2:B:901:PEP:H31	1.82	0.45
1:D:700:THR:HG21	1:D:703:LYS:CG	2.47	0.45
1:E:62:VAL:CG1	1:E:134:SER:HB3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:PRO:C	1:E:428:ARG:HG2	2.41	0.45
1:B:351:ASP:OD1	1:B:351:ASP:C	2.60	0.45
1:D:509:ASP:O	1:D:512:LEU:HB2	2.17	0.45
1:D:539:VAL:HG12	1:D:539:VAL:O	2.17	0.45
1:H:567:PHE:HB3	1:H:568[B]:HIS:CD2	2.52	0.45
1:C:134:SER:CB	1:D:740:THR:HG21	2.46	0.44
1:C:720:ILE:HG22	1:C:723:ARG:HG3	1.98	0.44
1:D:761:ALA:O	1:D:764:MET:HB2	2.17	0.44
1:E:396:VAL:HG12	1:E:396:VAL:O	2.16	0.44
1:E:543:VAL:CG2	1:E:734:TYR:CE1	3.00	0.44
3:A:902:TPP:HN42	3:A:902:TPP:C2	2.30	0.44
1:C:532:ILE:HG13	1:C:533:ALA:O	2.18	0.44
1:D:286:VAL:HG13	1:E:459:ILE:O	2.17	0.44
1:D:387:LYS:HE2	1:D:387:LYS:HB3	1.85	0.44
1:H:110:GLY:O	1:H:114:GLU:HG3	2.17	0.44
1:H:669:PHE:CD1	1:H:669:PHE:C	2.95	0.44
1:A:94:GLY:N	1:A:95:PRO:CD	2.80	0.44
1:A:296:PHE:CZ	1:A:298:THR:HG21	2.52	0.44
1:C:722:ASP:O	1:C:722:ASP:CG	2.60	0.44
1:C:802:VAL:HG12	1:C:806:VAL:HG21	1.99	0.44
1:E:768:ASP:HA	1:E:771:ALA:HB2	1.98	0.44
1:B:657:ALA:HA	1:B:801:TRP:CZ2	2.52	0.44
1:C:46:PRO:HB2	1:C:126:LEU:HD23	2.00	0.44
1:D:577:PHE:HB3	1:D:648:GLY:HA2	1.99	0.44
1:G:414:THR:HG22	1:G:585:LEU:HD21	1.99	0.44
1:G:583:MET:HE3	1:G:675:ALA:HB2	1.98	0.44
1:H:605:LYS:NZ	2:H:901:PEP:O1P	2.38	0.44
1:D:47:LEU:HD11	1:D:354:GLY:HA2	1.99	0.44
1:D:170:ASP:OD1	1:D:428:ARG:NH1	2.50	0.44
1:D:530:LYS:HB3	1:D:531:PRO:CD	2.47	0.44
1:E:10:TRP:CD2	1:E:278:LYS:HG3	2.52	0.44
1:E:722:ASP:OD1	1:E:722:ASP:C	2.60	0.44
1:C:43:ARG:HB2	1:C:58:LYS:HA	1.98	0.44
1:D:168:ILE:HD12	1:D:206:GLY:O	2.18	0.44
1:E:431:ARG:HD2	1:E:489:TYR:CE1	2.52	0.44
1:F:44:SER:O	1:F:56:ASP:HB3	2.17	0.44
1:F:695:PHE:CD1	1:F:695:PHE:C	2.95	0.44
1:G:430:PHE:HA	1:G:495:HIS:O	2.17	0.44
1:G:676:ASP:OD1	1:G:676:ASP:C	2.61	0.44
1:A:744:TYR:HB3	1:A:794:ASP:OD1	2.17	0.44
1:C:111:THR:HG23	1:C:370:ARG:NH1	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:PHE:CE1	1:D:156:GLU:HG3	2.53	0.44
1:D:483:GLU:O	1:D:487:GLU:HG3	2.18	0.44
1:E:578:ALA:HB1	1:E:584:LEU:HB2	1.98	0.44
1:F:163:HIS:HA	1:F:488:ALA:HB2	2.00	0.44
1:D:405:GLY:HA2	1:D:609:ALA:HB1	1.98	0.44
1:D:694:GLU:O	1:D:698:ILE:HG13	2.18	0.44
1:E:459:ILE:HG12	1:F:227:ARG:CZ	2.47	0.44
1:F:502:GLU:HA	1:F:539:VAL:HG13	1.99	0.44
1:G:126:LEU:HD12	1:G:126:LEU:HA	1.80	0.44
1:C:440:SER:O	1:C:605:LYS:HD2	2.18	0.44
1:D:547:ASP:HB2	1:D:741:THR:O	2.17	0.44
1:G:96:GLY:HA3	1:G:153:GLU:O	2.17	0.44
1:E:502:GLU:HA	1:E:539:VAL:HG13	2.00	0.43
1:C:707:PHE:HB3	1:C:731:VAL:HG22	2.00	0.43
1:D:375:PRO:HB2	1:D:382:ILE:HD11	2.00	0.43
1:E:198:LYS:HG3	1:F:224:ILE:HG23	2.00	0.43
1:B:442:ARG:CA	1:B:444:GLN:HE22	2.23	0.43
1:C:770:TYR:O	1:C:773:LYS:N	2.51	0.43
1:D:459:ILE:O	1:E:286:VAL:HG13	2.18	0.43
1:F:81:PHE:CD1	1:F:85:HIS:CD2	3.07	0.43
1:F:188:GLY:N	1:F:189:PRO:CD	2.81	0.43
1:B:459:ILE:O	1:H:284:ASP:HA	2.18	0.43
1:C:144:ALA:HB1	1:C:145:PRO:HD2	2.01	0.43
1:C:552:SER:HB2	1:C:553:HIS:ND1	2.33	0.43
1:D:700:THR:HG21	1:D:703:LYS:HG3	1.99	0.43
1:B:151:ILE:HG23	1:B:377:ALA:HA	2.00	0.43
1:E:19:GLU:OE2	1:E:261:ARG:NH1	2.51	0.43
1:E:697:ASP:OD1	1:E:697:ASP:C	2.62	0.43
1:H:442:ARG:HA	1:H:444:GLN:HE22	1.83	0.43
1:H:726:HIS:CD2	1:H:727:ASP:OD1	2.71	0.43
1:B:152:HIS:ND1	1:B:163:HIS:ND1	2.57	0.43
1:C:479:GLU:OE2	3:D:902:TPP:N1'	2.52	0.43
1:E:68:THR:N	1:E:69:PRO:HD2	2.33	0.43
1:F:490:LEU:HD23	1:F:494:ARG:O	2.18	0.43
1:F:652:THR:O	1:F:656:MET:HG2	2.18	0.43
1:G:144:ALA:HB1	1:G:145:PRO:HD2	1.99	0.43
1:C:9:PRO:HA	1:C:87:GLN:OE1	2.19	0.43
1:C:163:HIS:HA	1:C:488:ALA:CB	2.49	0.43
1:C:404:HIS:ND1	1:C:630:TRP:CE2	2.87	0.43
1:C:490:LEU:HA	1:C:494:ARG:O	2.18	0.43
1:D:705:VAL:HG11	1:D:729:PHE:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:ALA:HB1	1:E:145:PRO:HD2	2.00	0.43
1:E:648:GLY:O	1:E:651:PRO:HD2	2.18	0.43
1:F:99:GLY:N	1:F:100:PRO:HD2	2.34	0.43
1:B:151:ILE:CG2	1:B:377:ALA:HA	2.48	0.43
1:C:81:PHE:CD1	1:C:85:HIS:CD2	3.07	0.43
1:C:230:ASP:OD1	1:C:246:GLU:OE2	2.37	0.43
1:C:366:LYS:HE2	1:C:366:LYS:HA	2.01	0.43
1:C:589:GLU:O	1:C:593:LYS:HG3	2.18	0.43
1:D:34:TYR:CE2	1:D:346:PRO:HG3	2.54	0.43
1:F:396:VAL:HB	1:F:582:ASN:HD21	1.83	0.43
1:G:740:THR:HG22	5:G:1004:HOH:O	2.17	0.43
1:G:398:GLU:HG2	1:G:406:TRP:CZ2	2.54	0.43
1:G:773:LYS:CE	1:G:776:GLU:OE1	2.67	0.43
1:B:28:TYR:CD1	1:B:28:TYR:C	2.96	0.43
1:B:286:VAL:HG13	1:H:459:ILE:O	2.19	0.43
1:D:777:LEU:HD12	1:D:777:LEU:HA	1.91	0.43
1:G:502:GLU:OE2	1:G:710:HIS:NE2	2.45	0.43
1:G:547:ASP:O	1:G:740:THR:HA	2.19	0.43
1:A:313:THR:HG21	1:A:323:PRO:HB2	2.01	0.42
1:D:68:THR:HG22	1:D:72:ASN:ND2	2.33	0.42
1:D:188:GLY:O	1:D:189:PRO:C	2.60	0.42
1:D:486:LEU:O	1:D:487:GLU:C	2.62	0.42
1:D:611:TRP:C	1:D:612:LEU:HD23	2.43	0.42
1:D:722:ASP:OD1	1:D:722:ASP:C	2.62	0.42
1:E:218:LYS:HE2	1:E:221:ASN:HB2	2.00	0.42
1:E:369:LEU:HD12	1:E:369:LEU:HA	1.87	0.42
1:E:753:ASP:OD1	1:E:755:TYR:HB2	2.18	0.42
1:A:300:LYS:NZ	3:A:902:TPP:O1B	2.52	0.42
1:C:740:THR:HG21	1:D:134:SER:HA	1.99	0.42
1:E:740:THR:HG23	1:F:134:SER:HA	1.97	0.42
1:F:182:ASP:HB3	1:F:214:LEU:HD12	2.01	0.42
1:F:339:ASN:HB3	5:F:1086:HOH:O	2.18	0.42
1:F:576:TYR:HB3	1:F:587:ILE:HD13	2.01	0.42
1:G:479:GLU:OE2	3:H:902:TPP:N1'	2.52	0.42
1:H:547:ASP:HB2	1:H:741:THR:O	2.19	0.42
1:C:281:ALA:HA	1:C:284:ASP:O	2.19	0.42
1:D:652:THR:O	1:D:653:GLN:C	2.62	0.42
1:G:706:LEU:HD21	1:G:757:LEU:HD22	2.02	0.42
1:G:722:ASP:OD1	1:G:722:ASP:C	2.62	0.42
1:H:646:ALA:HA	1:H:708:ALA:O	2.19	0.42
1:C:62:VAL:CG1	1:C:134:SER:HB3	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:PHE:CZ	1:C:497:ILE:HG22	2.53	0.42
1:A:430:PHE:HA	1:A:495:HIS:O	2.20	0.42
1:E:293:MET:SD	1:E:293:MET:C	3.02	0.42
1:E:453:GLN:HG3	1:E:469:VAL:O	2.19	0.42
1:F:312:LYS:NZ	1:F:314:GLU:O	2.48	0.42
1:G:9:PRO:HB2	1:G:10:TRP:CD1	2.55	0.42
1:G:415:LEU:HD22	1:G:584:LEU:HD11	2.02	0.42
1:A:435:PRO:HA	1:A:476:GLN:O	2.19	0.42
1:B:9:PRO:HB2	1:B:10:TRP:CD1	2.55	0.42
1:C:643:VAL:HB	1:C:705:VAL:HG13	2.01	0.42
1:D:120:THR:O	1:D:125:GLY:HA3	2.20	0.42
1:F:311:LYS:O	1:F:313:THR:OG1	2.36	0.42
1:F:396:VAL:HB	1:F:582:ASN:ND2	2.34	0.42
1:F:702:ASP:OD1	1:F:702:ASP:N	2.53	0.42
1:H:65:TRP:O	1:H:69:PRO:HD2	2.19	0.42
1:A:65:TRP:HE1	1:A:304:CYS:HB3	1.85	0.42
1:A:459:ILE:O	1:F:284:ASP:HA	2.19	0.42
1:E:755:TYR:O	1:E:758:THR:HB	2.19	0.42
1:H:534:SER:HB3	1:H:597:LYS:HB2	2.00	0.42
1:H:681:GLN:O	1:H:723:ARG:NH2	2.53	0.42
1:B:577:PHE:CE1	1:B:602:ILE:HD13	2.55	0.42
1:C:235:GLU:CD	1:D:238:HIS:HD1	2.20	0.42
1:C:497:ILE:HG13	1:C:536:ASN:O	2.20	0.42
1:C:773:LYS:HA	1:C:773:LYS:HD3	1.85	0.42
1:D:99:GLY:N	1:D:100:PRO:CD	2.83	0.42
1:D:197:ASN:OD1	1:D:198:LYS:HE3	2.20	0.42
1:D:753:ASP:OD2	1:D:781:ARG:NE	2.52	0.42
1:E:440:SER:OG	2:E:901:PEP:O2P	2.38	0.42
1:F:62:VAL:HG12	1:F:134:SER:HB3	2.02	0.42
1:H:351:ASP:OD1	1:H:351:ASP:C	2.62	0.42
1:B:543:VAL:HG23	1:B:554:GLN:HB3	2.01	0.42
1:C:118:LYS:HG2	5:C:1041:HOH:O	2.19	0.42
1:C:677:LEU:O	1:C:677:LEU:HG	2.20	0.42
1:D:637:ASN:O	1:D:703:LYS:HE3	2.20	0.42
1:E:96:GLY:HA3	1:E:153:GLU:O	2.20	0.42
1:G:28:TYR:CD1	1:G:28:TYR:C	2.98	0.42
1:H:28:TYR:CD1	1:H:28:TYR:C	2.97	0.42
1:H:190:LEU:C	1:H:190:LEU:HD13	2.45	0.42
1:H:708:ALA:HB1	1:H:752:ILE:HD11	2.01	0.42
1:B:775:ASP:O	1:B:779:LYS:HG3	2.20	0.42
1:D:786:GLN:NE2	1:D:790:ASP:OD2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG21	1:A:610:THR:HG22	2.02	0.41
1:A:547:ASP:O	1:A:740:THR:HA	2.20	0.41
1:D:509:ASP:HA	1:D:512:LEU:HD12	2.01	0.41
1:E:804:SER:O	1:E:806:VAL:N	2.53	0.41
1:F:293:MET:SD	1:F:293:MET:C	3.03	0.41
1:H:547:ASP:O	1:H:740:THR:HA	2.20	0.41
1:C:213:HIS:CE1	1:C:215:ASN:HD22	2.38	0.41
1:D:630:TRP:CE3	1:D:631:ALA:HB2	2.55	0.41
3:G:902:TPP:C2	3:G:902:TPP:HN42	2.33	0.41
1:C:131:ARG:O	1:C:135:TYR:HB2	2.20	0.41
1:D:435:PRO:HA	1:D:476:GLN:O	2.20	0.41
1:D:725:ASN:OD1	1:D:728:ASN:ND2	2.46	0.41
1:H:535:MET:HE1	1:H:537:LEU:HB2	2.03	0.41
1:H:637:ASN:ND2	1:H:700:THR:HG22	2.34	0.41
1:H:645:ALA:HA	1:H:672:VAL:O	2.20	0.41
1:A:313:THR:CG2	1:A:323:PRO:HB3	2.50	0.41
1:B:78:ILE:O	1:B:82:ILE:HG13	2.20	0.41
1:B:650:VAL:N	1:B:651:PRO:CD	2.84	0.41
1:C:433:PHE:HB2	1:C:498:TRP:HB3	2.02	0.41
1:D:216:GLY:HA2	1:D:226:SER:CB	2.50	0.41
1:D:416:GLY:HA3	5:D:1008:HOH:O	2.20	0.41
1:D:202:PRO:HB2	1:D:281:ALA:CB	2.49	0.41
1:D:545:ARG:NH1	1:D:606:GLN:HB2	2.35	0.41
1:D:652:THR:O	1:D:655:ILE:N	2.45	0.41
1:D:720:ILE:O	1:D:720:ILE:CG1	2.68	0.41
1:F:540:SER:O	1:F:541:SER:C	2.63	0.41
1:G:45:ASN:N	1:G:46:PRO:CD	2.83	0.41
1:G:737:GLU:OE2	1:H:568[A]:HIS:ND1	2.54	0.41
1:B:650:VAL:HB	1:B:651:PRO:HD3	2.02	0.41
1:C:650:VAL:O	1:C:651:PRO:C	2.64	0.41
1:G:704:PRO:HB2	1:G:764:MET:HE2	2.03	0.41
1:B:644:LEU:HD11	1:B:662:LEU:HD12	2.03	0.41
1:C:655:ILE:CD1	1:C:708:ALA:HB3	2.51	0.41
1:D:643:VAL:HG21	1:D:700:THR:HG23	2.03	0.41
1:E:572:VAL:O	1:E:597:LYS:HA	2.21	0.41
1:G:198:LYS:HG3	1:H:224:ILE:HG23	2.03	0.41
1:G:219:ILE:O	1:G:317:TRP:HB2	2.20	0.41
1:A:134:SER:HB3	1:B:740:THR:HG21	2.03	0.41
1:D:237:PHE:CD1	1:D:293:MET:HE3	2.56	0.41
1:E:787:PHE:CE2	1:E:795:HIS:HA	2.56	0.41
1:F:742:THR:O	1:F:743:PRO:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:O	1:B:176:VAL:HA	2.21	0.41
1:C:419:THR:HA	1:C:422:ILE:HD12	2.02	0.41
1:C:504:PHE:CD1	1:D:156:GLU:HG3	2.56	0.41
1:C:708:ALA:HB2	1:C:757:LEU:HD11	2.03	0.41
1:C:742:THR:HG23	1:D:136:PRO:HG3	2.03	0.41
1:C:780:PHE:O	1:C:781:ARG:C	2.64	0.41
1:D:62:VAL:CG1	1:D:134:SER:HB3	2.51	0.41
1:D:201:ASN:HA	1:D:202:PRO:HD3	1.93	0.41
1:D:242:TYR:HA	1:D:291:TYR:O	2.21	0.41
1:D:406:TRP:CD2	1:D:406:TRP:C	2.98	0.41
1:D:433:PHE:HB2	1:D:498:TRP:HB3	2.03	0.41
1:D:644:LEU:O	1:D:671:VAL:HA	2.20	0.41
1:E:589:GLU:O	1:E:593:LYS:HG3	2.21	0.41
1:F:237:PHE:CD1	1:F:293:MET:HE3	2.56	0.41
1:F:720:ILE:O	1:F:722:ASP:N	2.54	0.41
1:H:13:LEU:HA	1:H:13:LEU:HD12	1.87	0.41
1:H:489:TYR:CE2	1:H:494:ARG:HB3	2.55	0.41
1:A:744:TYR:CE2	1:A:748:ARG:HD3	2.56	0.41
1:C:44:SER:HA	1:C:127:GLN:OE1	2.21	0.41
1:C:313:THR:O	1:C:319:SER:HB3	2.21	0.41
1:D:415:LEU:HB2	1:D:584:LEU:HD21	2.03	0.41
1:E:406:TRP:CG	1:E:407:GLY:N	2.89	0.41
1:F:384:ASN:HD22	1:F:384:ASN:HA	1.70	0.41
1:F:490:LEU:HA	1:F:494:ARG:O	2.20	0.41
1:D:632:SER:HB3	1:D:670:LYS:HA	2.03	0.40
1:E:313:THR:CG2	1:E:323:PRO:HB3	2.51	0.40
1:E:392:GLU:OE2	1:E:618:ARG:NH2	2.54	0.40
1:E:621:LEU:O	1:E:624:GLY:N	2.54	0.40
1:H:81:PHE:CD1	1:H:85:HIS:CD2	3.10	0.40
1:A:286:VAL:HA	1:A:469:VAL:HG11	2.03	0.40
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.84	0.40
1:A:499:SER:HA	1:A:538:LEU:O	2.22	0.40
1:D:67:THR:HG22	1:D:71:LEU:CD1	2.51	0.40
1:D:90:VAL:O	1:D:176:VAL:HA	2.21	0.40
1:E:151:ILE:CG2	1:E:377:ALA:HA	2.51	0.40
1:E:498:TRP:CE2	1:E:537:LEU:HD13	2.57	0.40
1:E:548:HIS:CD2	1:E:548:HIS:H	2.39	0.40
1:F:301:GLY:O	1:F:302:TRP:C	2.63	0.40
1:F:444:GLN:HE21	1:F:444:GLN:N	2.01	0.40
1:H:185:ALA:HA	1:H:190:LEU:HD12	2.02	0.40
1:B:39:GLN:HB3	1:B:133:PHE:CG	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ILE:O	1:C:317:TRP:HB2	2.21	0.40
1:C:681:GLN:HA	1:C:719:LEU:CD2	2.52	0.40
1:D:368:GLU:O	1:D:374:ASN:HA	2.21	0.40
1:D:415:LEU:HD22	1:D:584:LEU:HD11	2.03	0.40
1:H:274:ILE:HG13	1:H:292:PRO:HG2	2.04	0.40
1:C:404:HIS:HE1	1:C:616:GLU:OE2	2.04	0.40
1:C:515:HIS:O	1:C:519:LEU:HG	2.22	0.40
1:C:709:TYR:CE2	1:C:715:ASP:HB2	2.57	0.40
1:E:302:TRP:C	1:E:303:THR:HG23	2.46	0.40
1:E:505:VAL:O	1:E:508:ILE:HG13	2.22	0.40
1:E:734:TYR:CE2	1:E:736:GLU:HA	2.57	0.40
1:E:774:ILE:HG22	1:E:775:ASP:N	2.36	0.40
1:F:547:ASP:O	1:F:740:THR:HA	2.22	0.40
1:A:62:VAL:HG11	1:A:134:SER:HB3	2.03	0.40
1:B:391:LEU:HD12	1:B:391:LEU:HA	1.95	0.40
1:C:664:GLU:O	1:C:664:GLU:HG2	2.21	0.40
1:D:759:ALA:C	1:D:761:ALA:H	2.30	0.40
1:E:556:PRO:HD2	1:E:712:TYR:CE1	2.56	0.40
2:F:901:PEP:H32	2:F:901:PEP:O1P	2.22	0.40
1:G:437:GLU:OE2	3:H:902:TPP:H6'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	807/831 (97%)	758 (94%)	45 (6%)	4 (0%)	24	43
1	B	810/831 (98%)	766 (95%)	42 (5%)	2 (0%)	43	63
1	C	804/831 (97%)	698 (87%)	98 (12%)	8 (1%)	12	24
1	D	805/831 (97%)	715 (89%)	81 (10%)	9 (1%)	11	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	807/831 (97%)	725 (90%)	78 (10%)	4 (0%)	24	43
1	F	807/831 (97%)	745 (92%)	55 (7%)	7 (1%)	14	27
1	G	806/831 (97%)	737 (91%)	64 (8%)	5 (1%)	21	38
1	H	807/831 (97%)	748 (93%)	57 (7%)	2 (0%)	43	63
All	All	6453/6648 (97%)	5892 (91%)	520 (8%)	41 (1%)	21	38

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	66	GLY
1	D	652	THR
1	F	630	TRP
1	F	721	TYR
1	G	721	TYR
1	C	66	GLY
1	C	622	GLU
1	D	88	ASN
1	D	653	GLN
1	D	717	ARG
1	D	739	SER
1	D	748	ARG
1	E	387	LYS
1	F	358	ASP
1	H	771	ALA
1	A	302	TRP
1	A	702	ASP
1	A	766	ASP
1	B	88	ASN
1	C	390	ASN
1	E	725	ASN
1	E	771	ALA
1	F	303	THR
1	G	398	GLU
1	G	804	SER
1	H	564	ASN
1	A	442	ARG
1	C	54	ARG
1	C	774	ILE
1	F	442	ARG
1	F	568	HIS
1	G	807	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	302	TRP
1	C	524	ARG
1	C	630	TRP
1	D	162	SER
1	D	501	TYR
1	F	524	ARG
1	C	308	ILE
1	E	774	ILE
1	G	666	GLY

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	678/693 (98%)	656 (97%)	22 (3%)	34	62
1	B	680/693 (98%)	661 (97%)	19 (3%)	38	66
1	C	675/693 (97%)	617 (91%)	58 (9%)	10	21
1	D	676/693 (98%)	626 (93%)	50 (7%)	13	27
1	E	678/693 (98%)	645 (95%)	33 (5%)	22	45
1	F	678/693 (98%)	646 (95%)	32 (5%)	23	47
1	G	677/693 (98%)	645 (95%)	32 (5%)	23	47
1	H	678/693 (98%)	652 (96%)	26 (4%)	29	56
All	All	5420/5544 (98%)	5148 (95%)	272 (5%)	22	44

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	19	GLU
1	A	20	GLU
1	A	43	ARG
1	A	60	ARG
1	A	118	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	GLN
1	A	147	THR
1	A	198	LYS
1	A	286	VAL
1	A	366	LYS
1	A	369	LEU
1	A	444	GLN
1	A	477	LEU
1	A	532	ILE
1	A	534	SER
1	A	597	LYS
1	A	638	ASP
1	A	684	LYS
1	A	773	LYS
1	A	777	LEU
1	A	799	THR
1	B	61	LEU
1	B	147	THR
1	B	198	LYS
1	B	231	GLU
1	B	255	ASP
1	B	273	GLU
1	B	286	VAL
1	B	313	THR
1	B	369	LEU
1	B	410	GLU
1	B	444	GLN
1	B	477	LEU
1	B	526	ILE
1	B	668	LYS
1	B	684	LYS
1	B	693	GLU
1	B	751	ARG
1	B	777	LEU
1	B	808	THR
1	C	11	LYS
1	C	30	ARG
1	C	31	VAL
1	C	43	ARG
1	C	49	LYS
1	C	62	VAL
1	C	92	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	121	LYS
1	C	126	LEU
1	C	147	THR
1	C	168	ILE
1	C	265	GLU
1	C	274	ILE
1	C	286	VAL
1	C	306	LYS
1	C	330	THR
1	C	331	GLU
1	C	335	GLU
1	C	342	GLU
1	C	353	ASN
1	C	369	LEU
1	C	414	THR
1	C	444	GLN
1	C	470	SER
1	C	497	ILE
1	C	530	LYS
1	C	534	SER
1	C	547	ASP
1	C	548	HIS
1	C	565	LYS
1	C	566	CYS
1	C	569	ASN
1	C	579	THR
1	C	590	LYS
1	C	595	THR
1	C	602	ILE
1	C	612	LEU
1	C	638	ASP
1	C	642	VAL
1	C	643	VAL
1	C	644	LEU
1	C	653	GLN
1	C	654	GLU
1	C	655	ILE
1	C	687	ASP
1	C	719	LEU
1	C	722	ASP
1	C	727	ASP
1	C	754	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	757	LEU
1	C	764	MET
1	C	772	ASP
1	C	773	LYS
1	C	775	ASP
1	C	777	LEU
1	C	790	ASP
1	C	800	ASP
1	C	807	ASN
1	D	2	THR
1	D	43	ARG
1	D	50	GLU
1	D	60	ARG
1	D	126	LEU
1	D	147	THR
1	D	169	MET
1	D	286	VAL
1	D	313	THR
1	D	322	VAL
1	D	331	GLU
1	D	342	GLU
1	D	369	LEU
1	D	381	VAL
1	D	387	LYS
1	D	398	GLU
1	D	414	THR
1	D	426	ASN
1	D	429	ASP
1	D	442	ARG
1	D	444	GLN
1	D	477	LEU
1	D	495	HIS
1	D	499	SER
1	D	508	ILE
1	D	510	SER
1	D	547	ASP
1	D	548	HIS
1	D	560	SER
1	D	618	ARG
1	D	632	SER
1	D	635	LYS
1	D	644	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	655	ILE
1	D	659	SER
1	D	668	LYS
1	D	671	VAL
1	D	674	VAL
1	D	687	ASP
1	D	722	ASP
1	D	727	ASP
1	D	740	THR
1	D	752	ILE
1	D	758	THR
1	D	772	ASP
1	D	774	ILE
1	D	775	ASP
1	D	777	LEU
1	D	786	GLN
1	D	793	TYR
1	E	43	ARG
1	E	54	ARG
1	E	60	ARG
1	E	147	THR
1	E	190	LEU
1	E	198	LYS
1	E	255	ASP
1	E	331	GLU
1	E	369	LEU
1	E	371	ILE
1	E	382	ILE
1	E	383	ARG
1	E	387	LYS
1	E	402	TYR
1	E	414	THR
1	E	420	ARG
1	E	444	GLN
1	E	450	THR
1	E	477	LEU
1	E	508	ILE
1	E	547	ASP
1	E	548	HIS
1	E	618	ARG
1	E	665	LEU
1	E	684	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	697	ASP
1	E	719	LEU
1	E	731	VAL
1	E	746	MET
1	E	752	ILE
1	E	777	LEU
1	E	779	LYS
1	E	793	TYR
1	F	2	THR
1	F	11	LYS
1	F	23	GLU
1	F	54	ARG
1	F	67	THR
1	F	119	ILE
1	F	126	LEU
1	F	141	SER
1	F	147	THR
1	F	331	GLU
1	F	335	GLU
1	F	341	LEU
1	F	369	LEU
1	F	383	ARG
1	F	444	GLN
1	F	477	LEU
1	F	548	HIS
1	F	597	LYS
1	F	622	GLU
1	F	635	LYS
1	F	655	ILE
1	F	659	SER
1	F	670	LYS
1	F	716	VAL
1	F	719	LEU
1	F	735	GLU
1	F	749	VAL
1	F	773	LYS
1	F	777	LEU
1	F	779	LYS
1	F	808	THR
1	F	810	LYS
1	G	11	LYS
1	G	44	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	55	GLU
1	G	60	ARG
1	G	120	THR
1	G	147	THR
1	G	162	SER
1	G	192	THR
1	G	198	LYS
1	G	231	GLU
1	G	273	GLU
1	G	357	LYS
1	G	368	GLU
1	G	369	LEU
1	G	387	LYS
1	G	402	TYR
1	G	408	GLN
1	G	428	ARG
1	G	429	ASP
1	G	444	GLN
1	G	477	LEU
1	G	556	PRO
1	G	590	LYS
1	G	605	LYS
1	G	659	SER
1	G	693	GLU
1	G	706	LEU
1	G	740	THR
1	G	775	ASP
1	G	777	LEU
1	G	779	LYS
1	G	804	SER
1	H	35	LEU
1	H	47	LEU
1	H	55	GLU
1	H	119	ILE
1	H	147	THR
1	H	198	LYS
1	H	313	THR
1	H	324	LEU
1	H	369	LEU
1	H	381	VAL
1	H	408	GLN
1	H	444	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	465	GLU
1	H	526	ILE
1	H	534	SER
1	H	548	HIS
1	H	659	SER
1	H	661	LYS
1	H	693	GLU
1	H	719	LEU
1	H	751	ARG
1	H	752	ILE
1	H	772	ASP
1	H	773	LYS
1	H	777	LEU
1	H	799	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	79	ASN
1	A	105	GLN
1	A	127	GLN
1	A	444	GLN
1	A	549	ASN
1	A	571	HIS
1	A	673	ASN
1	B	14	ASN
1	B	39	GLN
1	B	59	HIS
1	B	256	HIS
1	B	339	ASN
1	B	444	GLN
1	B	549	ASN
1	B	569	ASN
1	B	571	HIS
1	B	807	ASN
1	C	88	ASN
1	C	171	ASN
1	C	285	ASN
1	C	374	ASN
1	C	376	ASN
1	C	425	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	444	GLN
1	C	466	HIS
1	C	513	ASN
1	C	549	ASN
1	C	554	GLN
1	C	571	HIS
1	D	14	ASN
1	D	59	HIS
1	D	142	HIS
1	D	384	ASN
1	D	444	GLN
1	D	513	ASN
1	D	546	GLN
1	D	548	HIS
1	D	549	ASN
1	D	571	HIS
1	D	730	ASN
1	D	732	HIS
1	D	786	GLN
1	D	791	ASN
1	E	64	HIS
1	E	384	ASN
1	E	404	HIS
1	E	444	GLN
1	E	480	HIS
1	E	548	HIS
1	E	549	ASN
1	E	673	ASN
1	E	732	HIS
1	E	750	ASN
1	E	786	GLN
1	F	39	GLN
1	F	256	HIS
1	F	384	ASN
1	F	444	GLN
1	F	481	GLN
1	F	513	ASN
1	F	549	ASN
1	F	596	ASN
1	F	673	ASN
1	F	750	ASN
1	F	807	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	14	ASN
1	G	39	GLN
1	G	79	ASN
1	G	213	HIS
1	G	384	ASN
1	G	404	HIS
1	G	408	GLN
1	G	444	GLN
1	G	472	GLN
1	G	548	HIS
1	G	549	ASN
1	G	637	ASN
1	H	142	HIS
1	H	256	HIS
1	H	408	GLN
1	H	444	GLN
1	H	481	GLN
1	H	495	HIS
1	H	549	ASN
1	H	564	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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEP	F	901	-	9,9,9	3.10	2 (22%)	11,13,13	2.25	6 (54%)
2	PEP	A	901	-	9,9,9	3.85	3 (33%)	11,13,13	1.61	2 (18%)
3	TPP	E	902	4	26,27,27	0.57	0	38,40,40	0.98	4 (10%)
2	PEP	D	901	-	9,9,9	3.19	3 (33%)	11,13,13	2.24	4 (36%)
2	PEP	H	901	-	9,9,9	2.68	3 (33%)	11,13,13	1.80	5 (45%)
2	PEP	E	901	-	9,9,9	2.23	2 (22%)	11,13,13	3.00	6 (54%)
3	TPP	G	902	4	26,27,27	0.60	0	38,40,40	0.99	3 (7%)
3	TPP	F	902	4	26,27,27	0.59	0	38,40,40	0.99	3 (7%)
3	TPP	H	902	4	26,27,27	0.52	0	38,40,40	0.96	2 (5%)
3	TPP	C	902	4	26,27,27	0.66	0	38,40,40	1.01	3 (7%)
2	PEP	C	901	-	9,9,9	3.15	3 (33%)	11,13,13	2.13	4 (36%)
2	PEP	G	901	-	9,9,9	3.00	3 (33%)	11,13,13	2.10	5 (45%)
2	PEP	B	901	-	9,9,9	2.53	2 (22%)	11,13,13	2.40	3 (27%)
3	TPP	B	902	4	26,27,27	0.80	1 (3%)	38,40,40	0.82	1 (2%)
3	TPP	D	902	4	26,27,27	0.65	0	38,40,40	1.02	3 (7%)
3	TPP	A	902	4	26,27,27	0.75	0	38,40,40	0.83	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEP	F	901	-	-	0/9/9/9	-
2	PEP	A	901	-	-	0/9/9/9	-
3	TPP	E	902	4	-	6/17/17/17	0/2/2/2
2	PEP	D	901	-	-	0/9/9/9	-
2	PEP	H	901	-	-	4/9/9/9	-
2	PEP	E	901	-	-	3/9/9/9	-
3	TPP	G	902	4	-	5/17/17/17	0/2/2/2
3	TPP	F	902	4	-	5/17/17/17	0/2/2/2
3	TPP	H	902	4	-	6/17/17/17	0/2/2/2
3	TPP	C	902	4	-	2/17/17/17	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEP	C	901	-	-	0/9/9/9	-
2	PEP	G	901	-	-	0/9/9/9	-
2	PEP	B	901	-	-	0/9/9/9	-
3	TPP	B	902	4	-	4/17/17/17	0/2/2/2
3	TPP	D	902	4	-	3/17/17/17	0/2/2/2
3	TPP	A	902	4	-	2/17/17/17	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	PEP	C2-C1	-10.75	1.38	1.49
2	D	901	PEP	C2-C1	-8.39	1.41	1.49
2	C	901	PEP	C2-C1	-8.32	1.41	1.49
2	F	901	PEP	C2-C1	-7.98	1.41	1.49
2	G	901	PEP	C2-C1	-7.61	1.41	1.49
2	H	901	PEP	C2-C1	-6.43	1.43	1.49
2	B	901	PEP	C2-C1	-6.20	1.43	1.49
2	E	901	PEP	C2-C1	-5.18	1.44	1.49
2	H	901	PEP	C3-C2	3.73	1.41	1.31
2	C	901	PEP	C3-C2	3.72	1.41	1.31
2	G	901	PEP	C3-C2	3.71	1.41	1.31
2	F	901	PEP	C3-C2	3.60	1.41	1.31
2	B	901	PEP	C3-C2	3.40	1.40	1.31
2	D	901	PEP	C3-C2	3.38	1.40	1.31
2	E	901	PEP	C3-C2	3.13	1.40	1.31
2	A	901	PEP	C3-C2	3.03	1.39	1.31
3	B	902	TPP	PA-O3A	2.47	1.62	1.59
2	D	901	PEP	O2'-C1	-2.33	1.24	1.30
2	C	901	PEP	O2'-C1	-2.26	1.24	1.30
2	A	901	PEP	O2'-C1	-2.23	1.24	1.30
2	G	901	PEP	O2'-C1	-2.14	1.24	1.30
2	H	901	PEP	O1-C1	2.09	1.27	1.22

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	PEP	O2-C2-C3	-7.45	110.62	124.85
2	D	901	PEP	O2-C2-C3	-4.66	115.94	124.85
2	B	901	PEP	O1-C1-C2	-4.64	114.80	121.79
2	C	901	PEP	O1-C1-C2	-4.56	114.91	121.79
2	B	901	PEP	O2-C2-C3	-4.19	116.85	124.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	PEP	O2-C2-C3	-4.11	116.99	124.85
2	B	901	PEP	O2'-C1-C2	3.95	120.66	113.91
2	C	901	PEP	O2'-C1-C2	3.76	120.32	113.91
2	G	901	PEP	O2-C2-C3	-3.73	117.72	124.85
2	E	901	PEP	C3-C2-C1	3.57	129.34	122.73
2	H	901	PEP	O2-C2-C3	-3.41	118.34	124.85
2	D	901	PEP	O1-C1-C2	-3.26	116.87	121.79
2	A	901	PEP	O3P-P-O2	3.08	114.28	105.32
2	G	901	PEP	O2P-P-O2	-2.99	96.63	105.32
2	F	901	PEP	O1-C1-C2	-2.92	117.39	121.79
2	F	901	PEP	O2P-P-O2	2.91	113.80	105.32
2	E	901	PEP	O2P-P-O2	-2.88	96.93	105.32
2	F	901	PEP	O2-P-O1P	-2.85	100.36	109.47
2	H	901	PEP	O2-P-O1P	-2.84	100.39	109.47
2	E	901	PEP	O3P-P-O2	2.81	113.51	105.32
2	G	901	PEP	O1-C1-C2	-2.81	117.55	121.79
3	C	902	TPP	O3B-PB-O2B	2.79	118.25	107.80
2	G	901	PEP	O2'-C1-C2	2.78	118.65	113.91
2	D	901	PEP	O3P-P-O2	2.69	113.16	105.32
2	D	901	PEP	O2'-C1-C2	2.64	118.41	113.91
2	E	901	PEP	O2'-C1-C2	2.58	118.31	113.91
2	C	901	PEP	O3P-P-O2	2.57	112.81	105.32
3	A	902	TPP	C2-S1-C5	-2.52	89.55	91.22
3	G	902	TPP	O2B-PB-O3A	2.52	113.08	104.64
2	A	901	PEP	O1-C1-C2	-2.51	118.00	121.79
2	G	901	PEP	O3P-P-O2	2.50	112.59	105.32
3	C	902	TPP	O2A-PA-O1A	2.49	124.03	112.44
2	H	901	PEP	O2P-P-O2	2.47	112.51	105.32
3	H	902	TPP	C2-S1-C5	-2.44	89.60	91.22
3	D	902	TPP	O2A-PA-O1A	2.40	123.63	112.44
2	F	901	PEP	C3-C2-C1	2.35	127.08	122.73
3	B	902	TPP	O3B-PB-O2B	2.35	116.61	107.80
3	E	902	TPP	O2A-PA-O7	-2.34	96.94	107.57
3	E	902	TPP	O2A-PA-O1A	2.34	123.33	112.44
3	E	902	TPP	O2A-PA-O3A	2.33	113.58	107.27
2	E	901	PEP	O1-C1-C2	-2.29	118.33	121.79
3	F	902	TPP	O7-PA-O1A	-2.27	99.94	108.94
3	G	902	TPP	C2-S1-C5	-2.22	89.74	91.22
3	F	902	TPP	O2A-PA-O3A	-2.19	101.36	107.27
3	F	902	TPP	O2A-PA-O1A	2.17	122.54	112.44
3	D	902	TPP	O2A-PA-O7	-2.16	97.77	107.57
3	E	902	TPP	O3A-PA-O1A	-2.13	104.30	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	901	PEP	O3P-P-O2	2.13	111.51	105.32
3	C	902	TPP	O2B-PB-O3A	-2.12	97.53	104.64
3	D	902	TPP	O3A-PA-O1A	-2.11	104.35	110.70
3	G	902	TPP	O2A-PA-O1A	2.09	122.19	112.44
3	A	902	TPP	O3B-PB-O2B	2.08	115.60	107.80
2	H	901	PEP	C3-C2-C1	2.06	126.54	122.73
3	H	902	TPP	O3A-PA-O1A	-2.06	104.52	110.70
2	F	901	PEP	O2'-C1-C2	2.04	117.39	113.91
2	C	901	PEP	O2-P-O1P	-2.04	102.95	109.47

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	901	PEP	O1-C1-C2-O2
2	E	901	PEP	O2'-C1-C2-O2
2	H	901	PEP	O2'-C1-C2-O2
3	C	902	TPP	C7-O7-PA-O2A
3	D	902	TPP	PA-O3A-PB-O3B
3	E	902	TPP	PA-O3A-PB-O2B
3	F	902	TPP	PA-O3A-PB-O3B
3	G	902	TPP	PA-O3A-PB-O2B
3	G	902	TPP	PA-O3A-PB-O3B
3	H	902	TPP	C4'-C5'-C7'-N3
3	G	902	TPP	PB-O3A-PA-O1A
3	E	902	TPP	C4'-C5'-C7'-N3
3	H	902	TPP	C6'-C5'-C7'-N3
3	B	902	TPP	PA-O3A-PB-O1B
3	H	902	TPP	PA-O3A-PB-O1B
3	D	902	TPP	PA-O3A-PB-O2B
3	C	902	TPP	C5-C6-C7-O7
3	E	902	TPP	PB-O3A-PA-O1A
3	G	902	TPP	C4'-C5'-C7'-N3
3	E	902	TPP	PB-O3A-PA-O2A
3	F	902	TPP	PB-O3A-PA-O1A
3	G	902	TPP	PB-O3A-PA-O2A
2	H	901	PEP	O1-C1-C2-C3
3	F	902	TPP	C4'-C5'-C7'-N3
3	A	902	TPP	PA-O3A-PB-O1B
3	D	902	TPP	PA-O3A-PB-O1B
3	E	902	TPP	PA-O3A-PB-O1B
3	A	902	TPP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	902	TPP	PA-O3A-PB-O2B
3	B	902	TPP	PA-O3A-PB-O3B
3	E	902	TPP	PA-O3A-PB-O3B
3	H	902	TPP	PA-O3A-PB-O2B
3	H	902	TPP	PA-O3A-PB-O3B
3	B	902	TPP	C5-C6-C7-O7
3	F	902	TPP	PA-O3A-PB-O1B
2	H	901	PEP	O1-C1-C2-O2
2	E	901	PEP	O2'-C1-C2-C3
2	H	901	PEP	O2'-C1-C2-C3
3	H	902	TPP	C5'-C7'-N3-C2
3	F	902	TPP	PB-O3A-PA-O2A

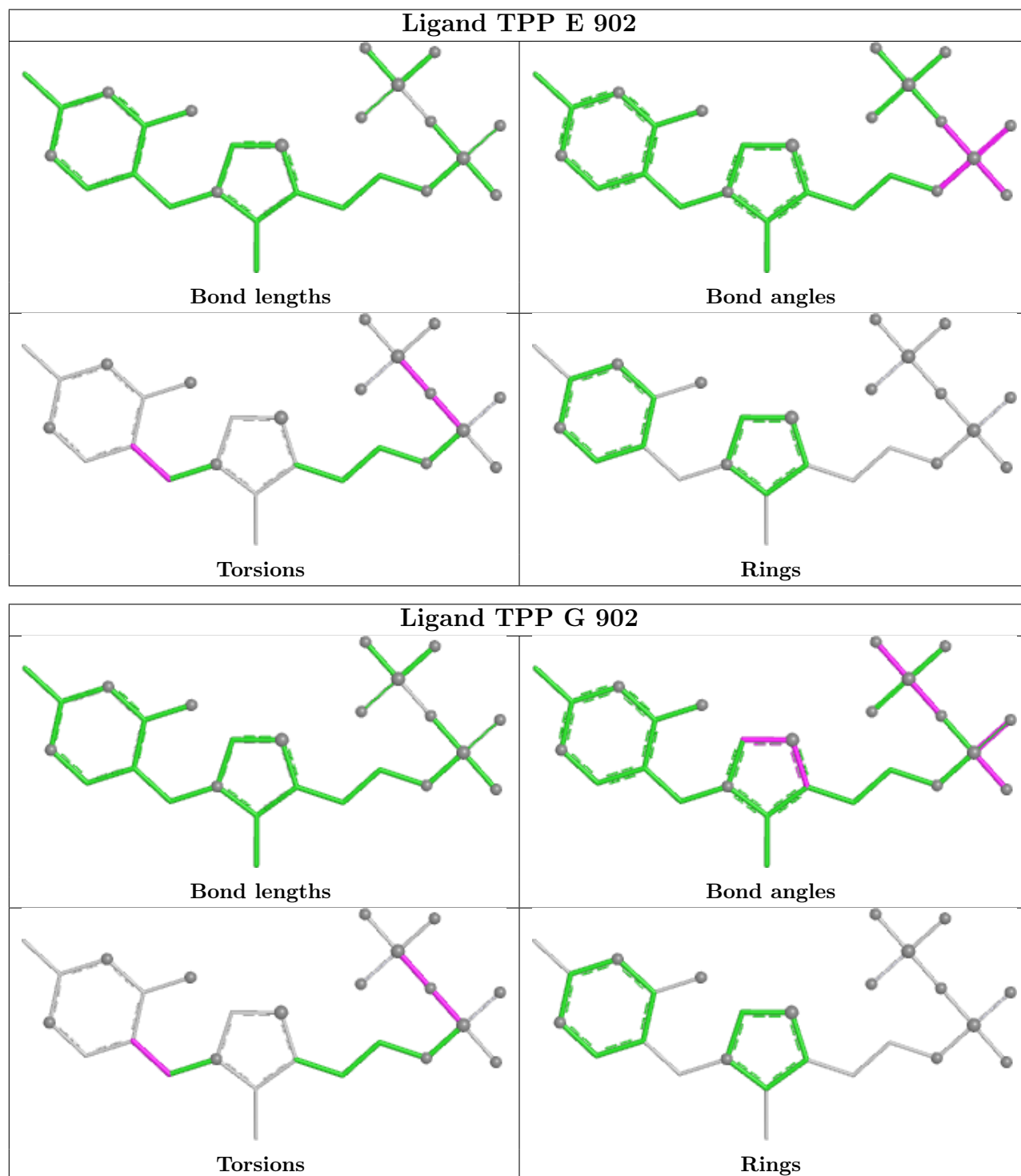
There are no ring outliers.

16 monomers are involved in 51 short contacts:

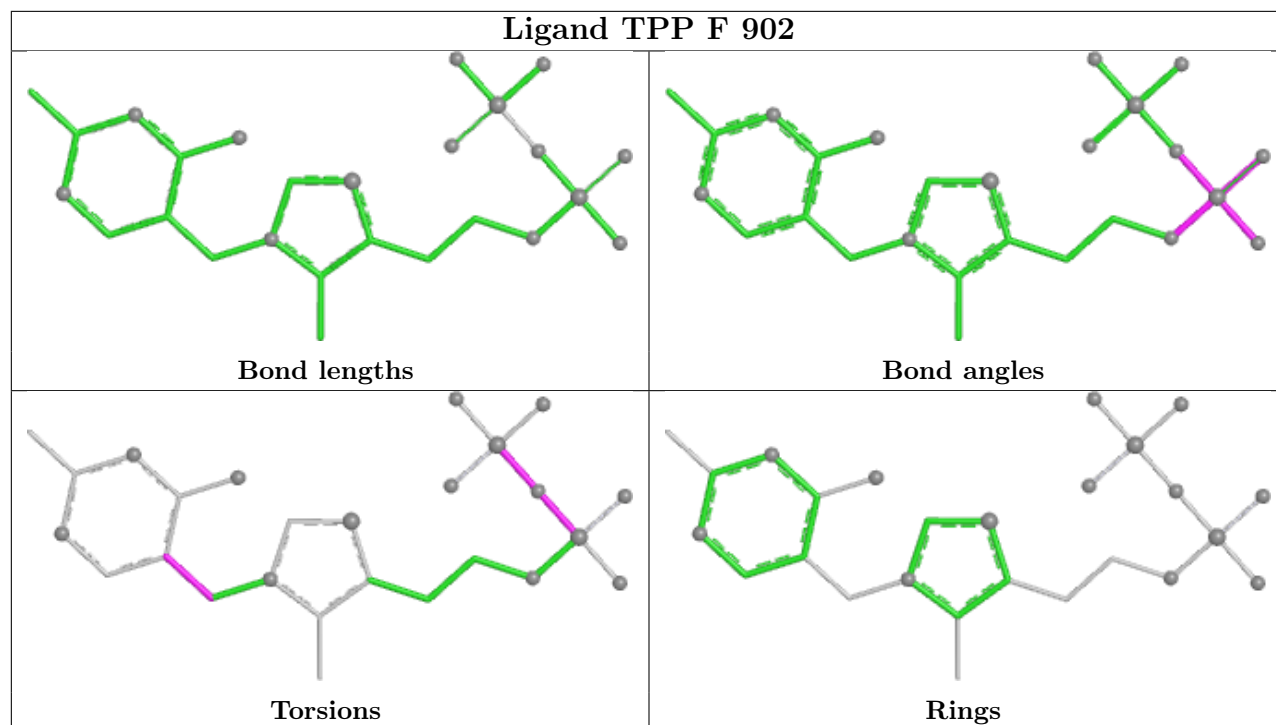
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	PEP	2	0
2	A	901	PEP	4	0
3	E	902	TPP	3	0
2	D	901	PEP	1	0
2	H	901	PEP	4	0
2	E	901	PEP	2	0
3	G	902	TPP	2	0
3	F	902	TPP	4	0
3	H	902	TPP	6	0
3	C	902	TPP	4	0
2	C	901	PEP	2	0
2	G	901	PEP	3	0
2	B	901	PEP	5	0
3	B	902	TPP	3	0
3	D	902	TPP	4	0
3	A	902	TPP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

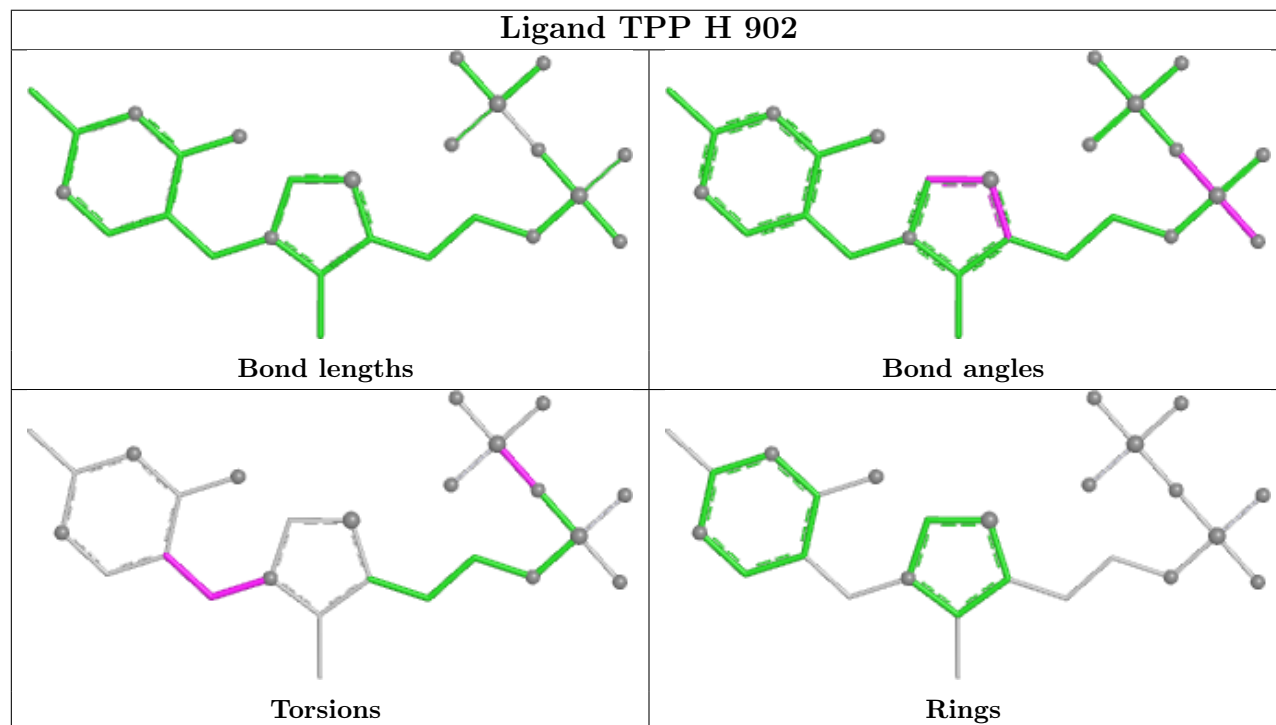
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



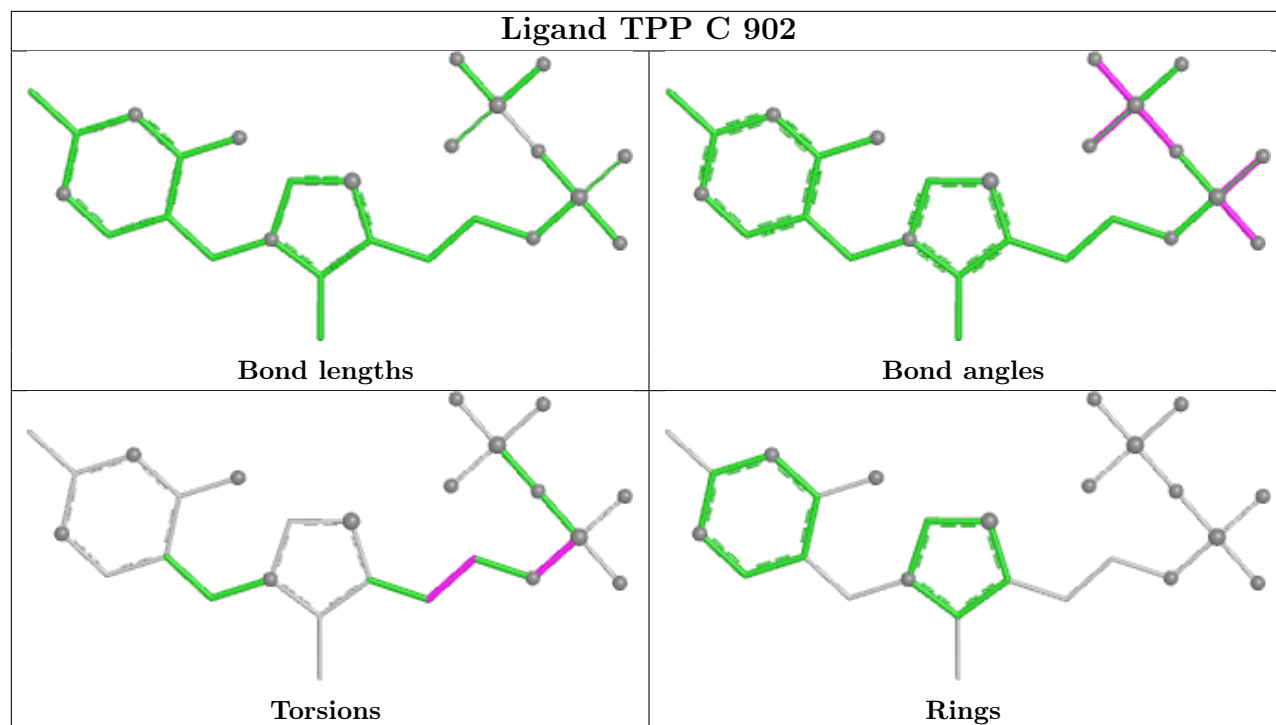
Ligand TPP F 902



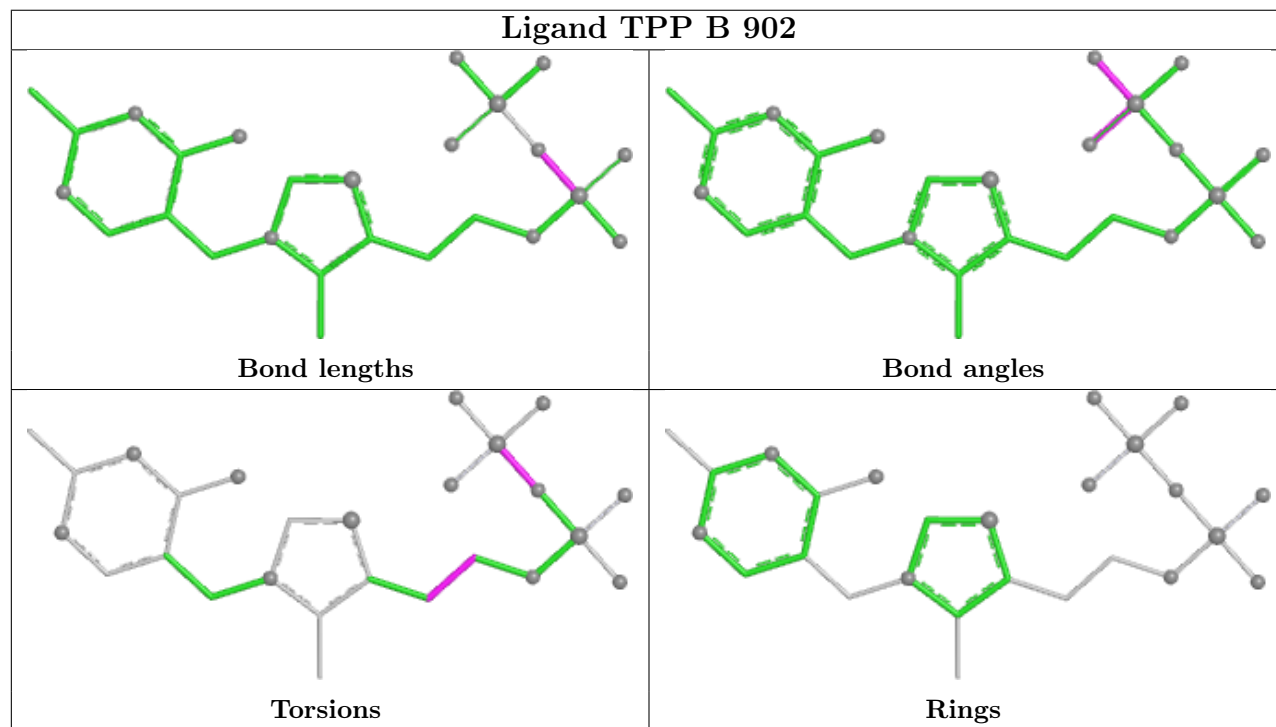
Ligand TPP H 902

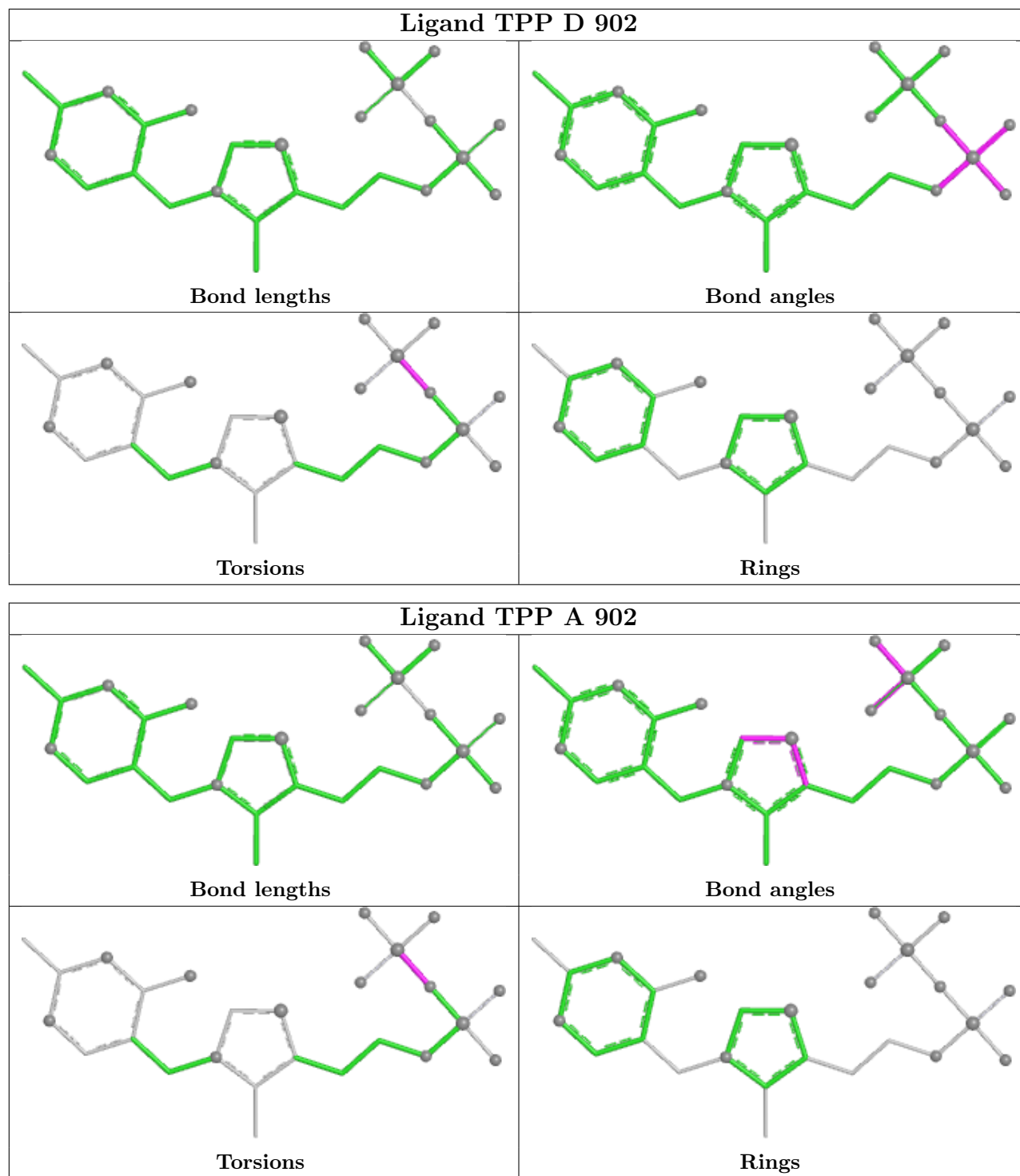


Ligand TPP C 902



Ligand TPP B 902





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	808/831 (97%)	-0.52	0	100	100	24, 44, 68, 135	1 (0%)
1	B	811/831 (97%)	-0.55	1 (0%)	92	90	24, 43, 70, 157	1 (0%)
1	C	806/831 (96%)	0.25	4 (0%)	87	85	43, 74, 108, 125	0
1	D	807/831 (97%)	0.20	5 (0%)	85	83	43, 71, 109, 132	0
1	E	809/831 (97%)	-0.03	2 (0%)	91	89	35, 58, 101, 158	0
1	F	809/831 (97%)	-0.04	2 (0%)	91	89	38, 62, 93, 144	0
1	G	807/831 (97%)	-0.29	1 (0%)	92	90	27, 51, 86, 119	1 (0%)
1	H	808/831 (97%)	-0.23	1 (0%)	92	90	33, 55, 83, 131	1 (0%)
All	All	6465/6648 (97%)	-0.15	16 (0%)	91	89	24, 57, 99, 158	4 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	738	GLY	3.6
1	D	626	ALA	3.1
1	D	627	ALA	2.8
1	F	642	VAL	2.6
1	C	399	VAL	2.4
1	B	810	LYS	2.4
1	E	672	VAL	2.3
1	D	714	HIS	2.3
1	C	762	LEU	2.2
1	E	669	PHE	2.2
1	D	672	VAL	2.2
1	F	810	LYS	2.1
1	H	568[A]	HIS	2.1
1	C	62	VAL	2.0
1	G	657	ALA	2.0
1	C	568	HIS	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 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.

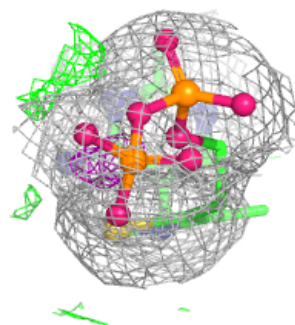
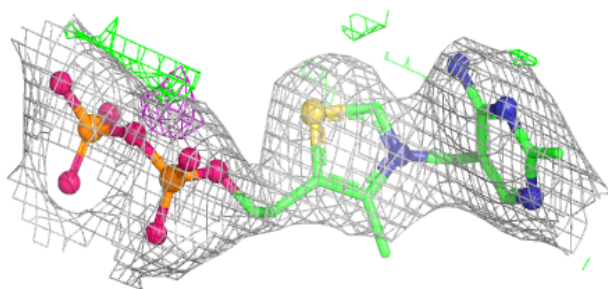
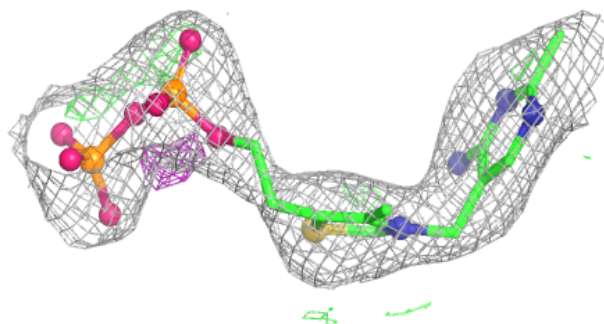
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEP	B	901	10/10	0.89	0.17	26,35,48,55	10
2	PEP	D	901	10/10	0.90	0.15	63,77,83,85	10
2	PEP	E	901	10/10	0.91	0.15	59,66,80,80	10
2	PEP	C	901	10/10	0.93	0.12	55,65,80,90	10
2	PEP	H	901	10/10	0.93	0.14	43,46,63,71	10
2	PEP	G	901	10/10	0.95	0.12	43,60,73,82	10
2	PEP	A	901	10/10	0.95	0.11	33,50,63,63	10
2	PEP	F	901	10/10	0.96	0.13	44,49,68,69	10
3	TPP	C	902	26/26	0.96	0.08	43,55,72,80	0
3	TPP	D	902	26/26	0.97	0.07	46,53,65,68	0
3	TPP	E	902	26/26	0.98	0.06	34,46,52,55	0
3	TPP	F	902	26/26	0.98	0.07	43,54,63,69	0
3	TPP	H	902	26/26	0.98	0.05	38,48,54,56	0
4	CA	D	903	1/1	0.98	0.08	71,71,71,71	0
4	CA	E	903	1/1	0.98	0.06	60,60,60,60	0
4	CA	H	903	1/1	0.98	0.05	74,74,74,74	0
4	CA	B	903	1/1	0.99	0.04	52,52,52,52	0
4	CA	C	903	1/1	0.99	0.04	77,77,77,77	0
3	TPP	B	902	26/26	0.99	0.05	29,36,41,43	0
3	TPP	G	902	26/26	0.99	0.05	32,44,49,55	0
4	CA	F	903	1/1	0.99	0.06	78,78,78,78	0
4	CA	G	903	1/1	0.99	0.08	52,52,52,52	0
3	TPP	A	902	26/26	0.99	0.05	27,35,48,59	0
4	CA	A	903	1/1	1.00	0.05	60,60,60,60	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.

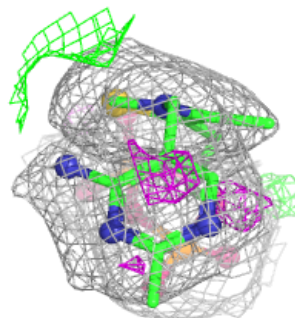
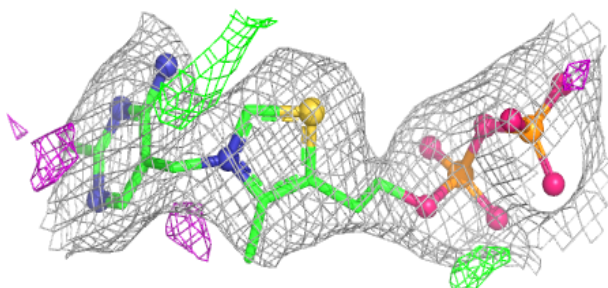
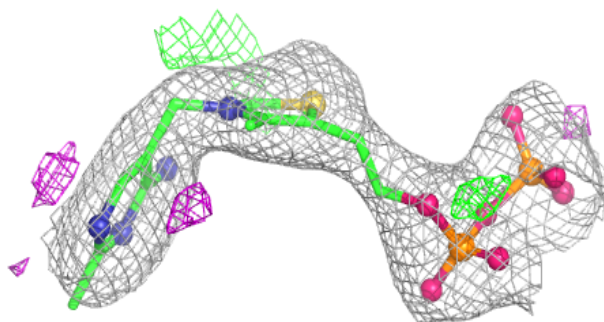
Electron density around TPP C 902:

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



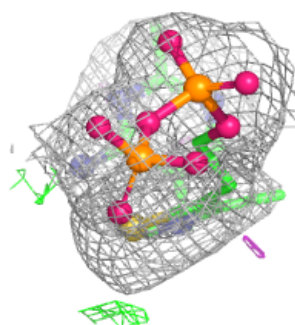
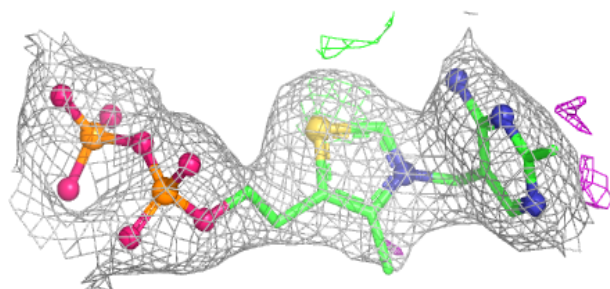
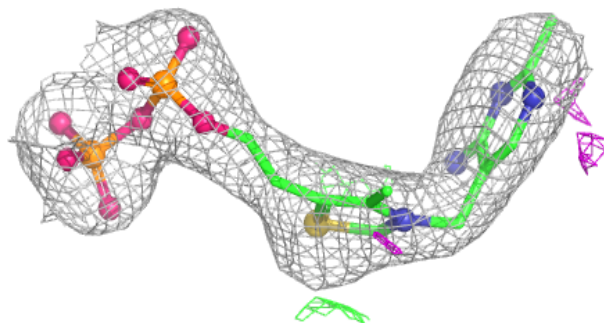
Electron density around TPP D 902:

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

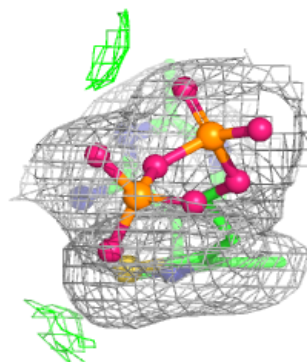
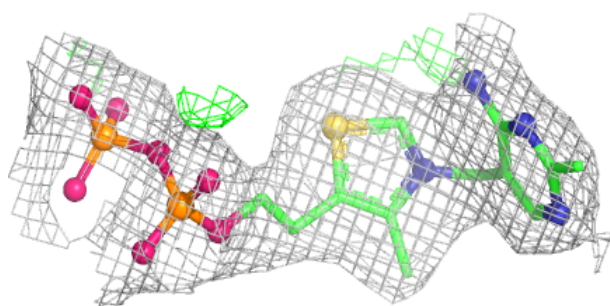
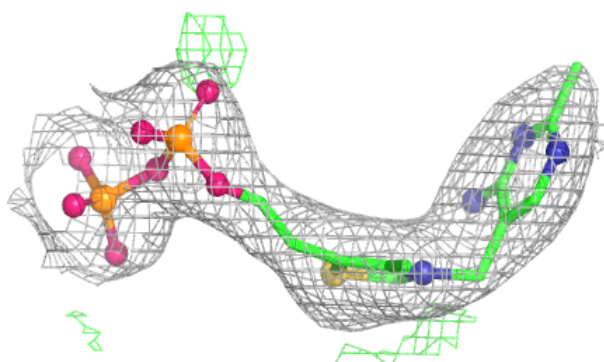


Electron density around TPP E 902:

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

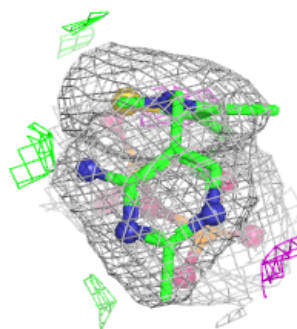
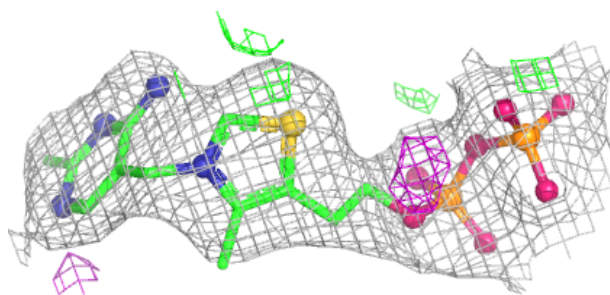
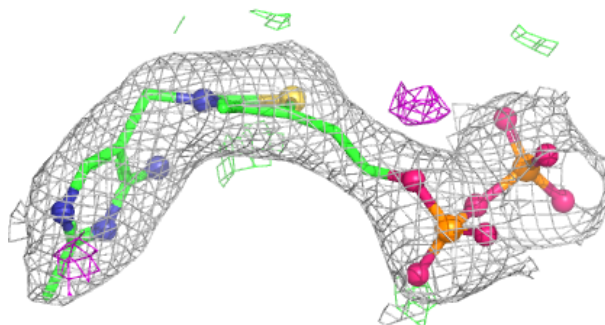
**Electron density around TPP F 902:**

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

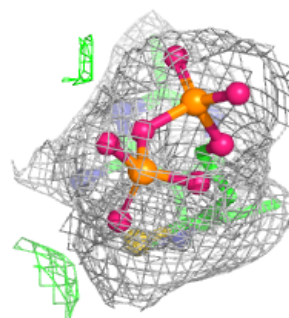
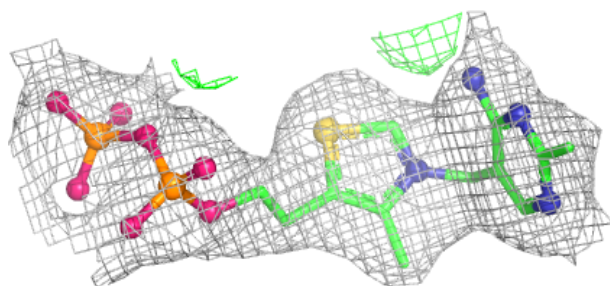
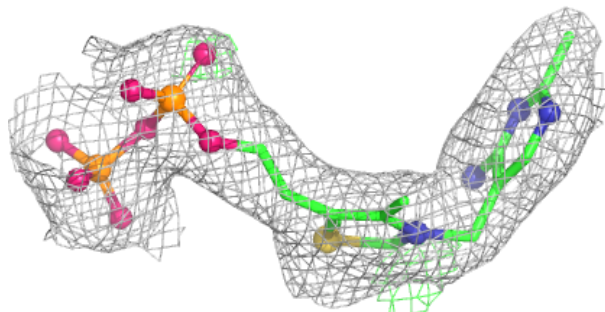


Electron density around TPP H 902:

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

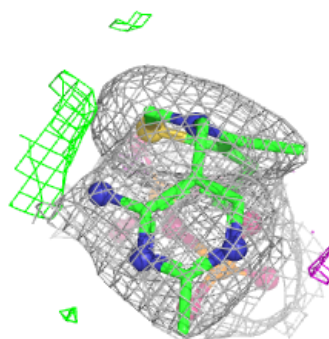
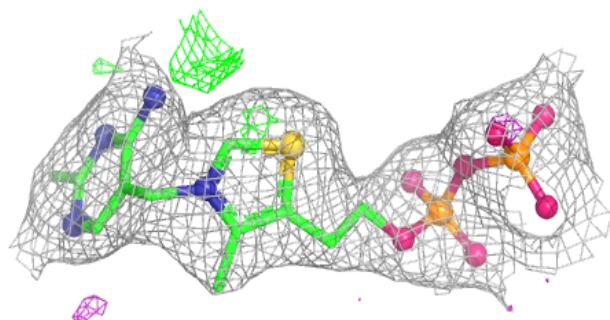
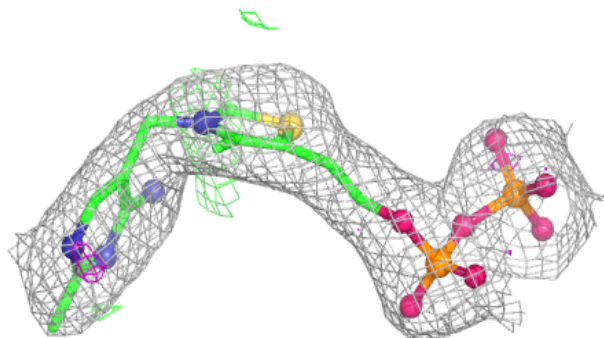
**Electron density around TPP B 902:**

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

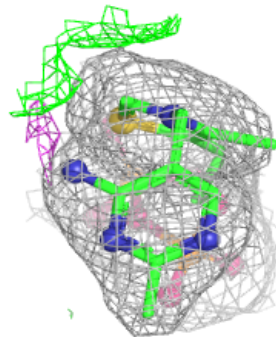
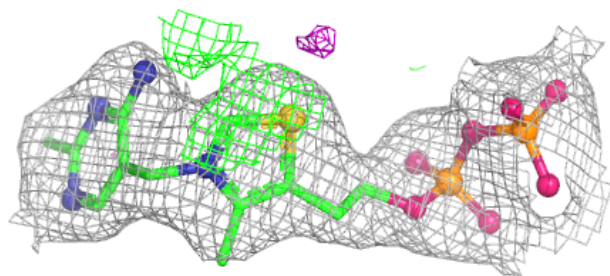
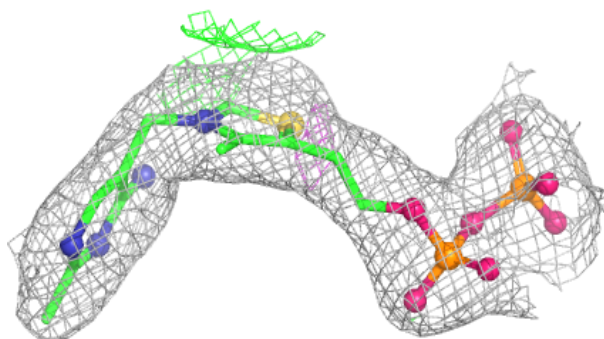


Electron density around TPP G 902:

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

**Electron density around TPP A 902:**

$2mF_o-DF_c$ (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.