



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 09:32 PM JST

PDB ID : 7C8I
Title : Ambient temperature structure of Bifidobacterium 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

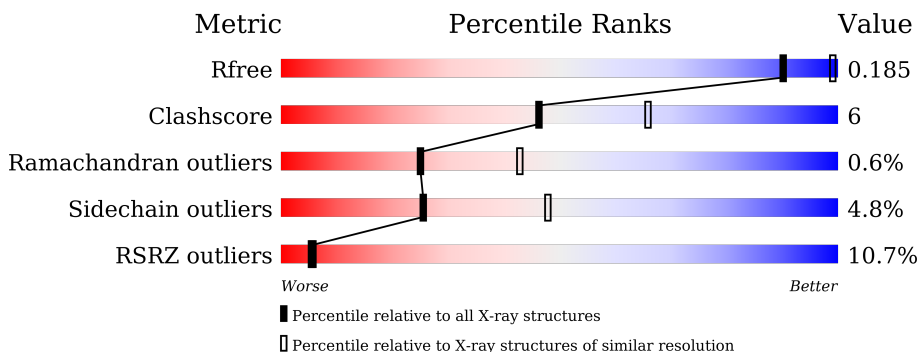
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	 5% 87% 9% ..
1	B	831	 6% 87% 10% .
1	C	831	 15% 74% 21% ..
1	D	831	 13% 71% 24% ..
1	E	831	 14% 79% 17% ..
1	F	831	 13% 80% 16% ..

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Mol	Chain	Length	Quality of chain
1	G	831	
1	H	831	

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 [i](#)

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

There are 48 discrepancies between the modelled and reference sequences:

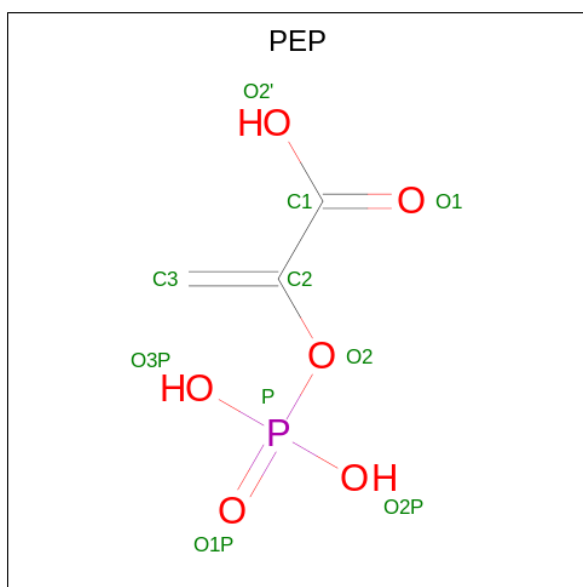
Chain	Residue	Modelled	Actual	Comment	Reference
A	826	HIS	-	expression tag	UNP Q6R2Q7
A	827	HIS	-	expression tag	UNP Q6R2Q7
A	828	HIS	-	expression tag	UNP Q6R2Q7
A	829	HIS	-	expression tag	UNP Q6R2Q7
A	830	HIS	-	expression tag	UNP Q6R2Q7
A	831	HIS	-	expression tag	UNP Q6R2Q7
B	826	HIS	-	expression tag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

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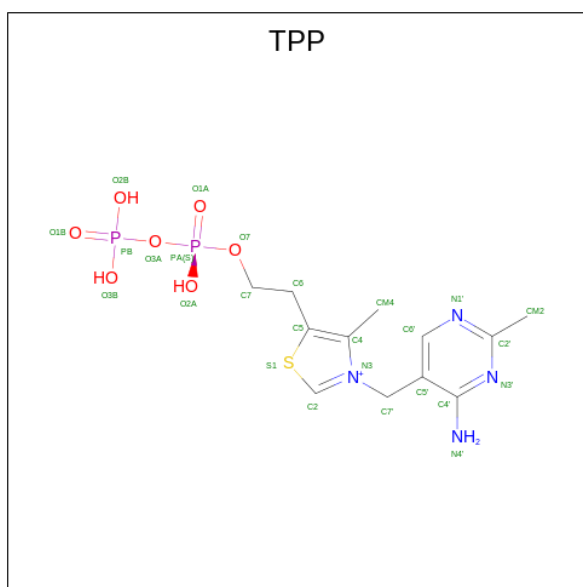
Chain	Residue	Modelled	Actual	Comment	Reference
C	827	HIS	-	expression tag	UNP Q6R2Q7
C	828	HIS	-	expression tag	UNP Q6R2Q7
C	829	HIS	-	expression tag	UNP Q6R2Q7
C	830	HIS	-	expression tag	UNP Q6R2Q7
C	831	HIS	-	expression tag	UNP Q6R2Q7
D	826	HIS	-	expression tag	UNP Q6R2Q7
D	827	HIS	-	expression tag	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 (three-letter code: PEP) (formula: C₃H₅O₆P).



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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
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 (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
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		

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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

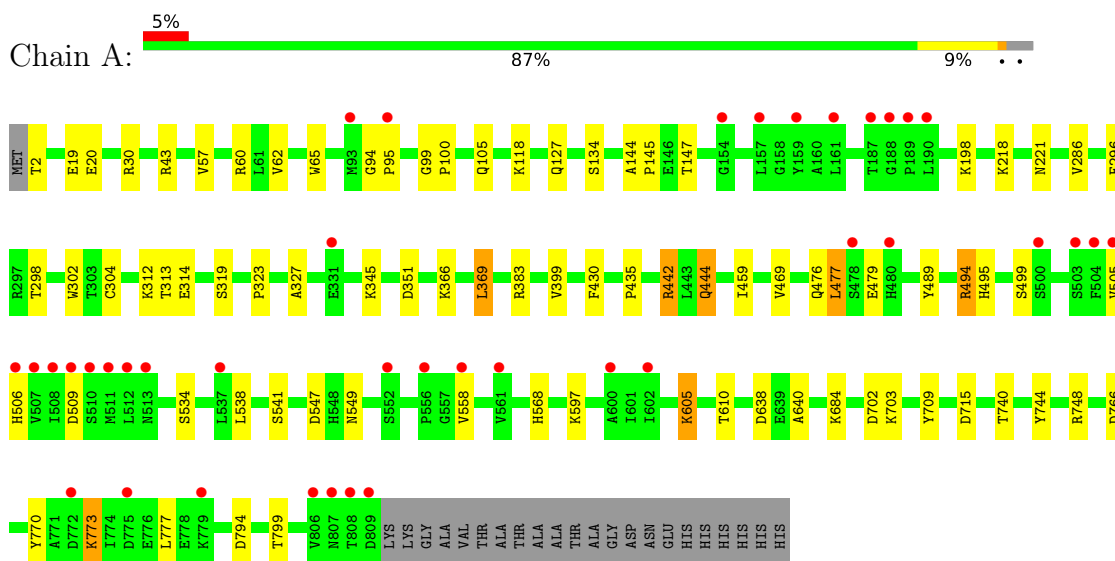
- Molecule 5 is water.

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

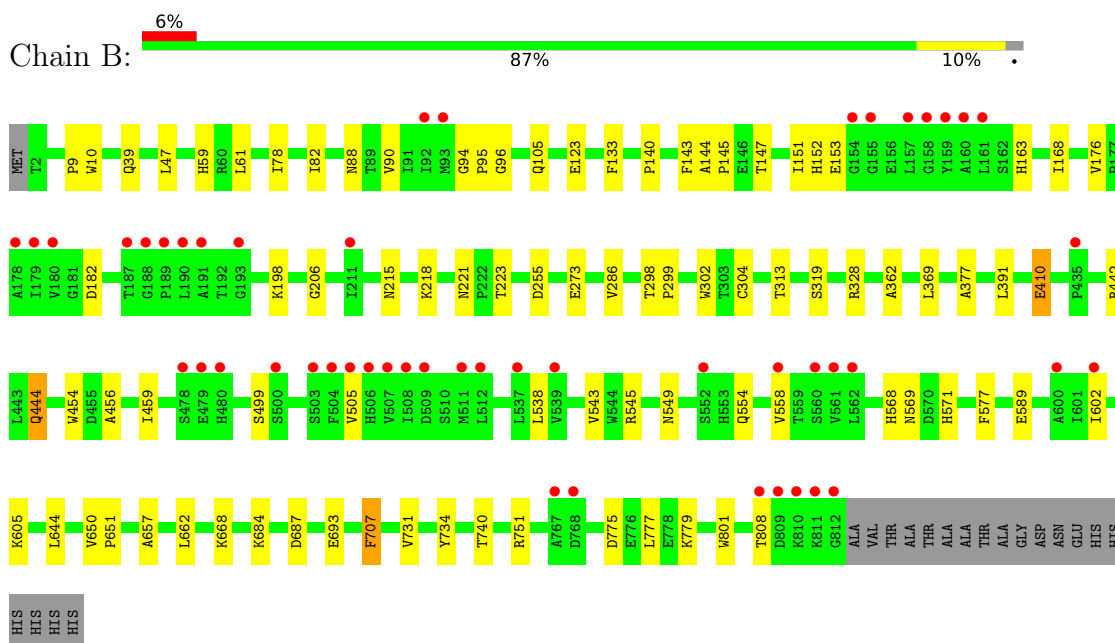
3 Residue-property plots [i](#)

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.

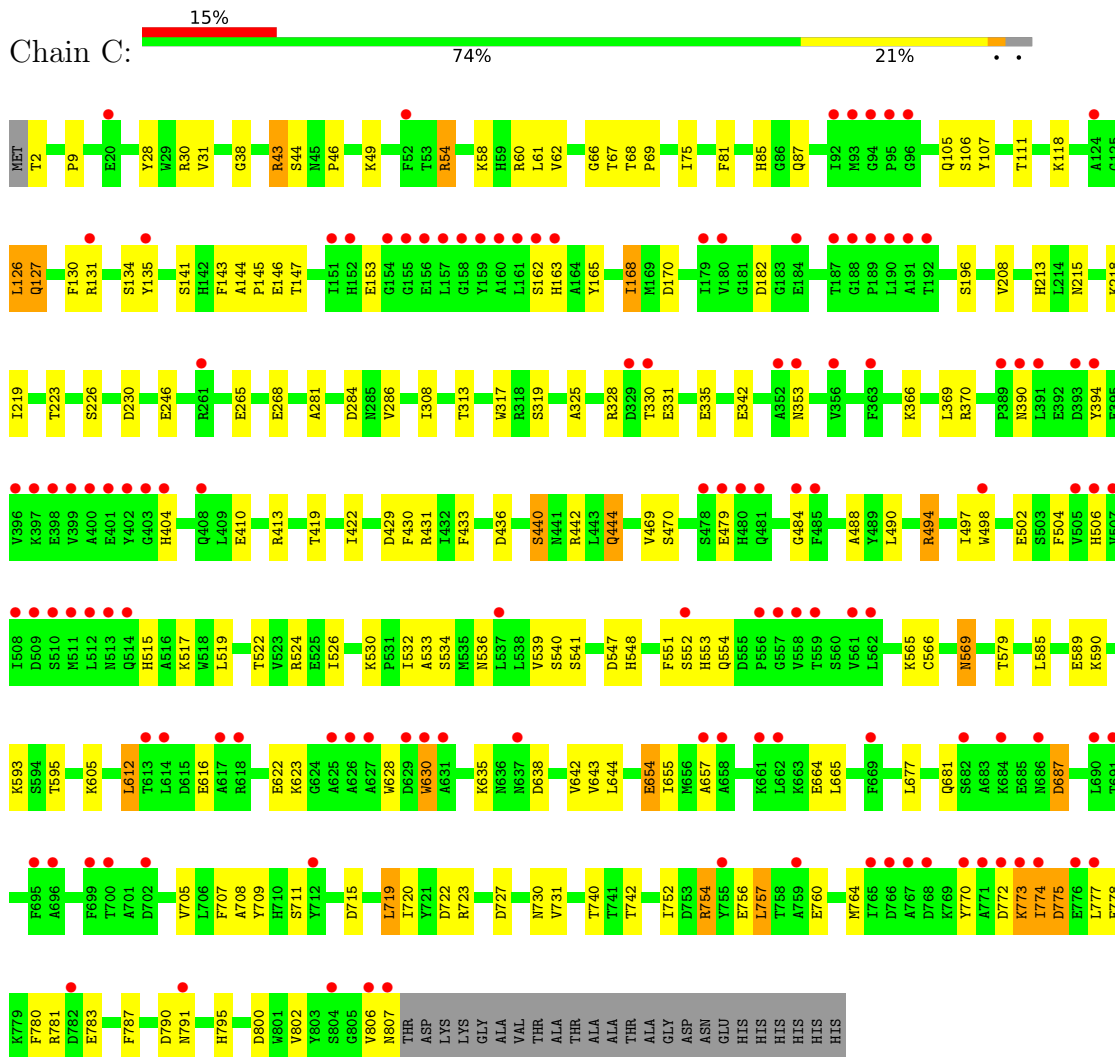
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



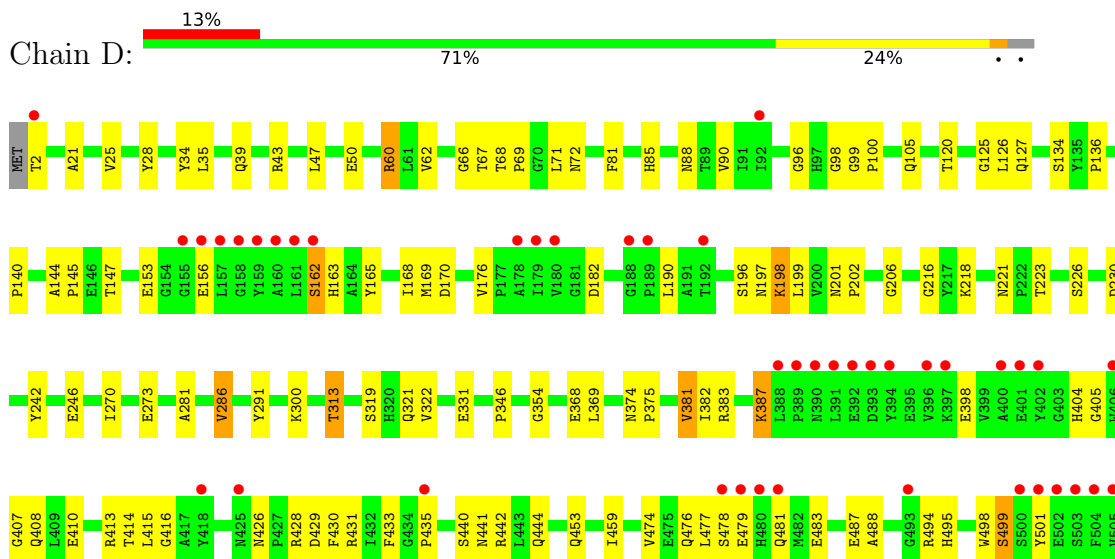
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

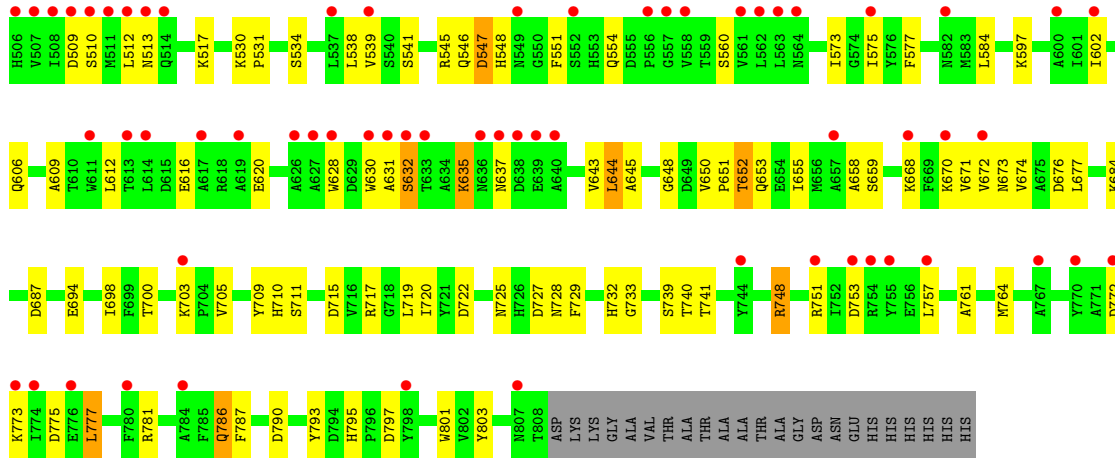


● Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

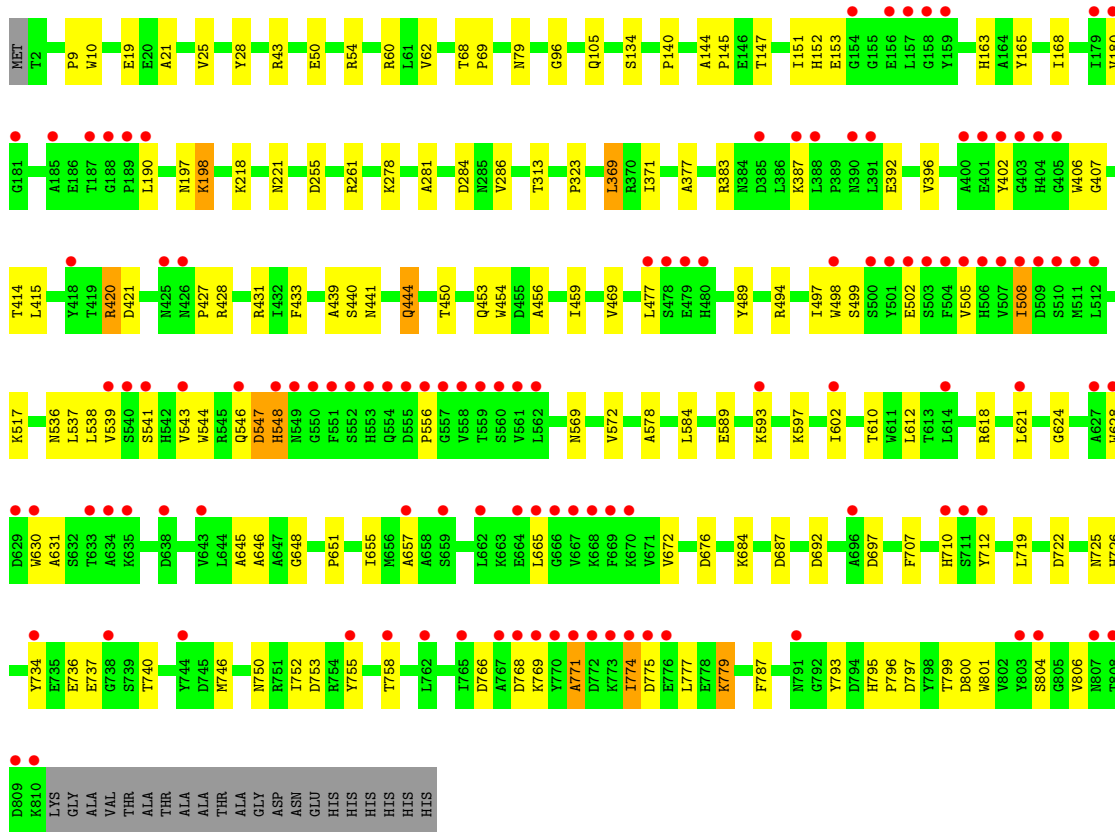
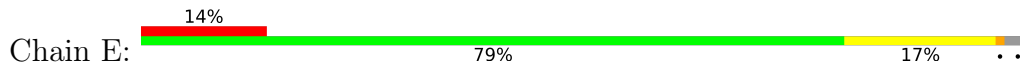


● Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

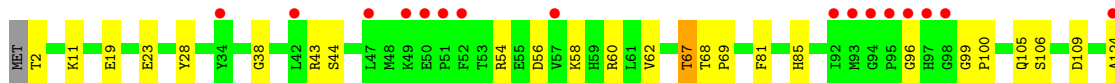
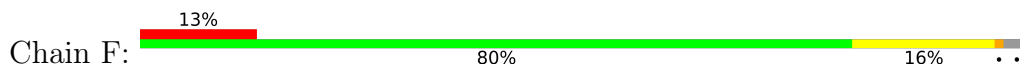


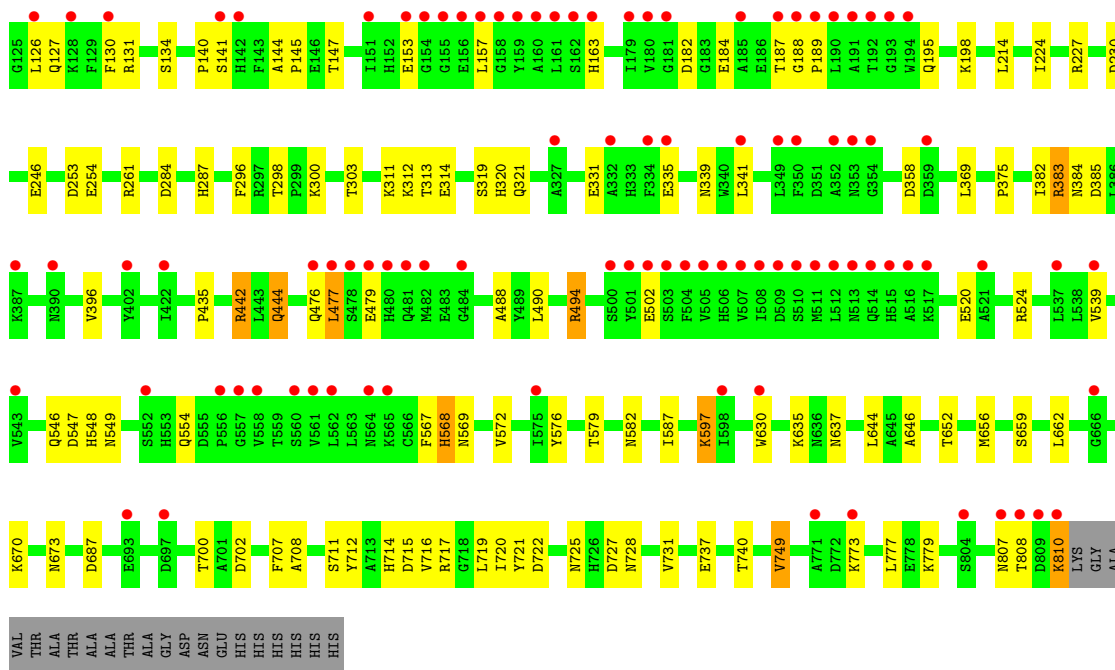


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

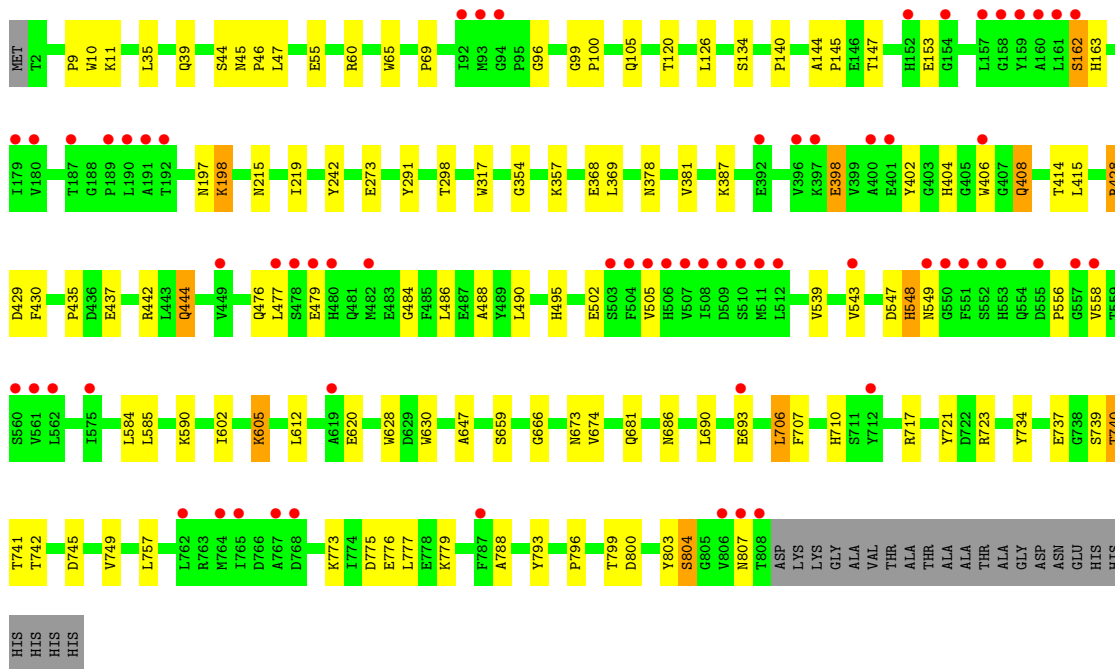
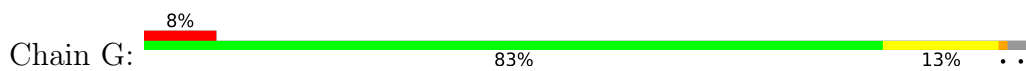


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

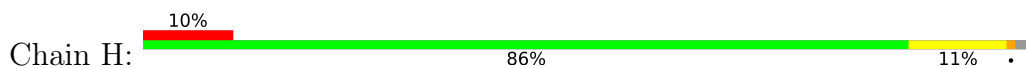


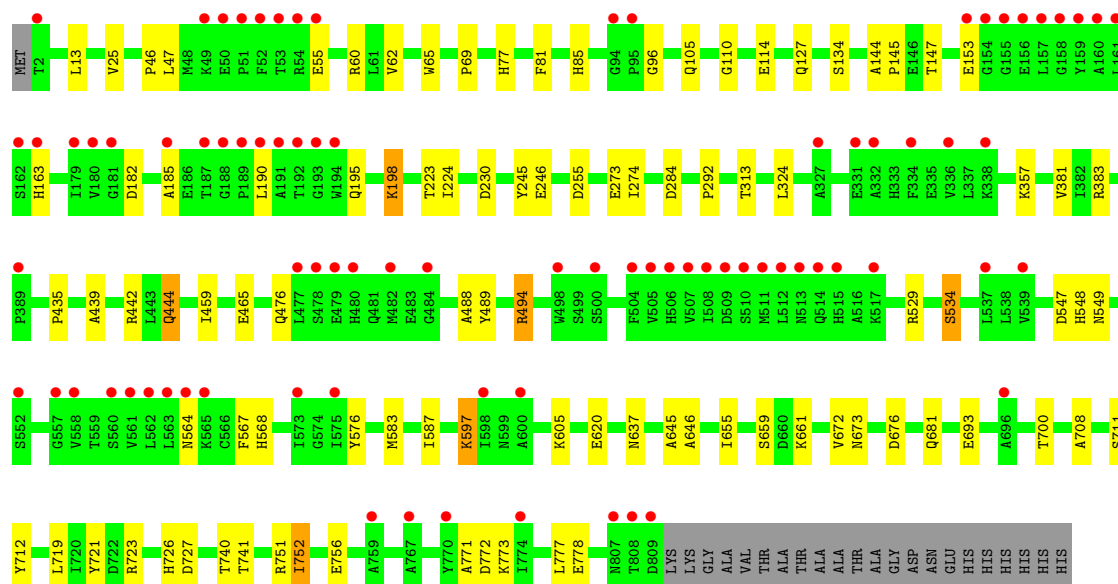


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



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





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 48.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.10-2.50) 99.9 (48.05-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.51Å)	Xtrriage
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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEP, TPP, 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	0.74	0/6614	0.89	1/8996 (0.0%)
1	B	0.72	1/6636 (0.0%)	0.88	0/9023
1	C	0.74	0/6588	0.87	1/8960 (0.0%)
1	D	0.74	0/6595	0.86	0/8970
1	E	0.74	0/6612	0.89	0/8992
1	F	0.72	0/6612	0.88	0/8992
1	G	0.73	0/6606	0.88	0/8985
1	H	0.73	0/6614	0.89	0/8996
All	All	0.73	1/52877 (0.0%)	0.88	2/71914 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	589	GLU	CD-OE1	5.81	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	LYS	CB-CA-C	5.42	121.23	110.40
1	A	383	ARG	NE-CZ-NH1	5.29	122.95	120.30

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	47	0
1	B	6458	0	6147	56	0
1	C	6411	0	6101	108	0
1	D	6418	0	6108	128	0
1	E	6435	0	6125	97	0
1	F	6435	0	6125	90	0
1	G	6428	0	6114	76	0
1	H	6436	0	6118	59	0
2	A	10	0	2	4	0
2	B	10	0	2	5	0
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	1	0
3	B	26	0	16	4	0
3	C	26	0	16	4	0
3	D	26	0	16	4	0
3	E	26	0	16	4	0
3	F	26	0	16	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	632	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 6.

All (632) 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
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	0.85
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:G:620:GLU:OE1	1:G:673:ASN:ND2	2.30	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: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: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:766:ASP:CG	1:E:769:LYS:HB3	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:547:ASP:CG	1:F:60:ARG:HH22	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ASP:OD2	1:D:431:ARG:NE	2.25	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:H:182:ASP:CG	1:H:223:THR:HG21	2.28	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: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
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:H:576:TYR:HB3	1:H:587:ILE:HD13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:569:ASN:OD1	1:C:687:ASP:CG	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:605:LYS:NZ	2:H:901:PEP:O1P	2.38	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
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: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: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:C:182:ASP:CG	1:C:223:THR:HG21	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:PRO:HA	5:B:1080:HOH:O	2.13	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
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: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:F:711:SER:OG	1:F:712:TYR:N	2.47	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: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

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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: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: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:E:676:ASP:OD1	1:E:676:ASP:C	2.53	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: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
1:C:38:GLY:HA3	1:C:130:PHE:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:190:LEU:HD13	1:D:190:LEU:C	2.36	0.46
1:F:28:TYR:CD1	1:F:28:TYR:C	2.89	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: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:737:GLU:HG3	1:H:568[B]:HIS:CE1	2.51	0.45
1:A:99:GLY:N	1:A:100:PRO:CD	2.79	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:D:720:ILE:O	1:D:720:ILE:CD1	2.63	0.45
1:F:43:ARG:O	1:F:127:GLN:NE2	2.49	0.45
1:C:75:ILE:HG21	1:C:105:GLN:HG3	1.98	0.45
1:F:195:GLN:OE1	1:F:198:LYS:NZ	2.48	0.45
1:A:477:LEU:HD22	3:B:902:TPP:HM41	1.99	0.45
1:A:709:TYR:CE2	1:A:715:ASP:HB2	2.51	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
1:C:106:SER:OG	1:C:111:THR:OG1	2.27	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: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:C:540:SER:O	1:C:541:SER:C	2.56	0.45
1:C:687:ASP:C	1:C:687:ASP:OD1	2.55	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
3:E:902:TPP:HM41	1:F:477:LEU:HD22	1.99	0.45
1:F:284:ASP:CG	1:F:287:HIS:HD1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:G:430:PHE:HA	1:G:495:HIS:O	2.17	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
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:182:ASP:CG	1:D:223:THR:HG21	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:162:SER:OG	5:D:1001:HOH:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:HG13	1:H:459:ILE:O	2.19	0.43
1:D:28:TYR:CD1	1:D:28:TYR:C	2.91	0.43
1:D:777:LEU:HD12	1:D:777:LEU:HA	1.91	0.43
1:F:253:ASP:O	1:F:254:GLU:C	2.57	0.43
1:F:714:HIS:O	1:F:715:ASP:C	2.57	0.43
1:G:442:ARG:C	1:G:444:GLN:NE2	2.72	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: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: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:G:706:LEU:HD21	1:G:757:LEU:HD22	2.02	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
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: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:D:98:GLY:C	1:D:100:PRO:HD2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:676:ASP:C	1:H:676:ASP:OD1	2.58	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:803:TYR:O	1:G:804:SER:C	2.58	0.41
1:B:650:VAL:HB	1:B:651:PRO:HD3	2.02	0.41
1:B:182:ASP:CG	1:B:223:THR:HG21	2.41	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:E:787:PHE:CE2	1:E:795:HIS:HA	2.56	0.41
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: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: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:427:PRO:C	1:E:428:ARG:HG2	2.41	0.41
1:E:589:GLU:O	1:E:593:LYS:HG3	2.21	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:28:TYR:CD1	1:C:28:TYR:C	2.94	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:28:TYR:CD1	1:E:28:TYR:C	2.94	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:A:351:ASP:OD1	1:A:351:ASP:C	2.59	0.40
1:D:632:SER:HB3	1:D:670:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:85:HIS:HE2	1:C:268:GLU:CD	2.23	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: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
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: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: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 [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	807/831 (97%)	758 (94%)	45 (6%)	4 (0%)	29	48
1	B	810/831 (98%)	766 (95%)	42 (5%)	2 (0%)	47	68
1	C	804/831 (97%)	698 (87%)	98 (12%)	8 (1%)	15	28
1	D	805/831 (97%)	715 (89%)	81 (10%)	9 (1%)	14	26
1	E	807/831 (97%)	725 (90%)	78 (10%)	4 (0%)	29	48
1	F	807/831 (97%)	745 (92%)	55 (7%)	7 (1%)	17	31
1	G	806/831 (97%)	737 (91%)	64 (8%)	5 (1%)	25	43
1	H	807/831 (97%)	748 (93%)	57 (7%)	2 (0%)	47	68
All	All	6453/6648 (97%)	5892 (91%)	520 (8%)	41 (1%)	25	43

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

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Mol	Chain	Res	Type
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
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 [i](#)

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%)	39 65
1	B	680/693 (98%)	664 (98%)	16 (2%)	49 74
1	C	675/693 (97%)	623 (92%)	52 (8%)	13 25
1	D	676/693 (98%)	628 (93%)	48 (7%)	14 28
1	E	678/693 (98%)	647 (95%)	31 (5%)	27 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	678/693 (98%)	647 (95%)	31 (5%)	27	50
1	G	677/693 (98%)	645 (95%)	32 (5%)	26	49
1	H	678/693 (98%)	652 (96%)	26 (4%)	33	58
All	All	5420/5544 (98%)	5162 (95%)	258 (5%)	25	48

All (258) 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	105	GLN
1	A	118	LYS
1	A	127	GLN
1	A	147	THR
1	A	198	LYS
1	A	366	LYS
1	A	369	LEU
1	A	444	GLN
1	A	477	LEU
1	A	494	ARG
1	A	534	SER
1	A	605	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	105	GLN
1	B	147	THR
1	B	198	LYS
1	B	255	ASP
1	B	273	GLU
1	B	369	LEU
1	B	410	GLU
1	B	444	GLN
1	B	668	LYS
1	B	684	LYS

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Mol	Chain	Res	Type
1	B	693	GLU
1	B	707	PHE
1	B	751	ARG
1	B	777	LEU
1	B	808	THR
1	C	30	ARG
1	C	31	VAL
1	C	43	ARG
1	C	49	LYS
1	C	107	TYR
1	C	126	LEU
1	C	127	GLN
1	C	147	THR
1	C	168	ILE
1	C	226	SER
1	C	265	GLU
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	440	SER
1	C	444	GLN
1	C	470	SER
1	C	494	ARG
1	C	530	LYS
1	C	534	SER
1	C	548	HIS
1	C	551	PHE
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	612	LEU
1	C	623	LYS
1	C	635	LYS
1	C	638	ASP
1	C	642	VAL
1	C	644	LEU

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Mol	Chain	Res	Type
1	C	654	GLU
1	C	687	ASP
1	C	719	LEU
1	C	722	ASP
1	C	727	ASP
1	C	754	ARG
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	105	GLN
1	D	126	LEU
1	D	127	GLN
1	D	147	THR
1	D	169	MET
1	D	198	LYS
1	D	286	VAL
1	D	313	THR
1	D	321	GLN
1	D	322	VAL
1	D	331	GLU
1	D	369	LEU
1	D	381	VAL
1	D	383	ARG
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	494	ARG

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Mol	Chain	Res	Type
1	D	499	SER
1	D	510	SER
1	D	547	ASP
1	D	548	HIS
1	D	551	PHE
1	D	560	SER
1	D	632	SER
1	D	635	LYS
1	D	644	LEU
1	D	659	SER
1	D	668	LYS
1	D	684	LYS
1	D	687	ASP
1	D	722	ASP
1	D	727	ASP
1	D	772	ASP
1	D	773	LYS
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	105	GLN
1	E	147	THR
1	E	198	LYS
1	E	255	ASP
1	E	369	LEU
1	E	383	ARG
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	494	ARG
1	E	508	ILE
1	E	547	ASP
1	E	548	HIS
1	E	665	LEU
1	E	684	LYS

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Mol	Chain	Res	Type
1	E	692	ASP
1	E	697	ASP
1	E	707	PHE
1	E	719	LEU
1	E	722	ASP
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	105	GLN
1	F	126	LEU
1	F	141	SER
1	F	147	THR
1	F	321	GLN
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	494	ARG
1	F	548	HIS
1	F	597	LYS
1	F	635	LYS
1	F	659	SER
1	F	670	LYS
1	F	716	VAL
1	F	719	LEU
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

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Mol	Chain	Res	Type
1	G	44	SER
1	G	55	GLU
1	G	60	ARG
1	G	105	GLN
1	G	120	THR
1	G	147	THR
1	G	162	SER
1	G	198	LYS
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	548	HIS
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	707	PHE
1	G	740	THR
1	G	775	ASP
1	G	777	LEU
1	G	779	LYS
1	H	47	LEU
1	H	55	GLU
1	H	105	GLN
1	H	147	THR
1	H	198	LYS
1	H	255	ASP
1	H	313	THR
1	H	324	LEU
1	H	357	LYS
1	H	381	VAL
1	H	383	ARG

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Mol	Chain	Res	Type
1	H	444	GLN
1	H	465	GLU
1	H	494	ARG
1	H	529	ARG
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	A	549	ASN
1	A	571	HIS
1	B	14	ASN
1	B	59	HIS
1	B	127	GLN
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	425	ASN
1	C	444	GLN
1	C	472	GLN
1	D	59	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

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Mol	Chain	Res	Type
1	D	730	ASN
1	D	786	GLN
1	D	791	ASN
1	E	384	ASN
1	E	404	HIS
1	E	444	GLN
1	E	480	HIS
1	E	548	HIS
1	E	750	ASN
1	E	786	GLN
1	F	39	GLN
1	F	384	ASN
1	F	444	GLN
1	F	513	ASN
1	F	549	ASN
1	F	673	ASN
1	G	14	ASN
1	G	132	GLN
1	G	384	ASN
1	G	404	HIS
1	G	408	GLN
1	G	444	GLN
1	G	548	HIS
1	G	549	ASN
1	G	730	ASN
1	H	59	HIS
1	H	408	GLN
1	H	444	GLN
1	H	549	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 monosaccharides in this entry.

5.6 Ligand geometry

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
3	TPP	B	902	4	22,27,27	0.78	0	29,40,40	1.20	3 (10%)
2	PEP	C	901	-	9,9,9	3.11	3 (33%)	11,13,13	2.10	3 (27%)
3	TPP	D	902	4	22,27,27	0.78	0	29,40,40	1.15	3 (10%)
2	PEP	A	901	-	9,9,9	3.82	3 (33%)	11,13,13	1.58	2 (18%)
3	TPP	C	902	4	22,27,27	0.88	1 (4%)	29,40,40	1.23	4 (13%)
2	PEP	G	901	-	9,9,9	2.96	2 (22%)	11,13,13	2.05	5 (45%)
3	TPP	G	902	4	22,27,27	0.62	0	29,40,40	1.10	2 (6%)
3	TPP	E	902	4	22,27,27	0.57	0	29,40,40	0.99	2 (6%)
2	PEP	H	901	-	9,9,9	2.64	2 (22%)	11,13,13	1.73	5 (45%)
2	PEP	E	901	-	9,9,9	2.19	2 (22%)	11,13,13	2.95	6 (54%)
2	PEP	F	901	-	9,9,9	3.06	2 (22%)	11,13,13	2.20	6 (54%)
3	TPP	H	902	4	22,27,27	0.72	0	29,40,40	0.95	0
2	PEP	D	901	-	9,9,9	3.17	3 (33%)	11,13,13	2.20	4 (36%)
3	TPP	F	902	4	22,27,27	0.63	0	29,40,40	1.02	3 (10%)
2	PEP	B	901	-	9,9,9	2.51	2 (22%)	11,13,13	2.39	3 (27%)
3	TPP	A	902	4	22,27,27	0.79	0	29,40,40	0.96	1 (3%)

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	TPP	B	902	4	-	3/16/17/17	0/2/2/2
2	PEP	C	901	-	-	0/9/9/9	-
3	TPP	D	902	4	-	3/16/17/17	0/2/2/2
2	PEP	A	901	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	C	902	4	-	3/16/17/17	0/2/2/2
2	PEP	G	901	-	-	0/9/9/9	-
3	TPP	G	902	4	-	6/16/17/17	0/2/2/2
3	TPP	E	902	4	-	7/16/17/17	0/2/2/2
2	PEP	H	901	-	-	4/9/9/9	-
2	PEP	E	901	-	-	3/9/9/9	-
2	PEP	F	901	-	-	0/9/9/9	-
3	TPP	H	902	4	-	6/16/17/17	0/2/2/2
2	PEP	D	901	-	-	0/9/9/9	-
3	TPP	F	902	4	-	5/16/17/17	0/2/2/2
2	PEP	B	901	-	-	0/9/9/9	-
3	TPP	A	902	4	-	3/16/17/17	0/2/2/2

All (20) 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	3.56	1.41	1.31
2	C	901	PEP	C3-C2	3.55	1.41	1.31
2	G	901	PEP	C3-C2	3.54	1.41	1.31
2	F	901	PEP	C3-C2	3.44	1.41	1.31
2	B	901	PEP	C3-C2	3.25	1.40	1.31
2	D	901	PEP	C3-C2	3.23	1.40	1.31
2	E	901	PEP	C3-C2	2.99	1.40	1.31
2	A	901	PEP	C3-C2	2.89	1.39	1.31
3	C	902	TPP	C6-C5	2.78	1.52	1.50
2	D	901	PEP	O2 ² -C1	-2.18	1.24	1.30
2	C	901	PEP	O2 ² -C1	-2.11	1.24	1.30
2	A	901	PEP	O2 ² -C1	-2.09	1.24	1.30

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	PEP	O2-C2-C3	-7.36	110.62	124.79
2	B	901	PEP	O1-C1-C2	-4.64	114.80	121.79
2	D	901	PEP	O2-C2-C3	-4.59	115.94	124.79
2	C	901	PEP	O1-C1-C2	-4.56	114.91	121.79
2	B	901	PEP	O2-C2-C3	-4.12	116.85	124.79
2	F	901	PEP	O2-C2-C3	-4.05	116.99	124.79
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	-3.67	117.72	124.79
2	E	901	PEP	C3-C2-C1	3.57	129.34	122.73
2	H	901	PEP	O2-C2-C3	-3.35	118.34	124.79
2	D	901	PEP	O1-C1-C2	-3.26	116.87	121.79
2	A	901	PEP	O3P-P-O2	2.96	114.28	105.25
3	B	902	TPP	C6-C5-C4	2.95	129.80	127.43
2	F	901	PEP	O1-C1-C2	-2.92	117.39	121.79
2	G	901	PEP	O2P-P-O2	-2.83	96.63	105.25
2	G	901	PEP	O1-C1-C2	-2.81	117.55	121.79
2	F	901	PEP	O2P-P-O2	2.80	113.80	105.25
2	G	901	PEP	O2'-C1-C2	2.78	118.65	113.91
3	C	902	TPP	O3B-PB-O2B	2.78	118.25	107.64
2	E	901	PEP	O2P-P-O2	-2.73	96.93	105.25
2	E	901	PEP	O3P-P-O2	2.71	113.51	105.25
3	F	902	TPP	C7'-N3-C2	-2.69	120.50	125.35
2	D	901	PEP	O2'-C1-C2	2.64	118.41	113.91
2	D	901	PEP	O3P-P-O2	2.60	113.16	105.25
2	E	901	PEP	O2'-C1-C2	2.58	118.31	113.91
2	F	901	PEP	O2-P-O1P	-2.52	100.36	109.32
3	G	902	TPP	O2B-PB-O3A	2.52	113.08	104.64
2	H	901	PEP	O2-P-O1P	-2.51	100.39	109.32
2	A	901	PEP	O1-C1-C2	-2.51	118.00	121.79
2	C	901	PEP	O3P-P-O2	2.48	112.81	105.25
3	D	902	TPP	C7'-N3-C2	-2.41	120.99	125.35
3	C	902	TPP	C7'-N3-C2	-2.41	121.00	125.35
2	G	901	PEP	O3P-P-O2	2.41	112.59	105.25
3	C	902	TPP	O2A-PA-O1A	2.38	124.03	112.24
2	H	901	PEP	O2P-P-O2	2.38	112.51	105.25
2	F	901	PEP	C3-C2-C1	2.35	127.08	122.73
3	B	902	TPP	O3B-PB-O2B	2.35	116.61	107.64
3	F	902	TPP	O7-PA-O1A	-2.34	99.94	109.07
3	E	902	TPP	O2A-PA-O7	-2.33	96.94	107.75
3	D	902	TPP	O2A-PA-O1A	2.30	123.63	112.24
2	E	901	PEP	O1-C1-C2	-2.29	118.33	121.79
3	E	902	TPP	O2A-PA-O1A	2.24	123.33	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	TPP	C5-C4-N3	2.23	112.03	107.57
3	D	902	TPP	O2A-PA-O7	-2.15	97.77	107.75
3	C	902	TPP	O2B-PB-O3A	-2.12	97.53	104.64
3	F	902	TPP	O2A-PA-O1A	2.08	122.54	112.24
3	A	902	TPP	O3B-PB-O2B	2.08	115.60	107.64
2	H	901	PEP	C3-C2-C1	2.06	126.54	122.73
2	H	901	PEP	O3P-P-O2	2.05	111.51	105.25
2	F	901	PEP	O2'-C1-C2	2.04	117.39	113.91
3	G	902	TPP	O2A-PA-O1A	2.01	122.19	112.24

There are no chirality outliers.

All (43) 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	C5-C6-C7-O7
3	D	902	TPP	PA-O3A-PB-O3B
3	E	902	TPP	C4'-C5'-C7'-N3
3	E	902	TPP	C4-C5-C6-C7
3	E	902	TPP	PA-O3A-PB-O2B
3	F	902	TPP	C4'-C5'-C7'-N3
3	F	902	TPP	C4-C5-C6-C7
3	F	902	TPP	PA-O3A-PB-O3B
3	G	902	TPP	C4'-C5'-C7'-N3
3	G	902	TPP	C4-C5-C6-C7
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	H	902	TPP	C4-C5-C6-C7
3	G	902	TPP	PB-O3A-PA-O1A
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	E	902	TPP	PB-O3A-PA-O1A
3	C	902	TPP	C7-O7-PA-O2A
3	A	902	TPP	C4-C5-C6-C7
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

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

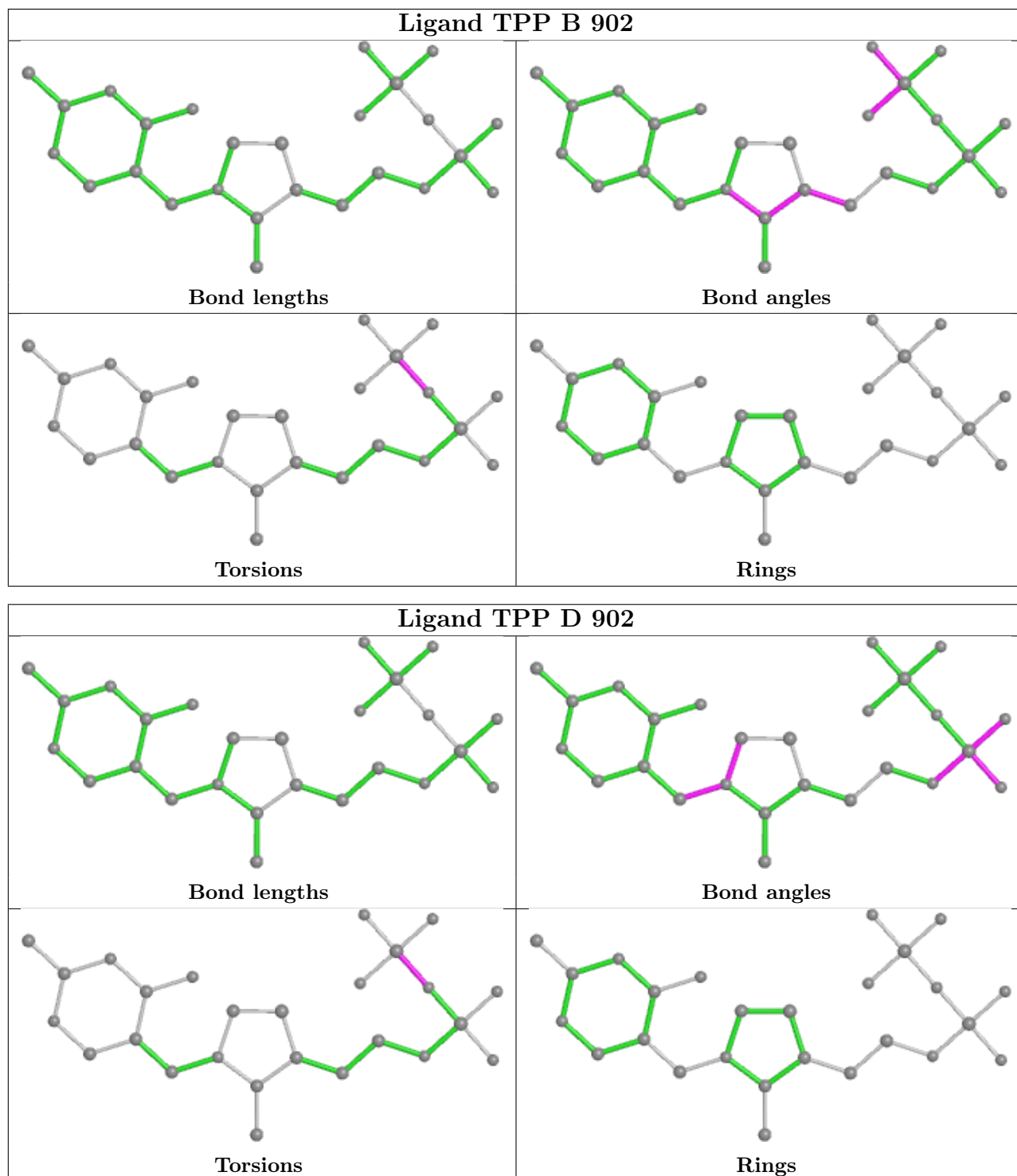
There are no ring outliers.

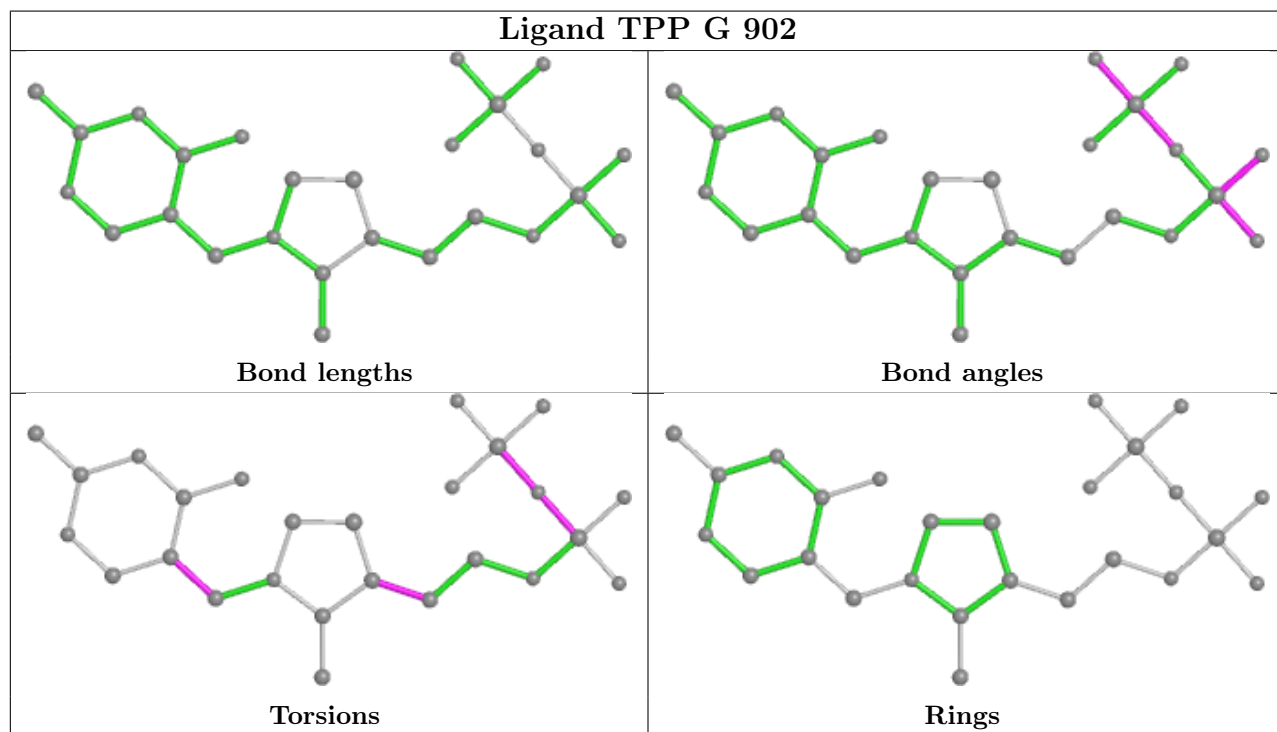
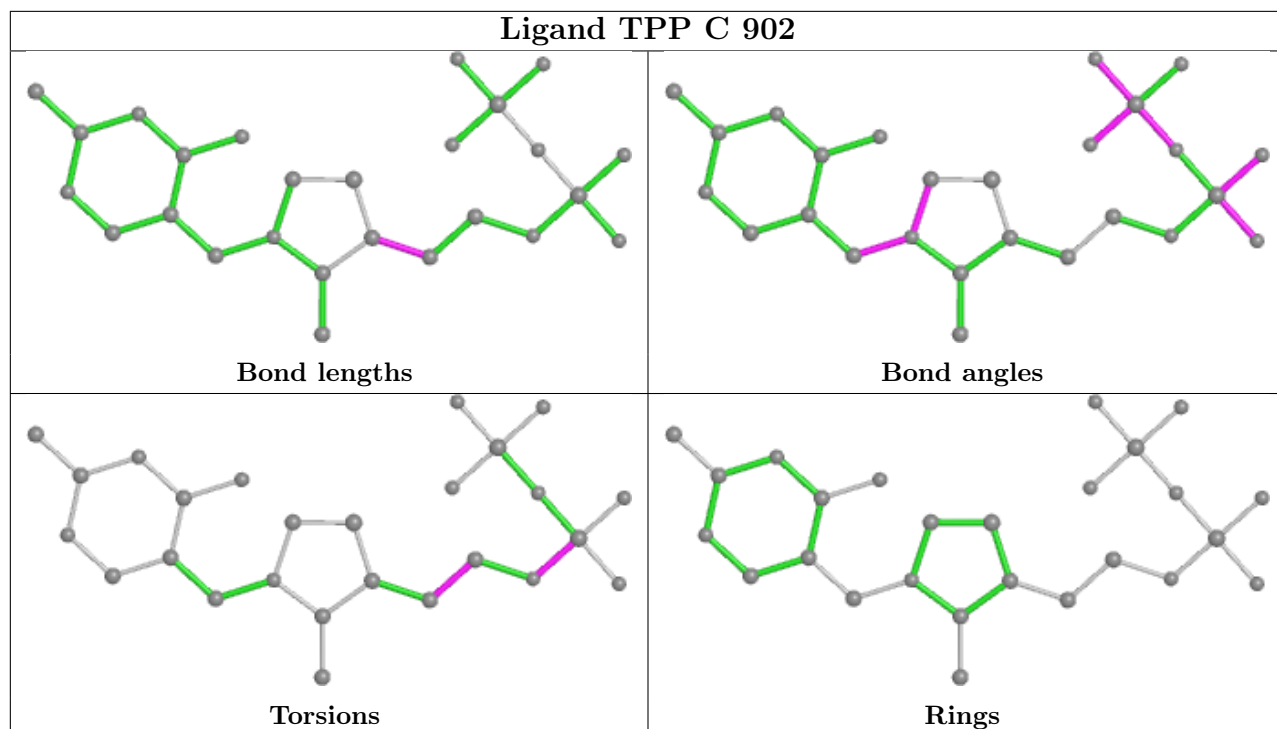
16 monomers are involved in 51 short contacts:

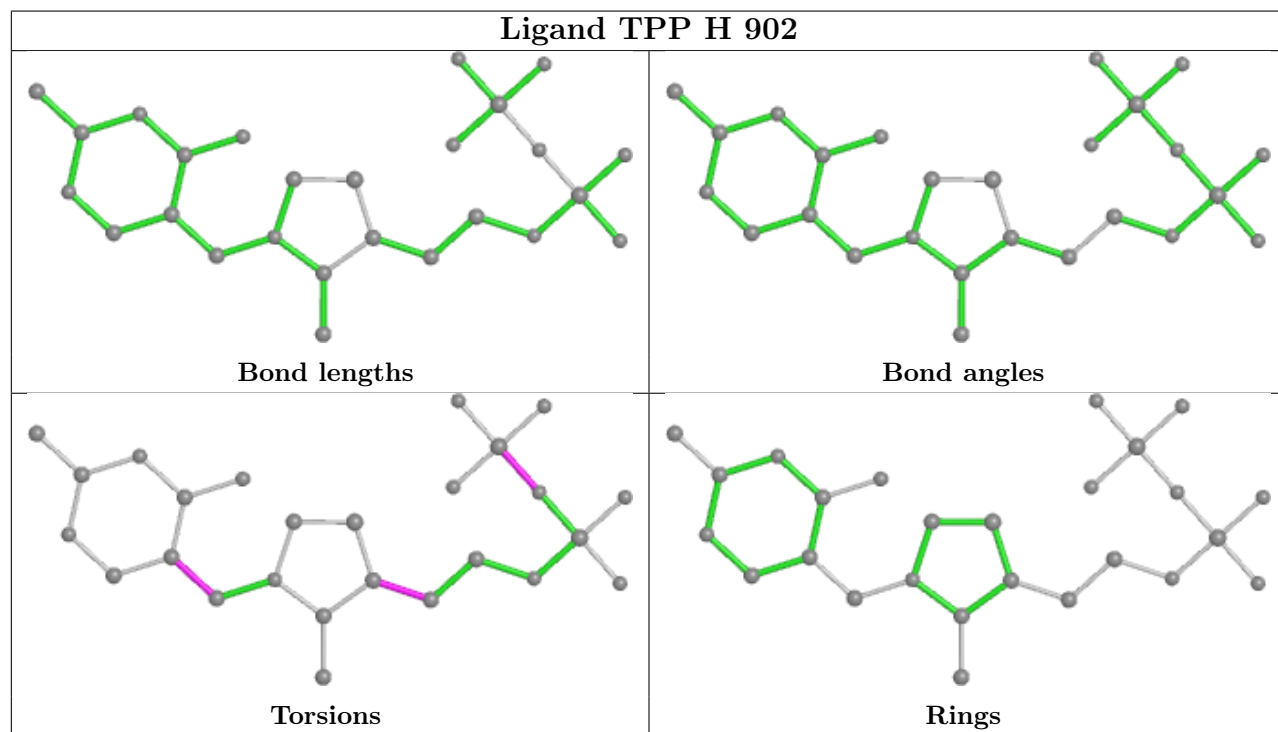
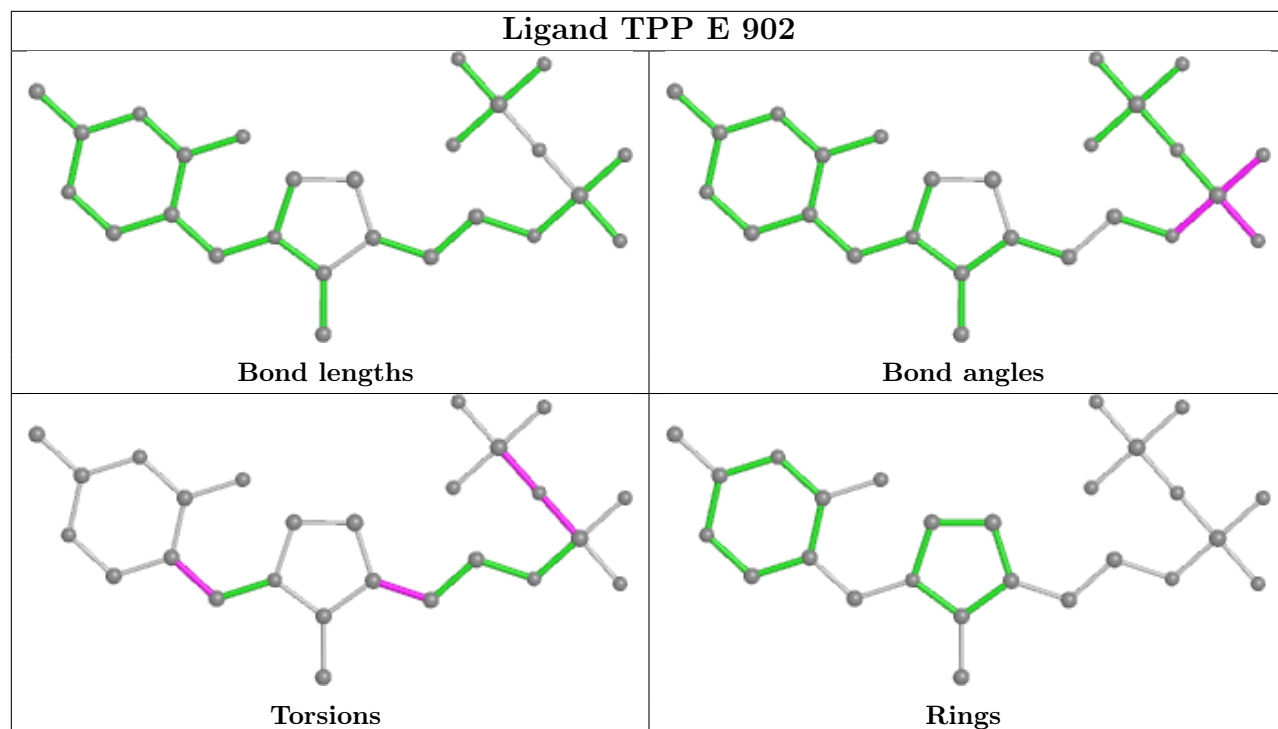
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	TPP	4	0
2	C	901	PEP	2	0
3	D	902	TPP	4	0
2	A	901	PEP	4	0
3	C	902	TPP	4	0
2	G	901	PEP	3	0
3	G	902	TPP	2	0
3	E	902	TPP	4	0
2	H	901	PEP	4	0
2	E	901	PEP	2	0
2	F	901	PEP	2	0
3	H	902	TPP	6	0
2	D	901	PEP	1	0
3	F	902	TPP	3	0
2	B	901	PEP	5	0
3	A	902	TPP	1	0

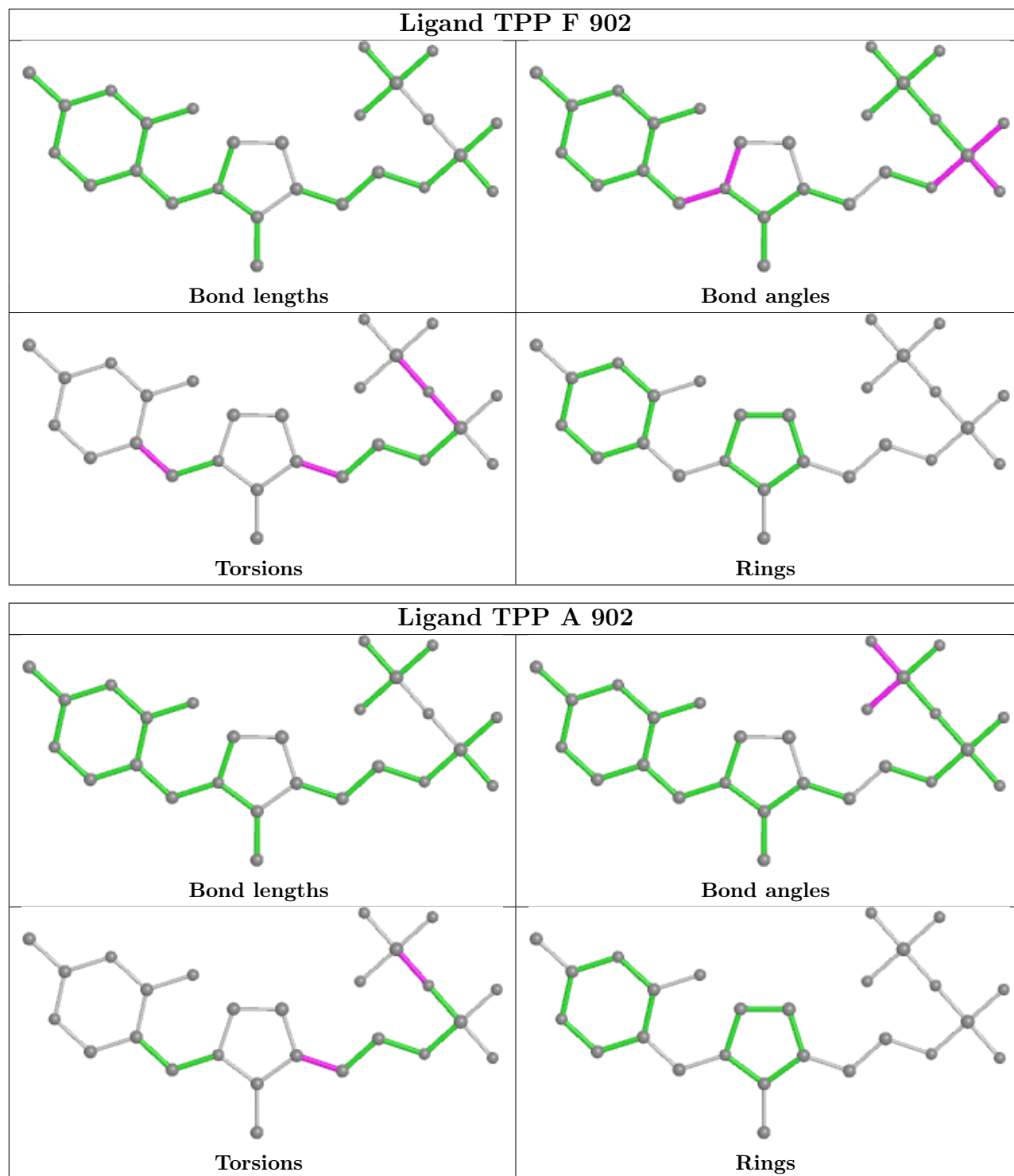
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

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%)	0.08	39 (4%) 30 32	29, 44, 68, 135	0
1	B	811/831 (97%)	0.10	49 (6%) 21 22	29, 43, 70, 157	0
1	C	806/831 (96%)	0.66	123 (15%) 2 1	43, 74, 108, 125	0
1	D	807/831 (97%)	0.54	105 (13%) 3 3	43, 71, 109, 132	0
1	E	809/831 (97%)	0.59	116 (14%) 2 2	35, 58, 101, 158	0
1	F	809/831 (97%)	0.60	112 (13%) 2 2	38, 62, 93, 144	0
1	G	807/831 (97%)	0.22	65 (8%) 12 12	29, 51, 86, 119	0
1	H	808/831 (97%)	0.37	84 (10%) 6 6	33, 55, 83, 131	0
All	All	6465/6648 (97%)	0.39	693 (10%) 6 5	29, 57, 99, 158	0

All (693) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	507	VAL	7.6
1	E	808	THR	7.5
1	F	157	LEU	7.1
1	C	399	VAL	7.1
1	F	512	LEU	6.4
1	E	507	VAL	6.2
1	E	809	ASP	6.1
1	E	508	ILE	6.1
1	C	507	VAL	6.0
1	F	507	VAL	6.0
1	H	512	LEU	5.8
1	C	159	TYR	5.8
1	E	503	SER	5.8
1	E	558	VAL	5.7
1	C	157	LEU	5.7
1	E	505	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	508	ILE	5.6
1	F	808	THR	5.6
1	D	506	HIS	5.4
1	C	696	ALA	5.4
1	H	157	LEU	5.4
1	H	507	VAL	5.3
1	F	156	GLU	5.3
1	F	561	VAL	5.3
1	H	508	ILE	5.3
1	C	561	VAL	5.2
1	E	633	THR	5.2
1	E	506	HIS	5.2
1	G	507	VAL	5.1
1	E	630	TRP	5.0
1	H	159	TYR	5.0
1	G	508	ILE	5.0
1	E	561	VAL	5.0
1	C	657	ALA	5.0
1	C	508	ILE	5.0
1	E	668	LYS	5.0
1	H	510	SER	4.9
1	C	189	PRO	4.9
1	F	159	TYR	4.9
1	D	508	ILE	4.9
1	C	768	ASP	4.8
1	D	562	LEU	4.8
1	F	190	LEU	4.7
1	H	511	MET	4.7
1	F	505	VAL	4.7
1	D	510	SER	4.7
1	G	552	SER	4.7
1	F	506	HIS	4.6
1	F	809	ASP	4.6
1	A	507	VAL	4.6
1	E	402	TYR	4.6
1	E	504	PHE	4.6
1	F	189	PRO	4.5
1	D	561	VAL	4.5
1	E	669	PHE	4.5
1	F	510	SER	4.5
1	B	508	ILE	4.5
1	D	503	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	808	THR	4.4
1	E	556	PRO	4.4
1	F	480	HIS	4.4
1	F	160	ALA	4.4
1	E	157	LEU	4.4
1	E	774	ILE	4.4
1	F	158	GLY	4.3
1	C	510	SER	4.3
1	E	557	GLY	4.3
1	H	558	VAL	4.3
1	E	552	SER	4.2
1	E	403	GLY	4.2
1	G	504	PHE	4.2
1	D	480	HIS	4.2
1	D	512	LEU	4.2
1	C	511	MET	4.2
1	H	561	VAL	4.2
1	E	635	LYS	4.2
1	C	161	LEU	4.1
1	D	158	GLY	4.1
1	A	508	ILE	4.1
1	F	155	GLY	4.1
1	E	772	ASP	4.1
1	F	511	MET	4.1
1	E	510	SER	4.1
1	H	505	VAL	4.1
1	H	562	LEU	4.1
1	E	773	LYS	4.1
1	G	505	VAL	4.0
1	E	562	LEU	4.0
1	D	159	TYR	4.0
1	D	558	VAL	4.0
1	E	555	ASP	4.0
1	C	394	TYR	4.0
1	E	770	TYR	4.0
1	E	502	GLU	4.0
1	G	506	HIS	4.0
1	C	512	LEU	4.0
1	C	124	ALA	4.0
1	H	506	HIS	3.9
1	E	187	THR	3.9
1	C	558	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	350	PHE	3.8
1	C	626	ALA	3.8
1	D	505	VAL	3.8
1	H	509	ASP	3.8
1	D	539	VAL	3.8
1	C	480	HIS	3.8
1	D	157	LEU	3.8
1	G	512	LEU	3.8
1	H	808	THR	3.8
1	E	425	ASN	3.8
1	F	509	ASP	3.8
1	C	158	GLY	3.8
1	C	772	ASP	3.8
1	C	156	GLU	3.8
1	B	507	VAL	3.8
1	C	770	TYR	3.7
1	F	95	PRO	3.7
1	D	703	LYS	3.7
1	D	400	ALA	3.7
1	A	558	VAL	3.7
1	G	561	VAL	3.7
1	E	549	ASN	3.7
1	H	156	GLU	3.7
1	H	190	LEU	3.7
1	E	543	VAL	3.7
1	G	503	SER	3.7
1	C	190	LEU	3.6
1	C	95	PRO	3.6
1	H	189	PRO	3.6
1	E	512	LEU	3.6
1	F	558	VAL	3.6
1	E	643	VAL	3.6
1	F	335	GLU	3.6
1	B	157	LEU	3.6
1	B	512	LEU	3.6
1	C	658	ALA	3.6
1	C	403	GLY	3.6
1	F	334	PHE	3.6
1	A	157	LEU	3.6
1	G	157	LEU	3.6
1	F	353	ASN	3.6
1	B	810	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	517	LYS	3.6
1	C	662	LEU	3.5
1	F	154	GLY	3.5
1	D	394	TYR	3.5
1	H	180	VAL	3.5
1	C	154	GLY	3.5
1	F	354	GLY	3.5
1	F	192	THR	3.5
1	B	159	TYR	3.5
1	A	512	LEU	3.5
1	G	511	MET	3.5
1	A	561	VAL	3.5
1	G	762	LEU	3.5
1	E	767	ALA	3.5
1	E	553	HIS	3.5
1	F	514	GLN	3.5
1	C	700	THR	3.5
1	D	619	ALA	3.5
1	E	771	ALA	3.5
1	C	180	VAL	3.5
1	C	684	LYS	3.5
1	E	479	GLU	3.4
1	F	771	ALA	3.4
1	A	505	VAL	3.4
1	B	558	VAL	3.4
1	B	809	ASP	3.4
1	C	506	HIS	3.4
1	F	504	PHE	3.4
1	D	478	SER	3.4
1	F	124	ALA	3.4
1	H	517	LYS	3.4
1	B	505	VAL	3.4
1	C	152	HIS	3.4
1	F	478	SER	3.4
1	D	617	ALA	3.4
1	H	809	ASP	3.4
1	F	562	LEU	3.3
1	C	771	ALA	3.3
1	F	359	ASP	3.3
1	D	511	MET	3.3
1	B	480	HIS	3.3
1	E	807	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	190	LEU	3.3
1	C	625	ALA	3.3
1	C	479	GLU	3.3
1	E	554	GLN	3.3
1	G	558	VAL	3.3
1	C	478	SER	3.3
1	C	614	LEU	3.3
1	C	699	PHE	3.3
1	D	757	LEU	3.3
1	F	513	ASN	3.3
1	G	478	SER	3.3
1	D	552	SER	3.3
1	C	92	ILE	3.3
1	E	551	PHE	3.3
1	E	666	GLY	3.3
1	F	807	ASN	3.3
1	E	634	ALA	3.3
1	C	162	SER	3.3
1	E	762	LEU	3.2
1	G	477	LEU	3.2
1	C	765	ILE	3.2
1	E	404	HIS	3.2
1	A	509	ASP	3.2
1	H	480	HIS	3.2
1	D	626	ALA	3.2
1	G	787	PHE	3.2
1	C	390	ASN	3.2
1	C	393	ASP	3.2
1	H	537	LEU	3.2
1	C	160	ALA	3.2
1	E	158	GLY	3.2
1	B	180	VAL	3.2
1	D	479	GLU	3.2
1	E	602	ILE	3.2
1	E	480	HIS	3.2
1	C	402	TYR	3.1
1	D	563	LEU	3.2
1	G	400	ALA	3.1
1	H	53	THR	3.1
1	H	160	ALA	3.1
1	D	744	TYR	3.1
1	G	509	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	541	SER	3.1
1	C	637	ASN	3.1
1	H	54	ARG	3.1
1	C	773	LYS	3.1
1	D	418	TYR	3.1
1	D	493	GLY	3.1
1	H	478	SER	3.1
1	C	179	ILE	3.1
1	D	504	PHE	3.1
1	H	334	PHE	3.1
1	D	509	ASP	3.1
1	C	767	ALA	3.1
1	D	640	ALA	3.1
1	E	185	ALA	3.1
1	G	808	THR	3.1
1	B	189	PRO	3.1
1	E	769	LYS	3.1
1	C	807	ASN	3.1
1	G	557	GLY	3.1
1	H	564	ASN	3.1
1	A	159	TYR	3.1
1	E	712	TYR	3.1
1	D	798	TYR	3.1
1	E	418	TYR	3.1
1	D	614	LEU	3.1
1	E	665	LEU	3.1
1	G	480	HIS	3.1
1	A	189	PRO	3.0
1	E	189	PRO	3.0
1	F	575	ILE	3.0
1	E	621	LEU	3.0
1	G	160	ALA	3.0
1	H	158	GLY	3.0
1	F	153	GLU	3.0
1	D	537	LEU	3.0
1	F	187	THR	3.0
1	B	561	VAL	3.0
1	C	397	LYS	3.0
1	D	406	TRP	3.0
1	H	514	GLN	3.0
1	B	811	LYS	3.0
1	E	560	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	777	LEU	3.0
1	D	627	ALA	3.0
1	G	396	VAL	3.0
1	B	190	LEU	3.0
1	E	662	LEU	3.0
1	H	187	THR	3.0
1	C	617	ALA	3.0
1	F	477	LEU	3.0
1	F	482	MET	3.0
1	F	92	ILE	3.0
1	F	162	SER	3.0
1	B	191	ALA	3.0
1	E	810	LYS	3.0
1	C	155	GLY	3.0
1	F	94	GLY	3.0
1	H	513	ASN	3.0
1	A	602	ILE	2.9
1	D	388	LEU	2.9
1	F	126	LEU	2.9
1	C	94	GLY	2.9
1	C	396	VAL	2.9
1	C	509	ASP	2.9
1	C	562	LEU	2.9
1	F	539	VAL	2.9
1	E	478	SER	2.9
1	D	637	ASN	2.9
1	G	807	ASN	2.9
1	E	803	TYR	2.9
1	A	504	PHE	2.9
1	D	575	ILE	2.9
1	D	600	ALA	2.9
1	E	758	THR	2.9
1	D	754	ARG	2.9
1	H	163	HIS	2.9
1	B	179	ILE	2.9
1	G	551	PHE	2.9
1	G	189	PRO	2.9
1	E	477	LEU	2.9
1	F	47	LEU	2.9
1	H	50	GLU	2.9
1	H	563	LEU	2.9
1	H	155	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	52	PHE	2.9
1	H	774	ILE	2.9
1	F	327	ALA	2.9
1	C	557	GLY	2.8
1	D	393	ASP	2.8
1	E	500	SER	2.8
1	H	153	GLU	2.8
1	D	92	ILE	2.8
1	B	158	GLY	2.8
1	H	94	GLY	2.8
1	F	163	HIS	2.8
1	A	331	GLU	2.8
1	H	331	GLU	2.8
1	H	573	ILE	2.8
1	H	162	SER	2.8
1	F	402	TYR	2.8
1	C	389	PRO	2.8
1	D	189	PRO	2.8
1	B	92	ILE	2.8
1	H	52	PHE	2.8
1	E	667	VAL	2.8
1	D	402	TYR	2.8
1	C	20	GLU	2.8
1	B	509	ASP	2.8
1	C	151	ILE	2.8
1	D	602	ILE	2.8
1	D	657	ALA	2.8
1	F	188	GLY	2.8
1	F	161	LEU	2.8
1	A	552	SER	2.8
1	D	611	TRP	2.7
1	E	405	GLY	2.7
1	E	670	LYS	2.7
1	F	501	TYR	2.7
1	B	160	ALA	2.7
1	F	352	ALA	2.7
1	H	498	TRP	2.7
1	G	767	ALA	2.7
1	E	501	TYR	2.7
1	F	349	LEU	2.7
1	H	504	PHE	2.7
1	D	772	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	557	GLY	2.7
1	E	550	GLY	2.7
1	C	627	ALA	2.7
1	H	696	ALA	2.7
1	D	500	SER	2.7
1	F	500	SER	2.7
1	C	498	TRP	2.7
1	A	511	MET	2.7
1	F	557	GLY	2.7
1	C	661	LYS	2.7
1	H	49	LYS	2.7
1	D	784	ALA	2.7
1	E	391	LEU	2.7
1	C	630	TRP	2.7
1	E	768	ASP	2.7
1	A	190	LEU	2.7
1	C	404	HIS	2.7
1	C	537	LEU	2.7
1	D	780	PHE	2.7
1	F	341	LEU	2.7
1	G	562	LEU	2.7
1	A	809	ASP	2.7
1	C	505	VAL	2.6
1	C	261	ARG	2.6
1	E	559	THR	2.6
1	E	614	LEU	2.6
1	F	142	HIS	2.6
1	E	154	GLY	2.6
1	D	501	TYR	2.6
1	G	555	ASP	2.6
1	F	503	SER	2.6
1	D	631	ALA	2.6
1	C	391	LEU	2.6
1	E	664	GLU	2.6
1	E	734	TYR	2.6
1	A	510	SER	2.6
1	C	759	ALA	2.6
1	H	332	ALA	2.6
1	E	156	GLU	2.6
1	G	765	ILE	2.6
1	E	159	TYR	2.6
1	D	392	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	510	SER	2.6
1	D	807	ASN	2.6
1	E	509	ASP	2.6
1	G	161	LEU	2.6
1	D	389	PRO	2.6
1	H	482	MET	2.6
1	A	478	SER	2.6
1	C	163	HIS	2.6
1	H	500	SER	2.6
1	E	738	GLY	2.6
1	G	190	LEU	2.6
1	F	479	GLU	2.6
1	C	481	GLN	2.6
1	D	162	SER	2.6
1	D	582	ASN	2.6
1	C	131	ARG	2.6
1	D	767	ALA	2.6
1	B	539	VAL	2.6
1	F	180	VAL	2.6
1	H	336	VAL	2.6
1	H	179	ILE	2.6
1	H	515	HIS	2.6
1	D	753	ASP	2.6
1	B	808	THR	2.5
1	C	330	THR	2.5
1	E	400	ALA	2.5
1	F	185	ALA	2.5
1	G	192	THR	2.5
1	D	514	GLN	2.5
1	C	618	ARG	2.5
1	E	548	HIS	2.5
1	F	666	GLY	2.5
1	G	549	ASN	2.5
1	F	194	TRP	2.5
1	G	764	MET	2.5
1	C	691	THR	2.5
1	H	327	ALA	2.5
1	C	669	PHE	2.5
1	A	480	HIS	2.5
1	A	506	HIS	2.5
1	F	97	HIS	2.5
1	G	479	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	767	ALA	2.5
1	F	332	ALA	2.5
1	D	391	LEU	2.5
1	D	751	ARG	2.5
1	E	539	VAL	2.5
1	E	776	GLU	2.5
1	H	479	GLU	2.5
1	E	180	VAL	2.5
1	D	155	GLY	2.5
1	F	179	ILE	2.5
1	G	397	LYS	2.5
1	G	406	TRP	2.5
1	B	602	ILE	2.5
1	G	392	GLU	2.5
1	H	598	ILE	2.5
1	C	93	MET	2.5
1	F	387	LYS	2.5
1	C	556	PRO	2.5
1	F	697	ASP	2.5
1	D	192	THR	2.5
1	D	636	ASN	2.5
1	C	356	VAL	2.5
1	D	670	LYS	2.5
1	H	575	ILE	2.5
1	C	702	ASP	2.5
1	E	188	GLY	2.5
1	E	657	ALA	2.5
1	F	390	ASN	2.5
1	F	484	GLY	2.5
1	F	34	TYR	2.4
1	G	180	VAL	2.4
1	D	773	LYS	2.4
1	H	192	THR	2.4
1	H	477	LEU	2.4
1	H	770	TYR	2.4
1	E	511	MET	2.4
1	F	181	GLY	2.4
1	F	481	GLN	2.4
1	F	810	LYS	2.4
1	C	352	ALA	2.4
1	B	552	SER	2.4
1	D	180	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	711	SER	2.4
1	F	560	SER	2.4
1	D	397	LYS	2.4
1	F	93	MET	2.4
1	B	187	THR	2.4
1	C	192	THR	2.4
1	C	400	ALA	2.4
1	G	152	HIS	2.4
1	C	401	GLU	2.4
1	A	807	ASN	2.4
1	C	513	ASN	2.4
1	E	755	TYR	2.4
1	H	484	GLY	2.4
1	C	184	GLU	2.4
1	E	498	TRP	2.4
1	E	628	TRP	2.4
1	A	600	ALA	2.4
1	G	619	ALA	2.4
1	A	775	ASP	2.4
1	E	546	GLN	2.4
1	A	188	GLY	2.4
1	C	774	ILE	2.4
1	D	502	GLU	2.4
1	D	755	TYR	2.4
1	B	435	PRO	2.4
1	H	600	ALA	2.4
1	C	187	THR	2.4
1	A	503	SER	2.4
1	B	478	SER	2.4
1	C	514	GLN	2.4
1	C	690	LEU	2.4
1	F	96	GLY	2.4
1	G	158	GLY	2.4
1	E	593	LYS	2.4
1	B	511	MET	2.4
1	E	179	ILE	2.4
1	G	575	ILE	2.4
1	C	712	TYR	2.4
1	C	631	ALA	2.4
1	B	500	SER	2.4
1	F	42	LEU	2.4
1	H	557	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	95	PRO	2.3
1	F	422	ILE	2.3
1	G	768	ASP	2.3
1	C	191	ALA	2.3
1	E	696	ALA	2.3
1	D	632	SER	2.3
1	C	484	GLY	2.3
1	F	564	ASN	2.3
1	D	628	TRP	2.3
1	F	630	TRP	2.3
1	B	211	ILE	2.3
1	F	191	ALA	2.3
1	H	767	ALA	2.3
1	F	141	SER	2.3
1	A	513	ASN	2.3
1	H	188	GLY	2.3
1	H	807	ASN	2.3
1	G	482	MET	2.3
1	A	187	THR	2.3
1	C	613	THR	2.3
1	E	426	ASN	2.3
1	E	401	GLU	2.3
1	G	712	TYR	2.3
1	B	161	LEU	2.3
1	F	57	VAL	2.3
1	B	93	MET	2.3
1	G	93	MET	2.3
1	G	401	GLU	2.3
1	G	693	GLU	2.3
1	A	500	SER	2.3
1	B	193	GLY	2.3
1	G	162	SER	2.3
1	G	560	SER	2.3
1	C	329	ASP	2.3
1	C	782	ASP	2.3
1	G	159	TYR	2.3
1	A	161	LEU	2.3
1	B	506	HIS	2.3
1	F	537	LEU	2.3
1	H	161	LEU	2.3
1	A	537	LEU	2.3
1	D	156	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	779	LYS	2.2
1	B	154	GLY	2.2
1	B	812	GLY	2.2
1	D	396	VAL	2.2
1	C	629	ASP	2.2
1	E	804	SER	2.2
1	D	639	GLU	2.2
1	G	187	THR	2.2
1	C	806	VAL	2.2
1	G	806	VAL	2.2
1	D	401	GLU	2.2
1	B	504	PHE	2.2
1	D	160	ALA	2.2
1	B	537	LEU	2.2
1	C	686	ASN	2.2
1	H	154	GLY	2.2
1	C	552	SER	2.2
1	C	682	SER	2.2
1	F	552	SER	2.2
1	F	151	ILE	2.2
1	C	695	PHE	2.2
1	H	51	PRO	2.2
1	G	154	GLY	2.2
1	C	755	TYR	2.2
1	B	503	SER	2.2
1	E	540	SER	2.2
1	G	543	VAL	2.2
1	D	774	ILE	2.2
1	G	92	ILE	2.2
1	H	191	ALA	2.2
1	C	398	GLU	2.2
1	C	776	GLU	2.2
1	D	549	ASN	2.2
1	E	387	LYS	2.2
1	E	390	ASN	2.2
1	E	791	ASN	2.2
1	B	600	ALA	2.2
1	F	516	ALA	2.2
1	B	768	ASP	2.2
1	C	485	PHE	2.2
1	D	556	PRO	2.2
1	F	193	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	353	ASN	2.2
1	D	179	ILE	2.2
1	D	425	ASN	2.2
1	H	193	GLY	2.2
1	D	776	GLU	2.2
1	H	338	LYS	2.1
1	E	710	HIS	2.1
1	F	543	VAL	2.1
1	G	550	GLY	2.1
1	F	502	GLU	2.1
1	B	562	LEU	2.1
1	F	49	LYS	2.1
1	C	804	SER	2.1
1	C	791	ASN	2.1
1	D	390	ASN	2.1
1	D	513	ASN	2.1
1	D	770	TYR	2.1
1	B	188	GLY	2.1
1	D	630	TRP	2.1
1	E	181	GLY	2.1
1	H	55	GLU	2.1
1	C	52	PHE	2.1
1	F	130	PHE	2.1
1	G	553	HIS	2.1
1	B	155	GLY	2.1
1	F	128	LYS	2.1
1	F	565	LYS	2.1
1	G	191	ALA	2.1
1	D	633	THR	2.1
1	A	556	PRO	2.1
1	F	598	ILE	2.1
1	G	179	ILE	2.1
1	E	388	LEU	2.1
1	D	188	GLY	2.1
1	F	521	ALA	2.1
1	D	2	THR	2.1
1	C	766	ASP	2.1
1	E	629	ASP	2.1
1	C	188	GLY	2.1
1	G	94	GLY	2.1
1	C	408	GLN	2.1
1	A	806	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	185	ALA	2.1
1	F	693	GLU	2.1
1	A	772	ASP	2.1
1	H	565	LYS	2.1
1	H	560	SER	2.1
1	H	194	TRP	2.1
1	B	479	GLU	2.1
1	F	773	LYS	2.1
1	H	539	VAL	2.1
1	D	638	ASP	2.1
1	E	385	ASP	2.1
1	E	765	ILE	2.1
1	E	659	SER	2.1
1	H	552	SER	2.1
1	F	476	GLN	2.1
1	F	50	GLU	2.1
1	B	178	ALA	2.0
1	D	178	ALA	2.0
1	E	627	ALA	2.0
1	F	51	PRO	2.0
1	H	95	PRO	2.0
1	H	389	PRO	2.0
1	C	559	THR	2.0
1	F	515	HIS	2.0
1	E	638	ASP	2.0
1	H	759	ALA	2.0
1	G	449	VAL	2.0
1	H	2	THR	2.0
1	D	481	GLN	2.0
1	D	668	LYS	2.0
1	D	161	LEU	2.0
1	F	98	GLY	2.0
1	E	775	ASP	2.0
1	D	435	PRO	2.0
1	F	556	PRO	2.0
1	D	613	THR	2.0
1	D	564	ASN	2.0
1	D	672	VAL	2.0
1	A	154	GLY	2.0
1	B	560	SER	2.0
1	C	96	GLY	2.0
1	F	804	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	181	GLY	2.0
1	C	135	TYR	2.0
1	C	363	PHE	2.0
1	E	744	TYR	2.0
1	A	93	MET	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 monosaccharides 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.

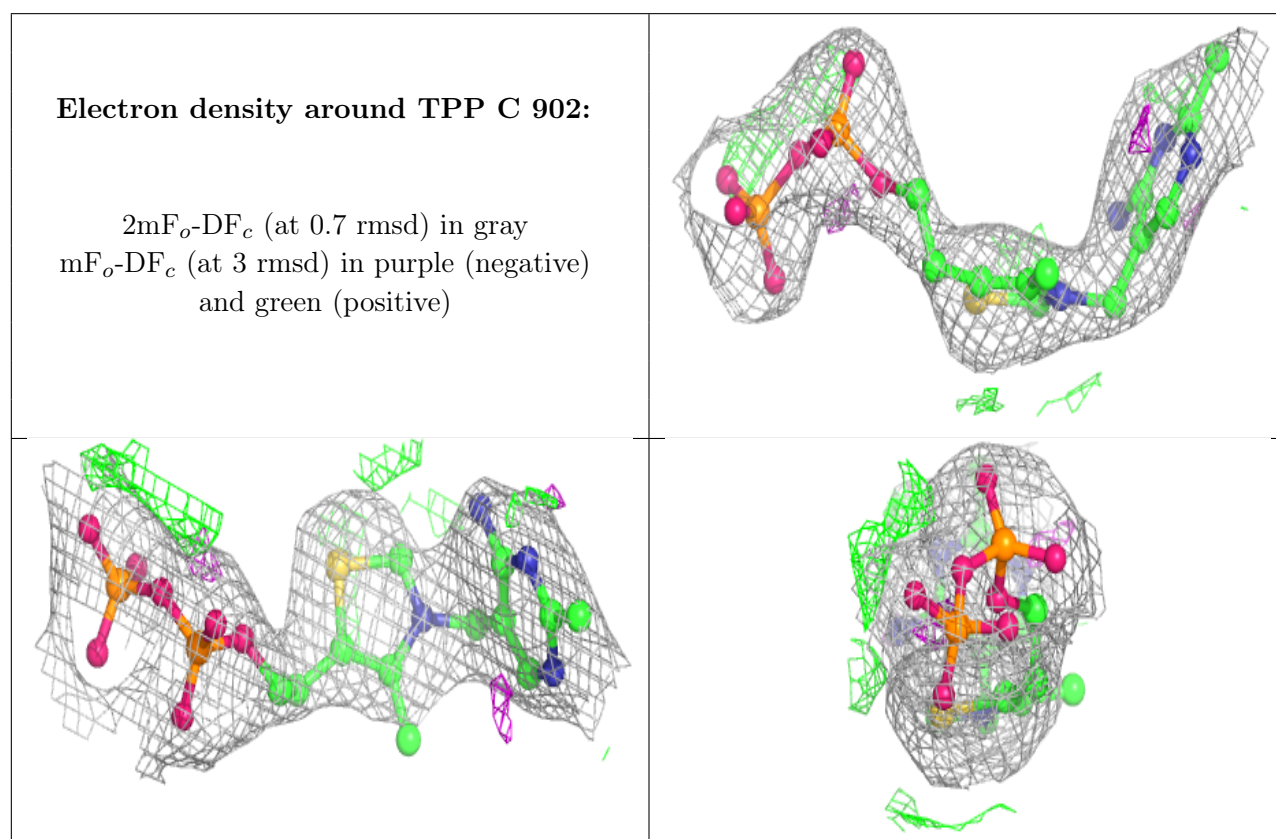
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEP	D	901	10/10	0.91	0.60	63,77,83,85	10
2	PEP	E	901	10/10	0.91	0.73	59,66,80,80	10
4	CA	D	903	1/1	0.93	0.06	71,71,71,71	0
2	PEP	A	901	10/10	0.94	0.54	33,50,63,63	10
2	PEP	B	901	10/10	0.94	0.58	26,35,48,55	10
2	PEP	G	901	10/10	0.94	0.54	43,60,73,82	10
2	PEP	C	901	10/10	0.94	0.48	55,65,80,90	10
4	CA	H	903	1/1	0.95	0.10	74,74,74,74	0
3	TPP	C	902	26/26	0.96	0.23	43,55,72,80	0
4	CA	C	903	1/1	0.96	0.09	77,77,77,77	0
2	PEP	F	901	10/10	0.96	0.59	44,49,68,69	10
4	CA	F	903	1/1	0.96	0.04	78,78,78,78	0
2	PEP	H	901	10/10	0.96	0.46	43,46,63,71	10
3	TPP	B	902	26/26	0.97	0.22	29,36,41,43	0
3	TPP	D	902	26/26	0.97	0.16	46,53,65,68	0
4	CA	E	903	1/1	0.97	0.09	60,60,60,60	0
3	TPP	F	902	26/26	0.97	0.25	43,54,63,69	0
4	CA	B	903	1/1	0.97	0.08	52,52,52,52	0

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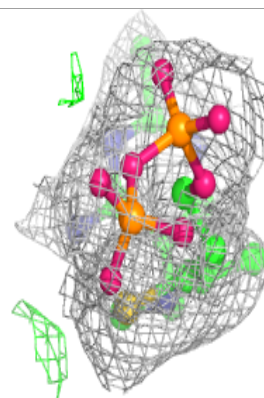
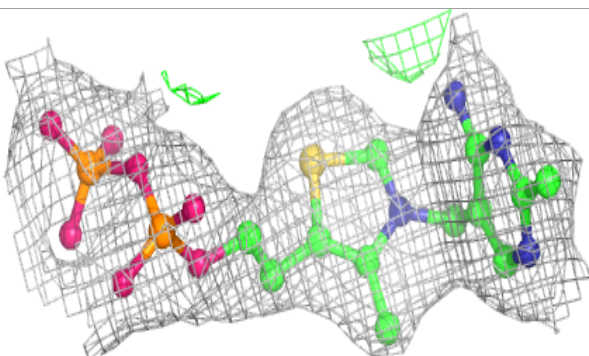
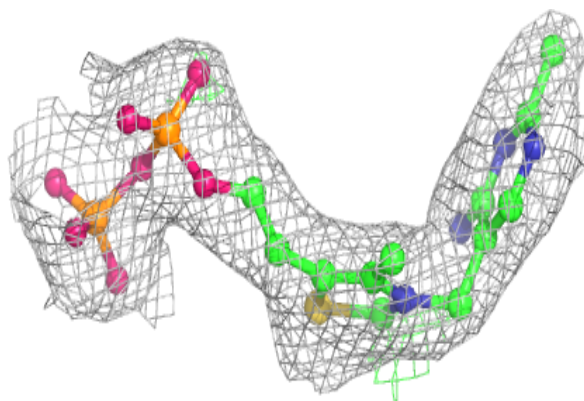
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TPP	A	902	26/26	0.98	0.21	27,35,48,59	0
3	TPP	G	902	26/26	0.98	0.18	32,44,49,55	0
3	TPP	H	902	26/26	0.98	0.21	38,48,54,56	0
4	CA	A	903	1/1	0.98	0.05	60,60,60,60	0
4	CA	G	903	1/1	0.98	0.06	52,52,52,52	0
3	TPP	E	902	26/26	0.98	0.20	34,46,52,55	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.

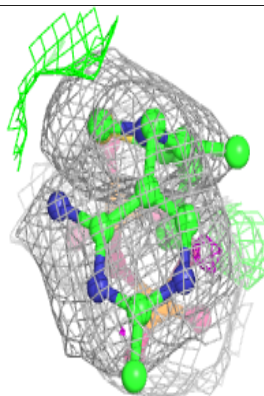
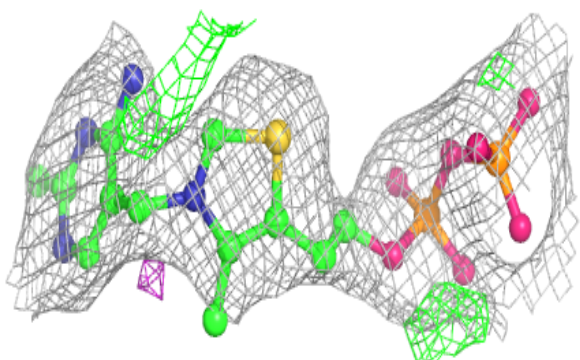
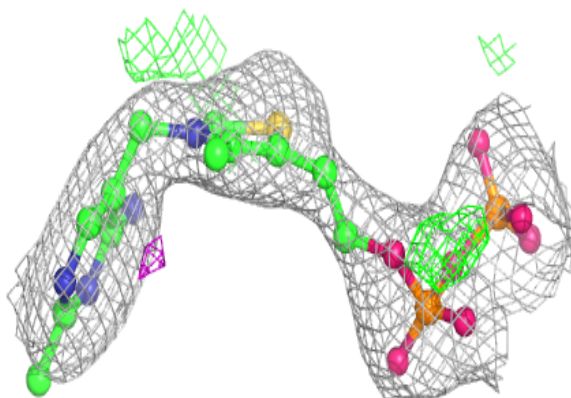


Electron density around TPP B 902:

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

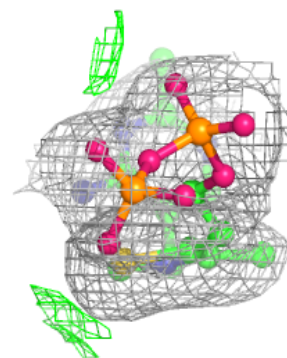
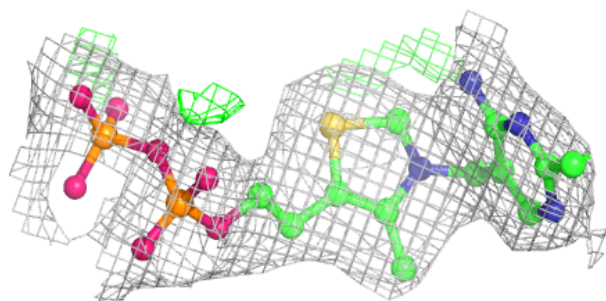
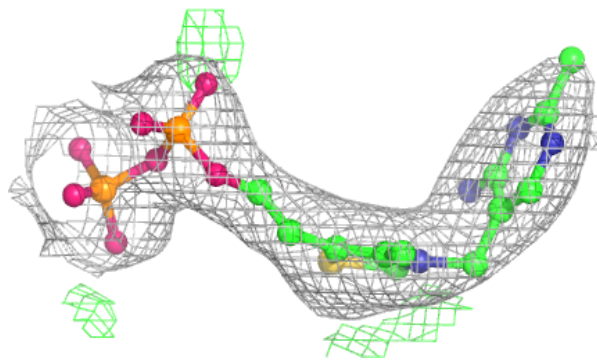
**Electron density around TPP D 902:**

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

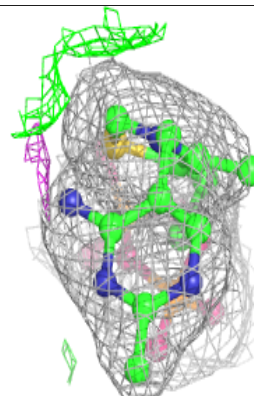
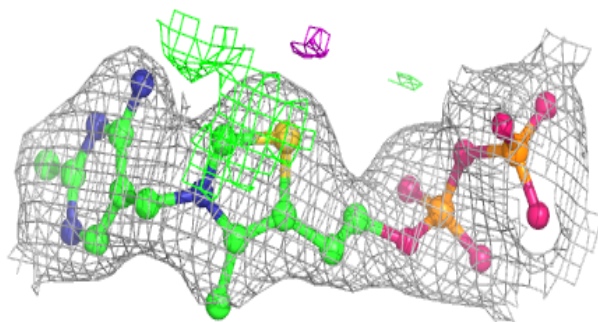
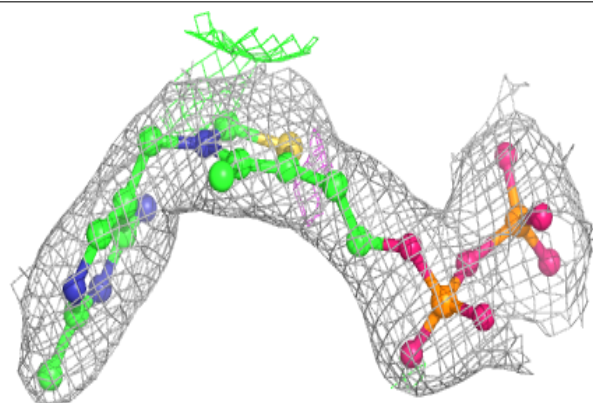


Electron density around TPP F 902:

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

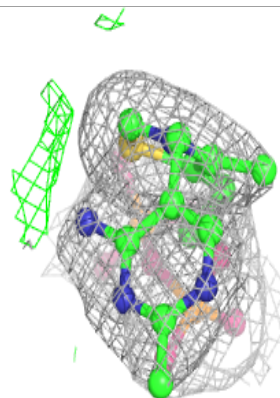
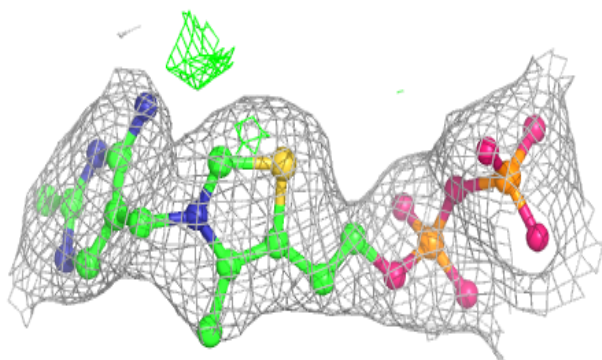
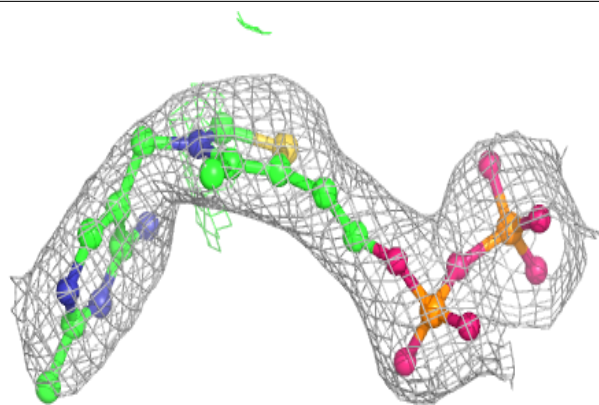
**Electron density around TPP A 902:**

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

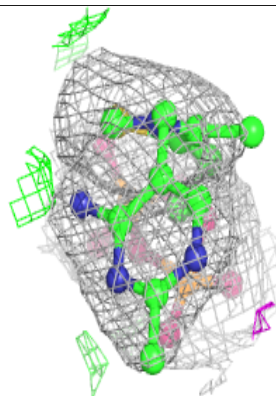
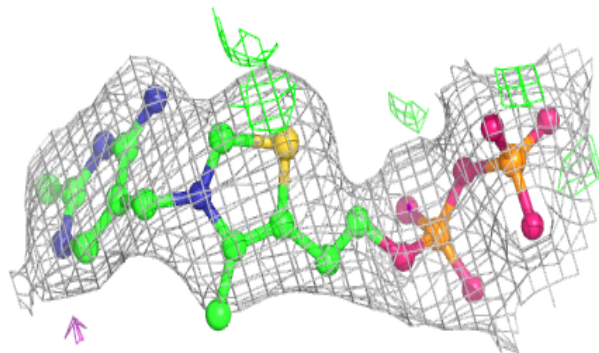
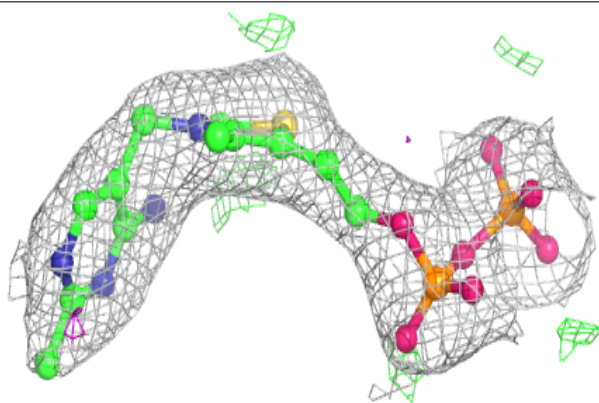


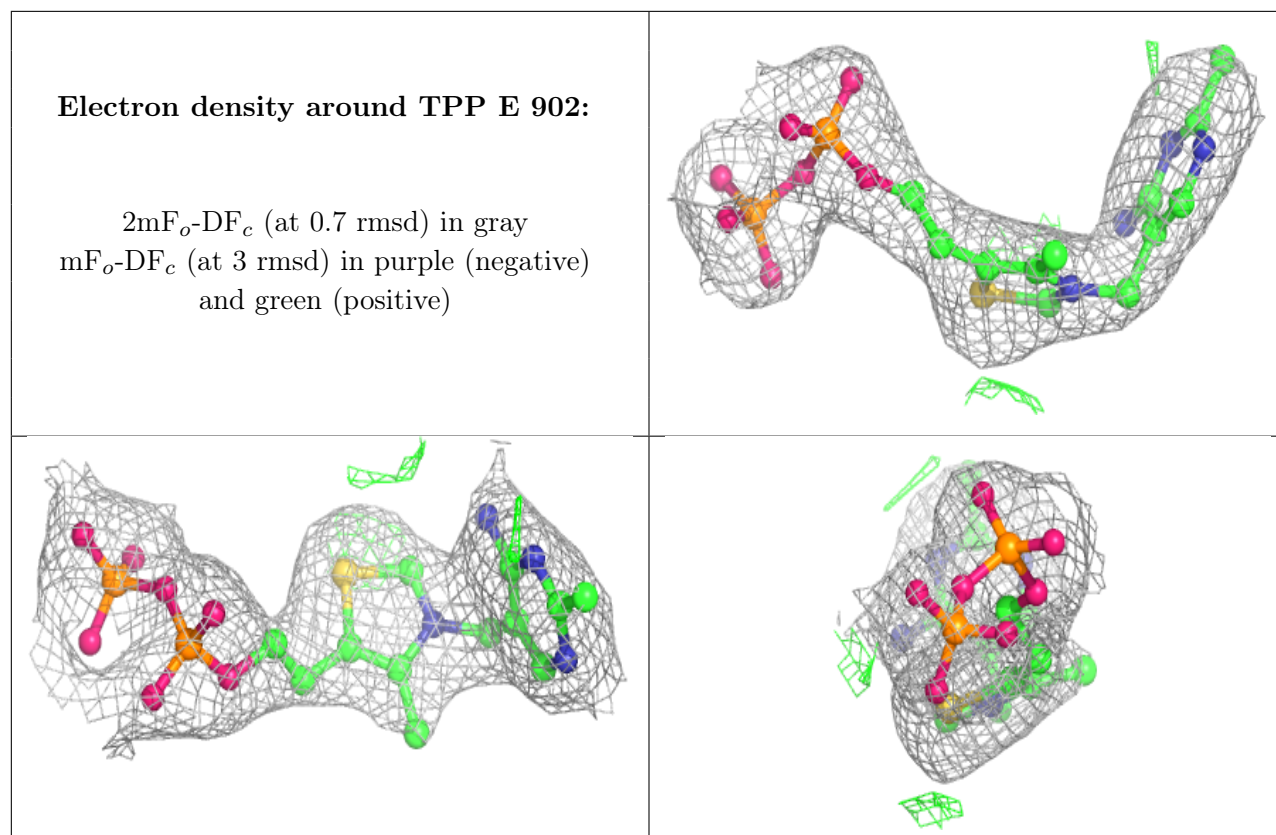
Electron density around TPP G 902:

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

**Electron density around TPP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.