



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:45 PM UTC

PDB ID : 3EXE / pdb_00003exe
Title : Crystal structure of the pyruvate dehydrogenase (E1p) component of human pyruvate dehydrogenase complex
Authors : Kato, M.; Wynn, R.M.; Chuang, J.L.; Tso, S.-C.; Machius, M.; Li, J.; Chuang, D.T.
Deposited on : 2008-10-16
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

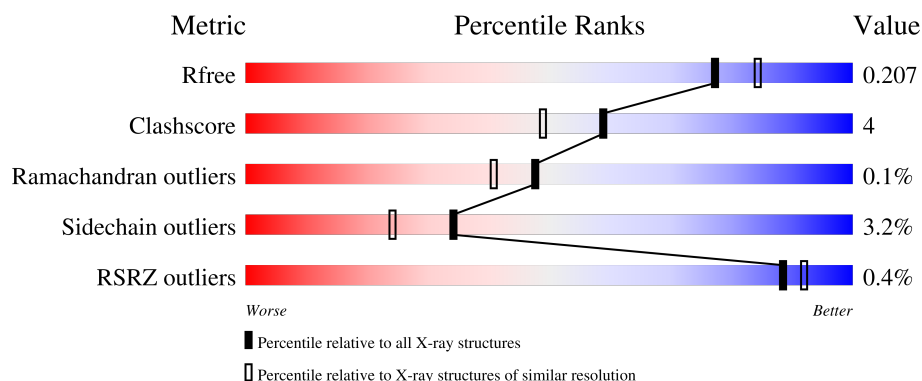
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	382	% 83% 12% 5%
1	C	382	 81% 13% • 5%
1	E	382	 78% 15% • 5%
1	G	382	% 81% 12% • 5%

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Mol	Chain	Length	Quality of chain
2	B	329	% 88% 12%
2	D	329	92% 7%
2	F	329	90% 9%
2	H	329	92% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23831 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 Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2836	1780	499	532	25			
1	C	362	Total	C	N	O	S	0	0	0
			2823	1772	496	531	24			
1	E	361	Total	C	N	O	S	0	0	0
			2818	1769	495	530	24			
1	G	362	Total	C	N	O	S	0	0	0
			2826	1774	496	531	25			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P08559
A	-19	GLY	-	expression tag	UNP P08559
A	-18	SER	-	expression tag	UNP P08559
A	-17	SER	-	expression tag	UNP P08559
A	-16	HIS	-	expression tag	UNP P08559
A	-15	HIS	-	expression tag	UNP P08559
A	-14	HIS	-	expression tag	UNP P08559
A	-13	HIS	-	expression tag	UNP P08559
A	-12	HIS	-	expression tag	UNP P08559
A	-11	HIS	-	expression tag	UNP P08559
A	-10	SER	-	expression tag	UNP P08559
A	-9	SER	-	expression tag	UNP P08559
A	-8	GLY	-	expression tag	UNP P08559
A	-7	LEU	-	expression tag	UNP P08559
A	-6	VAL	-	expression tag	UNP P08559
A	-5	PRO	-	expression tag	UNP P08559
A	-4	ARG	-	expression tag	UNP P08559
A	-3	GLY	-	expression tag	UNP P08559
A	-2	SER	-	expression tag	UNP P08559
A	-1	HIS	-	expression tag	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P08559
C	-20	MET	-	expression tag	UNP P08559
C	-19	GLY	-	expression tag	UNP P08559
C	-18	SER	-	expression tag	UNP P08559
C	-17	SER	-	expression tag	UNP P08559
C	-16	HIS	-	expression tag	UNP P08559
C	-15	HIS	-	expression tag	UNP P08559
C	-14	HIS	-	expression tag	UNP P08559
C	-13	HIS	-	expression tag	UNP P08559
C	-12	HIS	-	expression tag	UNP P08559
C	-11	HIS	-	expression tag	UNP P08559
C	-10	SER	-	expression tag	UNP P08559
C	-9	SER	-	expression tag	UNP P08559
C	-8	GLY	-	expression tag	UNP P08559
C	-7	LEU	-	expression tag	UNP P08559
C	-6	VAL	-	expression tag	UNP P08559
C	-5	PRO	-	expression tag	UNP P08559
C	-4	ARG	-	expression tag	UNP P08559
C	-3	GLY	-	expression tag	UNP P08559
C	-2	SER	-	expression tag	UNP P08559
C	-1	HIS	-	expression tag	UNP P08559
C	0	MET	-	expression tag	UNP P08559
E	-20	MET	-	expression tag	UNP P08559
E	-19	GLY	-	expression tag	UNP P08559
E	-18	SER	-	expression tag	UNP P08559
E	-17	SER	-	expression tag	UNP P08559
E	-16	HIS	-	expression tag	UNP P08559
E	-15	HIS	-	expression tag	UNP P08559
E	-14	HIS	-	expression tag	UNP P08559
E	-13	HIS	-	expression tag	UNP P08559
E	-12	HIS	-	expression tag	UNP P08559
E	-11	HIS	-	expression tag	UNP P08559
E	-10	SER	-	expression tag	UNP P08559
E	-9	SER	-	expression tag	UNP P08559
E	-8	GLY	-	expression tag	UNP P08559
E	-7	LEU	-	expression tag	UNP P08559
E	-6	VAL	-	expression tag	UNP P08559
E	-5	PRO	-	expression tag	UNP P08559
E	-4	ARG	-	expression tag	UNP P08559
E	-3	GLY	-	expression tag	UNP P08559
E	-2	SER	-	expression tag	UNP P08559
E	-1	HIS	-	expression tag	UNP P08559

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	expression tag	UNP P08559
G	-20	MET	-	expression tag	UNP P08559
G	-19	GLY	-	expression tag	UNP P08559
G	-18	SER	-	expression tag	UNP P08559
G	-17	SER	-	expression tag	UNP P08559
G	-16	HIS	-	expression tag	UNP P08559
G	-15	HIS	-	expression tag	UNP P08559
G	-14	HIS	-	expression tag	UNP P08559
G	-13	HIS	-	expression tag	UNP P08559
G	-12	HIS	-	expression tag	UNP P08559
G	-11	HIS	-	expression tag	UNP P08559
G	-10	SER	-	expression tag	UNP P08559
G	-9	SER	-	expression tag	UNP P08559
G	-8	GLY	-	expression tag	UNP P08559
G	-7	LEU	-	expression tag	UNP P08559
G	-6	VAL	-	expression tag	UNP P08559
G	-5	PRO	-	expression tag	UNP P08559
G	-4	ARG	-	expression tag	UNP P08559
G	-3	GLY	-	expression tag	UNP P08559
G	-2	SER	-	expression tag	UNP P08559
G	-1	HIS	-	expression tag	UNP P08559
G	0	MET	-	expression tag	UNP P08559

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	D	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	F	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	H	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

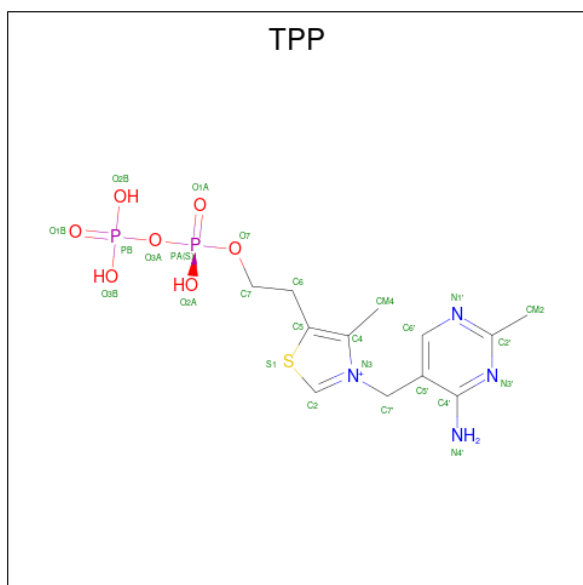
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	K	0	0
			1	1		
6	D	1	Total	K	0	0
			1	1		
6	F	1	Total	K	0	0
			1	1		
6	H	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	329	Total	O	0	0
			329	329		

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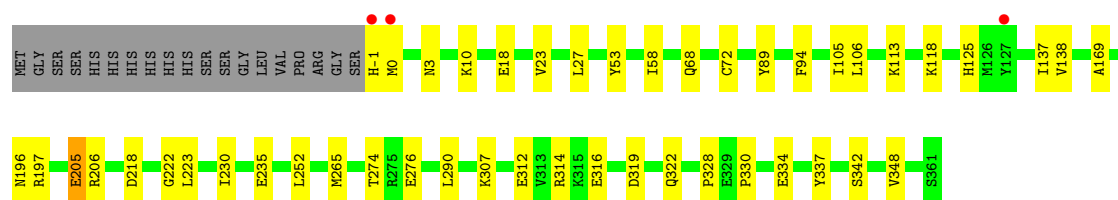
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	257	Total 257	O 257	0	0
7	C	301	Total 301	O 301	0	0
7	D	289	Total 289	O 289	0	0
7	E	287	Total 287	O 287	0	0
7	F	255	Total 255	O 255	0	0
7	G	317	Total 317	O 317	0	0
7	H	281	Total 281	O 281	0	0

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.

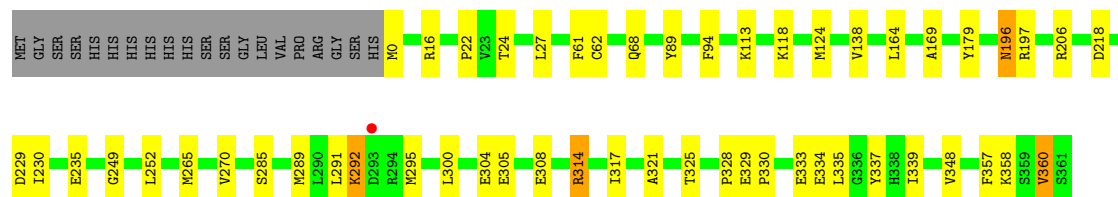
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain A: 



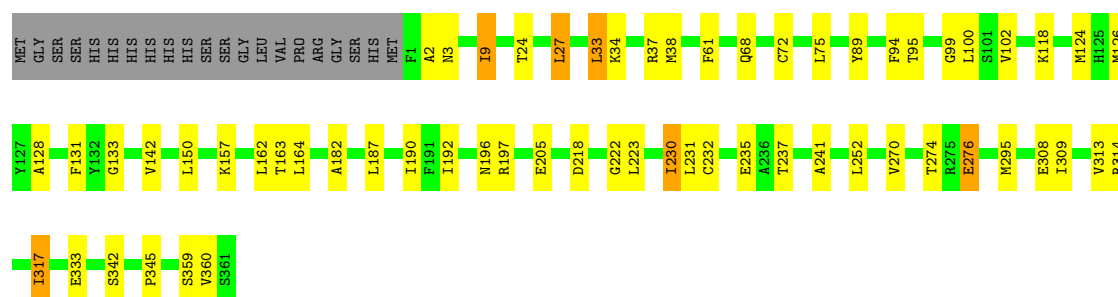
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain C: 

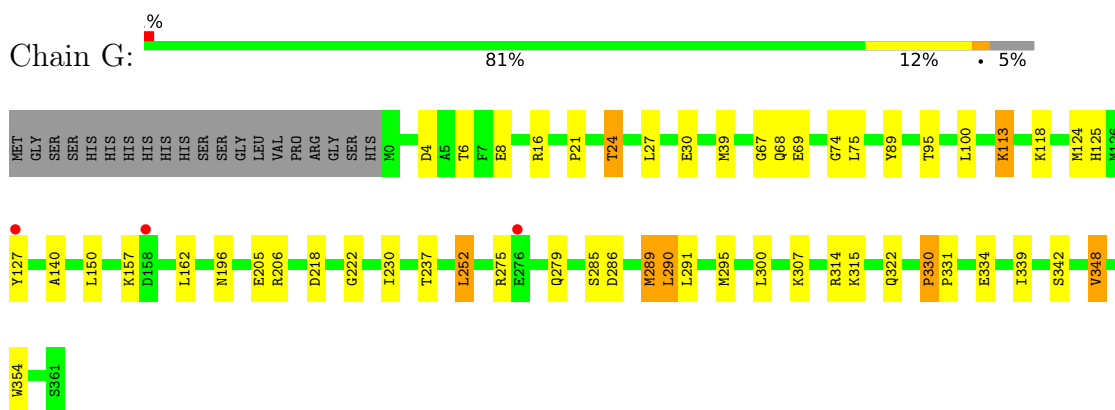


- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

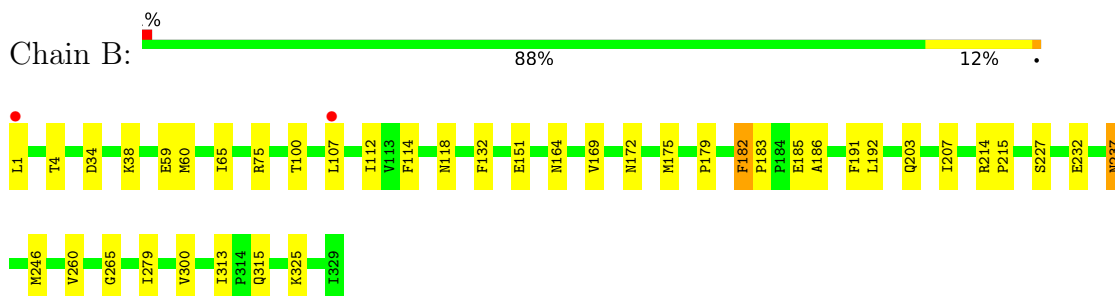
Chain E: 



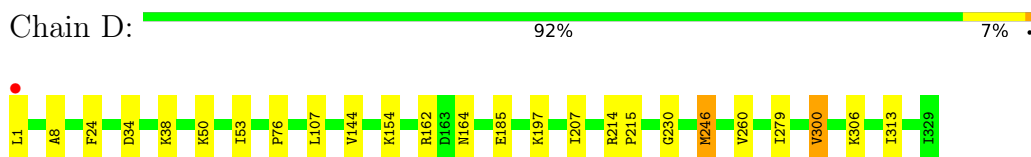
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial



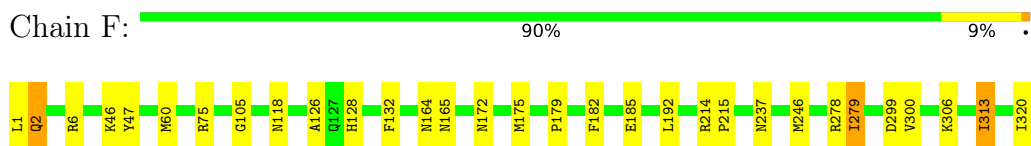
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



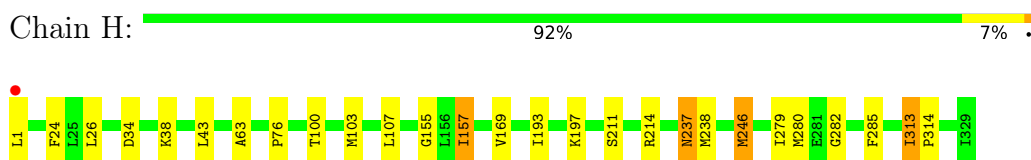
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.57Å 129.62Å 124.30Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 50.00 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.98) 98.7 (50.00-1.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.158 , 0.206 0.159 , 0.207	Depositor DCC
R_{free} test set	11272 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k 0.013 for -h,l,k 0.127 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23831	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: GOL, TPP, MN, K

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	1.22	6/2893 (0.2%)	1.07	0/3895
1	C	1.18	2/2879 (0.1%)	1.10	8/3877 (0.2%)
1	E	1.15	2/2874 (0.1%)	1.08	2/3870 (0.1%)
1	G	1.14	4/2882 (0.1%)	1.06	4/3880 (0.1%)
2	B	1.22	4/2574 (0.2%)	1.12	6/3488 (0.2%)
2	D	1.29	1/2574 (0.0%)	1.13	5/3488 (0.1%)
2	F	1.12	2/2574 (0.1%)	1.10	2/3488 (0.1%)
2	H	1.20	2/2574 (0.1%)	1.13	6/3488 (0.2%)
All	All	1.19	23/21824 (0.1%)	1.10	33/29474 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	PRO	CA-C	8.12	1.56	1.51
1	G	125	HIS	C-O	7.79	1.33	1.23
2	B	300	VAL	CA-CB	6.82	1.64	1.54
1	C	330	PRO	CA-C	6.78	1.55	1.51
1	A	105	ILE	CA-CB	6.25	1.61	1.54
2	D	144	VAL	CA-CB	6.24	1.62	1.54
2	H	169	VAL	CA-CB	6.10	1.61	1.53
1	E	270	VAL	CA-CB	5.72	1.62	1.54
1	A	58	ILE	C-O	-5.43	1.18	1.24
2	F	320	ILE	CA-CB	5.38	1.61	1.54
2	B	65	ILE	CA-CB	5.33	1.61	1.54
1	A	58	ILE	CA-CB	5.30	1.61	1.54
1	G	21	PRO	CA-C	5.29	1.54	1.51
2	B	169	VAL	CA-CB	5.27	1.60	1.53
1	A	137	ILE	CA-CB	5.25	1.60	1.54
2	F	165	ASN	N-CA	5.23	1.49	1.46
2	H	157	ILE	CA-CB	5.20	1.61	1.54
2	B	169	VAL	C-O	5.19	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	182	ALA	CA-CB	5.16	1.61	1.53
1	A	106	LEU	C-O	-5.07	1.18	1.24
1	G	74	GLY	N-CA	5.04	1.52	1.45
1	G	140	ALA	N-CA	5.03	1.52	1.46
1	C	196	ASN	CA-CB	5.01	1.60	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	182	PHE	CA-C-N	7.24	124.87	119.66
2	F	182	PHE	C-N-CA	7.24	124.87	119.66
1	E	2	ALA	N-CA-C	-6.28	101.81	110.35
2	D	246	MET	CG-SD-CE	-6.22	87.20	100.90
2	H	282	GLY	CA-C-N	6.21	125.83	119.56
2	H	282	GLY	C-N-CA	6.21	125.83	119.56
2	H	63	ALA	N-CA-C	-6.15	104.65	111.36
1	C	249	GLY	CA-C-N	6.11	126.08	120.03
1	C	249	GLY	C-N-CA	6.11	126.08	120.03
1	C	329	GLU	CA-C-N	-6.10	115.21	119.66
1	C	329	GLU	C-N-CA	-6.10	115.21	119.66
1	C	16	ARG	CG-CD-NE	-6.09	98.61	112.00
2	H	100	THR	N-CA-C	6.08	117.99	111.36
1	G	16	ARG	CG-CD-NE	-6.01	98.77	112.00
2	D	164	ASN	N-CA-C	5.89	120.09	113.02
1	G	330	PRO	O-C-N	5.83	123.99	121.31
2	B	100	THR	N-CA-C	5.76	117.64	111.36
2	D	300	VAL	CA-C-N	-5.71	114.08	119.85
2	D	300	VAL	C-N-CA	-5.71	114.08	119.85
2	B	182	PHE	CA-C-N	5.66	126.21	120.38
2	B	182	PHE	C-N-CA	5.66	126.21	120.38
2	B	59	GLU	N-CA-C	5.63	117.86	111.11
2	B	151	GLU	CB-CA-C	-5.60	102.09	110.88
1	E	99	GLY	N-CA-C	5.52	122.30	114.85
1	C	89	TYR	CA-CB-CG	-5.43	104.12	113.90
1	C	179	TYR	CB-CA-C	-5.42	102.37	110.88
1	G	315	LYS	N-CA-C	5.33	117.09	111.28
2	B	265	GLY	N-CA-C	5.28	120.59	112.51
2	H	214	ARG	CA-C-N	-5.24	114.42	119.87
2	H	214	ARG	C-N-CA	-5.24	114.42	119.87
2	D	162	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	C	270	VAL	N-CA-C	5.10	118.09	113.20
1	G	67	GLY	N-CA-C	-5.02	107.92	113.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2836	0	2791	26	0
1	C	2823	0	2777	30	0
1	E	2818	0	2775	36	0
1	G	2826	0	2784	31	0
2	B	2519	0	2517	20	0
2	D	2519	0	2517	12	0
2	F	2519	0	2517	24	0
2	H	2519	0	2517	12	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	26	0	16	3	0
4	C	26	0	16	0	0
4	E	26	0	16	1	0
4	G	26	0	16	2	0
5	A	6	0	8	0	0
5	C	6	0	8	1	0
5	E	6	0	8	0	0
5	G	6	0	8	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	A	329	0	0	10	0
7	B	257	0	0	5	0
7	C	301	0	0	8	0
7	D	289	0	0	3	0
7	E	287	0	0	5	0
7	F	255	0	0	3	0
7	G	317	0	0	5	0
7	H	281	0	0	1	0
All	All	23831	0	21291	186	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 4.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:HB2	7:A:4036:HOH:O	1.40	1.17
1:G:68:GLN:HE22	1:G:196:ASN:HD22	1.13	0.94
1:E:118:LYS:HE3	2:F:105:GLY:O	1.68	0.92
1:C:68:GLN:HE22	1:C:196:ASN:HD22	1.08	0.91
1:E:276:GLU:HG2	7:E:3567:HOH:O	1.72	0.90
1:E:68:GLN:HE22	1:E:196:ASN:HD22	1.17	0.88
1:C:24:THR:HG22	7:C:3224:HOH:O	1.75	0.87
1:A:3:ASN:HB3	7:A:4259:HOH:O	1.75	0.85
2:F:118:ASN:HD21	2:F:132:PHE:H	1.25	0.85
1:G:286:ASP:HB3	1:G:289:MET:HG2	1.57	0.84
2:D:313:ILE:HG22	7:D:3163:HOH:O	1.76	0.83
1:E:308:GLU:HG3	7:E:4113:HOH:O	1.80	0.80
1:A:68:GLN:HE22	1:A:196:ASN:HD22	1.27	0.79
1:A:312:GLU:O	1:A:316:GLU:HG2	1.83	0.79
1:E:68:GLN:NE2	1:E:196:ASN:HD22	1.81	0.78
2:B:118:ASN:HD21	2:B:132:PHE:H	1.31	0.78
1:G:68:GLN:NE2	1:G:196:ASN:HD22	1.81	0.78
1:G:206:ARG:HD2	7:G:3503:HOH:O	1.84	0.78
1:A:113:LYS:HE2	1:A:328:PRO:HG2	1.66	0.76
2:H:313:ILE:HG12	2:H:314:PRO:HD2	1.66	0.76
1:A:23:VAL:HG22	7:A:3671:HOH:O	1.86	0.75
1:C:113:LYS:HE2	1:C:328:PRO:HG2	1.69	0.74
1:C:68:GLN:NE2	1:C:196:ASN:HD22	1.85	0.74
1:C:291:LEU:HG	1:C:295:MET:HE2	1.71	0.73
2:F:75:ARG:HH12	2:F:164:ASN:ND2	1.88	0.71
2:B:313:ILE:HD13	7:B:3722:HOH:O	1.90	0.71
1:A:314:ARG:HG2	7:A:3507:HOH:O	1.89	0.71
1:E:274:THR:OG1	1:E:276:GLU:HG3	1.93	0.68
1:C:358:LYS:HD3	1:C:360:VAL:CG1	2.23	0.68
1:G:275:ARG:O	1:G:279:GLN:HG3	1.94	0.68
2:H:246:MET:CE	2:H:279:ILE:HG12	2.25	0.67
1:A:206:ARG:HD2	7:A:3061:HOH:O	1.95	0.67
1:G:285:SER:HB3	7:G:3912:HOH:O	1.99	0.63
1:C:321:ALA:O	1:C:325:THR:HG23	1.99	0.62
1:A:235:GLU:HG2	7:A:3336:HOH:O	2.00	0.62
1:E:95:THR:CG2	1:E:100:LEU:HD12	2.30	0.61
1:E:9:ILE:HB	1:E:232:CYS:SG	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:PRO:HB3	1:E:360:VAL:HG12	1.82	0.61
1:E:37:ARG:HD3	7:E:3978:HOH:O	2.00	0.60
2:F:118:ASN:HD21	2:F:132:PHE:N	1.96	0.60
2:H:246:MET:HE1	2:H:279:ILE:HG12	1.84	0.60
1:C:358:LYS:HD3	1:C:360:VAL:HG12	1.83	0.59
1:A:10:LYS:HE3	7:A:2992:HOH:O	2.02	0.59
1:E:314:ARG:HD2	7:E:3859:HOH:O	2.01	0.59
1:A:68:GLN:NE2	1:A:196:ASN:HD22	2.00	0.59
1:E:128:ALA:HB3	1:E:131:PHE:HB3	1.83	0.59
2:H:155:GLY:HA3	2:H:193:ILE:HD12	1.85	0.58
1:C:118:LYS:HB2	7:C:3482:HOH:O	2.05	0.57
1:G:113:LYS:NZ	1:G:113:LYS:HB2	2.20	0.57
1:C:0:MET:N	7:C:4166:HOH:O	2.37	0.56
1:C:334:GLU:HG2	1:C:337:TYR:CE2	2.41	0.56
2:D:185:GLU:H	2:D:185:GLU:CD	2.13	0.56
2:B:172:ASN:HD22	2:B:175:MET:H	1.55	0.55
1:C:206:ARG:HD2	7:C:3848:HOH:O	2.07	0.55
2:D:246:MET:HE1	2:D:279:ILE:HG12	1.89	0.55
1:G:322:GLN:HG3	7:G:4225:HOH:O	2.04	0.55
1:A:89:TYR:HH	4:A:1005:TPP:H71	1.72	0.55
1:A:290:LEU:HB3	7:A:4188:HOH:O	2.07	0.54
1:G:291:LEU:HG	1:G:295:MET:HE2	1.87	0.54
2:B:214:ARG:HB3	2:B:215:PRO:HD3	1.89	0.54
1:E:33:LEU:HD13	1:E:295:MET:HE1	1.90	0.54
1:E:34:LYS:O	1:E:38:MET:HG3	2.08	0.54
1:E:89:TYR:OH	4:E:1011:TPP:H71	2.08	0.53
2:B:60:MET:HE2	7:D:3957:HOH:O	2.07	0.53
1:G:222:GLY:HA2	1:G:252:LEU:O	2.09	0.52
1:G:89:TYR:OH	4:G:1008:TPP:H71	2.09	0.52
1:A:-1:HIS:N	7:A:3867:HOH:O	2.42	0.52
1:E:196:ASN:O	1:E:197:ARG:HB2	2.10	0.52
1:G:127:TYR:CD1	1:G:127:TYR:N	2.77	0.52
2:B:107:LEU:HD12	7:B:3942:HOH:O	2.10	0.51
2:F:214:ARG:HB3	2:F:215:PRO:HD3	1.92	0.51
1:G:68:GLN:HE22	1:G:196:ASN:ND2	1.96	0.51
1:G:150:LEU:C	1:G:150:LEU:HD23	2.36	0.51
2:H:313:ILE:HG12	2:H:314:PRO:CD	2.40	0.51
2:D:34:ASP:O	2:D:38:LYS:HA	2.11	0.51
2:B:207:ILE:HD11	2:B:260:VAL:HG23	1.93	0.50
1:C:339:ILE:CD1	1:C:348:VAL:HG21	2.41	0.50
1:E:274:THR:CB	1:E:276:GLU:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ASN:HD21	2:B:132:PHE:N	2.04	0.50
1:G:314:ARG:NH2	7:G:3263:HOH:O	2.24	0.50
1:G:118:LYS:O	1:G:330:PRO:HG3	2.12	0.49
2:H:34:ASP:O	2:H:38:LYS:HA	2.12	0.49
2:F:2:GLN:CG	2:F:179:PRO:HB2	2.42	0.49
1:E:61:PHE:CD2	1:E:124:MET:HE2	2.48	0.49
1:C:62:CYS:HB3	1:C:265:MET:HG2	1.95	0.49
2:F:313:ILE:HD11	7:F:3595:HOH:O	2.12	0.49
2:B:75:ARG:HH12	2:B:164:ASN:ND2	2.10	0.48
1:E:72:CYS:HA	1:E:94:PHE:CE1	2.48	0.48
1:G:289:MET:HE2	1:G:290:LEU:HD13	1.95	0.48
2:D:214:ARG:HB3	2:D:215:PRO:HD3	1.95	0.48
1:A:89:TYR:OH	4:A:1005:TPP:H71	2.13	0.48
5:C:1102:GOL:H12	2:D:53:ILE:HG23	1.94	0.48
1:C:308:GLU:HG3	7:C:3611:HOH:O	2.14	0.47
2:D:207:ILE:HD11	2:D:260:VAL:HG23	1.95	0.47
2:F:246:MET:HE1	2:F:279:ILE:HG12	1.95	0.47
1:A:72:CYS:HA	1:A:94:PHE:CE1	2.50	0.47
2:F:278:ARG:NH1	2:F:278:ARG:HG3	2.29	0.47
2:F:237:ASN:C	2:F:237:ASN:HD22	2.22	0.47
1:G:4:ASP:OD1	1:G:4:ASP:C	2.57	0.46
1:E:309:ILE:O	1:E:313:VAL:HG23	2.15	0.46
1:C:61:PHE:CD2	1:C:124:MET:HE2	2.51	0.46
1:E:102:VAL:HG11	1:E:317:ILE:HD12	1.97	0.46
2:B:237:ASN:ND2	7:B:2508:HOH:O	2.49	0.46
1:E:61:PHE:HD2	1:E:124:MET:HE2	1.81	0.46
2:F:75:ARG:HH12	2:F:164:ASN:HD21	1.61	0.46
2:F:128:HIS:CE1	1:G:124:MET:HE1	2.51	0.46
1:G:162:LEU:HD12	1:G:162:LEU:N	2.31	0.46
1:E:75:LEU:HD23	1:E:237:THR:OG1	2.16	0.46
1:A:196:ASN:O	1:A:197:ARG:HB2	2.14	0.46
2:F:300:VAL:HG12	1:G:339:ILE:HD11	1.99	0.45
1:A:53:TYR:CG	1:A:265:MET:HG3	2.51	0.45
1:G:6:THR:HG23	1:G:24:THR:HG23	1.98	0.45
1:A:274:THR:OG1	1:A:276:GLU:HG2	2.16	0.45
2:D:230:GLY:HA2	7:D:3955:HOH:O	2.16	0.45
1:E:27:LEU:HG	1:E:231:LEU:HD21	1.98	0.45
1:C:334:GLU:HB2	7:C:3666:HOH:O	2.15	0.45
1:C:335:LEU:HD13	1:C:357:PHE:CZ	2.52	0.45
1:C:196:ASN:O	1:C:197:ARG:HB2	2.17	0.45
2:F:6:ARG:HD2	7:F:2865:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:H	1:A:205:GLU:CD	2.24	0.44
1:E:150:LEU:C	1:E:150:LEU:HD23	2.42	0.44
1:G:331:PRO:HG2	1:G:334:GLU:HG3	1.99	0.44
2:B:34:ASP:O	2:B:38:LYS:HA	2.18	0.44
2:B:186:ALA:HA	2:B:191:PHE:CG	2.51	0.44
1:E:126:MET:O	1:E:133:GLY:HA2	2.17	0.44
2:B:315:GLN:HG2	7:B:3791:HOH:O	2.18	0.44
1:A:125:HIS:O	7:A:3062:HOH:O	2.21	0.44
1:E:150:LEU:HA	1:E:187:LEU:HD22	2.00	0.44
1:G:39:MET:HG2	1:G:69:GLU:HB3	1.99	0.44
2:H:237:ASN:ND2	7:H:2794:HOH:O	2.50	0.44
1:A:222:GLY:HA2	1:A:252:LEU:O	2.18	0.43
1:C:22:PRO:HD2	1:C:235:GLU:HG3	2.00	0.43
1:C:289:MET:SD	1:C:292:LYS:NZ	2.74	0.43
2:F:60:MET:HE2	7:F:2863:HOH:O	2.17	0.43
1:E:68:GLN:HE22	1:E:196:ASN:ND2	1.98	0.43
1:E:164:LEU:HG	1:E:192:ILE:HB	1.99	0.43
2:F:299:ASP:HB3	1:G:348:VAL:HG12	2.00	0.43
1:C:304:GLU:HG2	7:C:2895:HOH:O	2.17	0.43
2:F:2:GLN:HG3	2:F:179:PRO:HB2	1.99	0.43
1:G:95:THR:HG22	1:G:100:LEU:HB2	1.99	0.43
1:C:314:ARG:HG3	7:C:2596:HOH:O	2.18	0.43
2:H:246:MET:HE2	2:H:279:ILE:HG12	2.00	0.43
2:D:8:ALA:HB1	2:D:154:LYS:HB2	2.00	0.43
1:G:205:GLU:HG3	7:G:2713:HOH:O	2.18	0.43
2:B:227:SER:HB2	2:B:232:GLU:OE2	2.19	0.43
2:F:126:ALA:HB3	2:H:103:MET:SD	2.59	0.42
1:G:75:LEU:HD23	1:G:237:THR:OG1	2.20	0.42
2:H:24:PHE:CZ	2:H:76:PRO:HB3	2.54	0.42
1:C:339:ILE:HD12	1:C:348:VAL:HG21	2.00	0.42
1:A:138:VAL:HG13	1:A:169:ALA:HB2	2.01	0.42
2:F:46:LYS:HE2	2:F:47:TYR:CZ	2.54	0.42
1:E:162:LEU:HD12	1:E:162:LEU:N	2.34	0.42
2:B:182:PHE:HA	2:B:183:PRO:HD2	1.76	0.42
1:C:113:LYS:O	1:C:118:LYS:HD3	2.19	0.42
1:C:138:VAL:HG13	1:C:169:ALA:HB2	2.02	0.42
1:G:289:MET:HG3	1:G:290:LEU:N	2.35	0.42
4:G:1008:TPP:H2	4:G:1008:TPP:HN42	1.84	0.42
1:E:142:VAL:HA	1:E:163:THR:CG2	2.50	0.42
2:F:246:MET:CE	2:F:279:ILE:HG12	2.50	0.41
1:G:6:THR:CG2	1:G:24:THR:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:GLN:NE2	7:B:4063:HOH:O	2.52	0.41
2:B:237:ASN:C	2:B:237:ASN:HD22	2.28	0.41
2:B:246:MET:CE	2:B:279:ILE:HG12	2.51	0.41
2:F:278:ARG:HG3	2:F:278:ARG:HH11	1.86	0.41
1:C:61:PHE:HD2	1:C:124:MET:HE2	1.85	0.41
1:C:333:GLU:H	1:C:333:GLU:CD	2.29	0.41
2:F:237:ASN:C	2:F:237:ASN:ND2	2.77	0.41
1:E:230:ILE:HD13	1:E:230:ILE:O	2.20	0.41
1:E:157:LYS:HB2	7:E:3528:HOH:O	2.20	0.41
2:B:112:ILE:HD13	2:B:114:PHE:CZ	2.56	0.41
2:H:211:SER:C	2:H:238:MET:HE3	2.46	0.41
1:A:334:GLU:HG2	1:A:337:TYR:CE2	2.56	0.41
1:E:190:ILE:HD11	1:E:241:ALA:HA	2.03	0.41
1:E:222:GLY:HA2	1:E:252:LEU:O	2.21	0.41
2:F:325:LYS:HG2	1:G:354:TRP:CZ2	2.56	0.41
2:B:4:THR:HA	2:B:179:PRO:HA	2.03	0.40
2:D:50:LYS:O	2:D:50:LYS:HG2	2.21	0.40
4:A:1005:TPP:HN42	4:A:1005:TPP:H2	1.86	0.40
2:F:172:ASN:HD22	2:F:175:MET:H	1.70	0.40
1:A:348:VAL:HG11	2:D:300:VAL:HG13	2.04	0.40
1:C:94:PHE:CZ	1:C:164:LEU:HD21	2.56	0.40
2:H:280:MET:HA	2:H:285:PHE:CD1	2.56	0.40
1:A:113:LYS:O	1:A:118:LYS:HG2	2.22	0.40
1:C:229:ASP:OD1	1:C:229:ASP:C	2.64	0.40
2:D:24:PHE:CZ	2:D:76:PRO:HB3	2.56	0.40
1:E:345:PRO:HA	1:E:359:SER:O	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	361/382 (94%)	349 (97%)	11 (3%)	1 (0%)	36	27
1	C	360/382 (94%)	350 (97%)	9 (2%)	1 (0%)	36	27
1	E	359/382 (94%)	348 (97%)	10 (3%)	1 (0%)	36	27
1	G	360/382 (94%)	347 (96%)	12 (3%)	1 (0%)	36	27
2	B	327/329 (99%)	317 (97%)	10 (3%)	0	100	100
2	D	327/329 (99%)	316 (97%)	11 (3%)	0	100	100
2	F	327/329 (99%)	317 (97%)	10 (3%)	0	100	100
2	H	327/329 (99%)	316 (97%)	11 (3%)	0	100	100
All	All	2748/2844 (97%)	2660 (97%)	84 (3%)	4 (0%)	48	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ASP
1	C	218	ASP
1	E	218	ASP
1	G	218	ASP

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	296/312 (95%)	287 (97%)	9 (3%)	36	27
1	C	294/312 (94%)	284 (97%)	10 (3%)	32	22
1	E	294/312 (94%)	281 (96%)	13 (4%)	25	14
1	G	295/312 (95%)	281 (95%)	14 (5%)	23	12
2	B	268/268 (100%)	263 (98%)	5 (2%)	50	44
2	D	268/268 (100%)	264 (98%)	4 (2%)	57	52
2	F	268/268 (100%)	260 (97%)	8 (3%)	36	27
2	H	268/268 (100%)	259 (97%)	9 (3%)	32	22
All	All	2251/2320 (97%)	2179 (97%)	72 (3%)	34	24

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	18	GLU
1	A	27	LEU
1	A	205	GLU
1	A	223	LEU
1	A	230	ILE
1	A	307	LYS
1	A	322	GLN
1	A	342	SER
2	B	1	LEU
2	B	185	GLU
2	B	192	LEU
2	B	237	ASN
2	B	325	LYS
1	C	27	LEU
1	C	230	ILE
1	C	252	LEU
1	C	285	SER
1	C	292	LYS
1	C	300	LEU
1	C	305	GLU
1	C	314	ARG
1	C	317	ILE
1	C	360	VAL
2	D	1	LEU
2	D	107	LEU
2	D	197	LYS
2	D	306	LYS
1	E	3	ASN
1	E	9	ILE
1	E	24	THR
1	E	27	LEU
1	E	33	LEU
1	E	205	GLU
1	E	223	LEU
1	E	230	ILE
1	E	235	GLU
1	E	276	GLU
1	E	317	ILE
1	E	333	GLU
1	E	342	SER
2	F	1	LEU

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Mol	Chain	Res	Type
2	F	2	GLN
2	F	185	GLU
2	F	192	LEU
2	F	279	ILE
2	F	306	LYS
2	F	313	ILE
2	F	325	LYS
1	G	8	GLU
1	G	24	THR
1	G	27	LEU
1	G	30	GLU
1	G	113	LYS
1	G	157	LYS
1	G	230	ILE
1	G	252	LEU
1	G	289	MET
1	G	290	LEU
1	G	300	LEU
1	G	307	LYS
1	G	342	SER
1	G	348	VAL
2	H	1	LEU
2	H	26	LEU
2	H	43	LEU
2	H	107	LEU
2	H	157	ILE
2	H	197	LYS
2	H	237	ASN
2	H	246	MET
2	H	313	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	130	ASN
1	A	297	ASN
1	A	353	GLN
2	B	32	GLN
2	B	118	ASN
2	B	164	ASN
2	B	172	ASN

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Mol	Chain	Res	Type
2	B	237	ASN
2	B	328	ASN
1	C	55	GLN
1	C	68	GLN
1	C	322	GLN
2	D	187	GLN
2	D	237	ASN
2	D	328	ASN
1	E	68	GLN
1	E	80	ASN
1	E	130	ASN
1	E	279	GLN
1	E	297	ASN
1	E	353	GLN
2	F	2	GLN
2	F	32	GLN
2	F	118	ASN
2	F	164	ASN
2	F	172	ASN
2	F	237	ASN
1	G	51	GLN
1	G	55	GLN
1	G	68	GLN
1	G	299	ASN
1	G	322	GLN
2	H	237	ASN
2	H	257	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
5	GOL	G	1104	-	5,5,5	0.55	0	5,5,5	0.83	0
5	GOL	A	1101	-	5,5,5	0.34	0	5,5,5	0.86	0
4	TPP	G	1008	3	26,27,27	1.61	6 (23%)	38,40,40	1.99	10 (26%)
4	TPP	A	1005	3	26,27,27	1.53	4 (15%)	38,40,40	2.00	10 (26%)
4	TPP	E	1011	3	26,27,27	1.98	7 (26%)	38,40,40	1.72	10 (26%)
5	GOL	E	1103	-	5,5,5	0.36	0	5,5,5	0.88	0
5	GOL	C	1102	-	5,5,5	0.71	0	5,5,5	0.92	0
4	TPP	C	1002	3	26,27,27	1.73	6 (23%)	38,40,40	1.90	10 (26%)

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
5	GOL	G	1104	-	-	0/4/4/4	-
5	GOL	A	1101	-	-	0/4/4/4	-
4	TPP	G	1008	3	-	3/17/17/17	0/2/2/2
4	TPP	A	1005	3	-	4/17/17/17	0/2/2/2
4	TPP	E	1011	3	-	1/17/17/17	0/2/2/2
5	GOL	E	1103	-	-	0/4/4/4	-
5	GOL	C	1102	-	-	2/4/4/4	-
4	TPP	C	1002	3	-	2/17/17/17	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1011	TPP	C2'-N1'	4.16	1.40	1.34
4	E	1011	TPP	C2'-N3'	3.85	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1011	TPP	C5-S1	-3.77	1.62	1.72
4	C	1002	TPP	C2-N3	3.61	1.41	1.32
4	E	1011	TPP	C2-N3	3.58	1.41	1.32
4	G	1008	TPP	C5-S1	-3.42	1.63	1.72
4	A	1005	TPP	C2-N3	3.40	1.40	1.32
4	C	1002	TPP	C2'-N1'	3.07	1.39	1.34
4	C	1002	TPP	C4'-N3'	2.97	1.39	1.35
4	C	1002	TPP	C5-S1	-2.93	1.65	1.72
4	A	1005	TPP	PA-O3A	2.90	1.62	1.59
4	A	1005	TPP	C2'-N1'	2.90	1.38	1.34
4	E	1011	TPP	C4'-N3'	2.80	1.38	1.35
4	G	1008	TPP	C2-N3	2.76	1.39	1.32
4	C	1002	TPP	C5-C4	2.69	1.40	1.35
4	G	1008	TPP	C2'-N1'	2.69	1.38	1.34
4	E	1011	TPP	C5-C4	2.63	1.40	1.35
4	G	1008	TPP	C7'-C5'	2.54	1.55	1.51
4	A	1005	TPP	C2'-N3'	2.50	1.38	1.34
4	C	1002	TPP	C6'-N1'	2.47	1.39	1.34
4	E	1011	TPP	C6'-N1'	2.47	1.39	1.34
4	G	1008	TPP	C4'-N3'	2.13	1.37	1.35
4	G	1008	TPP	PA-O2A	-2.01	1.46	1.55

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1005	TPP	C6'-N1'-C2'	5.55	125.19	116.07
4	A	1005	TPP	N1'-C2'-N3'	-4.90	117.38	125.53
4	G	1008	TPP	N1'-C2'-N3'	-4.86	117.45	125.53
4	C	1002	TPP	C2-S1-C5	4.84	94.42	91.22
4	E	1011	TPP	C6'-C5'-C4'	4.56	121.15	115.55
4	G	1008	TPP	C6'-N1'-C2'	4.28	123.10	116.07
4	C	1002	TPP	O2A-PA-O3A	4.17	118.53	107.27
4	A	1005	TPP	C5'-C7'-N3	-3.78	104.82	112.97
4	G	1008	TPP	C5'-C7'-N3	-3.76	104.88	112.97
4	C	1002	TPP	C5'-C7'-N3	-3.75	104.90	112.97
4	A	1005	TPP	C5'-C6'-N1'	-3.74	117.75	123.83
4	A	1005	TPP	CM2-C2'-N3'	3.73	122.70	117.13
4	G	1008	TPP	CM2-C2'-N3'	3.70	122.66	117.13
4	C	1002	TPP	C6'-N1'-C2'	3.55	121.91	116.07
4	C	1002	TPP	N1'-C2'-N3'	-3.48	119.73	125.53
4	G	1008	TPP	C4-C5-S1	3.36	115.80	110.56
4	C	1002	TPP	C5'-C6'-N1'	-3.22	118.60	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1008	TPP	CM4-C4-N3	3.15	127.83	120.57
4	E	1011	TPP	C5'-C7'-N3	-3.13	106.22	112.97
4	G	1008	TPP	O2A-PA-O3A	3.11	115.68	107.27
4	E	1011	TPP	C5'-C6'-N1'	-3.07	118.83	123.83
4	E	1011	TPP	CM2-C2'-N1'	2.85	120.23	117.20
4	A	1005	TPP	C4-C5-S1	2.81	114.95	110.56
4	C	1002	TPP	CM2-C2'-N1'	2.77	120.15	117.20
4	A	1005	TPP	CM4-C4-N3	2.75	126.91	120.57
4	E	1011	TPP	C2-S1-C5	2.74	93.03	91.22
4	C	1002	TPP	C6'-C5'-C4'	2.63	118.78	115.55
4	G	1008	TPP	C5'-C6'-N1'	-2.61	119.59	123.83
4	A	1005	TPP	CM2-C2'-N1'	2.54	119.91	117.20
4	G	1008	TPP	CM2-C2'-N1'	2.52	119.88	117.20
4	A	1005	TPP	O3A-PA-O1A	-2.49	103.21	110.70
4	E	1011	TPP	N1'-C2'-N3'	-2.39	121.55	125.53
4	G	1008	TPP	O3A-PA-O1A	-2.36	103.61	110.70
4	A	1005	TPP	C6'-C5'-C4'	2.35	118.44	115.55
4	E	1011	TPP	CM4-C4-N3	2.29	125.84	120.57
4	E	1011	TPP	C6'-N1'-C2'	2.24	119.76	116.07
4	C	1002	TPP	O3A-PA-O1A	-2.23	104.00	110.70
4	E	1011	TPP	C6-C5-S1	-2.18	115.79	120.90
4	E	1011	TPP	O3A-PA-O1A	-2.09	104.42	110.70
4	C	1002	TPP	CM4-C4-N3	2.09	125.38	120.57

There are no chirality outliers.

All (12) torsion outliers are listed below:

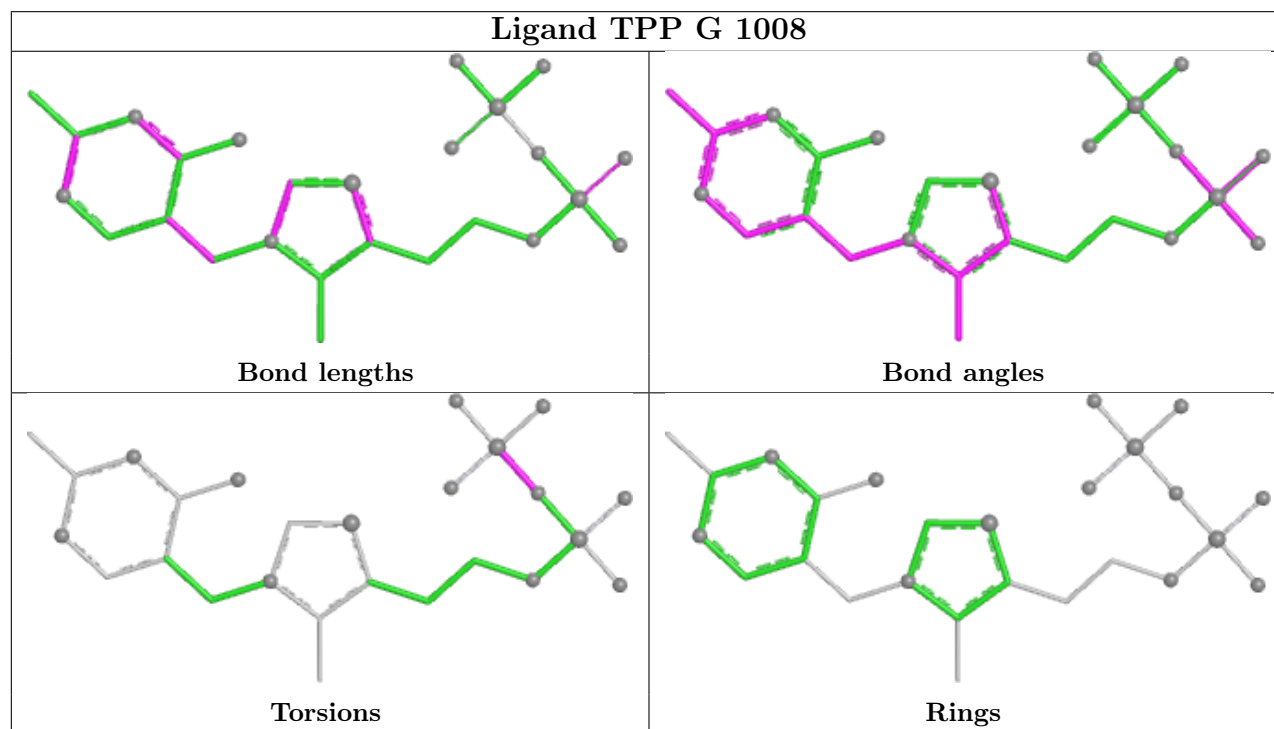
Mol	Chain	Res	Type	Atoms
4	C	1002	TPP	PA-O3A-PB-O2B
4	E	1011	TPP	PA-O3A-PB-O2B
5	C	1102	GOL	C1-C2-C3-O3
5	C	1102	GOL	O2-C2-C3-O3
4	C	1002	TPP	C5-C6-C7-O7
4	G	1008	TPP	PA-O3A-PB-O1B
4	A	1005	TPP	PA-O3A-PB-O1B
4	A	1005	TPP	PA-O3A-PB-O2B
4	A	1005	TPP	PA-O3A-PB-O3B
4	G	1008	TPP	PA-O3A-PB-O2B
4	G	1008	TPP	PA-O3A-PB-O3B
4	A	1005	TPP	C5-C6-C7-O7

There are no ring outliers.

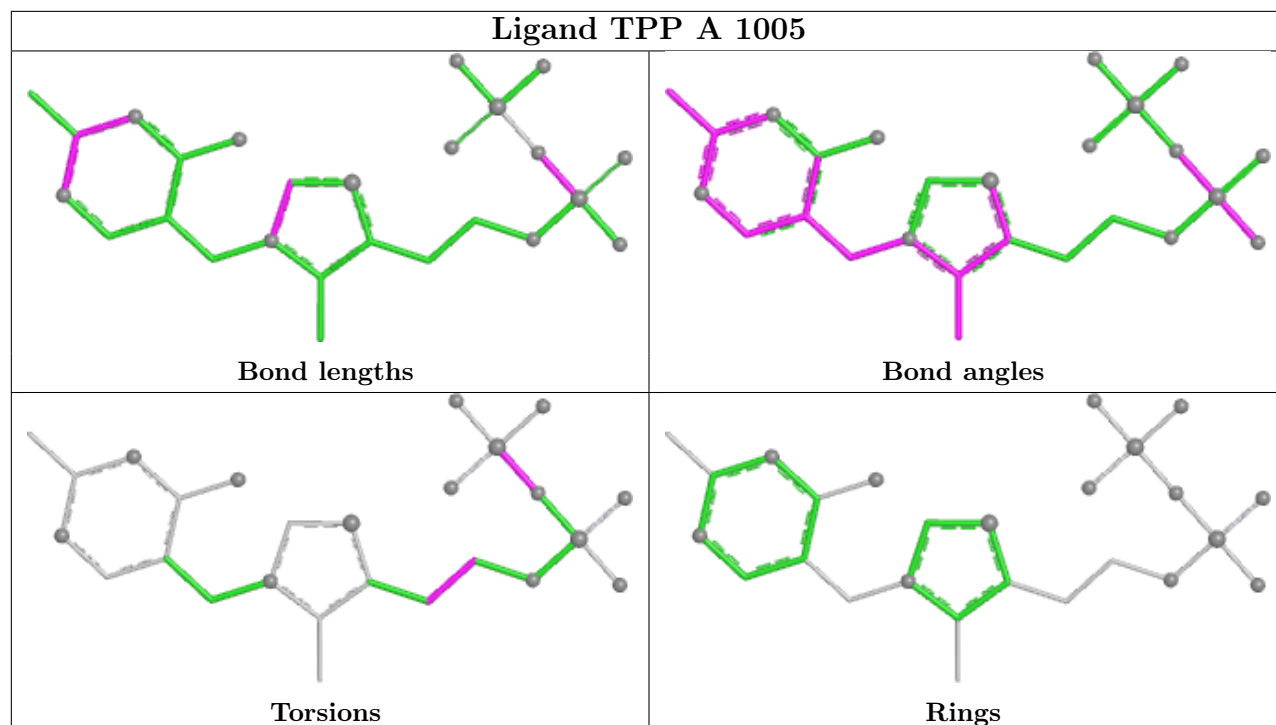
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1008	TPP	2	0
4	A	1005	TPP	3	0
4	E	1011	TPP	1	0
5	C	1102	GOL	1	0

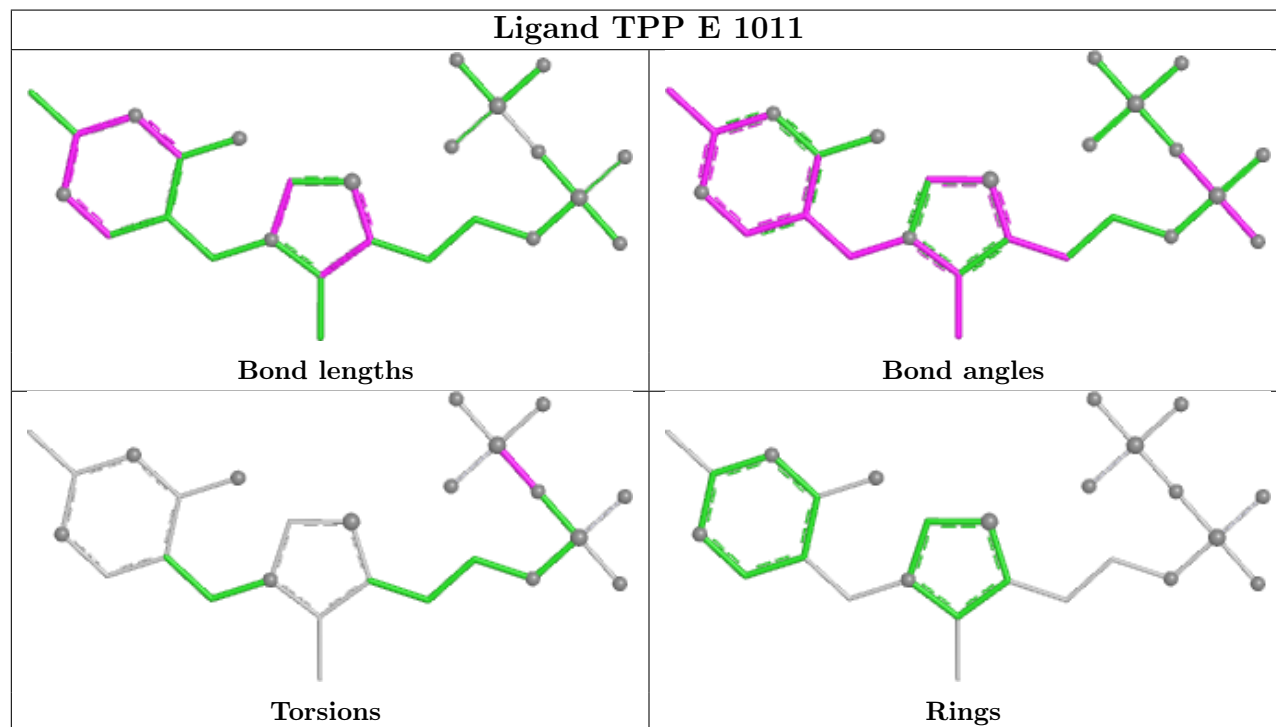
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

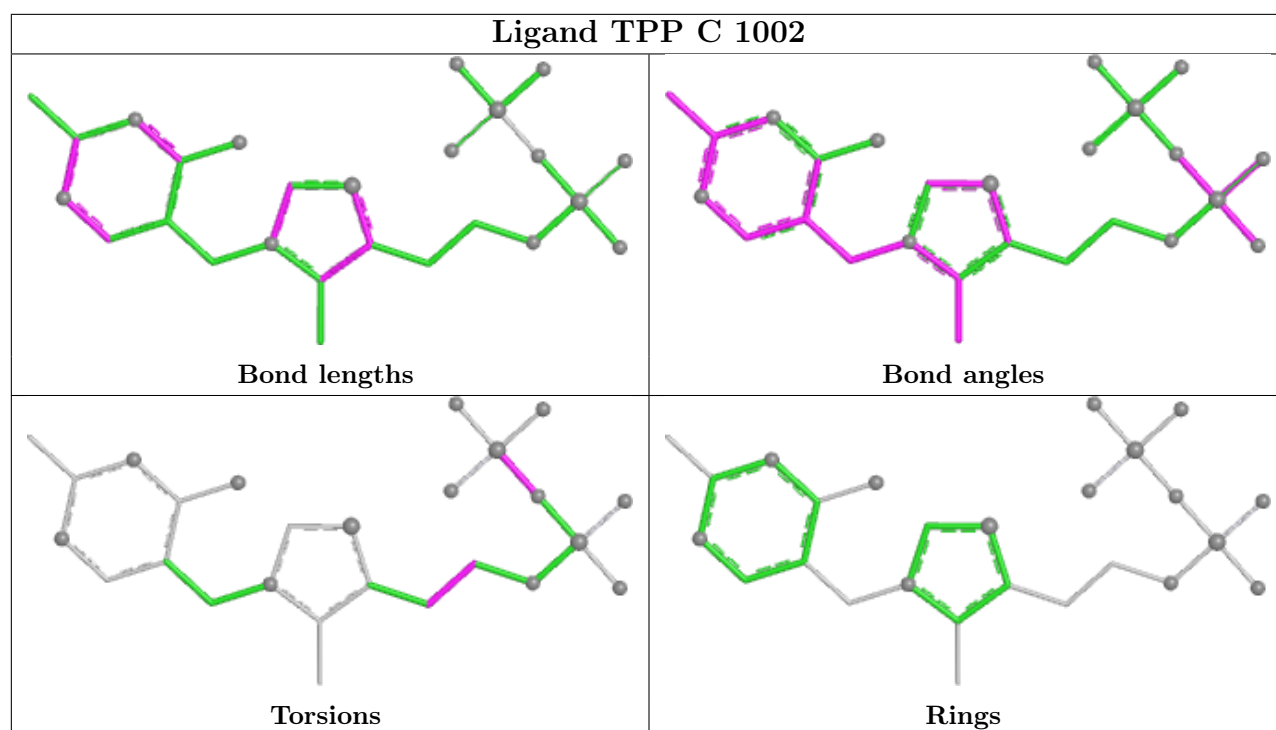


Ligand TPP A 1005



Ligand TPP E 1011





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	363/382 (95%)	-0.23	3 (0%) 82 87	9, 17, 26, 40	0
1	C	362/382 (94%)	-0.27	1 (0%) 90 93	12, 17, 26, 34	0
1	E	361/382 (94%)	-0.13	0 100 100	12, 17, 26, 35	0
1	G	362/382 (94%)	-0.15	3 (0%) 82 87	11, 17, 25, 33	0
2	B	329/329 (100%)	-0.39	2 (0%) 85 90	12, 16, 25, 36	0
2	D	329/329 (100%)	-0.43	1 (0%) 90 93	11, 16, 24, 34	0
2	F	329/329 (100%)	-0.34	0 100 100	10, 16, 24, 33	0
2	H	329/329 (100%)	-0.28	1 (0%) 90 93	12, 16, 24, 31	0
All	All	2764/2844 (97%)	-0.27	11 (0%) 88 92	9, 16, 26, 40	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	LEU	3.2
2	D	1	LEU	2.7
1	A	127	TYR	2.5
1	C	293	ASP	2.5
1	G	127	TYR	2.4
2	B	107	LEU	2.3
2	B	1	LEU	2.3
1	A	0	MET	2.3
1	A	-1	HIS	2.3
1	G	276	GLU	2.1
1	G	158	ASP	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

There are no oligosaccharides in this entry.

6.4 Ligands

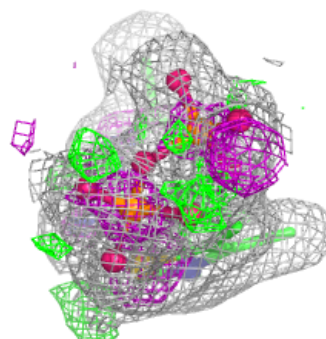
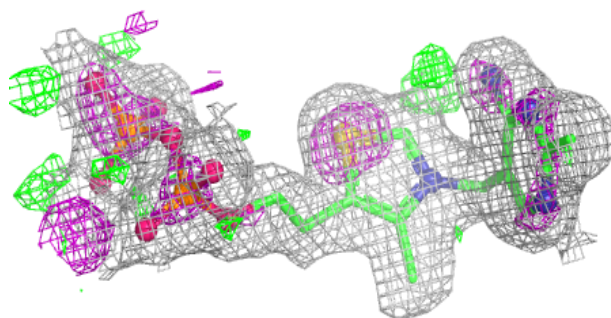
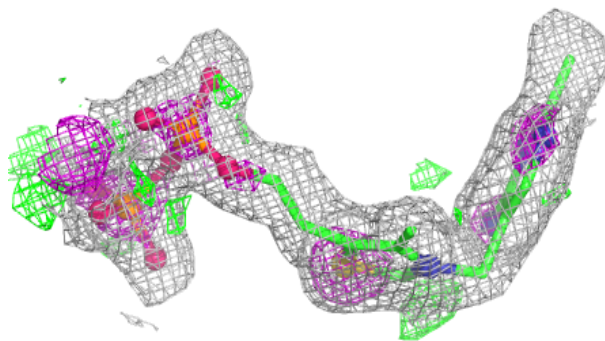
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	GOL	E	1103	6/6	0.82	0.20	35,40,42,43	0
5	GOL	G	1104	6/6	0.85	0.14	31,35,37,40	0
5	GOL	C	1102	6/6	0.87	0.16	26,32,33,34	0
5	GOL	A	1101	6/6	0.88	0.13	32,33,34,34	0
6	K	H	1012	1/1	0.94	0.19	34,34,34,34	0
4	TPP	G	1008	26/26	0.97	0.07	7,11,15,16	0
4	TPP	E	1011	26/26	0.97	0.07	6,11,16,19	0
4	TPP	C	1002	26/26	0.98	0.07	6,9,14,18	0
6	K	B	1003	1/1	0.98	0.15	34,34,34,34	0
6	K	F	1009	1/1	0.98	0.21	40,40,40,40	0
4	TPP	A	1005	26/26	0.98	0.07	5,9,14,16	0
6	K	D	1006	1/1	0.99	0.20	27,27,27,27	0
3	MN	E	1010	1/1	0.99	0.09	12,12,12,12	0
3	MN	C	1001	1/1	0.99	0.09	10,10,10,10	0
3	MN	A	1004	1/1	1.00	0.10	10,10,10,10	0
3	MN	G	1007	1/1	1.00	0.09	12,12,12,12	0

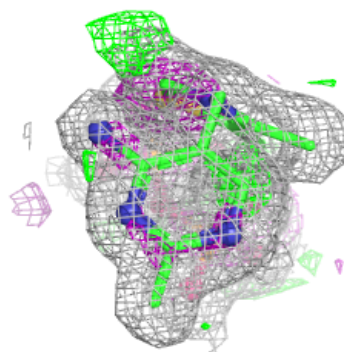
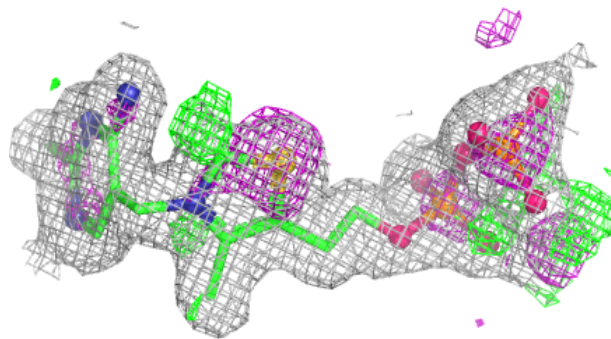
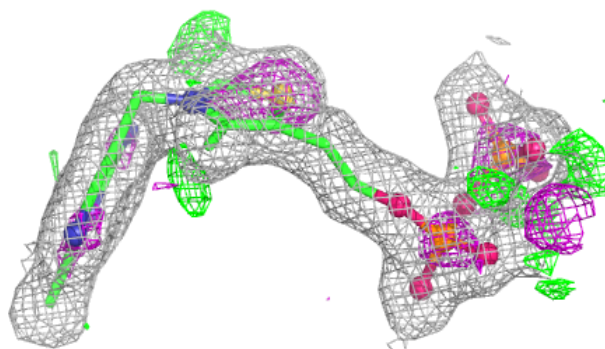
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP G 1008:

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

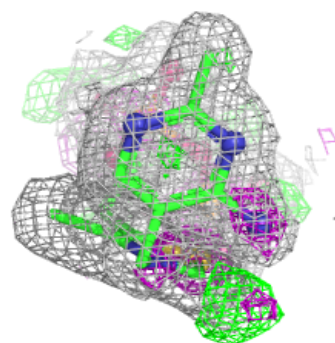
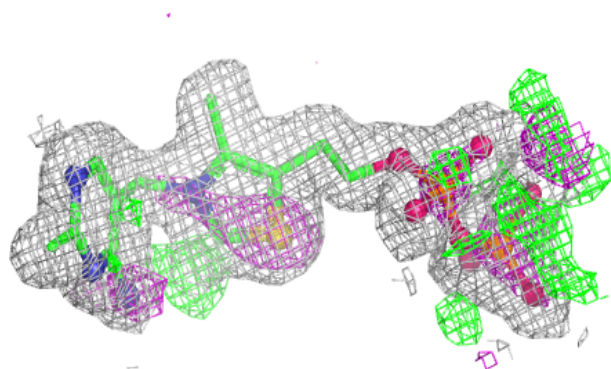
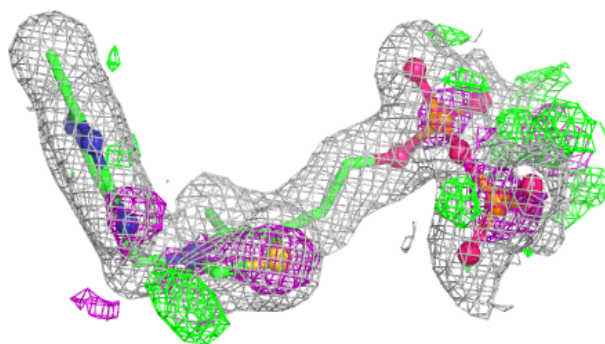
**Electron density around TPP E 1011:**

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

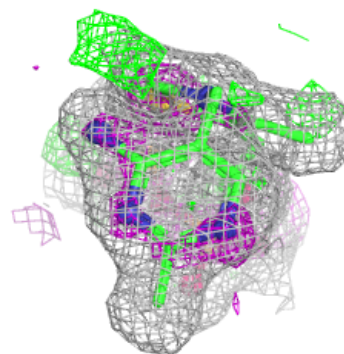
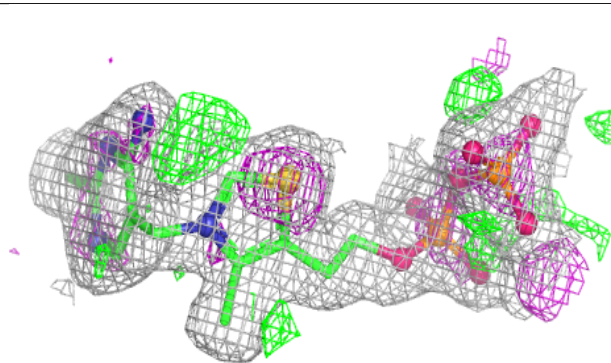
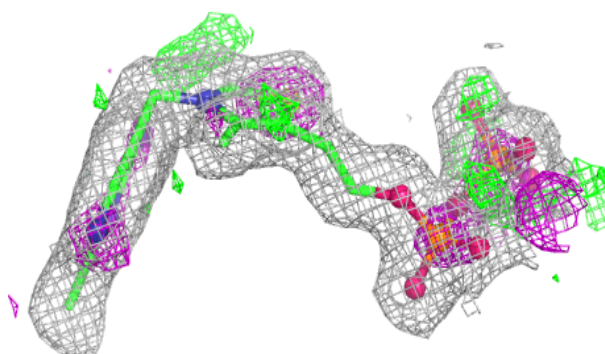


Electron density around TPP C 1002:

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

**Electron density around TPP A 1005:**

$2mF_o-DF_c$ (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.