



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:54 PM UTC

PDB ID : 9S01 / pdb_00009s01
Title : PYCR1 in complex with L-tartrate
Authors : Ragin-Oh, W.; Czerwonka, D.; Ruszkowski, M.
Deposited on : 2025-07-16
Resolution : 1.65 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

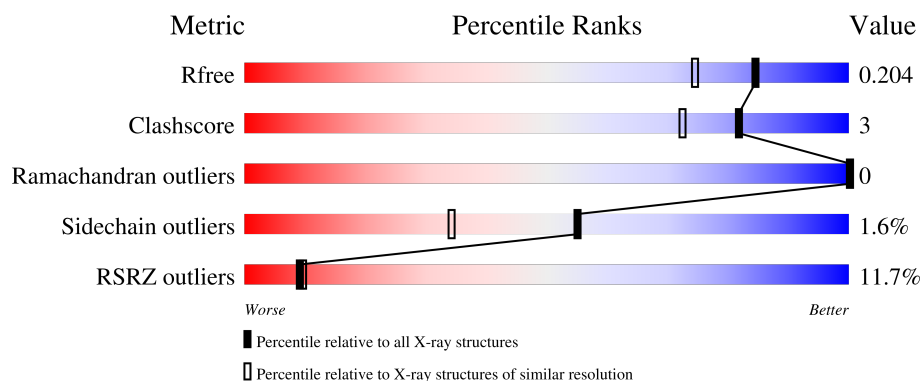
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	342	
1	B	342	
1	C	342	
1	D	342	
1	E	342	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10910 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 Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	5	0
			2029	1276	360	378	15			
1	B	278	Total	C	N	O	S	0	6	0
			2067	1303	363	386	15			
1	C	273	Total	C	N	O	S	0	4	0
			2029	1276	360	378	15			
1	D	275	Total	C	N	O	S	0	4	0
			2033	1278	361	380	14			
1	E	273	Total	C	N	O	S	0	5	0
			2032	1277	363	378	14			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P32322
A	-21	HIS	-	expression tag	UNP P32322
A	-20	HIS	-	expression tag	UNP P32322
A	-19	HIS	-	expression tag	UNP P32322
A	-18	HIS	-	expression tag	UNP P32322
A	-17	HIS	-	expression tag	UNP P32322
A	-16	HIS	-	expression tag	UNP P32322
A	-15	SER	-	expression tag	UNP P32322
A	-14	SER	-	expression tag	UNP P32322
A	-13	GLY	-	expression tag	UNP P32322
A	-12	VAL	-	expression tag	UNP P32322
A	-11	ASP	-	expression tag	UNP P32322
A	-10	LEU	-	expression tag	UNP P32322
A	-9	GLY	-	expression tag	UNP P32322
A	-8	THR	-	expression tag	UNP P32322
A	-7	GLU	-	expression tag	UNP P32322
A	-6	ASN	-	expression tag	UNP P32322
A	-5	ASN	-	expression tag	UNP P32322
A	-4	LEU	-	expression tag	UNP P32322

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP P32322
A	-2	PHE	-	expression tag	UNP P32322
A	-1	GLN	-	expression tag	UNP P32322
B	-22	MET	-	initiating methionine	UNP P32322
B	-21	HIS	-	expression tag	UNP P32322
B	-20	HIS	-	expression tag	UNP P32322
B	-19	HIS	-	expression tag	UNP P32322
B	-18	HIS	-	expression tag	UNP P32322
B	-17	HIS	-	expression tag	UNP P32322
B	-16	HIS	-	expression tag	UNP P32322
B	-15	SER	-	expression tag	UNP P32322
B	-14	SER	-	expression tag	UNP P32322
B	-13	GLY	-	expression tag	UNP P32322
B	-12	VAL	-	expression tag	UNP P32322
B	-11	ASP	-	expression tag	UNP P32322
B	-10	LEU	-	expression tag	UNP P32322
B	-9	GLY	-	expression tag	UNP P32322
B	-8	THR	-	expression tag	UNP P32322
B	-7	GLU	-	expression tag	UNP P32322
B	-6	ASN	-	expression tag	UNP P32322
B	-5	ASN	-	expression tag	UNP P32322
B	-4	LEU	-	expression tag	UNP P32322
B	-3	TYR	-	expression tag	UNP P32322
B	-2	PHE	-	expression tag	UNP P32322
B	-1	GLN	-	expression tag	UNP P32322
C	-22	MET	-	initiating methionine	UNP P32322
C	-21	HIS	-	expression tag	UNP P32322
C	-20	HIS	-	expression tag	UNP P32322
C	-19	HIS	-	expression tag	UNP P32322
C	-18	HIS	-	expression tag	UNP P32322
C	-17	HIS	-	expression tag	UNP P32322
C	-16	HIS	-	expression tag	UNP P32322
C	-15	SER	-	expression tag	UNP P32322
C	-14	SER	-	expression tag	UNP P32322
C	-13	GLY	-	expression tag	UNP P32322
C	-12	VAL	-	expression tag	UNP P32322
C	-11	ASP	-	expression tag	UNP P32322
C	-10	LEU	-	expression tag	UNP P32322
C	-9	GLY	-	expression tag	UNP P32322
C	-8	THR	-	expression tag	UNP P32322
C	-7	GLU	-	expression tag	UNP P32322
C	-6	ASN	-	expression tag	UNP P32322

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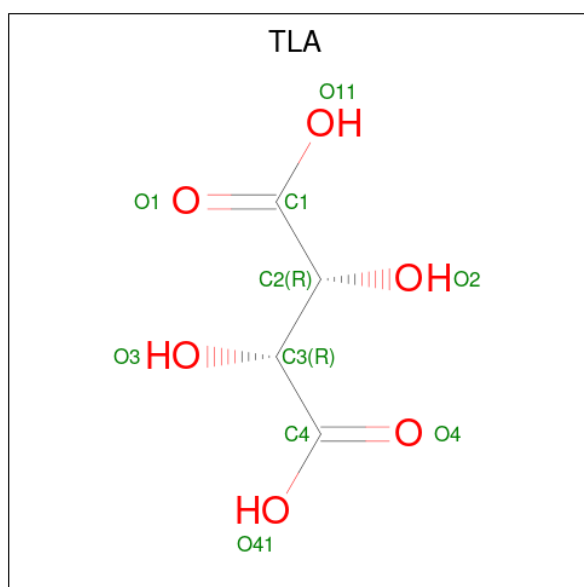
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASN	-	expression tag	UNP P32322
C	-4	LEU	-	expression tag	UNP P32322
C	-3	TYR	-	expression tag	UNP P32322
C	-2	PHE	-	expression tag	UNP P32322
C	-1	GLN	-	expression tag	UNP P32322
D	-22	MET	-	initiating methionine	UNP P32322
D	-21	HIS	-	expression tag	UNP P32322
D	-20	HIS	-	expression tag	UNP P32322
D	-19	HIS	-	expression tag	UNP P32322
D	-18	HIS	-	expression tag	UNP P32322
D	-17	HIS	-	expression tag	UNP P32322
D	-16	HIS	-	expression tag	UNP P32322
D	-15	SER	-	expression tag	UNP P32322
D	-14	SER	-	expression tag	UNP P32322
D	-13	GLY	-	expression tag	UNP P32322
D	-12	VAL	-	expression tag	UNP P32322
D	-11	ASP	-	expression tag	UNP P32322
D	-10	LEU	-	expression tag	UNP P32322
D	-9	GLY	-	expression tag	UNP P32322
D	-8	THR	-	expression tag	UNP P32322
D	-7	GLU	-	expression tag	UNP P32322
D	-6	ASN	-	expression tag	UNP P32322
D	-5	ASN	-	expression tag	UNP P32322
D	-4	LEU	-	expression tag	UNP P32322
D	-3	TYR	-	expression tag	UNP P32322
D	-2	PHE	-	expression tag	UNP P32322
D	-1	GLN	-	expression tag	UNP P32322
E	-22	MET	-	initiating methionine	UNP P32322
E	-21	HIS	-	expression tag	UNP P32322
E	-20	HIS	-	expression tag	UNP P32322
E	-19	HIS	-	expression tag	UNP P32322
E	-18	HIS	-	expression tag	UNP P32322
E	-17	HIS	-	expression tag	UNP P32322
E	-16	HIS	-	expression tag	UNP P32322
E	-15	SER	-	expression tag	UNP P32322
E	-14	SER	-	expression tag	UNP P32322
E	-13	GLY	-	expression tag	UNP P32322
E	-12	VAL	-	expression tag	UNP P32322
E	-11	ASP	-	expression tag	UNP P32322
E	-10	LEU	-	expression tag	UNP P32322
E	-9	GLY	-	expression tag	UNP P32322
E	-8	THR	-	expression tag	UNP P32322

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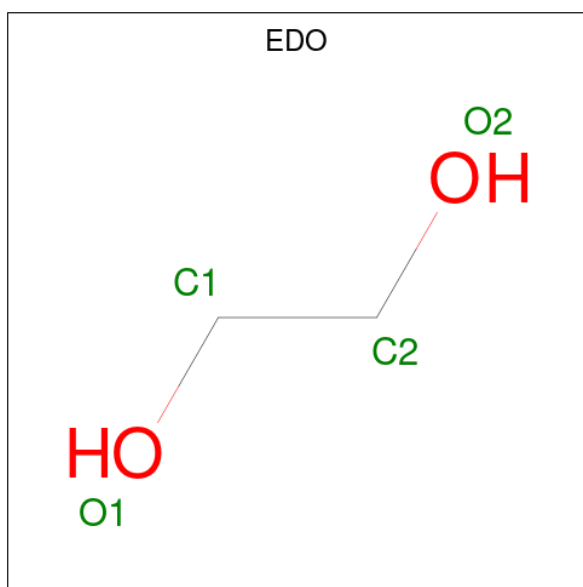
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	GLU	-	expression tag	UNP P32322
E	-6	ASN	-	expression tag	UNP P32322
E	-5	ASN	-	expression tag	UNP P32322
E	-4	LEU	-	expression tag	UNP P32322
E	-3	TYR	-	expression tag	UNP P32322
E	-2	PHE	-	expression tag	UNP P32322
E	-1	GLN	-	expression tag	UNP P32322

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	C	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

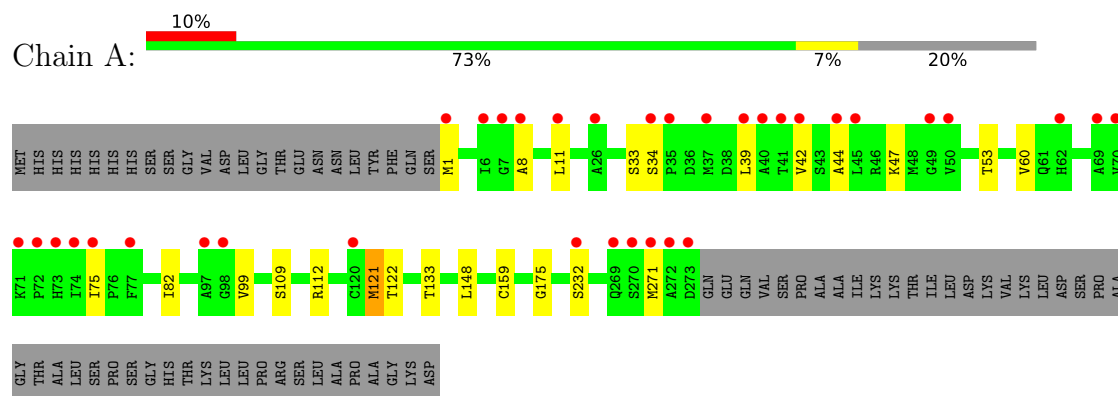
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		
4	B	132	Total	O	0	0
			132	132		
4	C	145	Total	O	0	0
			145	145		
4	D	160	Total	O	0	0
			160	160		
4	E	106	Total	O	0	0
			106	106		

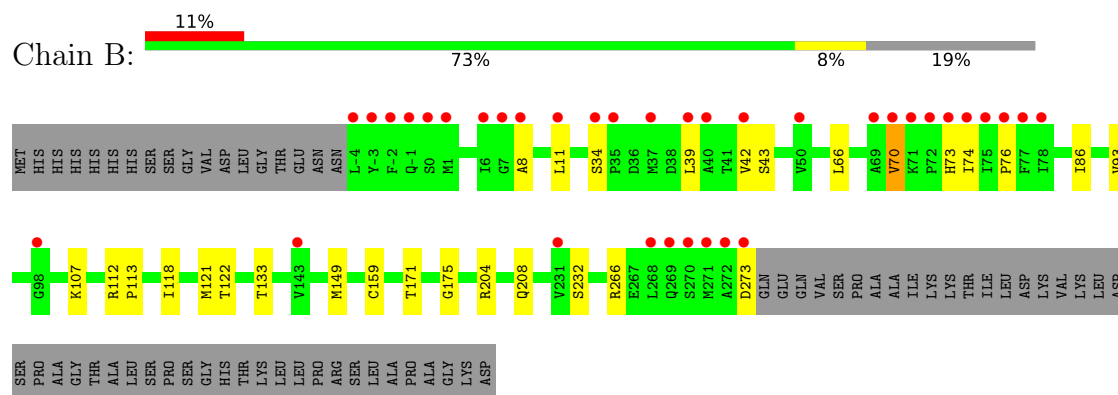
3 Residue-property plots [i](#)

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.

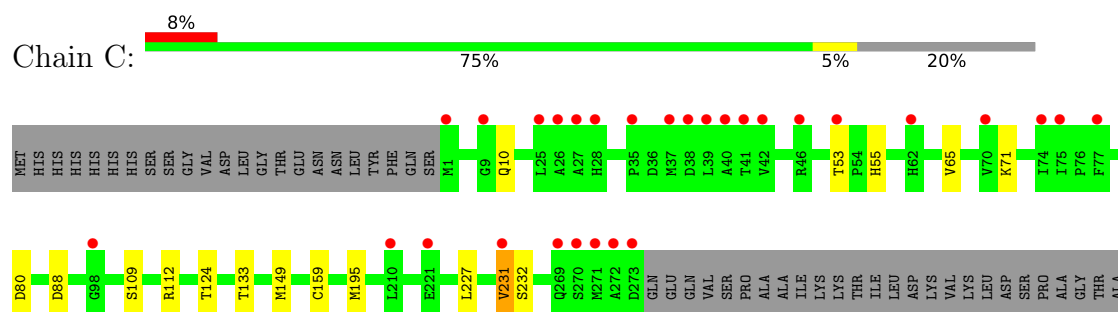
- Molecule 1: Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial



- Molecule 1: Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial



- Molecule 1: Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial



LEU
SER
PRO
SER
GLY
HIS
THR
LYS
LEU
LEU
PRO
ARG
SER
LEU
ALA
PRO
ALA
GLY
LYS
ASP

- Molecule 1: Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial

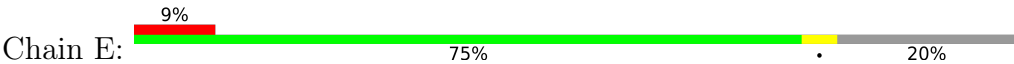


MET
HIS
HIS
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HIS
HIS
SER
SER
VAL
ASP
LEU
GLY
THR
GLU
ASN
ASN
LEU
TYR
PHE
Q-1
S0
I6
G7
A8
V24
S34
P35
D36
M37
D38
L39
A40
T41
V42
S43
K57
V60
A69
V70
K71
P72
H73
I74
I75
P76
F77
I78
I79
D80
E81
I82

A97
G98
V99
S109
R112
T133
V143
L153
V231
T265
R266
Q269
S270
M271
A272
D273
GLN
GLU
GLN
VAL
SER
PRO
ALA
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LYS
LYS
THR
ILE
LEU
ASP
LYS
VAL
LYS
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ASP
SER
PRO
ALA
GLY
THR
ALA
LEU
SER
PRO
GLY
HIS
THR
LYS
LEU

PRO
ARG
SER
LEU
ALA
PRO
ALA
GLY
ASP

- Molecule 1: Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial



MET
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
VAL
ASP
LEU
GLY
THR
GLU
ASN
ASN
LEU
TYR
PHE
GLN
SER
M1
L11
A12
F13
V24
L25
A26
S34
P35
D36
M37
D38
L39
A40
T41
V42
S43
A44
L45
R46
K47
L52
H62
V65
H73
I74
I78
I79
D80

G98
R112
C120
T133
V143
M149
C159
R204
Q208
A209
L210
L268
Q269
S270
M271
A272
D273
GLN
GLN
GLN
VAL
SER
PRO
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SER
GLY
HIS
THR

LYS
LEU
LEU
PRO
ARG
SER
LEU
ALA
PRO
ALA
GLY
LYS
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.20Å 88.11Å 116.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.21 – 1.65 37.21 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.21-1.65) 99.9 (37.21-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.182 , 0.204 0.183 , 0.204	Depositor DCC
R_{free} test set	2000 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10910	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: EDO, TLA

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	0.17	0/2063	0.38	0/2791
1	B	0.17	0/2100	0.38	0/2842
1	C	0.18	0/2063	0.39	0/2791
1	D	0.19	0/2070	0.38	0/2801
1	E	0.16	0/2066	0.37	0/2795
All	All	0.17	0/10362	0.38	0/14020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2029	0	2085	12	0
1	B	2067	0	2104	17	0
1	C	2029	0	2085	9	0
1	D	2033	0	2091	9	0
1	E	2032	0	2089	6	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	6	2	0
3	B	4	0	6	1	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	131	0	0	1	0
4	B	132	0	0	0	0
4	C	145	0	0	1	0
4	D	160	0	0	0	0
4	E	106	0	0	0	0
All	All	10910	0	10490	52	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 3.

All (52) 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:A:402:EDO:H11	1:D:266:ARG:HH22	1.39	0.87
1:B:76:PRO:HA	1:B:107:LYS:HE2	1.63	0.81
1:B:121[A]:MET:HE3	1:B:175:GLY:HA3	1.68	0.75
1:D:133:THR:HG21	1:D:153:LEU:HD13	1.68	0.73
1:B:8:ALA:HB3	1:B:34:SER:HB2	1.73	0.71
1:C:53:THR:HG22	1:C:55:HIS:H	1.54	0.71
1:E:13:PHE:HB2	1:E:41:THR:HG23	1.75	0.69
1:B:70:VAL:HG23	1:B:74:ILE:HB	1.76	0.67
1:A:8:ALA:HB3	1:A:34:SER:HB2	1.77	0.66
1:C:124:THR:HG21	1:D:231:VAL:HG12	1.78	0.65
1:B:121[A]:MET:HE2	1:B:171:THR:HG23	1.78	0.64
1:C:88:ASP:OD1	1:C:112:ARG:NH2	2.39	0.56
1:A:75:ILE:HG21	1:A:99:VAL:HG11	1.89	0.54
1:E:204[B]:ARG:NH1	1:E:208:GLN:HB2	2.22	0.53
1:B:39:LEU:HB2	1:B:42:VAL:HG23	1.90	0.53
1:E:74:ILE:HG22	1:E:78:ILE:HD13	1.92	0.52
1:C:10:GLN:NE2	4:C:503:HOH:O	2.44	0.51
1:B:93:VAL:HG21	1:B:149[B]:MET:HE2	1.92	0.51
1:B:11:LEU:HD11	1:B:122:THR:HG23	1.94	0.50
1:E:204[B]:ARG:HH12	1:E:208:GLN:HB2	1.76	0.50
1:E:65:VAL:HG11	1:E:149[B]:MET:HE1	1.94	0.50
1:B:118:ILE:HD13	1:B:149[B]:MET:HG2	1.94	0.49
1:D:109:SER:HA	1:D:112:ARG:O	2.12	0.49
1:A:109:SER:HA	1:A:112:ARG:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:NZ	1:D:81:GLU:O	2.48	0.47
1:A:60:VAL:HG21	1:A:82:ILE:HB	1.96	0.46
1:C:65:VAL:HG11	1:C:149[B]:MET:HE1	1.96	0.46
1:C:109:SER:HA	1:C:112:ARG:O	2.15	0.46
1:A:1:MET:N	4:A:502:HOH:O	2.49	0.46
1:B:112:ARG:HG2	1:B:113:PRO:HD2	1.98	0.46
1:A:39:LEU:HB2	1:A:42:VAL:HG23	1.99	0.44
1:A:133:THR:O	1:A:159:CYS:HA	2.17	0.44
1:D:75:ILE:HG21	1:D:99:VAL:HG11	1.99	0.44
1:B:118:ILE:CD1	1:B:149[B]:MET:HG2	2.47	0.44
1:A:1:MET:HE1	1:A:148:LEU:HD11	2.00	0.44
1:A:44:ALA:HA	1:A:47:LYS:HE2	2.00	0.44
1:B:204:ARG:HH12	1:B:208:GLN:HB2	1.83	0.43
1:B:266:ARG:HH12	3:B:401:EDO:H12	1.84	0.43
1:B:133:THR:O	1:B:159:CYS:HA	2.20	0.42
3:A:402:EDO:H12	1:C:195:MET:HA	2.02	0.42
1:D:60:VAL:HG21	1:D:82:ILE:HB	2.01	0.42
1:B:86:ILE:O	1:B:112:ARG:NE	2.53	0.41
1:D:8:ALA:HB3	1:D:34:SER:HB2	2.03	0.41
1:D:97:ALA:HB1	1:D:265:THR:HG23	2.03	0.41
1:C:227:LEU:O	1:C:231:VAL:HG12	2.20	0.41
1:E:133:THR:O	1:E:159:CYS:HA	2.21	0.40
1:A:33:SER:HA	1:A:53:THR:O	2.22	0.40
1:A:121[B]:MET:HE1	1:A:175:GLY:CA	2.51	0.40
1:A:11:LEU:HD11	1:A:122:THR:HG23	2.03	0.40
1:C:133:THR:O	1:C:159:CYS:HA	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	274/342 (80%)	269 (98%)	5 (2%)	0	100	100
1	B	278/342 (81%)	273 (98%)	5 (2%)	0	100	100
1	C	274/342 (80%)	270 (98%)	4 (2%)	0	100	100
1	D	275/342 (80%)	273 (99%)	2 (1%)	0	100	100
1	E	274/342 (80%)	271 (99%)	3 (1%)	0	100	100
All	All	1375/1710 (80%)	1356 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	215/270 (80%)	211 (98%)	4 (2%)	50	28
1	B	219/270 (81%)	214 (98%)	5 (2%)	44	21
1	C	215/270 (80%)	211 (98%)	4 (2%)	50	28
1	D	216/270 (80%)	216 (100%)	0	100	100
1	E	215/270 (80%)	210 (98%)	5 (2%)	44	21
All	All	1080/1350 (80%)	1062 (98%)	18 (2%)	55	32

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121[A]	MET
1	A	121[B]	MET
1	A	232	SER
1	A	271	MET
1	B	43	SER
1	B	70	VAL
1	B	73	HIS
1	B	232	SER
1	B	273	ASP
1	C	71	LYS

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Mol	Chain	Res	Type
1	C	80	ASP
1	C	231	VAL
1	C	232	SER
1	E	42	VAL
1	E	112	ARG
1	E	120	CYS
1	E	143	VAL
1	E	210[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	HIS
1	A	226	GLN
1	B	28	HIS
1	B	73	HIS
1	B	226	GLN
1	D	28	HIS
1	D	55	HIS
1	D	226	GLN
1	E	55	HIS
1	E	226	GLN
1	E	230	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	EDO	B	401	-	3,3,3	0.42	0	2,2,2	0.49	0
2	TLA	A	401	-	9,9,9	1.44	2 (22%)	12,12,12	1.37	2 (16%)
3	EDO	A	402	-	3,3,3	0.44	0	2,2,2	0.41	0
3	EDO	C	402	-	3,3,3	0.42	0	2,2,2	0.51	0
2	TLA	B	402	-	9,9,9	1.36	1 (11%)	12,12,12	1.33	2 (16%)
2	TLA	C	401	-	9,9,9	1.35	1 (11%)	12,12,12	1.46	2 (16%)
3	EDO	D	401	-	3,3,3	0.41	0	2,2,2	0.43	0

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	EDO	B	401	-	-	1/1/1/1	-
2	TLA	A	401	-	-	0/12/12/12	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
2	TLA	B	402	-	-	4/12/12/12	-
2	TLA	C	401	-	-	2/12/12/12	-
3	EDO	D	401	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	TLA	O41-C4	-2.10	1.23	1.30
2	C	401	TLA	O41-C4	-2.10	1.23	1.30
2	A	401	TLA	C3-C4	2.06	1.55	1.52
2	A	401	TLA	O41-C4	-2.04	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TLA	O4-C4-C3	-2.54	114.86	121.62
2	B	402	TLA	O4-C4-C3	-2.38	115.28	121.62
2	B	402	TLA	O1-C1-C2	-2.34	115.37	121.62
2	C	401	TLA	O1-C1-C2	-2.34	115.39	121.62
2	C	401	TLA	O4-C4-C3	-2.32	115.43	121.62
2	A	401	TLA	O1-C1-C2	-2.08	116.08	121.62

There are no chirality outliers.

All (10) torsion outliers are listed below:

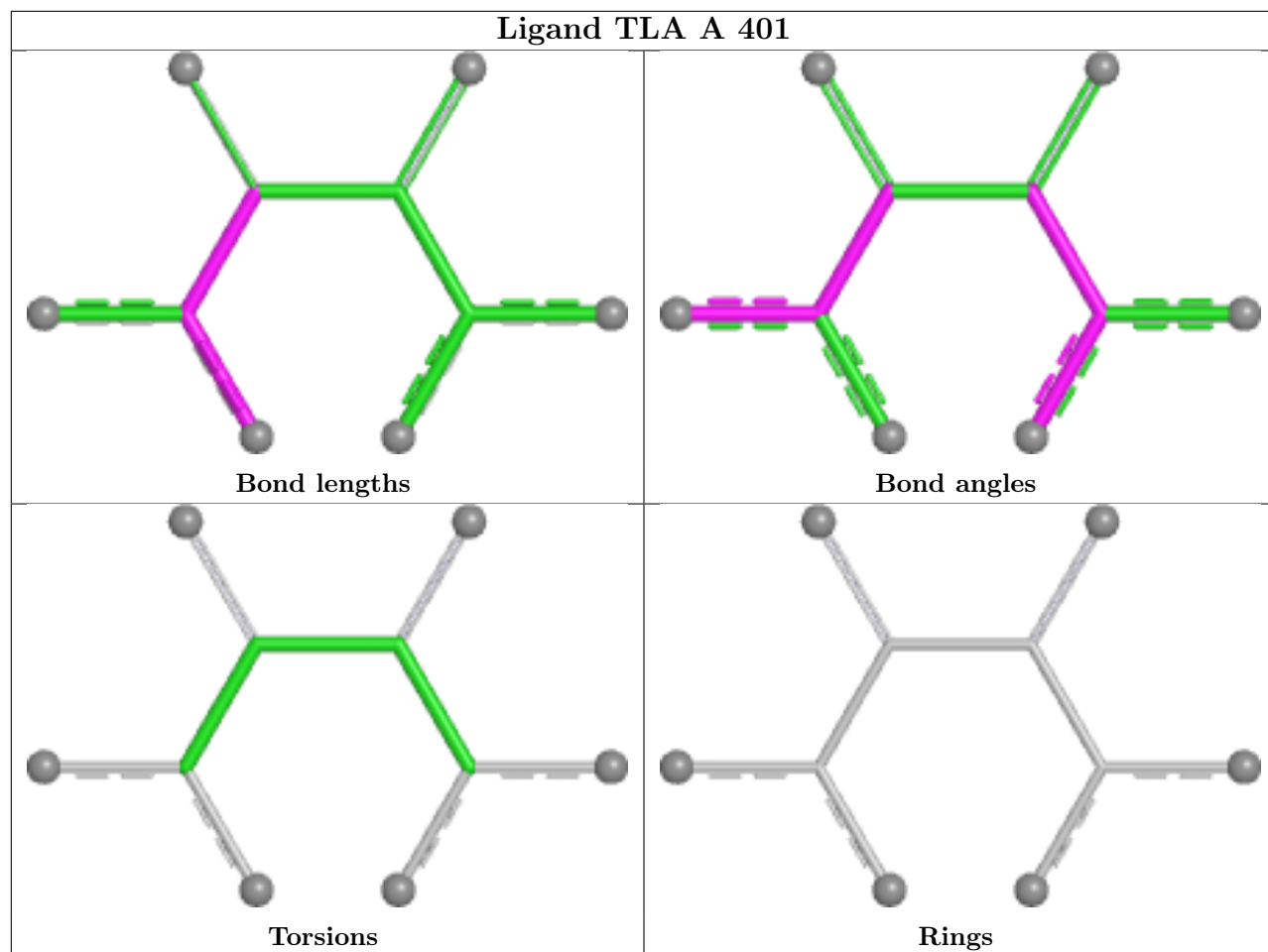
Mol	Chain	Res	Type	Atoms
2	B	402	TLA	C1-C2-C3-O3
3	A	402	EDO	O1-C1-C2-O2
2	B	402	TLA	O2-C2-C3-C4
2	B	402	TLA	O2-C2-C3-O3
2	C	401	TLA	C2-C3-C4-O4
2	B	402	TLA	C1-C2-C3-C4
2	C	401	TLA	O3-C3-C4-O4
3	B	401	EDO	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2
3	D	401	EDO	O1-C1-C2-O2

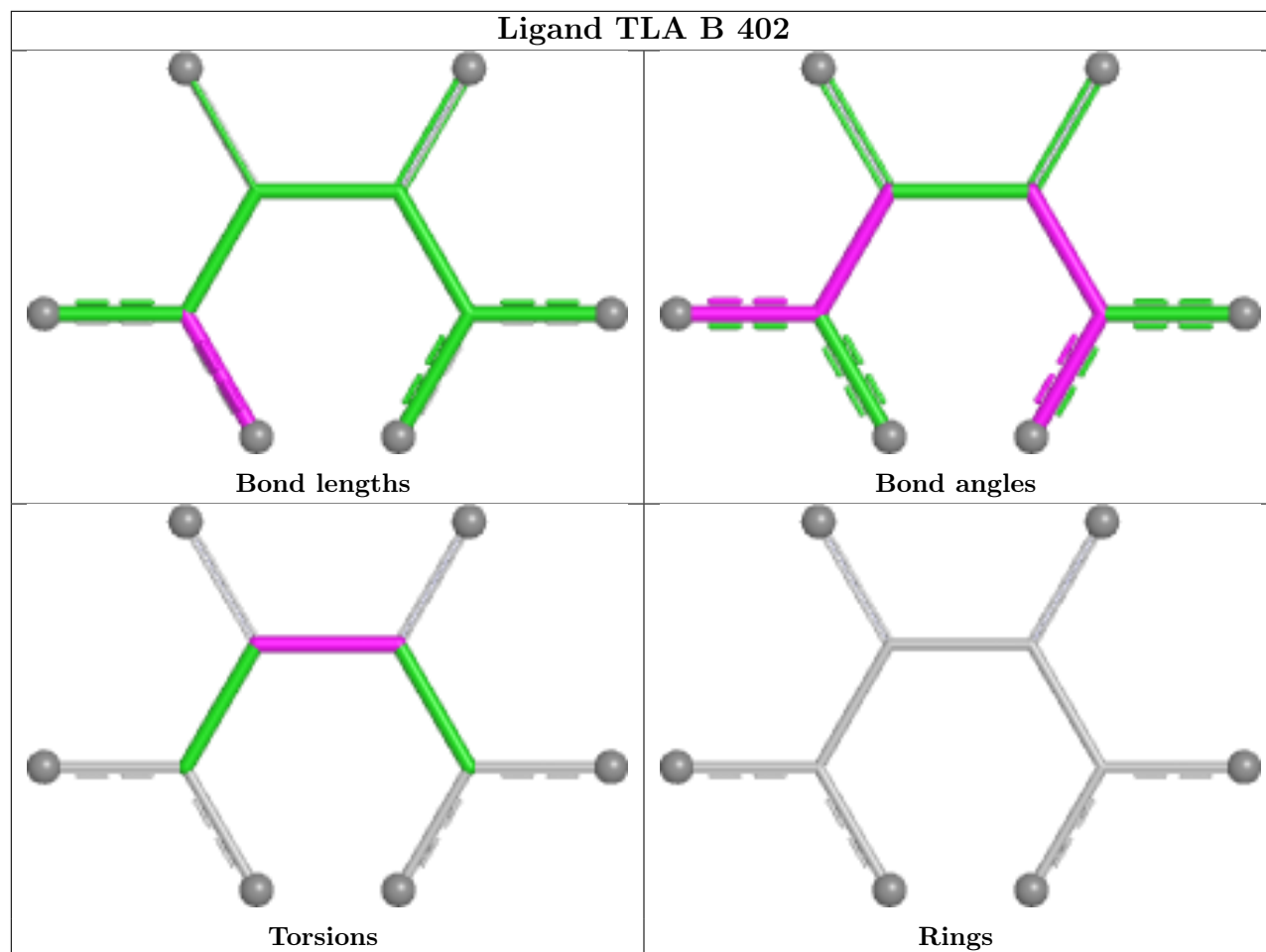
There are no ring outliers.

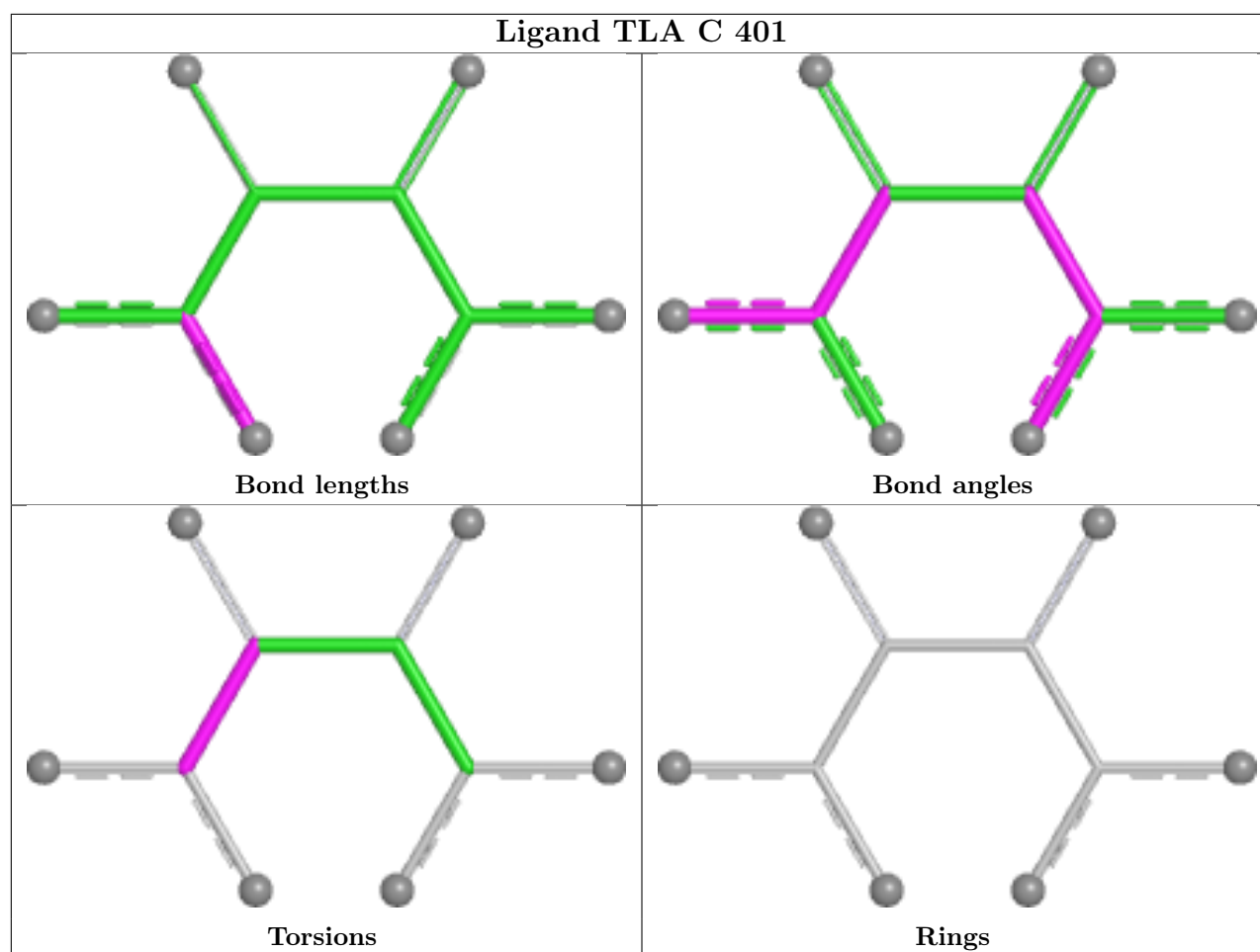
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	EDO	1	0
3	A	402	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/342 (79%)	0.69	35 (12%) 7 8	17, 45, 105, 187	3 (1%)
1	B	278/342 (81%)	0.66	36 (12%) 7 8	17, 45, 104, 167	2 (0%)
1	C	273/342 (79%)	0.54	29 (10%) 11 12	18, 42, 91, 206	4 (1%)
1	D	275/342 (80%)	0.57	30 (10%) 10 11	20, 43, 84, 137	2 (0%)
1	E	273/342 (79%)	0.61	30 (10%) 10 11	19, 44, 96, 188	3 (1%)
All	All	1372/1710 (80%)	0.61	160 (11%) 9 10	17, 44, 96, 206	14 (1%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	42	VAL	7.2
1	D	70	VAL	7.1
1	D	74	ILE	6.5
1	A	75	ILE	6.2
1	B	8	ALA	6.2
1	E	37	MET	6.1
1	B	74	ILE	5.8
1	B	75	ILE	5.6
1	E	39	LEU	5.6
1	C	39	LEU	5.5
1	A	70	VAL	5.4
1	B	70	VAL	5.4
1	B	72	PRO	5.4
1	B	77	PHE	5.3
1	A	8	ALA	5.3
1	E	143	VAL	5.2
1	B	-4	LEU	5.1
1	A	42	VAL	5.1
1	E	41	THR	5.0
1	D	8	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	40	ALA	4.7
1	D	143	VAL	4.5
1	D	39	LEU	4.5
1	E	273	ASP	4.5
1	E	272	ALA	4.4
1	B	35	PRO	4.4
1	A	35	PRO	4.3
1	D	42	VAL	4.3
1	D	77	PHE	4.3
1	A	272	ALA	4.2
1	D	72	PRO	4.1
1	B	73	HIS	4.1
1	B	98	GLY	4.1
1	E	35	PRO	4.0
1	B	0	SER	4.0
1	B	37	MET	4.0
1	B	69	ALA	4.0
1	E	40	ALA	4.0
1	C	273	ASP	4.0
1	D	273	ASP	3.9
1	A	74	ILE	3.9
1	A	69	ALA	3.9
1	C	41	THR	3.9
1	D	37	MET	3.8
1	D	69	ALA	3.8
1	A	39	LEU	3.8
1	C	272	ALA	3.8
1	B	-3	TYR	3.7
1	B	143	VAL	3.6
1	B	39	LEU	3.5
1	D	73	HIS	3.5
1	B	40	ALA	3.4
1	D	272	ALA	3.4
1	D	75	ILE	3.4
1	B	273	ASP	3.4
1	A	40	ALA	3.3
1	C	26	ALA	3.3
1	A	26	ALA	3.3
1	A	72	PRO	3.2
1	C	38	ASP	3.2
1	D	40	ALA	3.2
1	D	7	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	6[A]	ILE	3.2
1	C	74	ILE	3.2
1	E	269	GLN	3.2
1	B	42	VAL	3.2
1	D	71	LYS	3.1
1	B	50	VAL	3.1
1	B	76	PRO	3.1
1	E	74	ILE	3.1
1	B	-2	PHE	3.1
1	B	272	ALA	3.1
1	C	42	VAL	3.0
1	D	35	PRO	3.0
1	A	1	MET	3.0
1	D	34	SER	3.0
1	B	231	VAL	2.9
1	B	270	SER	2.9
1	C	270	SER	2.9
1	C	271	MET	2.9
1	D	270	SER	2.9
1	B	71	LYS	2.9
1	B	78	ILE	2.9
1	C	77	PHE	2.9
1	C	27	ALA	2.9
1	A	271	MET	2.9
1	A	71	LYS	2.9
1	A	270	SER	2.9
1	B	34	SER	2.9
1	A	7	GLY	2.8
1	D	98	GLY	2.8
1	A	73	HIS	2.8
1	E	11	LEU	2.8
1	A	77	PHE	2.8
1	A	45	LEU	2.8
1	E	271	MET	2.8
1	A	62	HIS	2.8
1	A	11	LEU	2.7
1	A	50	VAL	2.7
1	A	41	THR	2.7
1	A	44	ALA	2.7
1	C	37	MET	2.6
1	C	98	GLY	2.6
1	A	120	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	35	PRO	2.6
1	C	231	VAL	2.6
1	A	98	GLY	2.5
1	A	273	ASP	2.5
1	C	62	HIS	2.5
1	A	37	MET	2.5
1	C	53	THR	2.5
1	C	1	MET	2.5
1	A	34	SER	2.5
1	E	34	SER	2.5
1	E	25	LEU	2.4
1	E	45	LEU	2.4
1	E	47	LYS	2.4
1	D	-1	GLN	2.4
1	A	97	ALA	2.4
1	D	80	ASP	2.4
1	A	232	SER	2.4
1	C	269	GLN	2.4
1	D	76	PRO	2.4
1	B	11	LEU	2.4
1	C	25	LEU	2.4
1	C	210[A]	LEU	2.4
1	C	70	VAL	2.4
1	E	36	ASP	2.3
1	D	24	VAL	2.3
1	C	28	HIS	2.3
1	A	269	GLN	2.3
1	B	7	GLY	2.3
1	E	38	ASP	2.3
1	E	73	HIS	2.3
1	E	268	LEU	2.2
1	E	43	SER	2.2
1	E	44	ALA	2.2
1	D	0	SER	2.2
1	B	271	MET	2.2
1	E	52	LEU	2.2
1	D	6	ILE	2.2
1	D	43	SER	2.2
1	E	98	GLY	2.1
1	B	268	LEU	2.1
1	B	1	MET	2.1
1	E	80	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	221	GLU	2.1
1	D	269	GLN	2.1
1	A	49	GLY	2.1
1	E	1	MET	2.1
1	D	78	ILE	2.1
1	E	26	ALA	2.1
1	E	62	HIS	2.1
1	B	-1	GLN	2.0
1	B	269	GLN	2.0
1	C	9	GLY	2.0
1	A	6	ILE	2.0
1	C	46	ARG	2.0
1	C	75	ILE	2.0
1	E	24	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

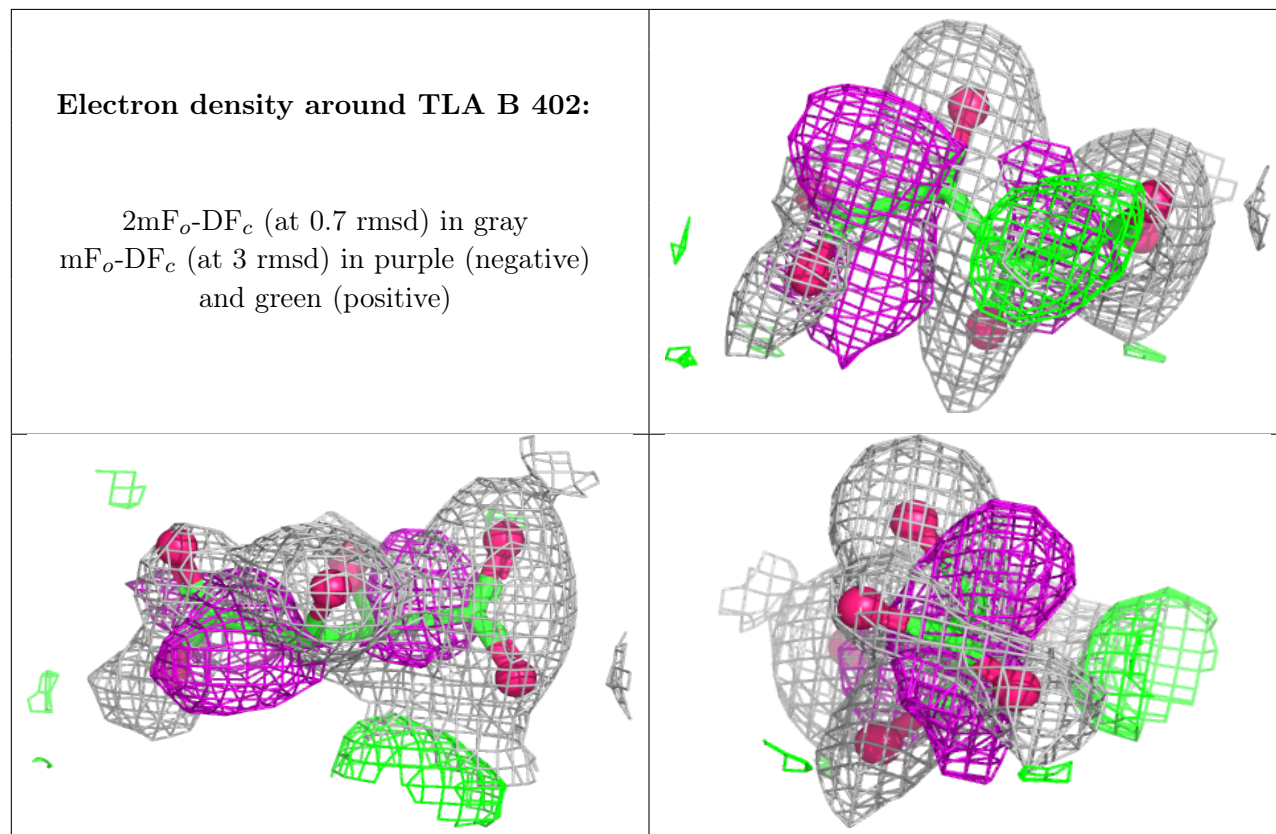
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	402	4/4	0.79	0.18	40,49,59,65	0
2	TLA	B	402	10/10	0.81	0.15	39,60,72,83	0
2	TLA	C	401	10/10	0.84	0.15	34,57,65,69	0
3	EDO	D	401	4/4	0.85	0.18	50,50,57,73	0
3	EDO	B	401	4/4	0.86	0.17	51,51,56,67	0
3	EDO	C	402	4/4	0.88	0.16	44,54,54,65	0
2	TLA	A	401	10/10	0.89	0.11	35,48,55,55	0

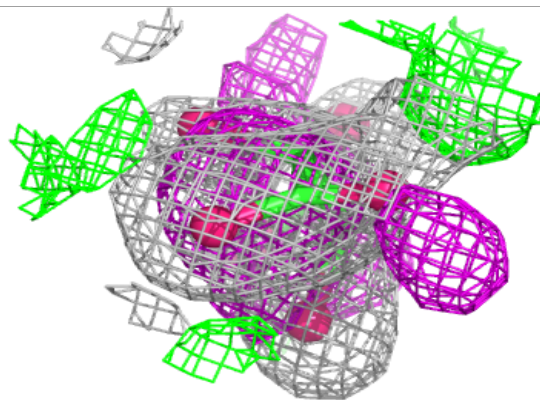
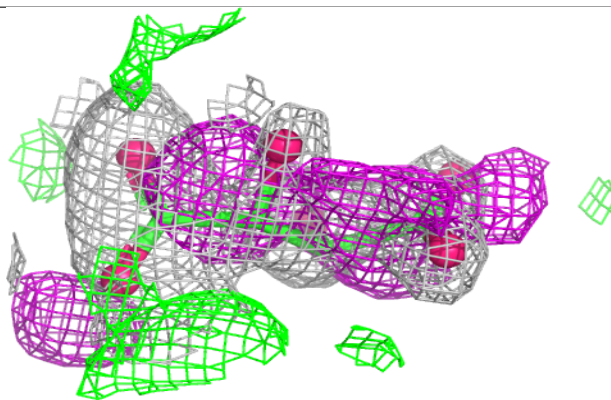
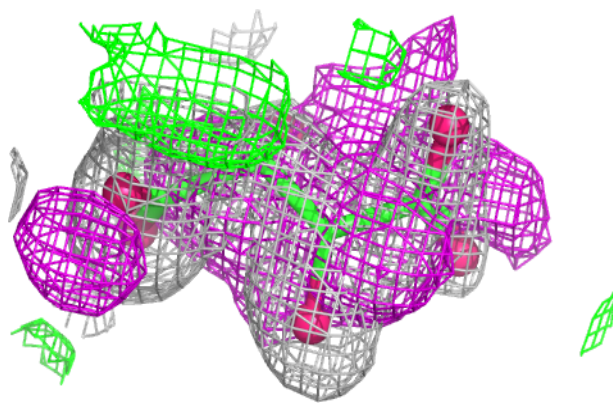
The following is a graphical depiction of the model fit to experimental electron density of all

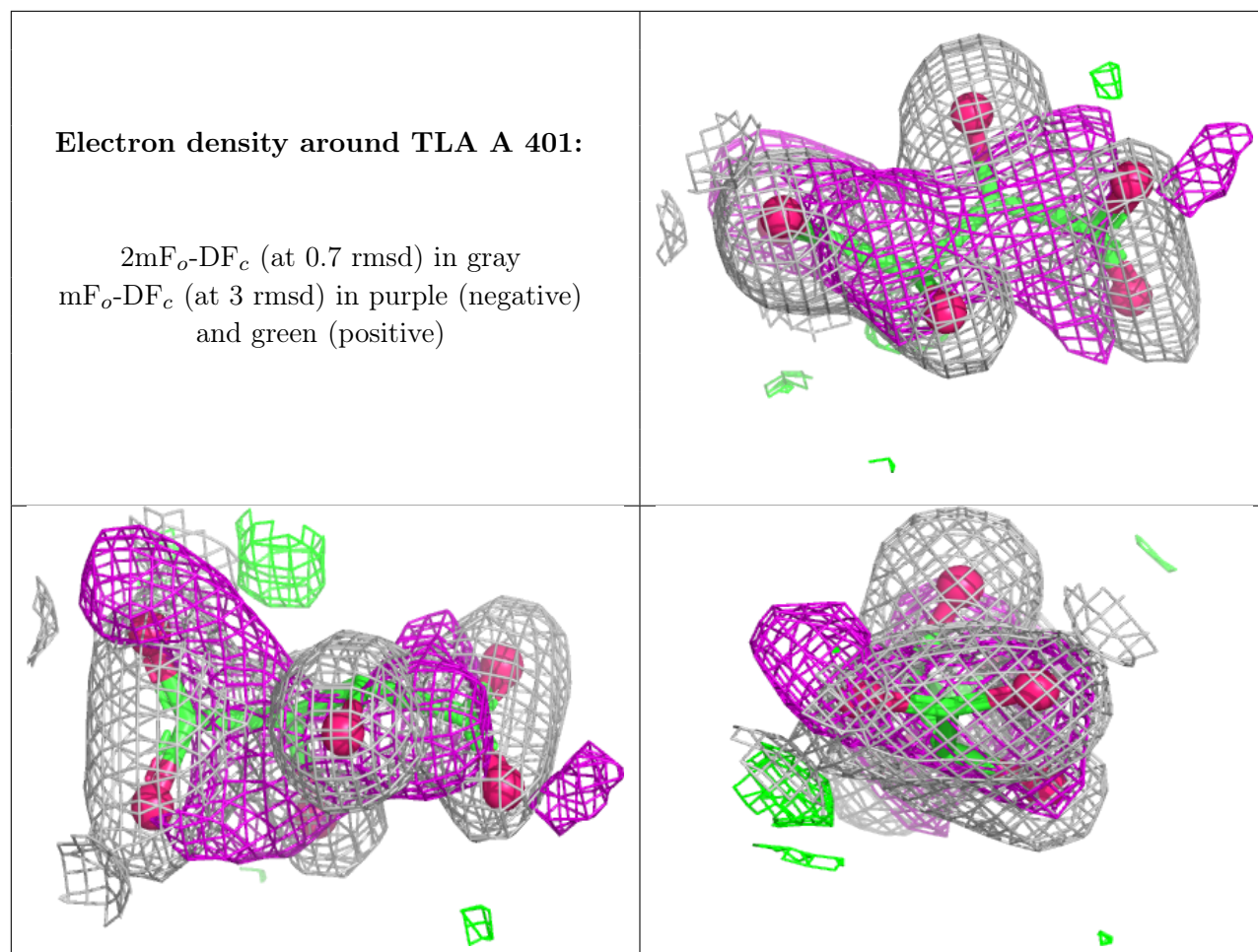
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around TLA C 401:

$2mF_o-DF_c$ (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.