



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2025 – 04:12 pm BST

PDB ID : 9S04 / pdb_00009s04
Title : PYCR1 in complex with 1-(2,4-Difluorophenyl)-2-(1H-1,2,4-triazol-1-yl)ethanone
Authors : Ragin-Oh, W.; Czerwonka, D.; Ruszkowski, M.
Deposited on : 2025-07-16
Resolution : 1.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

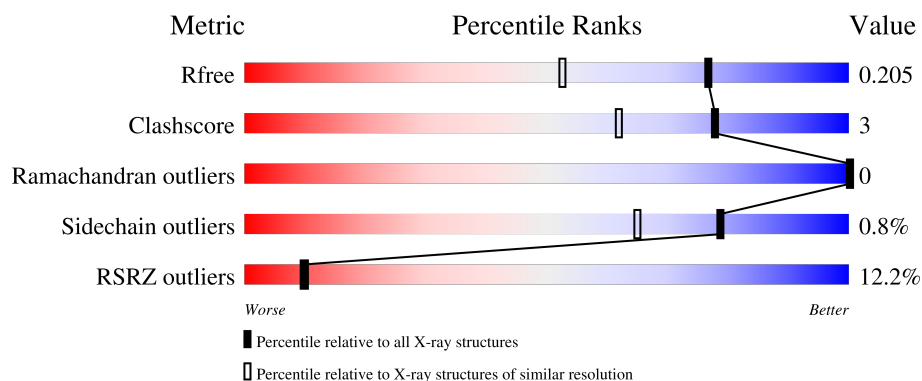
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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}	164625	7165 (1.60-1.56)
Clashscore	180529	1026 (1.58-1.58)
Ramachandran outliers	177936	1005 (1.58-1.58)
Sidechain outliers	177891	1004 (1.58-1.58)
RSRZ outliers	164620	7163 (1.60-1.56)

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	<div> <div>8%</div> <div>75%</div> <div>5%</div> <div>20%</div> </div>
1	B	342	<div> <div>8%</div> <div>76%</div> <div>•</div> <div>20%</div> </div>
1	C	342	<div> <div>12%</div> <div>72%</div> <div>7%</div> <div>20%</div> </div>
1	D	342	<div> <div>7%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
1	E	342	<div> <div>13%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11114 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	3	0
			2023	1275	358	376	14			
1	B	273	Total	C	N	O	S	0	3	0
			2026	1276	359	377	14			
1	C	273	Total	C	N	O	S	0	4	0
			2030	1278	361	377	14			
1	D	273	Total	C	N	O	S	0	2	0
			2018	1270	358	376	14			
1	E	273	Total	C	N	O	S	0	2	0
			2021	1271	359	377	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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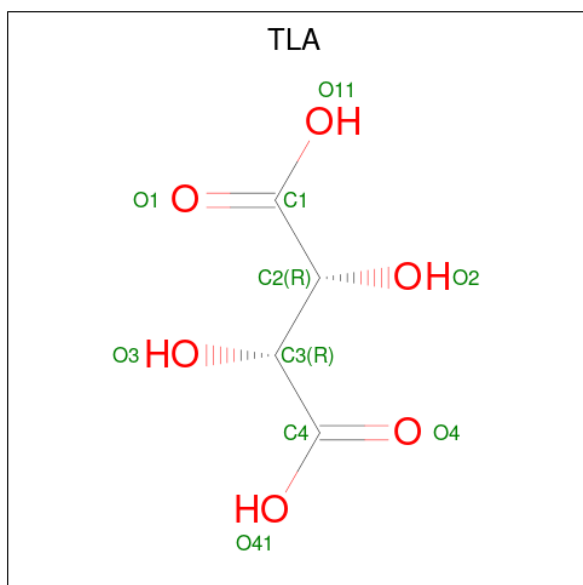
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASN	-	expression tag	UNP P32322
C	-4	LEU	-	expression tag	UNP P32322
C	-3	TYR	-	expression tag	UNP P32322
C	-2	PHE	-	expression tag	UNP P32322
C	-1	GLN	-	expression tag	UNP P32322
D	-22	MET	-	initiating methionine	UNP P32322
D	-21	HIS	-	expression 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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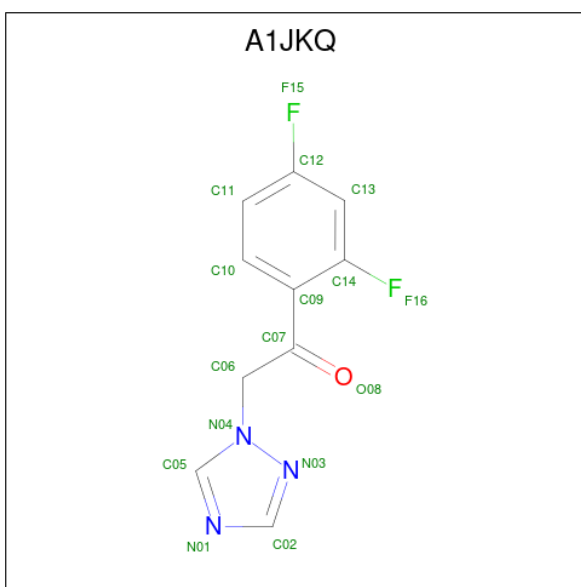
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	GLU	-	expression tag	UNP P32322
E	-6	ASN	-	expression tag	UNP P32322
E	-5	ASN	-	expression tag	UNP P32322
E	-4	LEU	-	expression tag	UNP P32322
E	-3	TYR	-	expression tag	UNP P32322
E	-2	PHE	-	expression tag	UNP P32322
E	-1	GLN	-	expression tag	UNP P32322

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



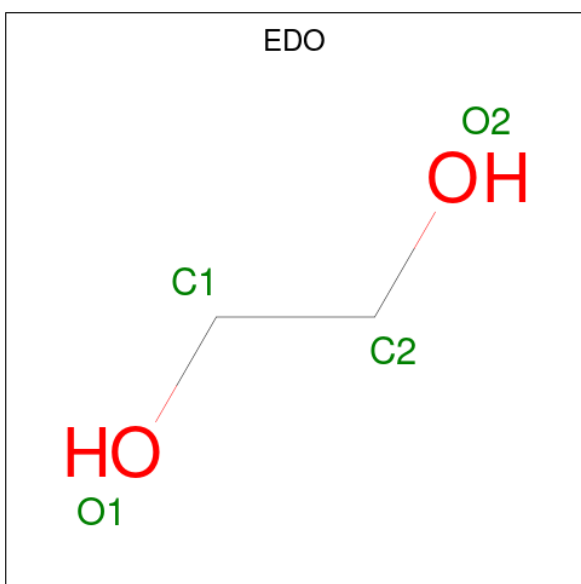
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	C	1	Total	C	O	0	0
			10	4	6		
2	D	1	Total	C	O	0	0
			10	4	6		
2	E	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is 1-[2,4-bis(fluoranyl)phenyl]-2-(1,2,4-triazol-1-yl)ethanone (CCD ID: A1JKQ) (formula: C₁₀H₇F₂N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			16	10	2	3	1		
3	B	1	Total	C	F	N	O	0	0
			16	10	2	3	1		
3	C	1	Total	C	F	N	O	0	0
			16	10	2	3	1		
3	D	1	Total	C	F	N	O	0	0
			16	10	2	3	1		
3	E	1	Total	C	F	N	O	0	0
			16	10	2	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

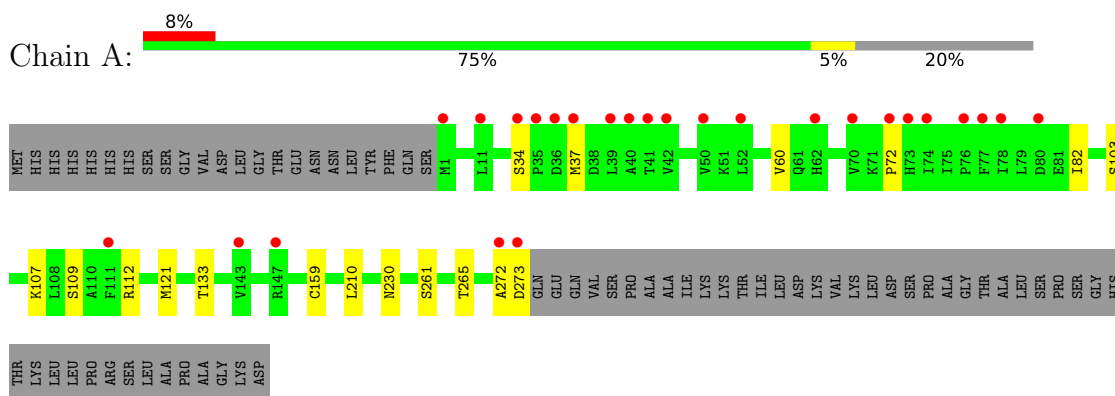
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	176	Total O 176 176	0	0
5	B	181	Total O 181 181	0	0
5	C	182	Total O 182 182	0	0
5	D	177	Total O 177 177	0	0
5	E	126	Total O 126 126	0	0

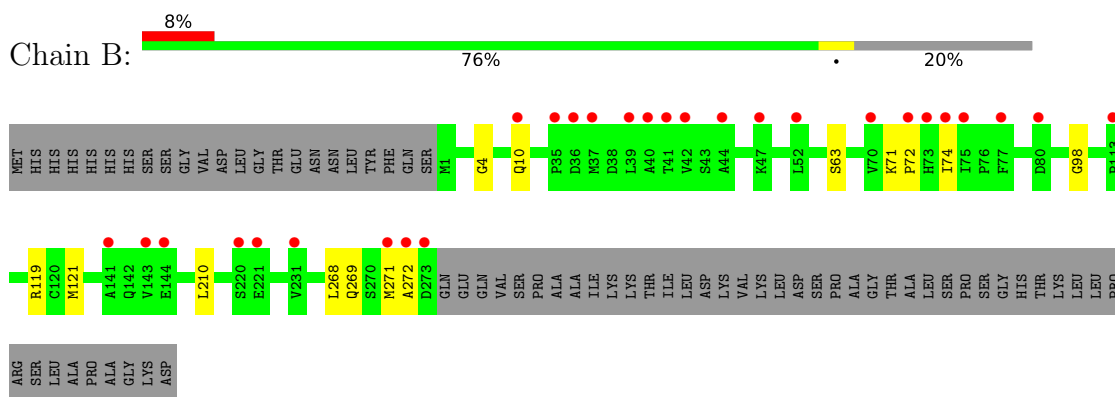
3 Residue-property plots [i](#)

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.

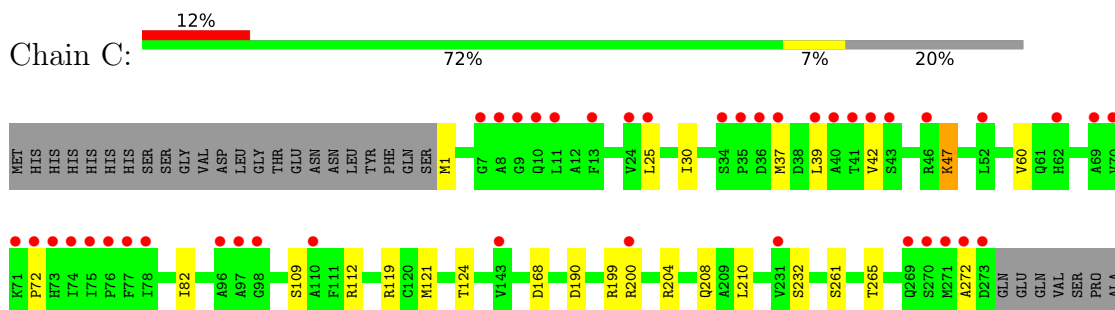
- Molecule 1: Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial



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



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



ALA
ILE
LYS
LYS
THR
ILE
LEU
ASP
LYS
VAL
LYS
LEU
ASP
SER
GLY
VAL
LEU
ASP
SER
PRO
ALA
GLY
THR
ALA
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
HIS
HIS
HIS
HIS
SER
SER
GLY
VAL
ASP
LEU
GLY
THR
GLU
ASN
THR
LEU
TYR
PHE
GLN
SER
M1
G7
A8
G9
Q10
A26
S34
P35
D36
M37
D38
L39
A40
T41
V42
V70
K71
P72
H73
I74
I75
P76
F77
I78
L79
D80
G98
S109
R112

R119
G120
M121
V143
E144
L210
S220
V231
S261
T265
L268
Q269
S270
M271
A272
D273
GLN
GLN
VAL
SER
PRO
ALA
ALA
ILE
LYS
LYS
THR
ILE
LEU
ASP
LYS
VAL
LYS
LEU
ASP
SER
PRO
ALA
GLY
THR
ALA
LEU
SER
PRO
GLY
HIS
THR
LYS
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
HIS
HIS
HIS
HIS
SER
SER
SER
GLY
VAL
ASP
LEU
GLY
THR
GLU
ASN
THR
LEU
TYR
PHE
GLN
SER
M1
G7
A8
G9
Q10
L11
L25
A26
A27
S34
P35
D36
M37
D38
L39
A40
T41
V42
S43
A44
L45
L52
V60
S63
A69
V70
K71
P72
H73
I74

L75
P76
F77
I78
L79
D80
E81
I82
G83
A84
L91
A97
G98
P113
M121
Y135
V143
E144
R147
D190
R199
R200
R204
Q208
V231
S261
T265
Q269
S270
M271
A272
D273
GLN
GLN
VAL
SER
PRO
ALA
ALA
ILE
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GLY
SER
GLY
HIS
THR
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	163.78Å 88.00Å 116.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.57 38.64 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.64-1.57) 100.0 (38.64-1.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.57Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.205 0.185 , 0.205	Depositor DCC
R_{free} test set	2000 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11114	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, A1JKQ, 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	0.26	0/2063	0.45	0/2792
1	B	0.27	0/2063	0.46	0/2792
1	C	0.26	0/2073	0.48	0/2806
1	D	0.26	0/2055	0.46	0/2781
1	E	0.24	0/2055	0.44	0/2781
All	All	0.26	0/10309	0.46	0/13952

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	2023	0	2089	10	0
1	B	2026	0	2088	10	0
1	C	2030	0	2098	17	0
1	D	2018	0	2078	13	0
1	E	2021	0	2077	10	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
2	D	10	0	4	0	0
2	E	10	0	4	0	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
3	E	16	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	12	0	18	0	0
5	A	176	0	0	0	0
5	B	181	0	0	3	0
5	C	182	0	0	4	0
5	D	177	0	0	4	0
5	E	126	0	0	0	0
All	All	11114	0	10486	55	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.

The worst 5 of 55 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:B:72:PRO:HB3	1:B:272:ALA:HB2	1.71	0.73
1:C:210:LEU:HD11	1:D:210:LEU:HD13	1.70	0.72
1:A:210[B]:LEU:HD13	1:B:210[B]:LEU:HD11	1.72	0.71
1:A:103:SER:O	1:A:107:LYS:HD3	1.97	0.64
1:A:210[A]:LEU:HD11	1:B:210[A]:LEU:HD13	1.79	0.63

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	274/342 (80%)	270 (98%)	4 (2%)	0	100	100
1	B	274/342 (80%)	270 (98%)	4 (2%)	0	100	100
1	C	275/342 (80%)	270 (98%)	5 (2%)	0	100	100
1	D	273/342 (80%)	269 (98%)	4 (2%)	0	100	100
1	E	273/342 (80%)	269 (98%)	4 (2%)	0	100	100
All	All	1369/1710 (80%)	1348 (98%)	21 (2%)	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%)	213 (99%)	2 (1%)	75	59
1	B	215/270 (80%)	214 (100%)	1 (0%)	86	78
1	C	216/270 (80%)	212 (98%)	4 (2%)	52	24
1	D	214/270 (79%)	213 (100%)	1 (0%)	86	78
1	E	214/270 (79%)	213 (100%)	1 (0%)	86	78
All	All	1074/1350 (80%)	1065 (99%)	9 (1%)	79	65

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	121	MET
1	E	121	MET
1	C	39	LEU
1	C	47	LYS
1	C	121	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	230	ASN
1	E	226	GLN
1	D	230	ASN
1	D	226	GLN
1	E	140	HIS

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](#)

16 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$
4	EDO	D	404	-	3,3,3	0.46	0	2,2,2	0.34	0
2	TLA	C	401	-	9,9,9	1.44	2 (22%)	12,12,12	1.47	2 (16%)
3	A1JKQ	B	402	-	15,17,17	1.30	3 (20%)	18,23,23	2.26	7 (38%)
2	TLA	E	401	-	9,9,9	1.50	2 (22%)	12,12,12	1.46	3 (25%)
3	A1JKQ	E	402	-	15,17,17	1.23	2 (13%)	18,23,23	2.37	8 (44%)
4	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.43	0
3	A1JKQ	A	402	-	15,17,17	1.26	2 (13%)	18,23,23	2.36	7 (38%)
3	A1JKQ	C	402	-	15,17,17	1.24	2 (13%)	18,23,23	2.41	9 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1JKQ	D	402	-	15,17,17	1.22	3 (20%)	18,23,23	2.32	8 (44%)
4	EDO	B	403	-	3,3,3	0.47	0	2,2,2	0.34	0
2	TLA	A	401	-	9,9,9	1.43	1 (11%)	12,12,12	1.62	4 (33%)
4	EDO	C	403	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	D	403	-	3,3,3	0.52	0	2,2,2	0.29	0
2	TLA	D	401	-	9,9,9	1.38	1 (11%)	12,12,12	1.38	2 (16%)
4	EDO	D	405	-	3,3,3	0.45	0	2,2,2	0.44	0
2	TLA	B	401	-	9,9,9	1.47	2 (22%)	12,12,12	1.39	2 (16%)

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
4	EDO	D	404	-	-	0/1/1/1	-
2	TLA	C	401	-	-	0/12/12/12	-
3	A1JKQ	B	402	-	-	0/7/8/8	0/2/2/2
2	TLA	E	401	-	-	0/12/12/12	-
3	A1JKQ	E	402	-	-	0/7/8/8	0/2/2/2
4	EDO	A	403	-	-	1/1/1/1	-
3	A1JKQ	A	402	-	-	0/7/8/8	0/2/2/2
3	A1JKQ	C	402	-	-	0/7/8/8	0/2/2/2
3	A1JKQ	D	402	-	-	0/7/8/8	0/2/2/2
4	EDO	B	403	-	-	1/1/1/1	-
2	TLA	A	401	-	-	0/12/12/12	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-
2	TLA	D	401	-	-	0/12/12/12	-
4	EDO	D	405	-	-	1/1/1/1	-
2	TLA	B	401	-	-	0/12/12/12	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1JKQ	C09-C07	2.73	1.54	1.48
3	A	402	A1JKQ	C09-C07	2.65	1.53	1.48
3	C	402	A1JKQ	C09-C07	2.52	1.53	1.48
3	D	402	A1JKQ	C09-C07	2.48	1.53	1.48
3	E	402	A1JKQ	C09-C07	2.48	1.53	1.48

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	A1JKQ	C05-N01-C02	4.52	107.43	102.34
3	A	402	A1JKQ	C05-N01-C02	4.36	107.25	102.34
3	B	402	A1JKQ	C05-N01-C02	4.28	107.17	102.34
3	C	402	A1JKQ	C13-C14-C09	-4.15	119.10	123.53
3	E	402	A1JKQ	C05-N01-C02	4.11	106.97	102.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

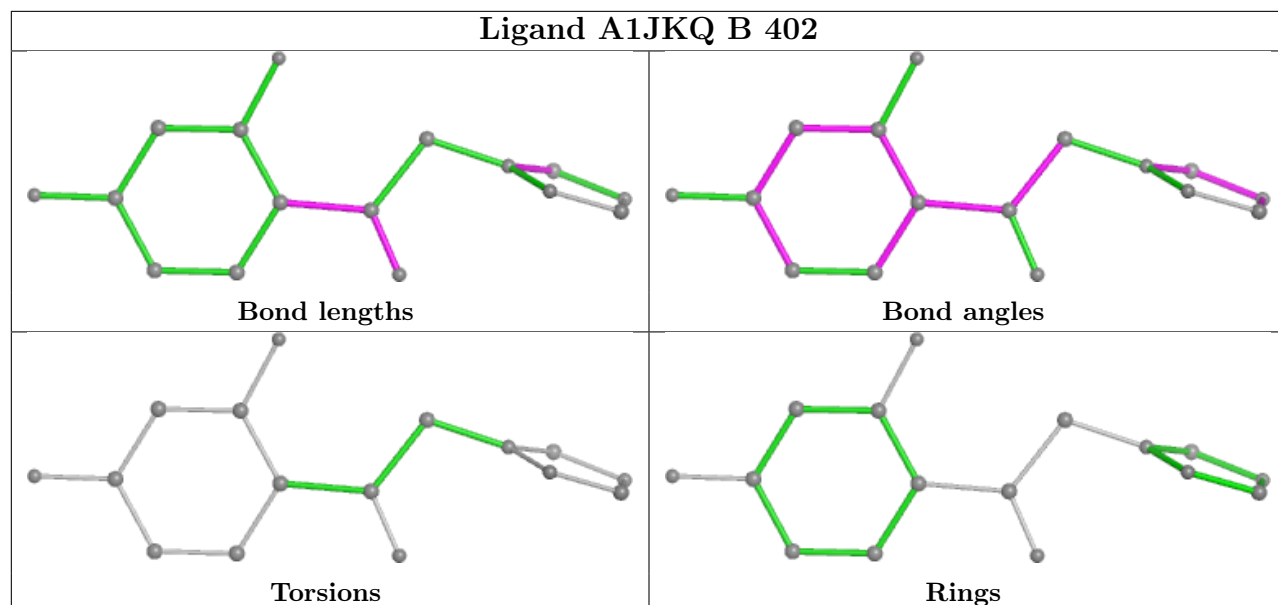
Mol	Chain	Res	Type	Atoms
4	A	403	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2
4	D	405	EDO	O1-C1-C2-O2

There are no ring outliers.

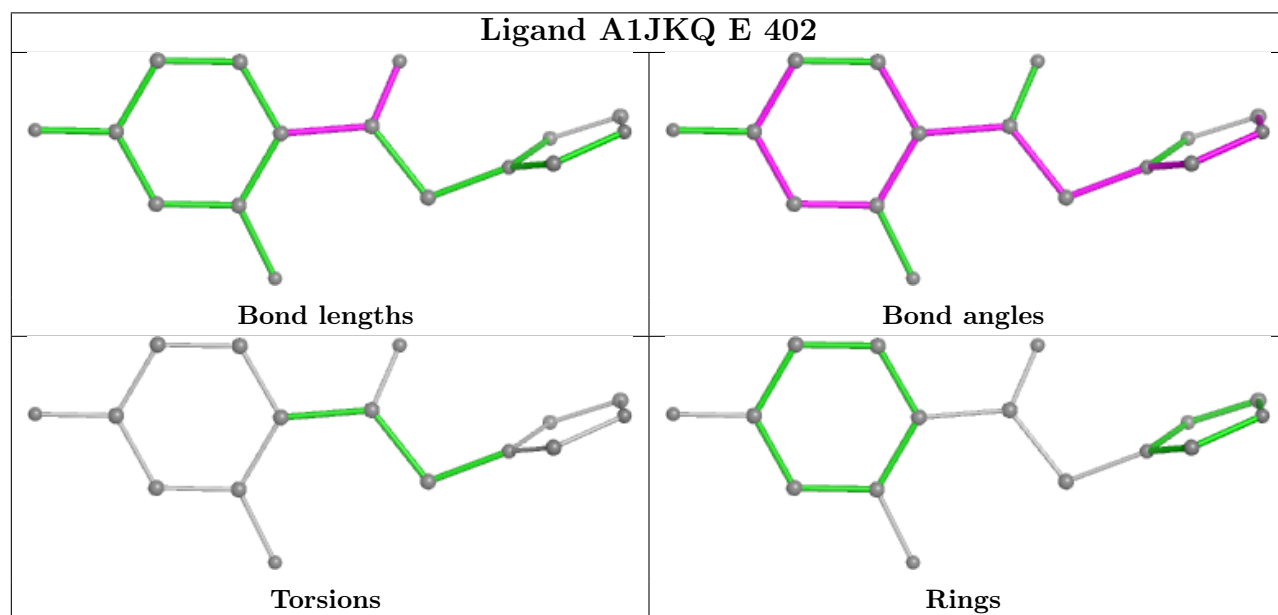
No monomer is involved in short contacts.

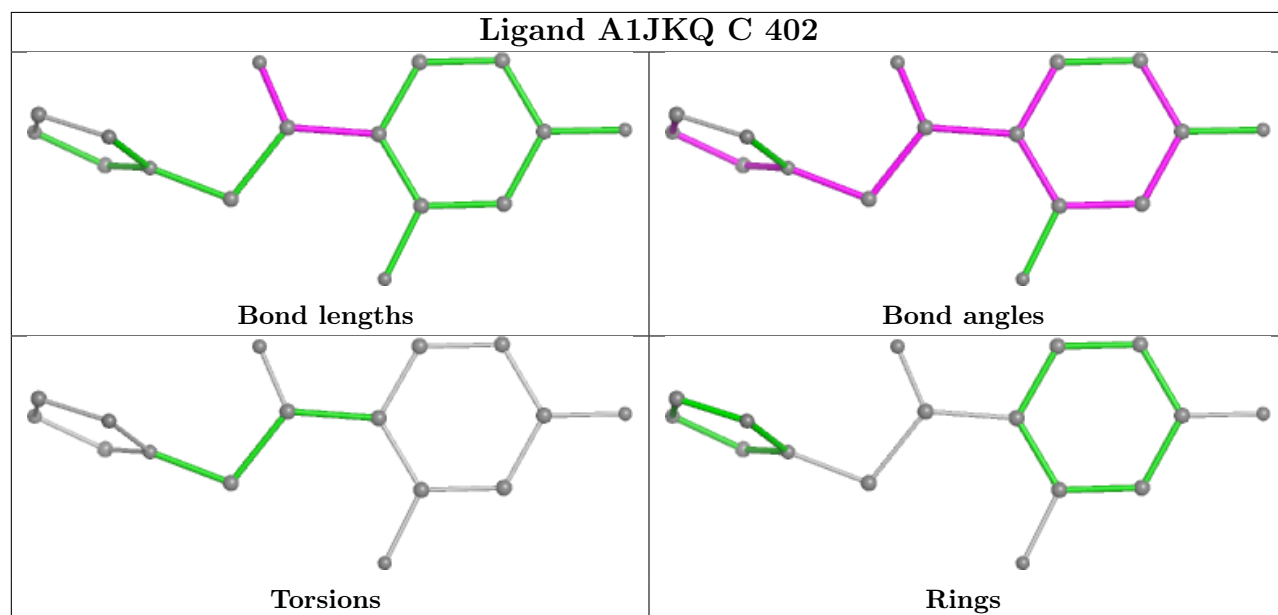
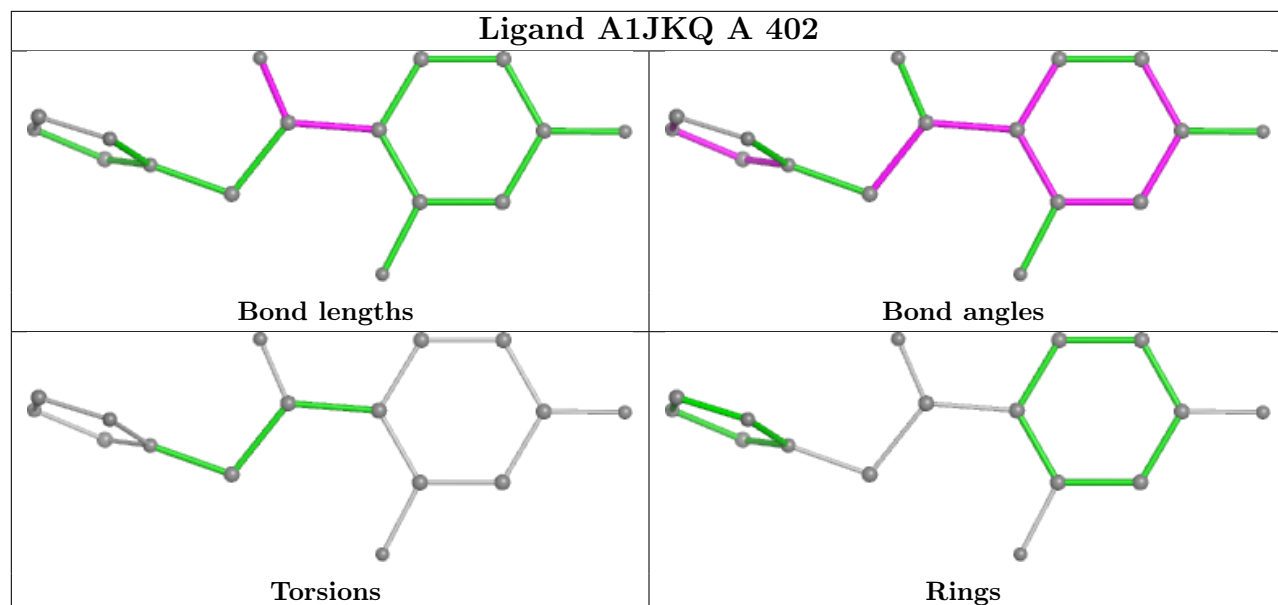
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

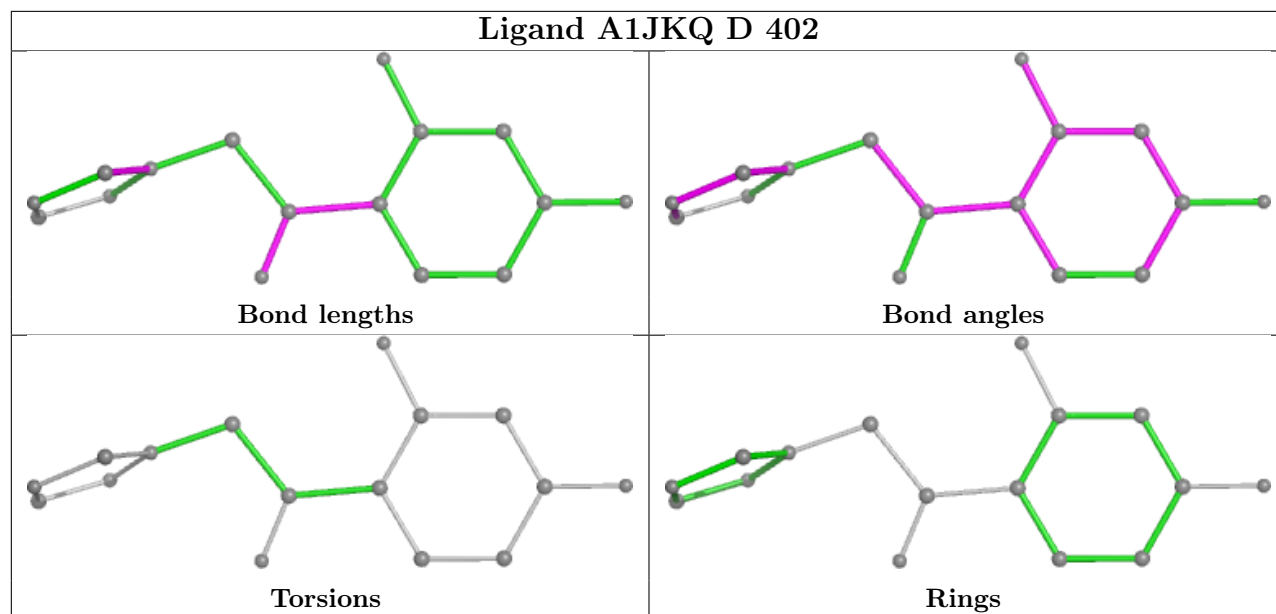
Ligand A1JKQ B 402



Ligand A1JKQ E 402







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	273/342 (79%)	0.59	26 (9%)	15 16	16, 37, 81, 132	3 (1%)
1	B	273/342 (79%)	0.60	28 (10%)	13 14	18, 37, 71, 98	3 (1%)
1	C	273/342 (79%)	0.74	42 (15%)	6 6	16, 37, 92, 135	4 (1%)
1	D	273/342 (79%)	0.53	25 (9%)	16 17	16, 38, 67, 115	2 (0%)
1	E	273/342 (79%)	0.88	46 (16%)	5 5	15, 43, 92, 132	2 (0%)
All	All	1365/1710 (79%)	0.67	167 (12%)	10 10	15, 39, 80, 135	14 (1%)

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	8.0
1	C	70	VAL	7.6
1	E	8	ALA	6.7
1	C	8	ALA	6.7
1	D	143	VAL	6.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

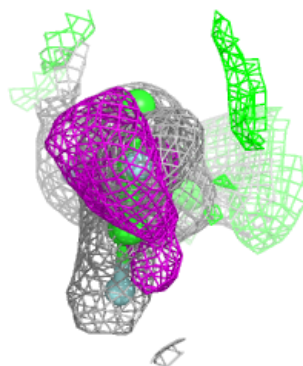
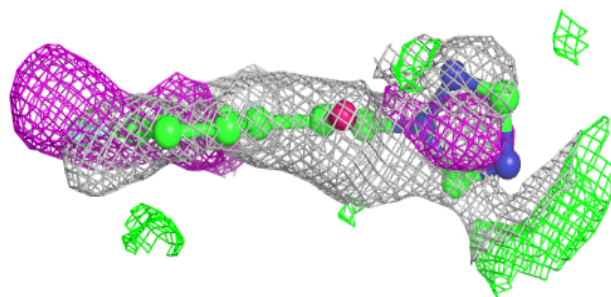
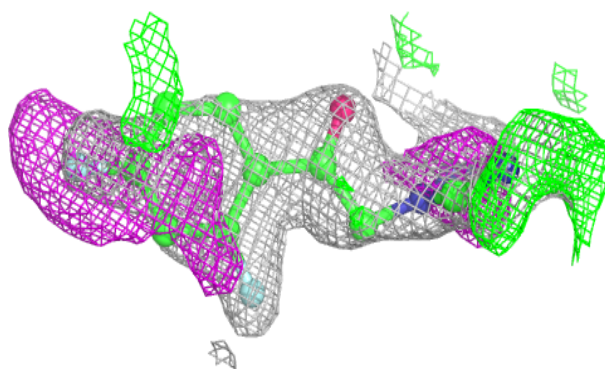
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	D	405	4/4	0.57	0.18	63,67,68,72	0
3	A1JKQ	E	402	16/16	0.61	0.21	55,68,80,83	0
3	A1JKQ	C	402	16/16	0.65	0.20	51,68,74,75	0
2	TLA	D	401	10/10	0.83	0.15	27,33,44,45	10
4	EDO	B	403	4/4	0.84	0.15	37,44,49,61	0
4	EDO	A	403	4/4	0.84	0.16	34,44,48,67	0
3	A1JKQ	A	402	16/16	0.85	0.14	47,54,58,59	0
2	TLA	E	401	10/10	0.85	0.14	32,51,57,61	0
4	EDO	D	403	4/4	0.86	0.15	47,55,62,68	0
3	A1JKQ	B	402	16/16	0.88	0.12	42,48,53,55	0
4	EDO	D	404	4/4	0.89	0.14	35,49,50,56	0
4	EDO	C	403	4/4	0.89	0.13	55,55,56,61	0
2	TLA	A	401	10/10	0.90	0.10	29,33,35,36	0
3	A1JKQ	D	402	16/16	0.90	0.11	37,46,51,54	0
2	TLA	B	401	10/10	0.90	0.11	31,37,41,48	0
2	TLA	C	401	10/10	0.92	0.09	30,34,38,41	0

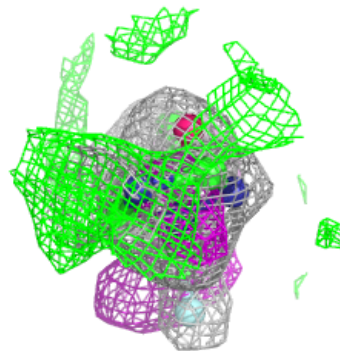
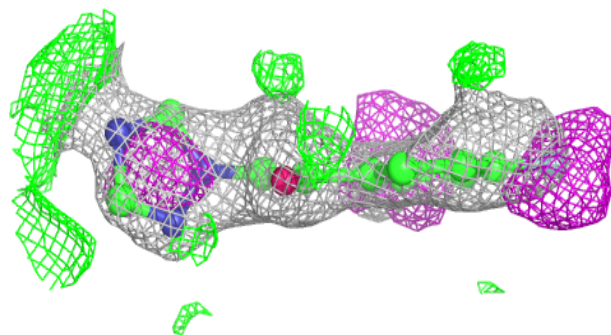
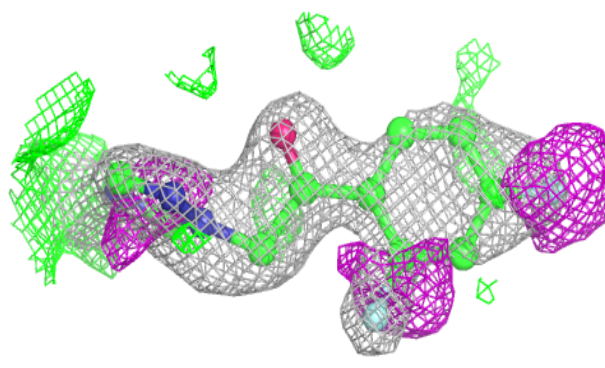
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JKQ E 402:

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

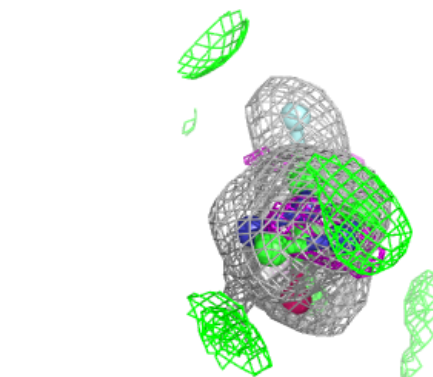
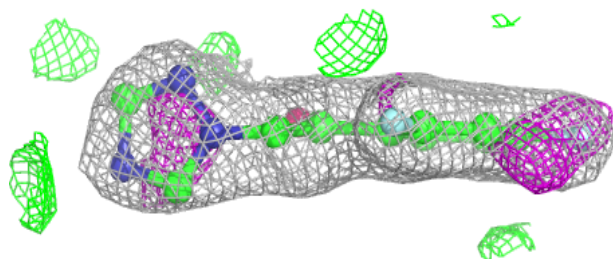
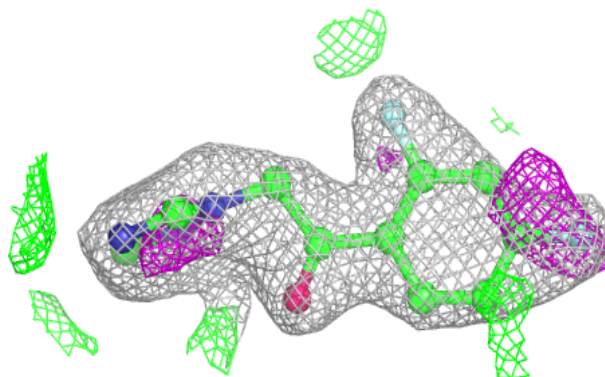
**Electron density around A1JKQ C 402:**

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

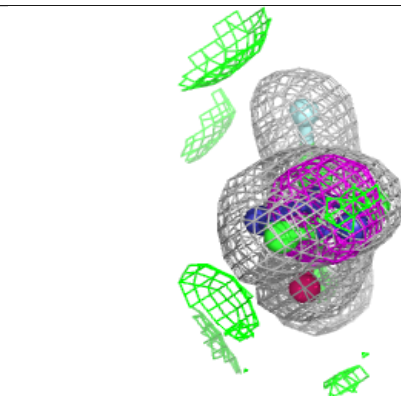
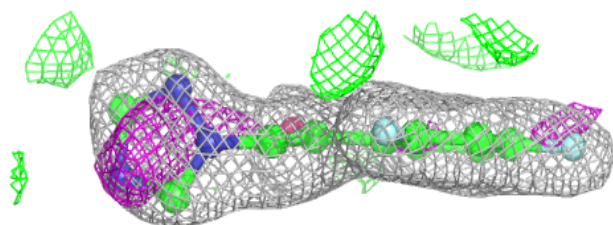
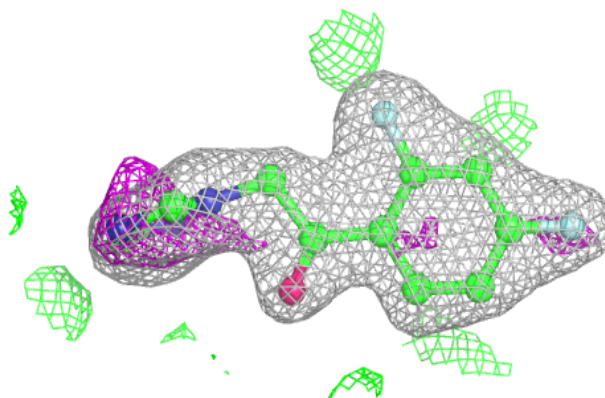


Electron density around A1JKQ A 402:

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

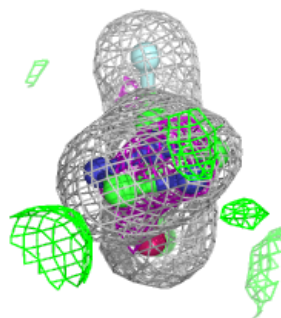
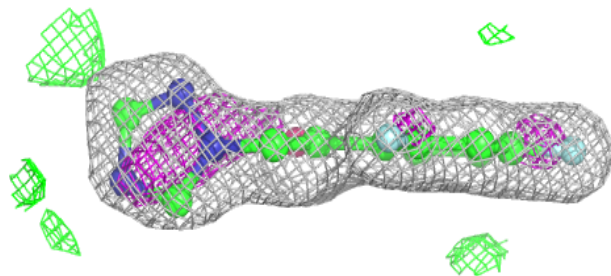
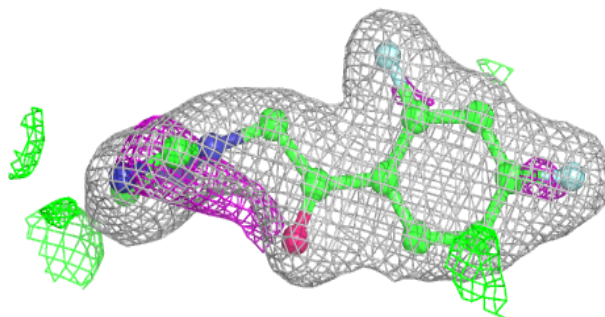
**Electron density around A1JKQ B 402:**

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



Electron density around A1JKQ D 402:

$2mF_o - DF_c$ (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.