



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2025 – 04:14 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

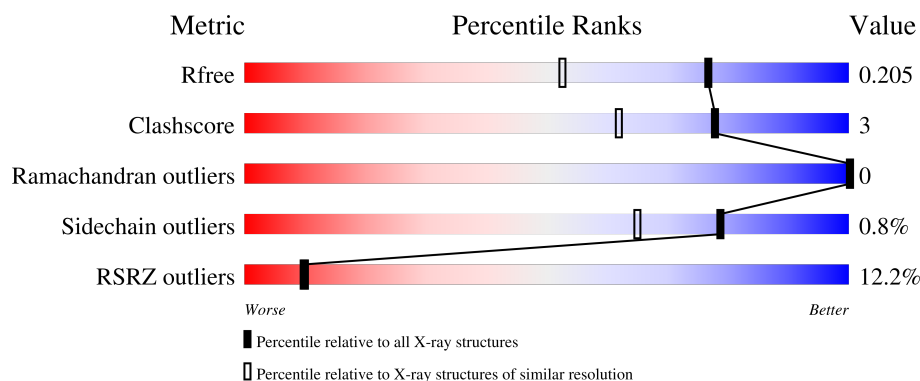
# 1 Overall quality at a glance

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  $\geq 3$ , 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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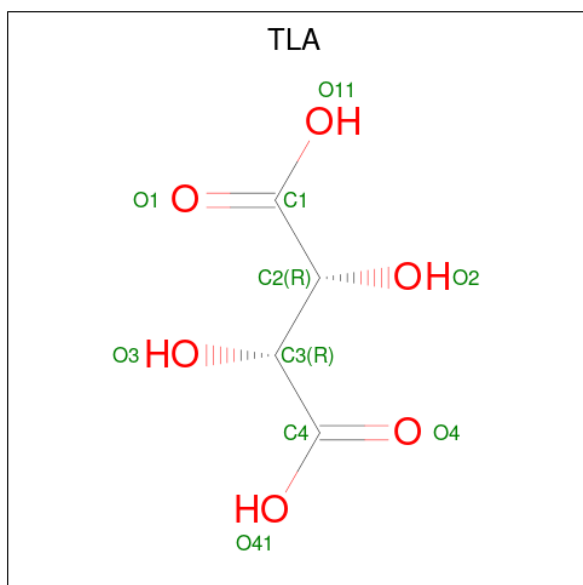
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASN	-	expression tag	UNP P32322
C	-4	LEU	-	expression tag	UNP P32322
C	-3	TYR	-	expression tag	UNP P32322
C	-2	PHE	-	expression tag	UNP P32322
C	-1	GLN	-	expression tag	UNP P32322
D	-22	MET	-	initiating methionine	UNP P32322
D	-21	HIS	-	expression 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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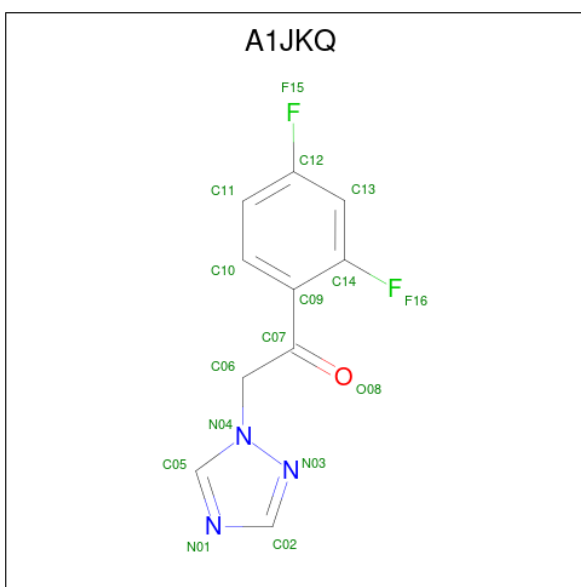
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	GLU	-	expression tag	UNP P32322
E	-6	ASN	-	expression tag	UNP P32322
E	-5	ASN	-	expression tag	UNP P32322
E	-4	LEU	-	expression tag	UNP P32322
E	-3	TYR	-	expression tag	UNP P32322
E	-2	PHE	-	expression tag	UNP P32322
E	-1	GLN	-	expression tag	UNP P32322

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



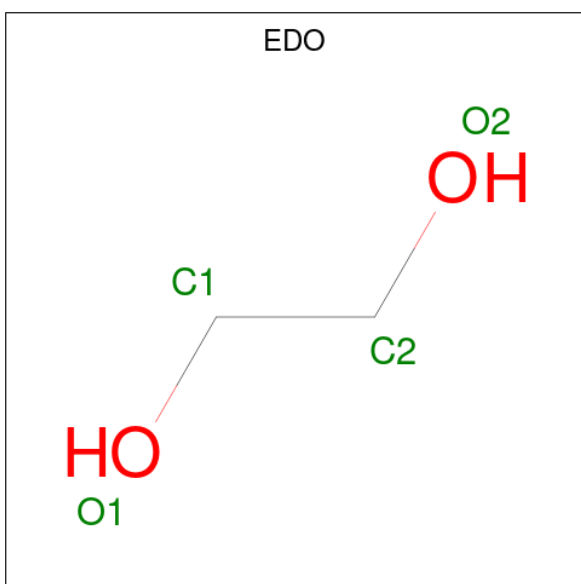
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	E	1	Total C O 10 4 6	0	0

- Molecule 3 is 1-[2,4-bis(fluoranyl)phenyl]-2-(1,2,4-triazol-1-yl)ethanone (CCD ID: A1JKQ) (formula: C<sub>10</sub>H<sub>7</sub>F<sub>2</sub>N<sub>3</sub>O) (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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

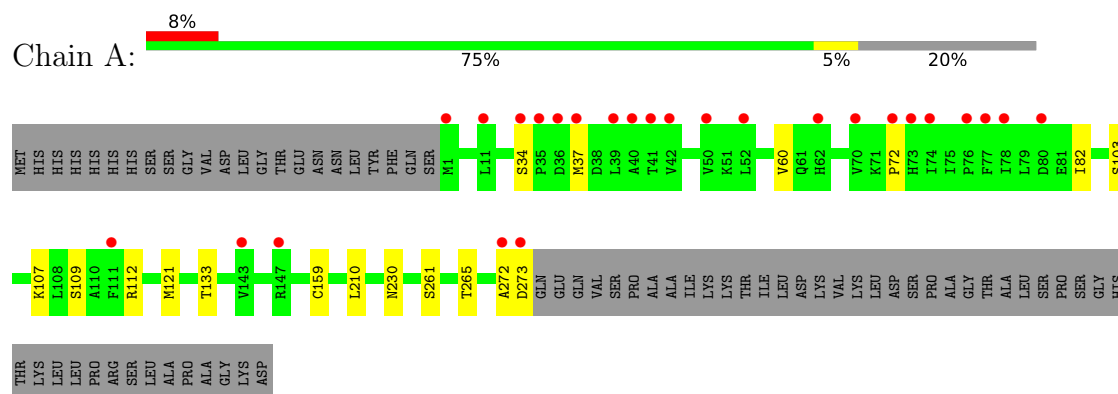
- Molecule 5 is water.

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

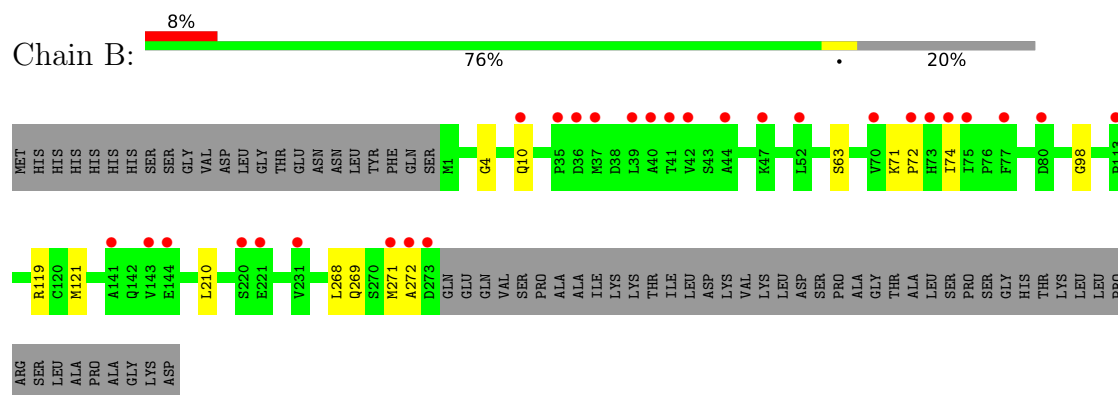
### 3 Residue-property plots [i](#)

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.

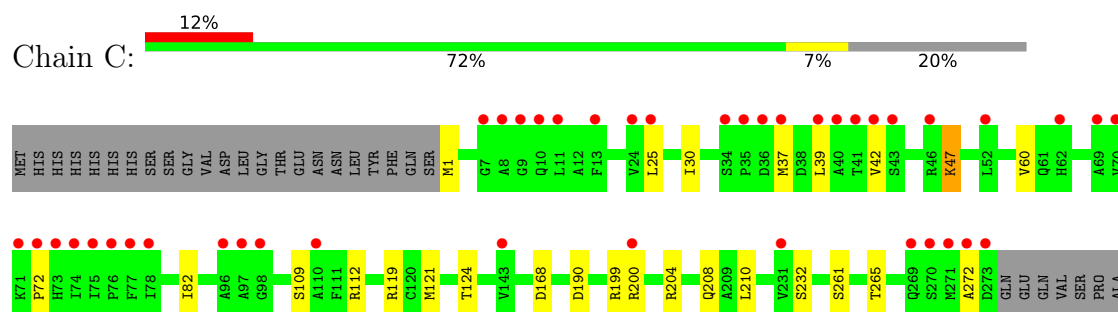
- Molecule 1: Isoform 3 of Pyrroline-5-carboxylate reductase 1, mitochondrial



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

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


Chain D:  7% 74% 6% 20%

MET HIS HIS HIS HIS HIS HIS SER SER VAL ASP LEU 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 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 ASP SER PRO ALA THR ALA LEU SER PRO SER 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

Chain E:  13% 74% 6% 20%

MET HIS HIS HIS HIS HIS HIS SER SER VAL ASP LEU LEU GLY THR GLU ASN THR 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

I75 P76 F77 I78 L79 D80 E81 I82 G83 A84 I91 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 LYS LYS THR ILE

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

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

All (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
1:E:37:MET:HE3	1:E:42:VAL:HG22	1.80	0.63
1:C:37:MET:HE3	1:C:42:VAL:HG22	1.83	0.61
1:A:72:PRO:HB3	1:A:272:ALA:HB2	1.82	0.60
1:C:1:MET:N	5:C:503:HOH:O	2.34	0.59
1:C:168:ASP:HB3	5:C:634:HOH:O	2.03	0.57
1:C:261:SER:O	1:C:265:THR:HG23	2.04	0.57
1:C:124[B]:THR:HG21	1:D:231:VAL:HG12	1.87	0.55
1:E:261:SER:O	1:E:265:THR:HG23	2.07	0.54
1:D:119:ARG:NH2	5:D:504:HOH:O	2.41	0.53
1:E:72:PRO:HB2	1:E:272:ALA:HB2	1.89	0.53
1:C:204[B]:ARG:HH12	1:C:208:GLN:HB2	1.75	0.51
1:D:72:PRO:HB3	1:D:272:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204[B]:ARG:NH1	1:C:208:GLN:HB2	2.26	0.50
1:C:200:ARG:NH1	5:C:501:HOH:O	2.22	0.50
1:B:268:LEU:HA	1:B:271:MET:HE2	1.93	0.49
1:C:119:ARG:NH2	5:C:504:HOH:O	2.44	0.49
1:E:1:MET:HE2	1:E:25:LEU:HD21	1.95	0.49
1:B:119:ARG:NH2	5:B:504:HOH:O	2.46	0.48
1:A:261:SER:O	1:A:265:THR:HG23	2.14	0.47
1:A:34:SER:HB3	1:A:37:MET:HB2	1.97	0.47
1:D:74:ILE:HD12	5:D:574:HOH:O	2.14	0.47
1:B:71:LYS:HD3	5:B:644:HOH:O	2.15	0.46
1:B:98:GLY:HA2	1:B:269:GLN:HB2	1.97	0.46
1:C:25:LEU:CD1	1:C:30:ILE:HD11	2.46	0.46
1:D:34:SER:HB3	1:D:37:MET:HB2	1.98	0.45
1:D:37:MET:HG2	1:D:42:VAL:HG23	1.98	0.45
1:B:74:ILE:HD12	5:B:568:HOH:O	2.17	0.45
1:C:190:ASP:OD1	1:C:199[B]:ARG:NH1	2.39	0.45
1:C:47:LYS:NZ	1:C:47:LYS:HA	2.33	0.44
1:A:60:VAL:HG21	1:A:82:ILE:HB	1.98	0.44
1:C:60:VAL:HG21	1:C:82:ILE:HB	1.98	0.43
1:E:135:TYR:OH	1:E:147:ARG:NH2	2.51	0.43
1:C:72:PRO:HB3	1:C:272:ALA:HB2	2.00	0.43
1:E:37:MET:HE1	1:E:52:LEU:HD22	1.99	0.43
1:E:190:ASP:OD1	1:E:199[B]:ARG:NH1	2.39	0.43
1:D:71:LYS:HD3	5:D:641:HOH:O	2.19	0.43
1:D:98:GLY:HA2	1:D:269:GLN:HB2	2.00	0.42
1:C:109:SER:HA	1:C:112:ARG:O	2.20	0.42
1:D:109:SER:HA	1:D:112:ARG:O	2.20	0.42
1:A:230:ASN:HB3	1:B:10:GLN:NE2	2.34	0.42
1:D:268:LEU:HA	1:D:271:MET:HE2	2.01	0.42
1:E:204:ARG:HH12	1:E:208:GLN:HB2	1.85	0.41
1:A:109:SER:HA	1:A:112:ARG:O	2.19	0.41
1:D:261:SER:O	1:D:265:THR:HG23	2.19	0.41
1:D:35:PRO:HD3	5:D:598:HOH:O	2.20	0.41
1:A:133:THR:O	1:A:159:CYS:HA	2.20	0.41
1:B:4:GLY:HA3	1:B:63:SER:OG	2.21	0.41
1:E:60:VAL:HG21	1:E:82:ILE:HB	2.02	0.41
1:E:98:GLY:HA2	1:E:269:GLN:HB2	2.02	0.41
1:C:25:LEU:HD11	1:C:30:ILE:HD11	2.01	0.41

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%)	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

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	MET
1	A	273	ASP
1	B	121	MET
1	C	39	LEU
1	C	47	LYS
1	C	121	MET
1	C	232	SER
1	D	121	MET
1	E	121	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	GLN
1	C	219	HIS
1	D	219	HIS
1	D	226	GLN
1	D	230	ASN
1	E	140	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](#)

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%)
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
2	E	401	TLA	C3-C4	2.42	1.55	1.52
2	A	401	TLA	C3-C4	2.33	1.55	1.52
2	D	401	TLA	O11-C1	-2.27	1.23	1.30
2	C	401	TLA	O41-C4	-2.26	1.23	1.30
3	B	402	A1JKQ	C05-N04	-2.23	1.31	1.33
2	B	401	TLA	C3-C4	2.19	1.55	1.52
3	C	402	A1JKQ	O08-C07	-2.13	1.18	1.22
3	A	402	A1JKQ	O08-C07	-2.13	1.18	1.22
3	D	402	A1JKQ	O08-C07	-2.13	1.18	1.22
3	E	402	A1JKQ	O08-C07	-2.08	1.19	1.22
2	E	401	TLA	O41-C4	-2.06	1.23	1.30
2	B	401	TLA	O41-C4	-2.06	1.23	1.30
3	B	402	A1JKQ	O08-C07	-2.06	1.19	1.22
3	D	402	A1JKQ	C05-N04	-2.05	1.31	1.33
2	C	401	TLA	C3-C4	2.02	1.55	1.52

All (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
3	E	402	A1JKQ	C13-C14-C09	-4.04	119.22	123.53
3	C	402	A1JKQ	C05-N01-C02	4.02	106.87	102.34
3	A	402	A1JKQ	C13-C14-C09	-3.83	119.44	123.53
3	A	402	A1JKQ	C14-C13-C12	3.81	120.62	116.62
3	D	402	A1JKQ	N01-C05-N04	-3.80	107.64	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	A1JKQ	C14-C13-C12	3.75	120.56	116.62
3	B	402	A1JKQ	C14-C13-C12	3.75	120.56	116.62
3	B	402	A1JKQ	N01-C05-N04	-3.71	107.75	112.24
3	A	402	A1JKQ	N01-C05-N04	-3.69	107.78	112.24
3	E	402	A1JKQ	N01-C05-N04	-3.65	107.83	112.24
3	D	402	A1JKQ	C13-C14-C09	-3.64	119.65	123.53
3	E	402	A1JKQ	C14-C13-C12	3.59	120.39	116.62
3	C	402	A1JKQ	N01-C05-N04	-3.51	107.99	112.24
3	B	402	A1JKQ	C13-C14-C09	-3.42	119.88	123.53
3	C	402	A1JKQ	C06-C07-C09	3.36	124.23	118.33
3	D	402	A1JKQ	C14-C13-C12	3.32	120.11	116.62
2	A	401	TLA	O4-C4-C3	-3.22	113.17	121.63
3	A	402	A1JKQ	C06-C07-C09	3.12	123.80	118.33
3	E	402	A1JKQ	C06-C07-C09	3.03	123.65	118.33
3	D	402	A1JKQ	C06-C07-C09	2.95	123.50	118.33
2	E	401	TLA	O4-C4-C3	-2.89	114.03	121.63
2	C	401	TLA	O4-C4-C3	-2.76	114.37	121.63
3	B	402	A1JKQ	C06-C07-C09	2.67	123.01	118.33
3	B	402	A1JKQ	C11-C12-C13	-2.65	119.85	123.29
3	D	402	A1JKQ	C10-C09-C14	2.65	119.67	116.67
2	B	401	TLA	O4-C4-C3	-2.62	114.74	121.63
3	E	402	A1JKQ	C10-C09-C14	2.59	119.62	116.67
2	D	401	TLA	O4-C4-C3	-2.56	114.91	121.63
3	C	402	A1JKQ	C10-C09-C14	2.54	119.55	116.67
3	A	402	A1JKQ	C11-C12-C13	-2.47	120.09	123.29
3	C	402	A1JKQ	C07-C06-N04	-2.41	107.60	110.89
3	A	402	A1JKQ	C10-C09-C14	2.41	119.40	116.67
2	A	401	TLA	O41-C4-C3	2.40	119.75	113.27
2	E	401	TLA	O1-C1-C2	-2.37	115.40	121.63
2	D	401	TLA	O1-C1-C2	-2.32	115.52	121.63
3	E	402	A1JKQ	C11-C12-C13	-2.25	120.37	123.29
2	B	401	TLA	O1-C1-C2	-2.21	115.82	121.63
3	D	402	A1JKQ	C11-C12-C13	-2.21	120.42	123.29
3	C	402	A1JKQ	C11-C12-C13	-2.21	120.42	123.29
2	E	401	TLA	O41-C4-C3	2.20	119.21	113.27
3	B	402	A1JKQ	C10-C09-C14	2.18	119.14	116.67
2	A	401	TLA	O2-C2-C1	-2.15	106.16	110.66
2	C	401	TLA	O1-C1-C2	-2.14	116.00	121.63
2	A	401	TLA	O1-C1-C2	-2.09	116.13	121.63
3	C	402	A1JKQ	O08-C07-C06	-2.06	118.13	120.43
3	E	402	A1JKQ	C07-C06-N04	-2.05	108.09	110.89
3	D	402	A1JKQ	F16-C14-C09	2.03	123.11	119.67

There are no chirality outliers.

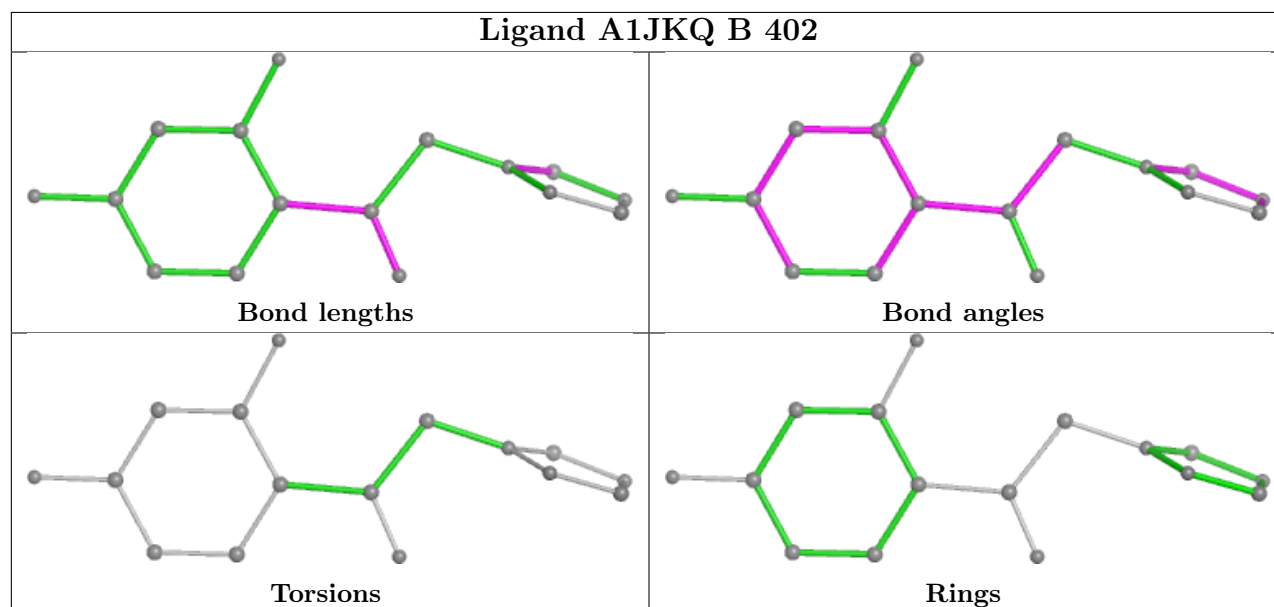
All (3) torsion outliers are listed below:

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

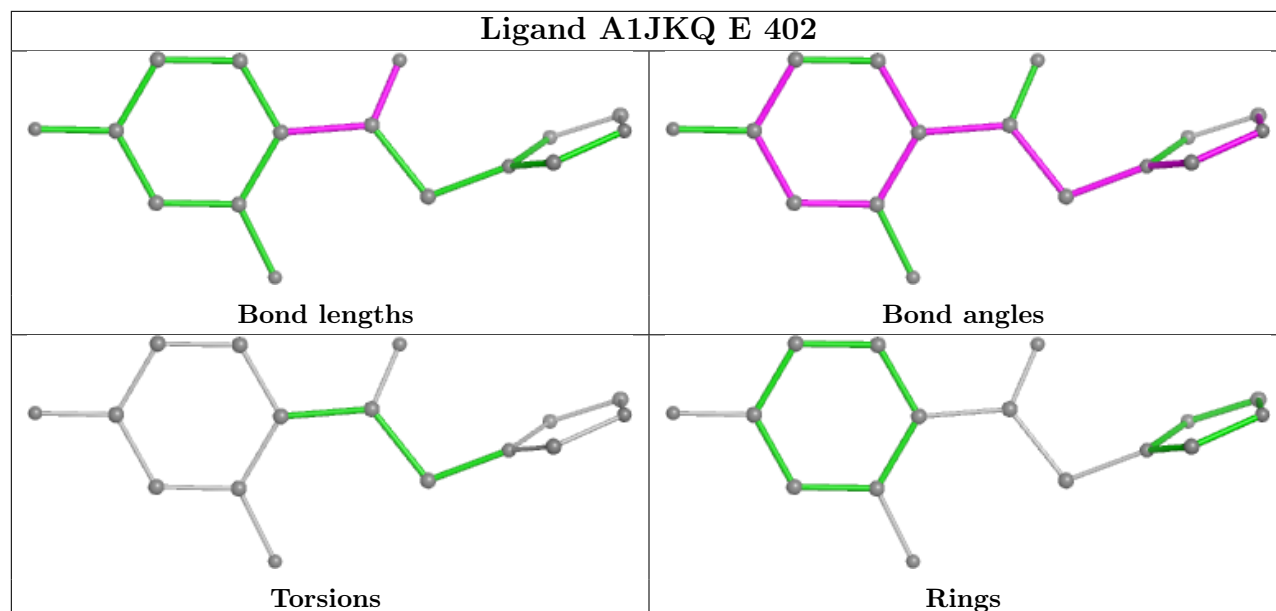
There are no ring outliers.

No monomer is involved in short contacts.

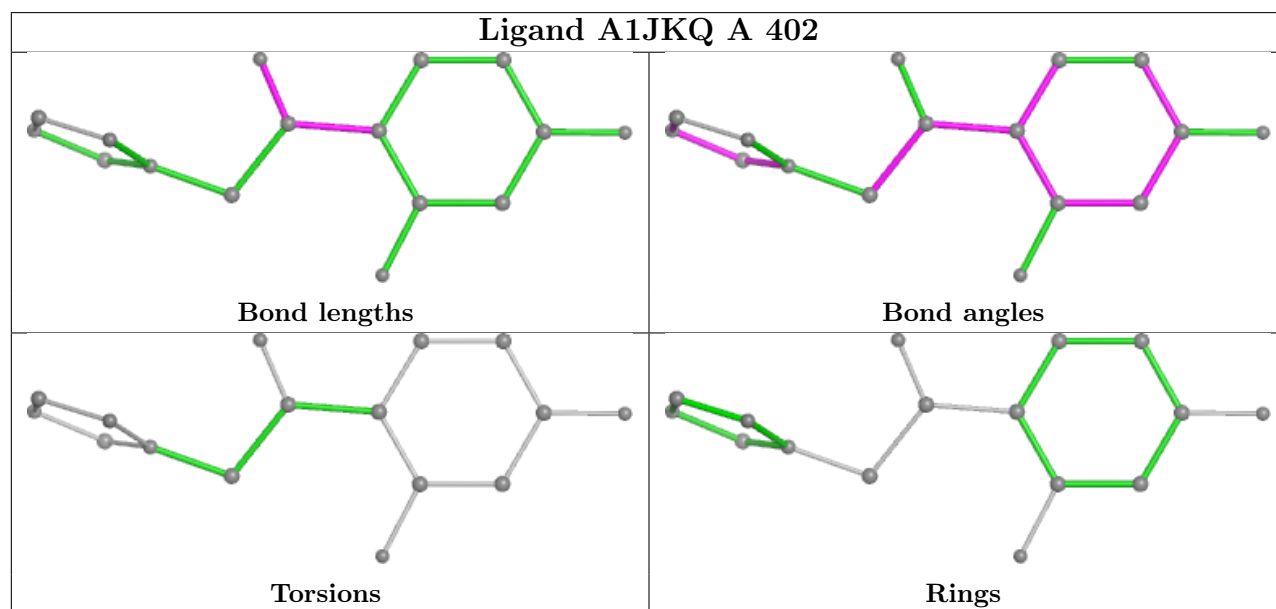
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

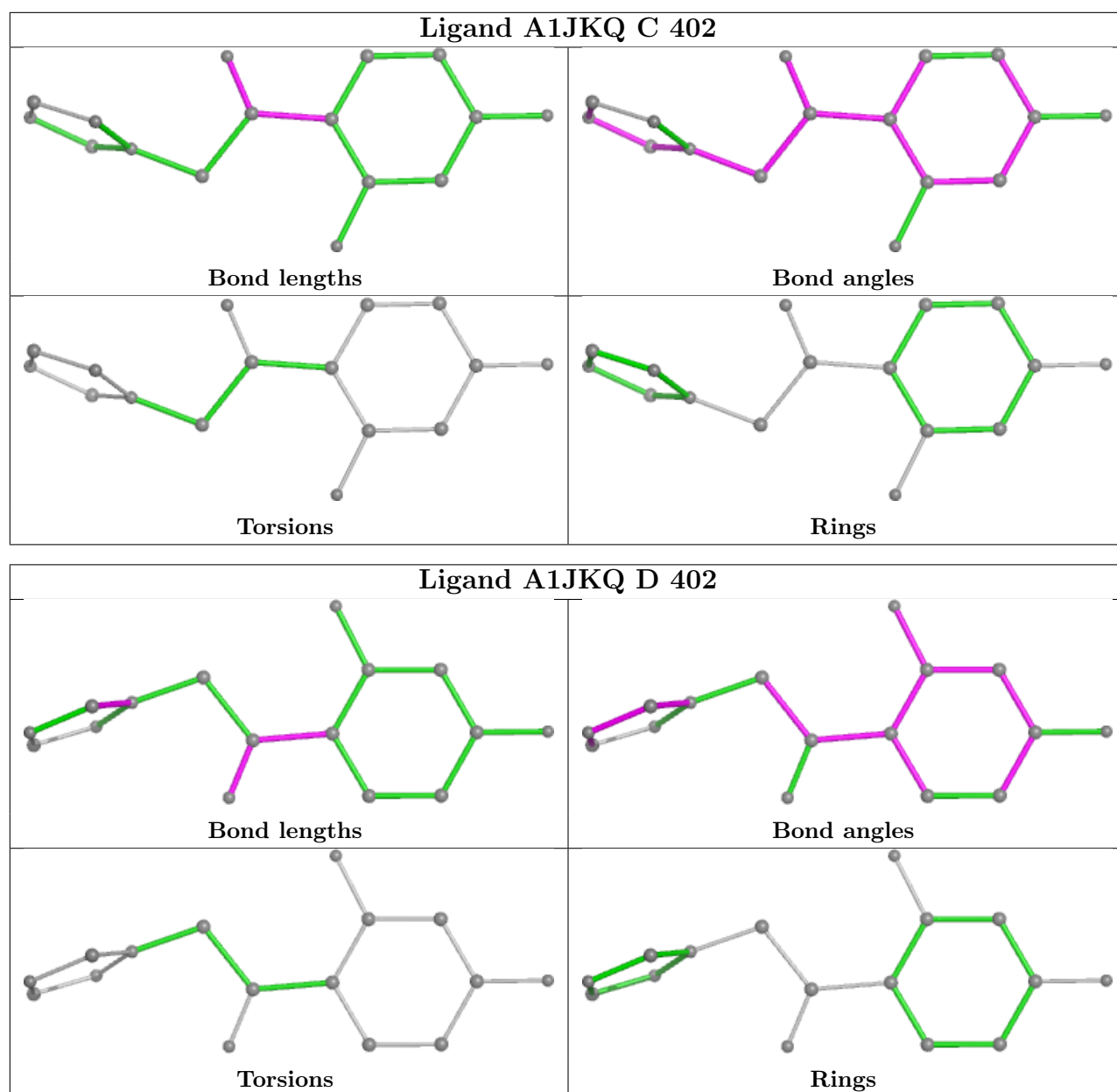


## Ligand A1JKQ E 402



## Ligand A1JKQ A 402





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	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%)

All (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
1	C	39	LEU	6.2
1	E	7	GLY	6.1
1	B	143	VAL	6.1
1	C	11	LEU	5.7
1	B	273	ASP	5.3
1	E	11	LEU	5.2
1	E	72	PRO	5.1
1	E	75	ILE	5.0
1	A	39	LEU	4.9
1	C	72	PRO	4.9
1	D	35	PRO	4.9
1	C	74	ILE	4.8
1	C	77	PHE	4.8
1	E	39	LEU	4.8
1	E	143	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	74	ILE	4.7
1	B	41	THR	4.6
1	E	77	PHE	4.5
1	E	41	THR	4.3
1	D	39	LEU	4.2
1	A	74	ILE	4.2
1	C	75	ILE	4.2
1	C	7	GLY	4.2
1	C	35	PRO	4.2
1	B	39	LEU	4.1
1	E	272	ALA	4.1
1	E	231	VAL	4.1
1	D	77	PHE	4.0
1	C	69	ALA	4.0
1	A	41	THR	4.0
1	C	40	ALA	4.0
1	E	9	GLY	3.9
1	E	98	GLY	3.9
1	C	42	VAL	3.9
1	C	272	ALA	3.9
1	A	77	PHE	3.9
1	E	76	PRO	3.8
1	C	270	SER	3.8
1	E	69	ALA	3.7
1	B	74	ILE	3.7
1	C	25	LEU	3.6
1	C	24	VAL	3.6
1	B	231	VAL	3.6
1	D	70	VAL	3.6
1	D	74	ILE	3.5
1	C	37	MET	3.5
1	C	273	ASP	3.5
1	B	70	VAL	3.5
1	E	273	ASP	3.5
1	D	41	THR	3.5
1	B	77	PHE	3.5
1	D	72	PRO	3.4
1	E	97	ALA	3.4
1	D	34	SER	3.4
1	B	35	PRO	3.4
1	C	41	THR	3.4
1	A	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	35	PRO	3.3
1	A	78	ILE	3.3
1	E	35	PRO	3.3
1	A	70	VAL	3.3
1	D	80	ASP	3.3
1	B	42	VAL	3.2
1	B	272	ALA	3.2
1	C	76	PRO	3.2
1	E	42	VAL	3.1
1	A	40	ALA	3.1
1	C	73	HIS	3.1
1	E	45	LEU	3.1
1	E	37	MET	3.0
1	A	11	LEU	3.0
1	C	34	SER	3.0
1	D	8	ALA	3.0
1	C	71	LYS	3.0
1	C	9	GLY	3.0
1	D	7	GLY	3.0
1	A	34	SER	2.9
1	B	72	PRO	2.9
1	A	273	ASP	2.9
1	C	46	ARG	2.9
1	A	80	ASP	2.9
1	B	73	HIS	2.8
1	D	78	ILE	2.8
1	C	200	ARG	2.8
1	A	272	ALA	2.8
1	C	98	GLY	2.8
1	D	36	ASP	2.8
1	D	272	ALA	2.8
1	B	37	MET	2.7
1	D	273	ASP	2.7
1	D	73	HIS	2.7
1	C	78	ILE	2.7
1	E	200	ARG	2.7
1	E	73	HIS	2.7
1	A	42	VAL	2.6
1	E	34	SER	2.6
1	D	75	ILE	2.6
1	A	76	PRO	2.6
1	E	71	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	36	ASP	2.6
1	A	62	HIS	2.5
1	B	271	MET	2.5
1	E	78	ILE	2.5
1	A	50	VAL	2.5
1	E	40	ALA	2.5
1	A	72	PRO	2.5
1	C	231	VAL	2.5
1	C	13	PHE	2.4
1	C	97	ALA	2.4
1	E	113	PRO	2.4
1	E	80	ASP	2.4
1	B	52	LEU	2.4
1	B	44	ALA	2.4
1	D	40	ALA	2.4
1	E	147	ARG	2.4
1	A	36	ASP	2.4
1	C	10	GLN	2.3
1	E	79	LEU	2.3
1	B	141	ALA	2.3
1	D	10	GLN	2.3
1	B	36	ASP	2.3
1	C	269	GLN	2.2
1	C	43	SER	2.2
1	E	1	MET	2.2
1	B	80	ASP	2.2
1	E	36	ASP	2.2
1	C	62	HIS	2.2
1	B	10	GLN	2.2
1	A	37	MET	2.2
1	D	37	MET	2.2
1	E	82	ILE	2.2
1	A	147	ARG	2.2
1	A	111	PHE	2.2
1	B	40	ALA	2.2
1	C	110	ALA	2.2
1	D	26	ALA	2.2
1	E	44	ALA	2.2
1	E	84	ALA	2.2
1	A	73	HIS	2.2
1	B	75	ILE	2.2
1	B	47	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	144	GLU	2.1
1	D	144	GLU	2.1
1	C	52	LEU	2.1
1	D	71	LYS	2.1
1	A	143	VAL	2.1
1	C	143	VAL	2.1
1	E	43	SER	2.1
1	E	270	SER	2.1
1	E	10	GLN	2.1
1	B	113	PRO	2.1
1	B	220	SER	2.1
1	D	220	SER	2.1
1	E	63	SER	2.1
1	E	27	ALA	2.1
1	C	271	MET	2.1
1	A	52	LEU	2.1
1	E	52	LEU	2.1
1	B	221	GLU	2.1
1	C	96	ALA	2.0
1	E	91	ILE	2.0
1	E	144	GLU	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, 95<sup>th</sup> 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.

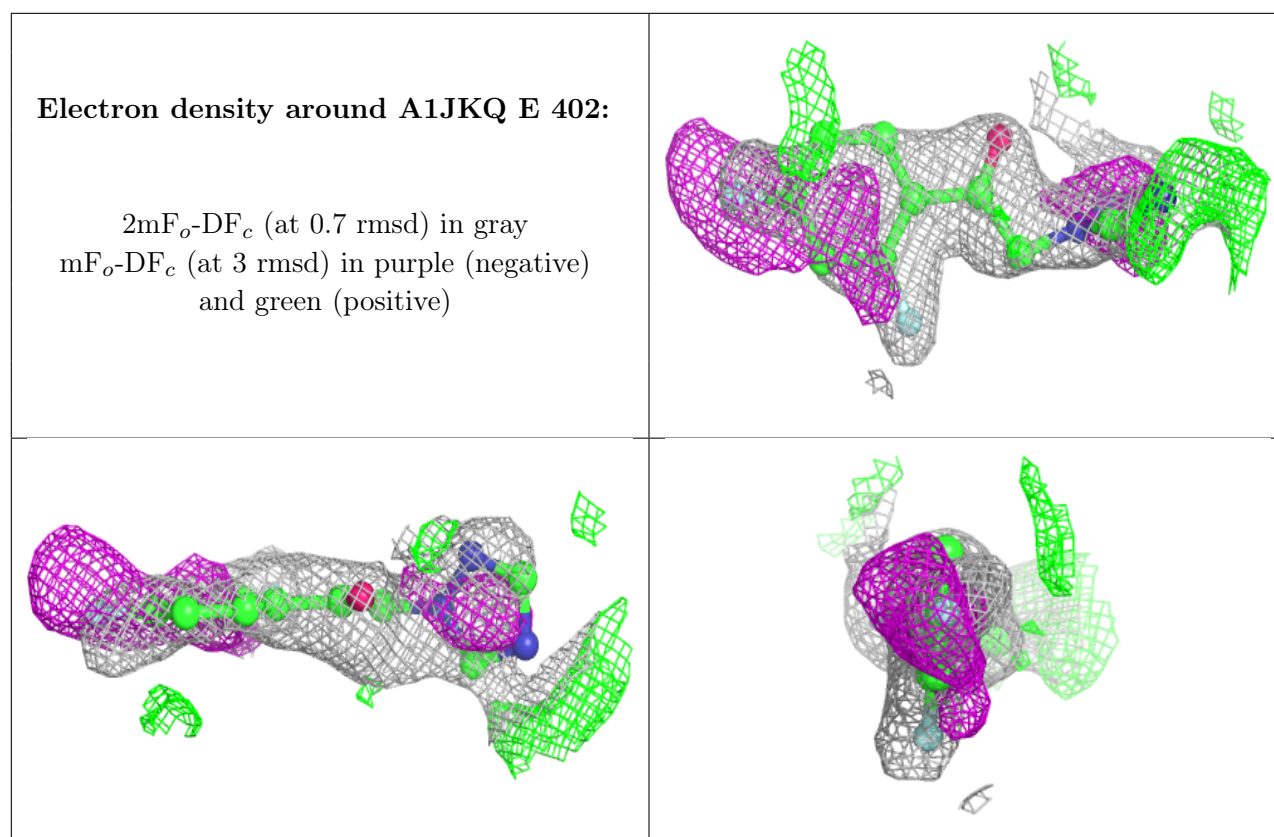
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	D	405	4/4	0.57	0.18	63,67,68,72	0
3	A1JKQ	E	402	16/16	0.61	0.21	55,68,80,83	0

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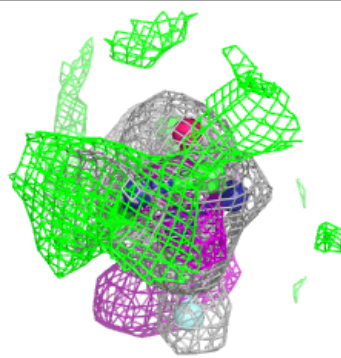
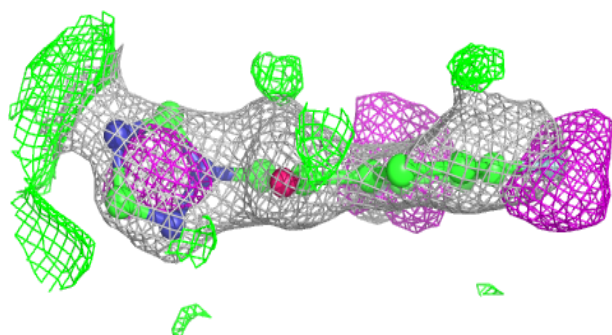
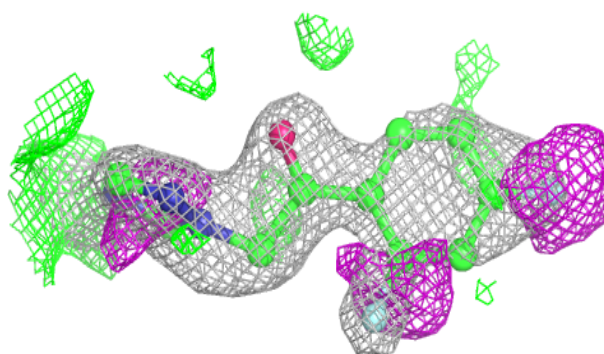
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1JKQ	C	402	16/16	0.65	0.20	51,68,74,75	0
2	TLA	D	401	10/10	0.83	0.15	27,33,44,45	10
4	EDO	B	403	4/4	0.84	0.15	37,44,49,61	0
4	EDO	A	403	4/4	0.84	0.16	34,44,48,67	0
3	A1JKQ	A	402	16/16	0.85	0.14	47,54,58,59	0
2	TLA	E	401	10/10	0.85	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.

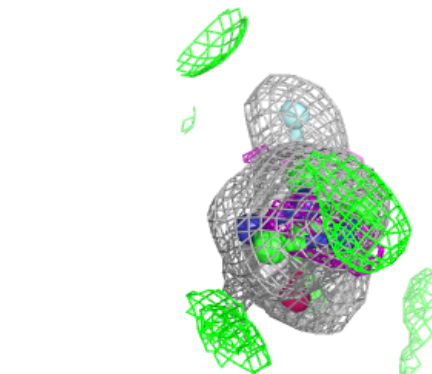
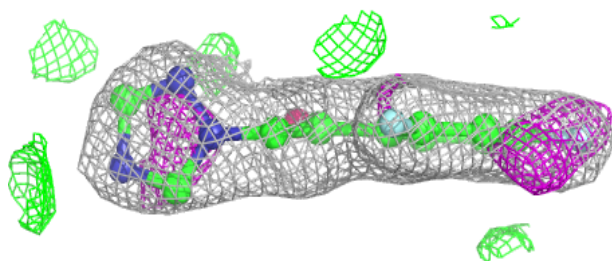
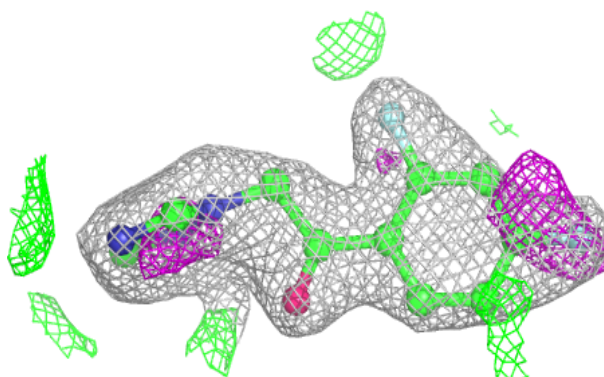


**Electron density around A1JKQ C 402:**

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

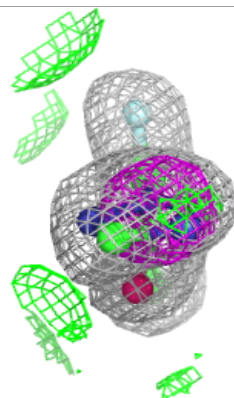
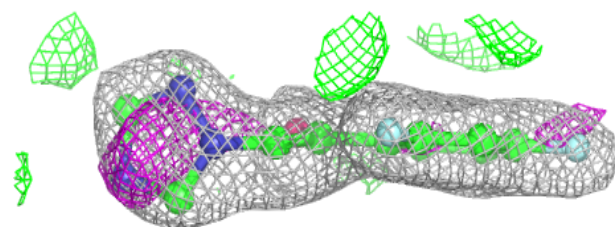
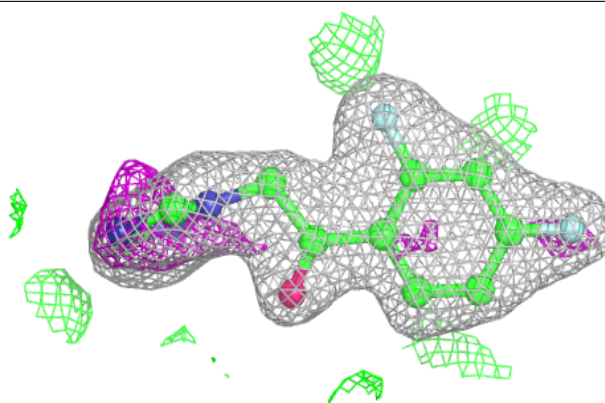
**Electron density around A1JKQ A 402:**

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

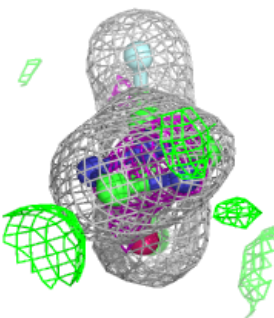
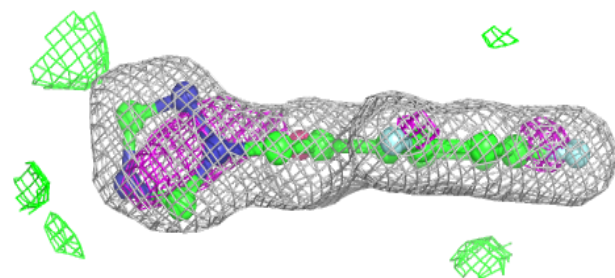
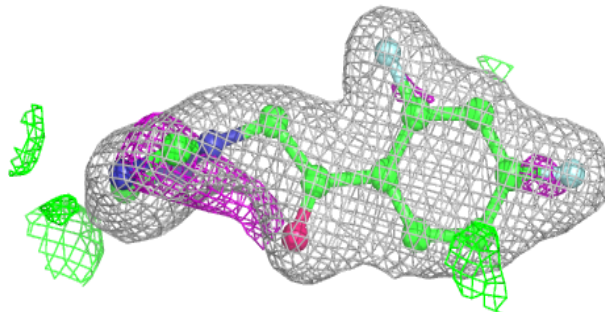


**Electron density around A1JKQ B 402:**

$2mF_o-DF_c$  (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.