



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 04:17 AM JST

PDB ID : 7EYT
Title : Fe(II)/(alpha)ketoglutarate-dependent dioxygenase SptF with andilesin C and NOG
Authors : Tao, H.; Mori, T.; Abe, I.
Deposited on : 2021-06-01
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

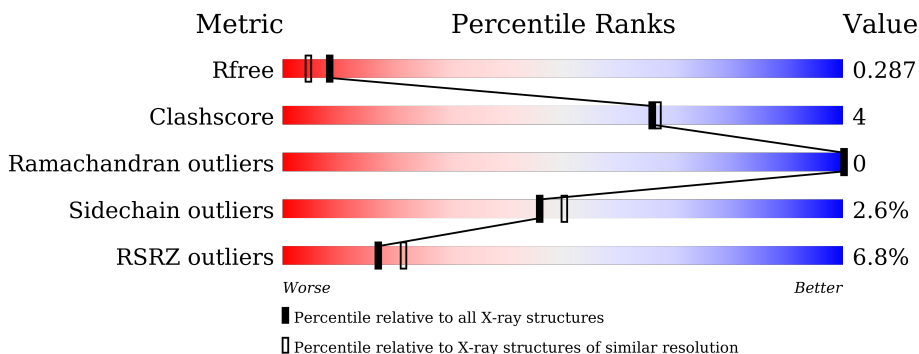
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	296	 6% 74% 13% 13%
1	B	296	 5% 83% 7% 10%
1	C	296	 8% 82% 11% 6%
1	D	296	 5% 80% 13% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9018 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 2-oxoglutarate/Fe(II)-dependent dioxygenase SptF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	277	2193	1389	388	401	15	0	0	0
1	A	258	2027	1287	357	368	15	0	0	0
1	B	267	2123	1348	370	390	15	0	1	0
1	D	276	2188	1385	385	403	15	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

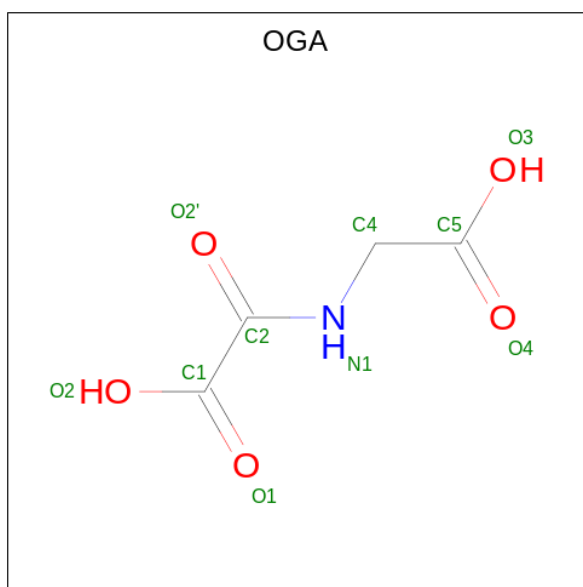
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A0A6J4CX17
C	284	LYS	-	expression tag	UNP A0A6J4CX17
C	285	LEU	-	expression tag	UNP A0A6J4CX17
C	286	ALA	-	expression tag	UNP A0A6J4CX17
C	287	ALA	-	expression tag	UNP A0A6J4CX17
C	288	ALA	-	expression tag	UNP A0A6J4CX17
C	289	LEU	-	expression tag	UNP A0A6J4CX17
C	290	GLU	-	expression tag	UNP A0A6J4CX17
C	291	HIS	-	expression tag	UNP A0A6J4CX17
C	292	HIS	-	expression tag	UNP A0A6J4CX17
C	293	HIS	-	expression tag	UNP A0A6J4CX17
C	294	HIS	-	expression tag	UNP A0A6J4CX17
C	295	HIS	-	expression tag	UNP A0A6J4CX17
C	296	HIS	-	expression tag	UNP A0A6J4CX17
A	1	MET	-	initiating methionine	UNP A0A6J4CX17
A	284	LYS	-	expression tag	UNP A0A6J4CX17
A	285	LEU	-	expression tag	UNP A0A6J4CX17
A	286	ALA	-	expression tag	UNP A0A6J4CX17
A	287	ALA	-	expression tag	UNP A0A6J4CX17
A	288	ALA	-	expression tag	UNP A0A6J4CX17
A	289	LEU	-	expression tag	UNP A0A6J4CX17

Continued on next page...

Continued from previous page...

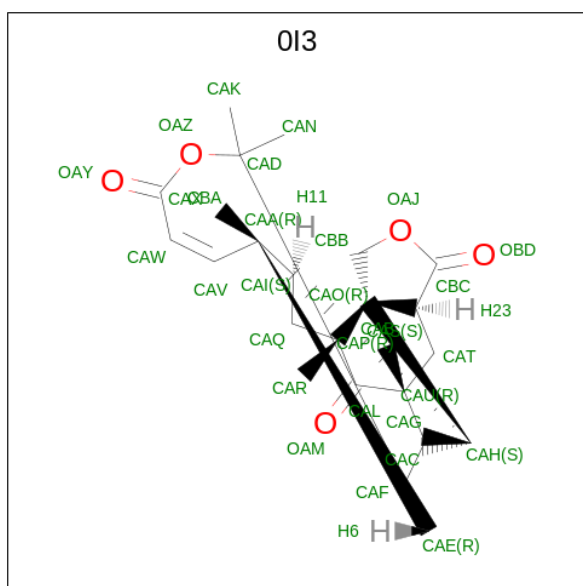
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLU	-	expression tag	UNP A0A6J4CX17
A	291	HIS	-	expression tag	UNP A0A6J4CX17
A	292	HIS	-	expression tag	UNP A0A6J4CX17
A	293	HIS	-	expression tag	UNP A0A6J4CX17
A	294	HIS	-	expression tag	UNP A0A6J4CX17
A	295	HIS	-	expression tag	UNP A0A6J4CX17
A	296	HIS	-	expression tag	UNP A0A6J4CX17
B	3	MET	-	initiating methionine	UNP A0A6J4CX17
B	286	LYS	-	expression tag	UNP A0A6J4CX17
B	287	LEU	-	expression tag	UNP A0A6J4CX17
B	288	ALA	-	expression tag	UNP A0A6J4CX17
B	289	ALA	-	expression tag	UNP A0A6J4CX17
B	290	ALA	-	expression tag	UNP A0A6J4CX17
B	291	LEU	-	expression tag	UNP A0A6J4CX17
B	292	GLU	-	expression tag	UNP A0A6J4CX17
B	293	HIS	-	expression tag	UNP A0A6J4CX17
B	294	HIS	-	expression tag	UNP A0A6J4CX17
B	295	HIS	-	expression tag	UNP A0A6J4CX17
B	296	HIS	-	expression tag	UNP A0A6J4CX17
B	297	HIS	-	expression tag	UNP A0A6J4CX17
B	298	HIS	-	expression tag	UNP A0A6J4CX17
D	3	MET	-	initiating methionine	UNP A0A6J4CX17
D	286	LYS	-	expression tag	UNP A0A6J4CX17
D	287	LEU	-	expression tag	UNP A0A6J4CX17
D	288	ALA	-	expression tag	UNP A0A6J4CX17
D	289	ALA	-	expression tag	UNP A0A6J4CX17
D	290	ALA	-	expression tag	UNP A0A6J4CX17
D	291	LEU	-	expression tag	UNP A0A6J4CX17
D	292	GLU	-	expression tag	UNP A0A6J4CX17
D	293	HIS	-	expression tag	UNP A0A6J4CX17
D	294	HIS	-	expression tag	UNP A0A6J4CX17
D	295	HIS	-	expression tag	UNP A0A6J4CX17
D	296	HIS	-	expression tag	UNP A0A6J4CX17
D	297	HIS	-	expression tag	UNP A0A6J4CX17
D	298	HIS	-	expression tag	UNP A0A6J4CX17

- Molecule 2 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	C	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 3 is Andilesin C (three-letter code: 0I3) (formula: $C_{25}H_{32}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			30	25	5		

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

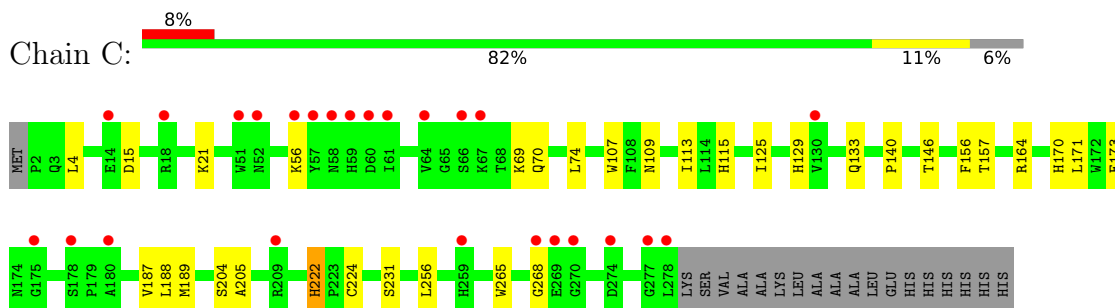
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	113	Total O 113 113	0	0
5	A	106	Total O 106 106	0	0
5	B	104	Total O 104 104	0	0
5	D	120	Total O 120 120	0	0

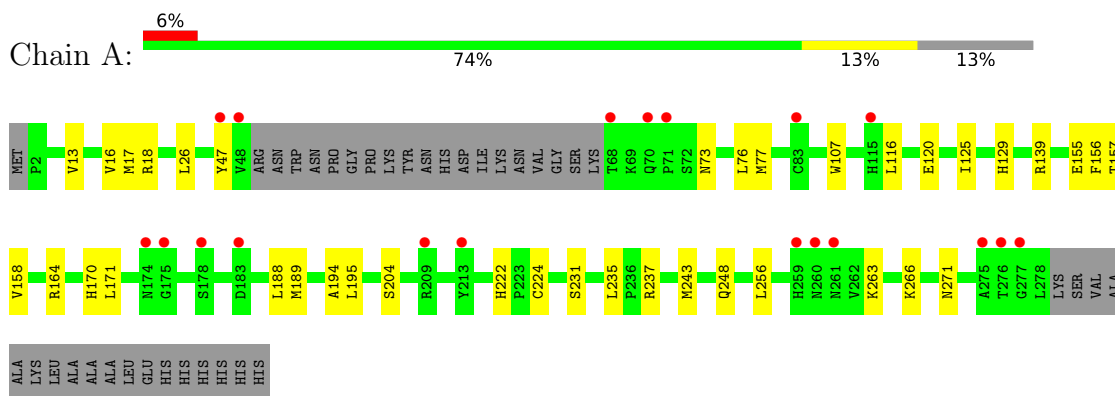
3 Residue-property plots [i](#)

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.

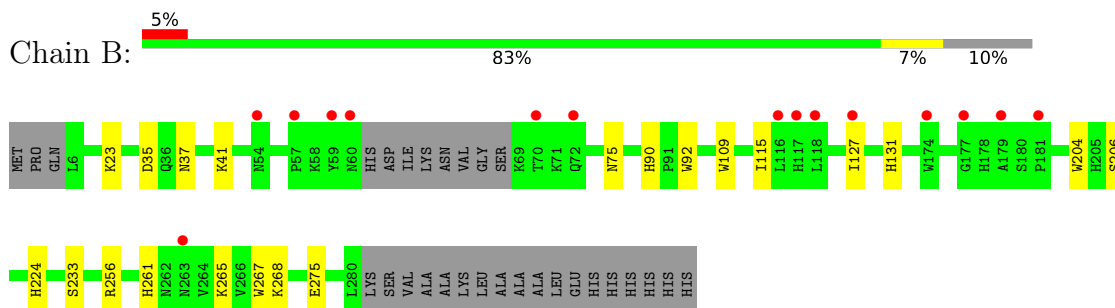
- Molecule 1: 2-oxoglutarate/Fe(II)-dependent dioxygenase SptF



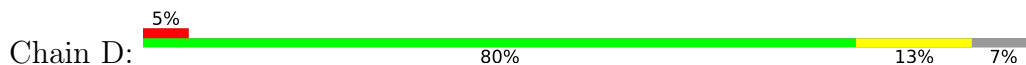
- Molecule 1: 2-oxoglutarate/Fe(II)-dependent dioxygenase SptF

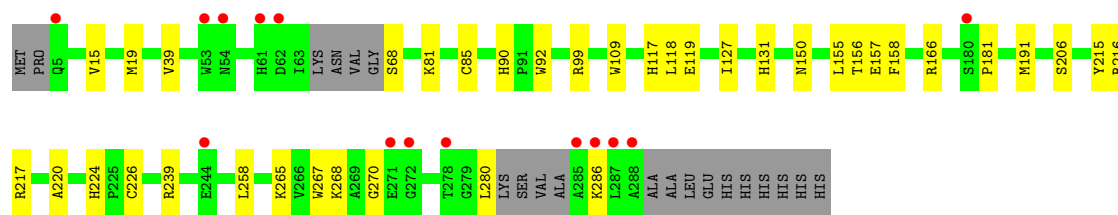


- Molecule 1: 2-oxoglutarate/Fe(II)-dependent dioxygenase SptF



- Molecule 1: 2-oxoglutarate/Fe(II)-dependent dioxygenase SptF





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.05Å 72.56Å 78.83Å 81.74° 84.19° 70.23°	Depositor
Resolution (Å)	48.42 – 2.10 48.42 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.42-2.10) 94.2 (48.42-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.236 , 0.286 0.236 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtrriage
Anisotropy	0.826	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9018	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0322e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 0I3, OGA, FE2

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	0.24	0/2088	0.47	0/2846
1	B	0.24	0/2189	0.47	0/2986
1	C	0.24	0/2261	0.47	0/3082
1	D	0.24	0/2254	0.47	0/3072
All	All	0.24	0/8792	0.47	0/11986

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	2027	0	1919	21	0
1	B	2123	0	1999	12	0
1	C	2193	0	2071	19	0
1	D	2188	0	2061	20	0
2	C	10	0	3	1	0
3	C	30	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	106	0	0	0	0
5	B	104	0	0	0	0
5	C	113	0	0	1	0
5	D	120	0	0	1	0
All	All	9018	0	8053	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:HE3	1:A:195:LEU:HB2	1.80	0.64
1:D:280:LEU:O	1:D:286:LYS:NZ	2.23	0.63
1:C:224:CYS:HB2	1:C:256:LEU:HD13	1.82	0.61
1:C:125:ILE:HA	1:C:204:SER:HB3	1.82	0.61
1:A:16:VAL:HG13	1:A:26:LEU:HD21	1.83	0.59
1:A:125:ILE:HA	1:A:204:SER:HB3	1.85	0.58
1:D:118:LEU:HD12	1:D:216:ARG:HD3	1.84	0.58
1:D:81:LYS:NZ	1:D:85:CYS:SG	2.77	0.58
1:C:146:THR:HG23	1:C:222:HIS:HB3	1.86	0.57
1:D:265:LYS:HB2	1:D:268:LYS:HD3	1.87	0.56
1:A:224:CYS:HB2	1:A:256:LEU:HD13	1.89	0.55
1:D:268:LYS:NZ	1:D:270:GLY:O	2.39	0.55
1:D:127:ILE:HA	1:D:206:SER:HB3	1.90	0.54
1:D:226:CYS:HB2	1:D:258:LEU:HD13	1.91	0.53
1:D:156:THR:HG23	1:D:217:ARG:HB2	1.89	0.53
1:C:140:PRO:HG3	1:C:173:GLU:HA	1.91	0.52
1:C:109:ASN:HD22	1:C:146:THR:HG21	1.73	0.52
1:D:90:HIS:CE1	1:D:92:TRP:HB2	2.44	0.52
1:D:118:LEU:HB2	1:D:216:ARG:HB3	1.92	0.51
1:A:47:TYR:CD2	1:A:77:MET:HG2	2.47	0.50
1:A:156:PHE:HB2	1:A:189:MET:HB2	1.92	0.50
1:D:158:PHE:HB2	1:D:191:MET:HB2	1.93	0.50
1:B:90:HIS:CE1	1:B:92:TRP:HB2	2.48	0.49
1:A:116:LEU:HD22	1:A:120:GLU:HG2	1.95	0.48
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.77	0.48
1:A:47:TYR:CG	1:A:77:MET:HG2	2.48	0.48
1:C:170:HIS:CE1	1:C:171:LEU:HG	2.49	0.48
1:A:263:LYS:NZ	1:A:271:ASN:OD1	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ILE:HD12	1:B:115:ILE:H	1.78	0.48
1:C:156:PHE:HB2	1:C:189:MET:HB2	1.96	0.47
1:A:13:VAL:O	1:A:17:MET:HG2	2.15	0.47
1:B:127:ILE:HG22	1:B:204:TRP:HE3	1.79	0.47
1:D:117:HIS:CE1	1:D:217:ARG:HG2	2.50	0.46
1:D:68:SER:N	5:D:412:HOH:O	2.48	0.46
1:C:133:GLN:HB2	1:B:261:HIS:NE2	2.31	0.46
1:A:157:THR:HA	1:A:188:LEU:HD22	1.98	0.46
1:C:265:TRP:CD2	1:B:233:SER:HB2	2.51	0.45
1:C:56:LYS:NZ	5:C:407:HOH:O	2.45	0.45
1:B:256:ARG:HG2	1:B:275:GLU:HB3	1.99	0.45
1:C:69:LYS:HB2	1:C:115:HIS:HB3	1.98	0.45
1:C:157:THR:HA	1:C:188:LEU:HD13	1.97	0.45
1:A:155:GLU:HG2	1:A:157:THR:HG23	1.99	0.45
1:A:231:SER:HB2	1:D:267:TRP:CD2	2.52	0.45
1:B:127:ILE:HA	1:B:206:SER:HB2	1.99	0.44
1:A:263:LYS:HB2	1:A:266:LYS:HD3	2.00	0.44
1:D:150:ASN:HD21	1:D:220:ALA:HB1	1.81	0.44
1:B:37:ASN:O	1:B:41:LYS:HG3	2.17	0.44
1:C:74:LEU:HD21	1:C:113:ILE:HG12	2.00	0.43
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.86	0.43
1:D:15:VAL:O	1:D:19:MET:HG2	2.18	0.43
1:C:70:GLN:HA	1:C:113:ILE:O	2.18	0.43
1:C:231:SER:HB2	1:B:267:TRP:CD2	2.54	0.43
1:A:189:MET:HE1	1:A:194:ALA:C	2.40	0.42
1:C:205:ALA:HB2	2:C:301:OGA:C5	2.50	0.42
1:B:35:ASP:N	1:B:35:ASP:OD1	2.45	0.42
1:A:170:HIS:CE1	1:A:171:LEU:HG	2.55	0.42
1:D:127:ILE:HG21	1:D:181:PRO:HG2	2.01	0.42
1:A:158:VAL:HG23	1:A:188:LEU:HD21	2.01	0.41
1:C:4:LEU:HD11	1:C:187:VAL:HG22	2.02	0.41
1:D:119:GLU:HG3	1:D:215:TYR:HE1	1.85	0.41
1:A:266:LYS:HB2	1:A:266:LYS:HE3	1.82	0.41
1:D:39:VAL:HB	1:D:155:LEU:HD23	2.02	0.41
1:C:56:LYS:HA	1:C:56:LYS:HD2	1.79	0.40
1:C:268:GLY:N	1:B:75:ASN:OD1	2.55	0.40
1:A:243:MET:HB2	1:A:248:GLN:HG3	2.04	0.40
1:A:76:LEU:HB2	1:A:235:LEU:HD11	2.02	0.40
1:B:265:LYS:HB2	1:B:268:LYS:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/296 (86%)	247 (97%)	7 (3%)	0	100	100
1	B	264/296 (89%)	261 (99%)	3 (1%)	0	100	100
1	C	275/296 (93%)	269 (98%)	6 (2%)	0	100	100
1	D	270/296 (91%)	262 (97%)	8 (3%)	0	100	100
All	All	1063/1184 (90%)	1039 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/261 (84%)	211 (97%)	7 (3%)	39	41
1	B	230/261 (88%)	226 (98%)	4 (2%)	60	67
1	C	236/261 (90%)	230 (98%)	6 (2%)	47	52
1	D	237/261 (91%)	230 (97%)	7 (3%)	41	44
All	All	921/1044 (88%)	897 (97%)	24 (3%)	46	50

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ASP
1	C	21	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	107	TRP
1	C	129	HIS
1	C	164	ARG
1	C	222	HIS
1	A	18	ARG
1	A	73	ASN
1	A	107	TRP
1	A	129	HIS
1	A	164	ARG
1	A	222	HIS
1	A	237	ARG
1	B	23	LYS
1	B	109	TRP
1	B	131	HIS
1	B	224	HIS
1	D	99	ARG
1	D	109	TRP
1	D	131	HIS
1	D	157	GLU
1	D	166	ARG
1	D	224	HIS
1	D	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OGA	C	301	4	9,9,9	1.49	2 (22%)	10,11,11	1.35	1 (10%)
3	0I3	C	302	-	32,35,35	3.03	7 (21%)	41,64,64	2.06	13 (31%)

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
2	OGA	C	301	4	-	0/8/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	0I3	CAU-CAL	-9.59	1.39	1.52
3	C	302	0I3	CAA-CAV	-9.23	1.39	1.51
3	C	302	0I3	CAS-CBC	-6.55	1.39	1.51
3	C	302	0I3	CAP-CAL	-4.96	1.40	1.53
3	C	302	0I3	CAW-CAX	-3.52	1.38	1.47
2	C	301	OGA	C2-C1	-3.06	1.50	1.54
3	C	302	0I3	OAZ-CAD	-2.88	1.44	1.48
2	C	301	OGA	O2-C1	-2.43	1.23	1.30
3	C	302	0I3	CAW-CAV	2.29	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	0I3	OBD-CBC-CAS	-4.44	121.85	129.12
3	C	302	0I3	CBB-OAJ-CBC	-3.97	104.98	110.20
3	C	302	0I3	OAZ-CAX-CAW	3.94	130.54	122.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	OI3	OAJ-CBB-CAO	-3.90	101.67	105.87
3	C	302	OI3	OAZ-CAX-OAY	-3.51	112.23	116.78
3	C	302	OI3	CAD-CAE-CAA	3.44	120.54	117.60
3	C	302	OI3	OAJ-CBC-OBD	3.29	124.83	121.42
3	C	302	OI3	CAU-CAT-CAS	-3.19	108.90	113.55
3	C	302	OI3	OAJ-CBC-CAS	2.97	113.30	110.03
2	C	301	OGA	O1-C1-C2	-2.65	116.29	122.18
3	C	302	OI3	CAF-CAE-CAA	-2.50	108.90	111.36
3	C	302	OI3	CAG-CAF-CAE	2.47	115.86	111.07
3	C	302	OI3	CAN-CAD-CAK	-2.27	106.46	109.92
3	C	302	OI3	CAK-CAD-CAE	-2.08	106.75	113.23

There are no chirality outliers.

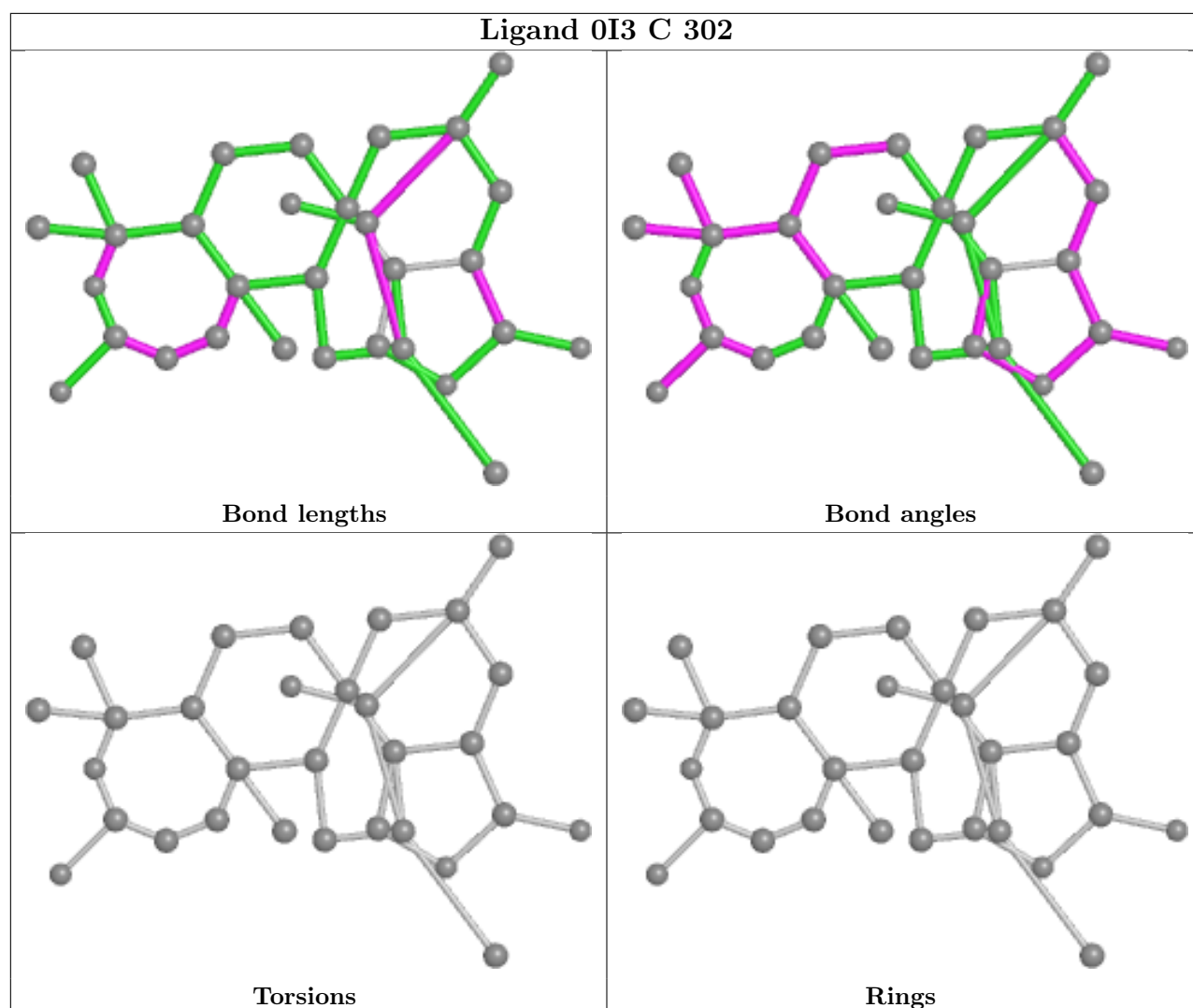
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	OGA	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	258/296 (87%)	0.64	19 (7%) 14 18	13, 28, 41, 49	0
1	B	267/296 (90%)	0.68	15 (5%) 24 29	19, 29, 41, 62	0
1	C	277/296 (93%)	0.78	25 (9%) 9 12	16, 29, 45, 51	0
1	D	276/296 (93%)	0.51	14 (5%) 28 33	15, 24, 36, 63	0
All	All	1078/1184 (91%)	0.65	73 (6%) 17 21	13, 27, 42, 63	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	57	TYR	4.7
1	A	174	ASN	4.5
1	D	285	ALA	4.4
1	C	66	SER	4.3
1	A	68	THR	4.3
1	C	259	HIS	4.1
1	C	59	HIS	4.1
1	B	116	LEU	3.9
1	C	269	GLU	3.9
1	C	270	GLY	3.6
1	D	272	GLY	3.6
1	C	268	GLY	3.6
1	C	18	ARG	3.5
1	B	118	LEU	3.5
1	A	47	TYR	3.5
1	C	52	ASN	3.4
1	B	70	THR	3.3
1	C	61	ILE	3.3
1	A	70	GLN	3.3
1	B	127	ILE	3.2
1	A	261	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	260	ASN	3.0
1	D	62	ASP	3.0
1	C	209	ARG	2.9
1	A	213	TYR	2.9
1	A	276	THR	2.9
1	D	287	LEU	2.9
1	A	277	GLY	2.9
1	B	177	GLY	2.9
1	B	54	ASN	2.8
1	B	60	ASN	2.8
1	C	175	GLY	2.8
1	C	67	LYS	2.7
1	C	278	LEU	2.7
1	D	271	GLU	2.7
1	C	64	VAL	2.6
1	C	60	ASP	2.6
1	D	54	ASN	2.6
1	D	61	HIS	2.6
1	C	58	ASN	2.6
1	D	286	LYS	2.5
1	A	71	PRO	2.5
1	B	72	GLN	2.5
1	A	83	CYS	2.5
1	C	14	GLU	2.4
1	D	5	GLN	2.4
1	C	56	LYS	2.4
1	A	209	ARG	2.4
1	C	180	ALA	2.4
1	A	275	ALA	2.4
1	B	179	ALA	2.4
1	B	117	HIS	2.4
1	B	59	TYR	2.4
1	B	181	PRO	2.3
1	D	244	GLU	2.3
1	D	180	SER	2.3
1	B	263	ASN	2.3
1	A	115	HIS	2.3
1	C	178	SER	2.3
1	B	57	PRO	2.3
1	C	274	ASP	2.2
1	A	48	VAL	2.2
1	C	277	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	259	HIS	2.1
1	C	130	VAL	2.1
1	A	183	ASP	2.1
1	A	178	SER	2.1
1	B	174	TRP	2.1
1	A	175	GLY	2.1
1	D	278	THR	2.1
1	C	51	TRP	2.0
1	D	288	ALA	2.0
1	D	53	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

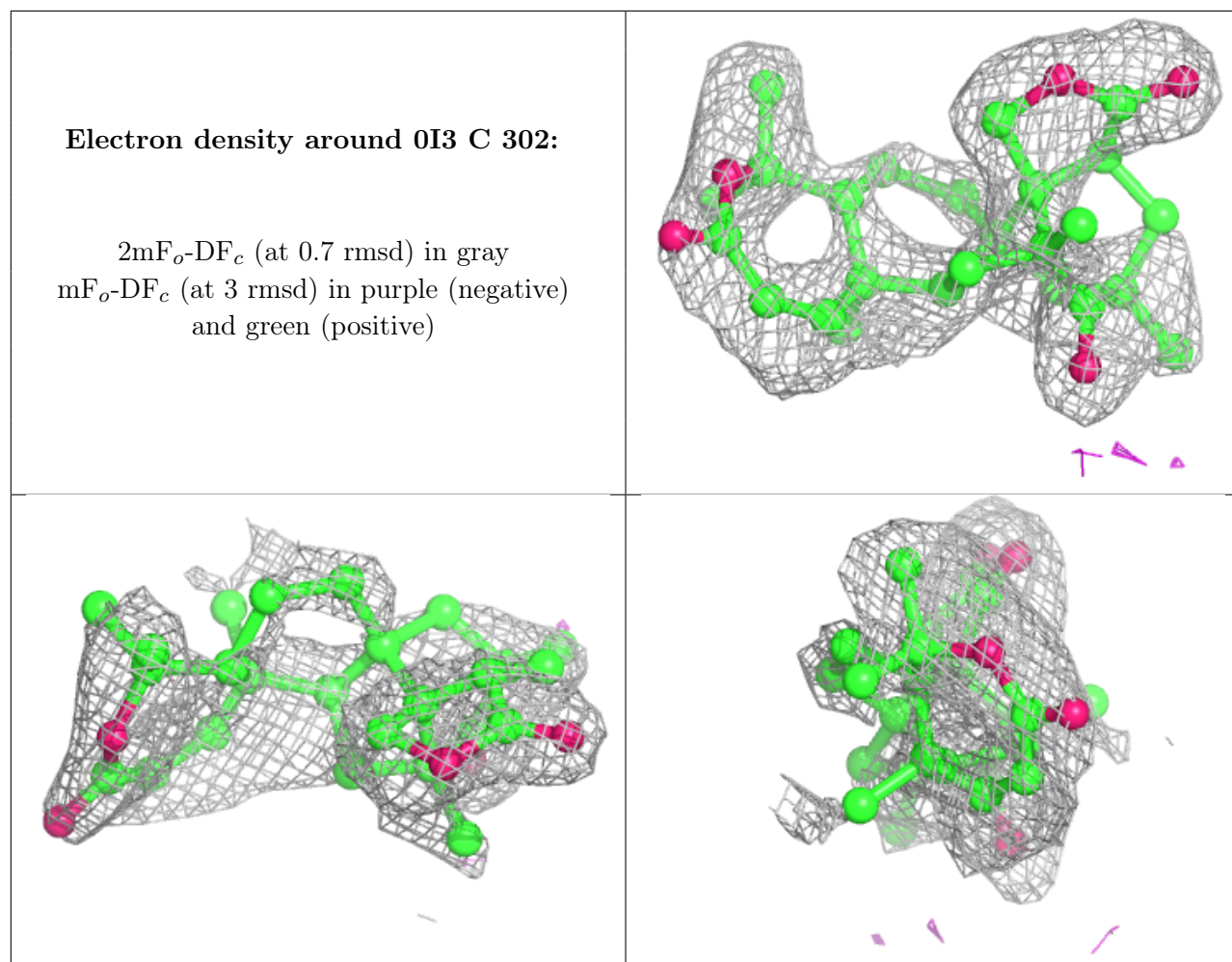
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	0I3	C	302	30/30	0.72	0.28	20,25,31,34	30
2	OGA	C	301	10/10	0.90	0.14	23,27,32,35	0
4	FE2	B	301	1/1	0.94	0.10	51,51,51,51	1
4	FE2	D	301	1/1	0.94	0.07	37,37,37,37	1
4	FE2	A	301	1/1	0.95	0.09	42,42,42,42	1
4	FE2	C	303	1/1	0.96	0.04	37,37,37,37	1

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.