



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:26 PM UTC

PDB ID : 6PLF / pdb_00006plf
Title : Crystal structure of human PHGDH complexed with Compound 1
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Deposited on : 2019-06-30
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

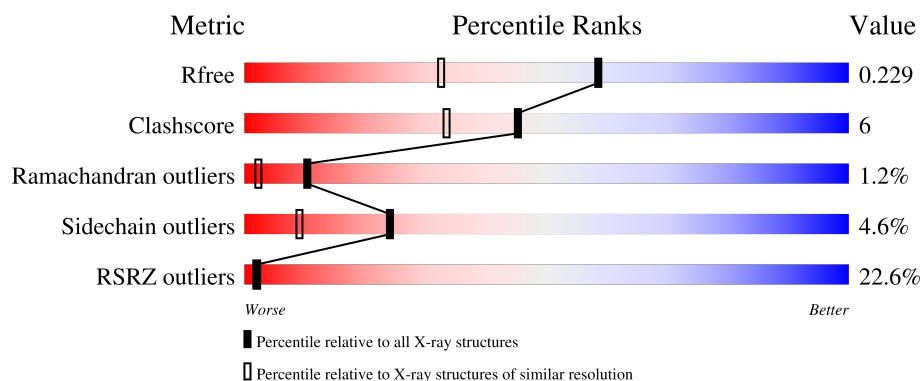
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	314	18% 81%14% . .
1	B	314	25% 79%12% . 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4806 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.

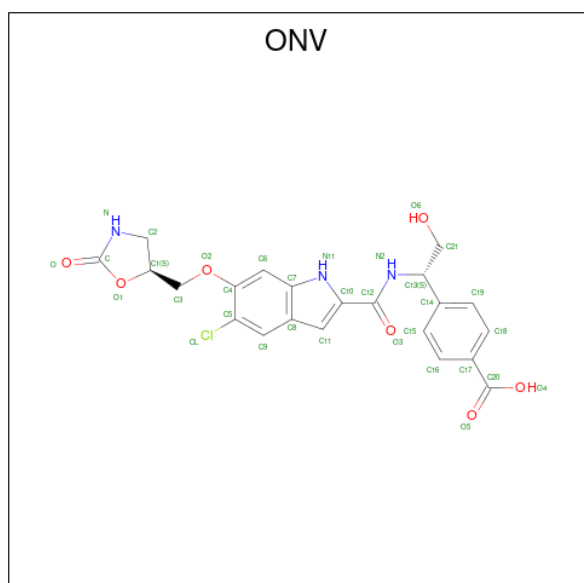
- Molecule 1 is a protein called D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	7	0
			2319	1439	413	447	20			
1	B	292	Total	C	N	O	S	0	5	0
			2118	1314	380	403	21			

There are 4 discrepancies between the modelled and reference sequences:

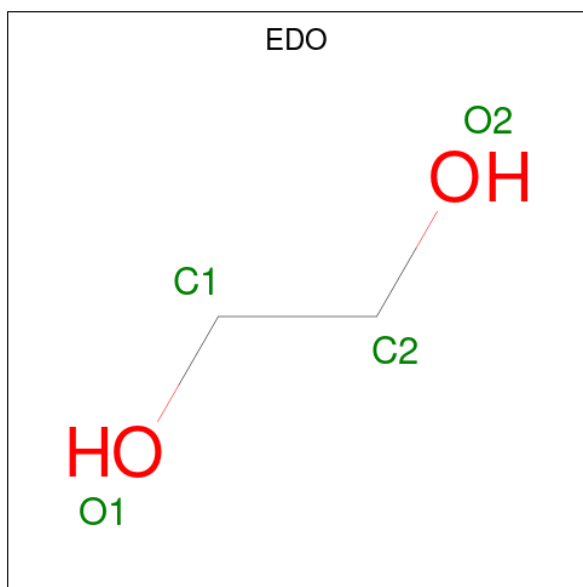
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP O43175
A	3	MET	-	expression tag	UNP O43175
B	2	SER	-	expression tag	UNP O43175
B	3	MET	-	expression tag	UNP O43175

- Molecule 2 is 4-{(1S)-1-[(5-chloro-6-{[(5S)-2-oxo-1,3-oxazolidin-5-yl]methoxy}-1H-indole-2-carbonyl)amino]-2-hydroxyethyl}benzoic acid (CCD ID: ONV) (formula: C₂₂H₂₀ClN₃O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			33	22	1	3	7		
2	B	1	Total	C	Cl	N	O	0	0
			33	22	1	3	7		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total	O	0	0
			138	138		
4	B	145	Total	O	0	0
			145	145		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.20Å 126.19Å 59.50Å 90.00° 99.76° 90.00°	Depositor
Resolution (Å)	40.37 – 1.70 40.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.37-1.70) 96.0 (40.37-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.184 , 0.223 0.194 , 0.229	Depositor DCC
R_{free} test set	3288 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4806	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 5.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ONV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	6/2351 (0.3%)	1.39	2/3178 (0.1%)
1	B	1.17	1/2148 (0.0%)	1.37	4/2911 (0.1%)
All	All	1.17	7/4499 (0.2%)	1.38	6/6089 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	ALA	C-O	7.06	1.32	1.24
1	A	115	MET	C-O	5.84	1.30	1.24
1	A	106	ALA	C-O	5.45	1.30	1.24
1	A	107	ALA	C-O	5.32	1.30	1.24
1	A	112	GLY	C-O	5.20	1.30	1.23
1	B	210	LEU	N-CA	5.07	1.50	1.45
1	A	149	GLY	C-O	5.02	1.29	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ILE	N-CA-C	-5.71	104.95	110.72
1	B	201	ASP	N-CA-C	-5.27	106.00	112.90
1	A	226	LYS	CB-CA-C	-5.15	100.40	109.62
1	B	221	THR	CB-CA-C	5.13	120.09	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ASN	CA-C-N	5.07	125.71	120.03
1	B	100	ASN	C-N-CA	5.07	125.71	120.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	25	ASP	Peptide
1	B	92	GLY	Peptide

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	2319	0	2356	29	0
1	B	2118	0	2073	25	0
2	A	33	0	0	0	0
2	B	33	0	0	1	0
3	A	12	0	18	0	0
3	B	8	0	12	2	0
4	A	138	0	0	4	0
4	B	145	0	0	4	0
All	All	4806	0	4459	53	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 6.

All (53) 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:268[A]:ARG:HH21	1:A:268[A]:ARG:CG	1.69	1.05
1:A:268[A]:ARG:HG2	1:A:268[A]:ARG:NH2	1.55	1.02
1:A:268[A]:ARG:HH21	1:A:268[A]:ARG:HG2	0.76	0.84
1:B:294:ARG:NH2	4:B:502:HOH:O	2.18	0.76
1:A:113[B]:MET:SD	1:A:234:CYS:SG	2.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113[B]:MET:SD	1:B:234:CYS:SG	2.89	0.69
1:A:175:ASP:O	4:A:501:HOH:O	2.11	0.67
1:B:120:GLN:HG2	3:B:403:EDO:H11	1.76	0.66
1:A:54:ARG:NE	1:A:292:GLN:OE1	2.31	0.64
1:A:115:MET:HE3	1:A:115:MET:HA	1.83	0.59
1:B:175:ASP:O	4:B:501:HOH:O	2.16	0.59
1:B:155[A]:ARG:H	1:B:155[A]:ARG:NE	2.03	0.56
1:A:54:ARG:NH2	1:A:55[B]:SER:OG	2.38	0.56
1:A:230:ARG:NH2	4:A:503:HOH:O	2.30	0.56
1:A:268[A]:ARG:CG	1:A:268[A]:ARG:NH2	2.40	0.55
1:B:155[A]:ARG:H	1:B:155[A]:ARG:CZ	2.20	0.55
1:A:64:ILE:HG23	1:A:93:ILE:HD12	1.88	0.54
1:B:74:GLY:C	1:B:299:ILE:HD11	2.32	0.54
1:B:23:LEU:O	1:B:28:LEU:CB	2.57	0.53
1:A:294:ARG:NH2	4:A:506:HOH:O	2.42	0.53
1:A:20:ARG:HG3	1:A:30:VAL:HG11	1.91	0.52
1:B:74:GLY:HA3	1:B:299:ILE:HD11	1.93	0.51
1:A:33:LYS:CB	1:A:36:LEU:CD1	2.88	0.51
1:B:74:GLY:CA	1:B:299:ILE:HD11	2.44	0.48
1:B:304:VAL:CG1	1:B:304:VAL:O	2.61	0.48
1:A:96:MET:HE2	1:A:302:GLN:OE1	2.14	0.47
1:B:85:LEU:O	1:B:89:THR:OG1	2.28	0.47
1:A:78:THR:HG23	1:A:102:ASN:HD22	1.80	0.46
1:B:238:GLY:HA2	1:B:263[A]:THR:HG22	1.97	0.46
1:A:173:GLY:O	1:A:190:GLN:HA	2.17	0.45
1:B:120:GLN:HG3	4:B:608:HOH:O	2.15	0.45
1:B:61:ALA:O	1:B:65:ASN:HB2	2.17	0.45
1:A:130:ASP:OD2	1:A:132:LYS:HE2	2.17	0.45
1:B:117:LEU:HA	3:B:403:EDO:H12	1.99	0.45
1:A:115:MET:HA	1:A:115:MET:CE	2.47	0.45
1:A:33:LYS:CB	1:A:36:LEU:HD11	2.47	0.45
1:A:33:LYS:CB	1:A:36:LEU:HD13	2.46	0.44
1:B:155[A]:ARG:HH22	2:B:401:ONV:C17	2.30	0.44
1:A:230:ARG:HD3	4:A:512:HOH:O	2.19	0.43
1:B:75:ARG:NH2	1:B:78:THR:O	2.49	0.43
1:B:115[B]:MET:HE1	1:B:119:ARG:HG3	2.01	0.43
1:B:68:GLU:O	1:B:69:LYS:C	2.62	0.42
1:A:45:LEU:HA	1:A:48:CYS:HB2	2.00	0.42
1:A:108:GLU:O	1:B:115[B]:MET:HE2	2.19	0.42
1:A:129:LYS:HE3	4:B:510:HOH:O	2.20	0.42
1:B:22:ILE:HG21	1:B:300:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ALA:HB3	1:B:63:VAL:HG22	2.02	0.41
1:A:10:LEU:HD22	1:A:44:GLU:HB2	2.03	0.41
1:A:64:ILE:HD13	1:A:88:ALA:HA	2.02	0.41
1:A:117:LEU:HD23	1:A:279[B]:ILE:HD12	2.02	0.41
1:B:116:CYS:HB3	1:B:279:ILE:HD13	2.01	0.41
1:B:103:SER:OG	1:B:155[A]:ARG:HG3	2.21	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	310/314 (99%)	288 (93%)	19 (6%)	3 (1%)	12	3
1	B	291/314 (93%)	264 (91%)	23 (8%)	4 (1%)	9	2
All	All	601/628 (96%)	552 (92%)	42 (7%)	7 (1%)	10	2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	LYS
1	A	8	LYS
1	B	14	SER
1	B	31	VAL
1	A	36	LEU
1	B	46	GLN
1	A	35	ASN

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	253/257 (98%)	241 (95%)	12 (5%)	23	9
1	B	216/257 (84%)	205 (95%)	11 (5%)	21	7
All	All	469/514 (91%)	446 (95%)	23 (5%)	24	8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	15	LEU
1	A	36	LEU
1	A	38	LYS
1	A	47	ASP
1	A	68	GLU
1	A	69	LYS
1	A	230	ARG
1	A	268[A]	ARG
1	A	268[B]	ARG
1	A	292	GLN
1	A	307	VAL
1	B	7	ARG
1	B	24	GLN
1	B	31	VAL
1	B	48	CYS
1	B	78	THR
1	B	83	VAL
1	B	89	THR
1	B	155[A]	ARG
1	B	155[B]	ARG
1	B	194	GLU
1	B	304	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	120	GLN
1	B	35	ASN
1	B	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	403	-	3,3,3	0.24	0	2,2,2	0.24	0
3	EDO	A	403	-	3,3,3	0.24	0	2,2,2	0.21	0
3	EDO	A	402	-	3,3,3	0.45	0	2,2,2	0.69	0
3	EDO	A	404	-	3,3,3	0.34	0	2,2,2	0.19	0
2	ONV	B	401	-	36,36,36	1.50	2 (5%)	49,51,51	1.62	11 (22%)
2	ONV	A	401	-	36,36,36	1.96	10 (27%)	49,51,51	2.45	16 (32%)
3	EDO	B	402	-	3,3,3	0.18	0	2,2,2	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	A	404	-	-	0/1/1/1	-
2	ONV	B	401	-	-	7/23/32/32	0/4/4/4
2	ONV	A	401	-	-	9/23/32/32	0/4/4/4
3	EDO	B	402	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ONV	O1-C	7.17	1.45	1.36
2	B	401	ONV	O1-C	5.61	1.43	1.36
2	B	401	ONV	C14-C13	-3.27	1.47	1.52
2	A	401	ONV	C6-C7	-3.05	1.34	1.39
2	A	401	ONV	C6-C4	-2.91	1.33	1.38
2	A	401	ONV	O1-C1	-2.85	1.42	1.46
2	A	401	ONV	C17-C20	2.71	1.55	1.49
2	A	401	ONV	C8-C11	-2.62	1.35	1.44
2	A	401	ONV	C5-CL	2.54	1.79	1.73
2	A	401	ONV	C9-C5	-2.50	1.34	1.38
2	A	401	ONV	C10-N11	-2.39	1.35	1.38
2	A	401	ONV	C18-C17	2.35	1.43	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ONV	O2-C4-C5	8.41	126.41	116.39
2	A	401	ONV	O2-C4-C6	-5.95	110.65	123.49
2	A	401	ONV	C9-C8-C7	4.66	122.01	119.13
2	A	401	ONV	C3-O2-C4	4.28	127.72	118.21
2	A	401	ONV	O4-C20-C17	4.10	125.35	114.84
2	A	401	ONV	C7-N11-C10	-4.01	104.71	109.01
2	A	401	ONV	O1-C1-C3	-3.99	100.92	109.10
2	A	401	ONV	O5-C20-C17	-3.74	111.64	121.46
2	B	401	ONV	C4-C5-CL	-3.71	115.20	119.44
2	B	401	ONV	C9-C8-C7	3.55	121.32	119.13
2	B	401	ONV	C8-C9-C5	-3.39	115.51	121.12
2	B	401	ONV	C21-C13-C14	-3.28	103.30	111.08
2	B	401	ONV	O2-C3-C1	3.22	115.22	107.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ONV	O2-C4-C5	2.95	119.90	116.39
2	A	401	ONV	C8-C9-C5	-2.90	116.31	121.12
2	B	401	ONV	O5-C20-C17	-2.87	113.94	121.46
2	A	401	ONV	C8-C7-N11	2.85	110.62	107.65
2	B	401	ONV	O4-C20-C17	2.81	122.06	114.84
2	A	401	ONV	C9-C5-CL	2.74	122.94	118.45
2	A	401	ONV	C6-C7-C8	-2.74	119.88	122.59
2	A	401	ONV	O3-C12-C10	-2.72	117.58	121.09
2	A	401	ONV	C4-C5-CL	-2.66	116.41	119.44
2	A	401	ONV	C6-C4-C5	2.61	122.81	119.29
2	B	401	ONV	C9-C5-C4	2.47	124.14	121.01
2	A	401	ONV	C21-C13-C14	-2.26	105.72	111.08
2	B	401	ONV	C18-C19-C14	-2.20	118.99	121.18
2	B	401	ONV	C15-C14-C13	-2.04	116.65	120.79

There are no chirality outliers.

All (18) torsion outliers are listed below:

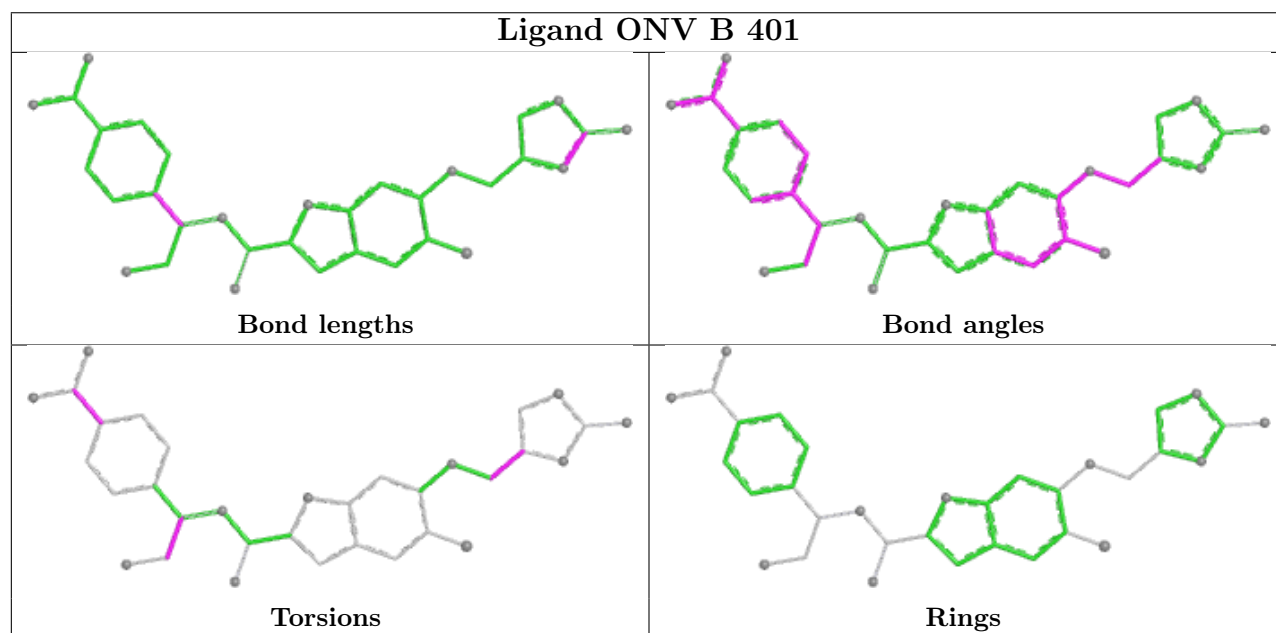
Mol	Chain	Res	Type	Atoms
2	A	401	ONV	C2-C1-C3-O2
2	A	401	ONV	C5-C4-O2-C3
2	A	401	ONV	C16-C17-C20-O4
2	A	401	ONV	C18-C17-C20-O4
2	A	401	ONV	C16-C17-C20-O5
2	B	401	ONV	C18-C17-C20-O4
2	A	401	ONV	C6-C4-O2-C3
2	A	401	ONV	C18-C17-C20-O5
2	B	401	ONV	C16-C17-C20-O4
2	B	401	ONV	O1-C1-C3-O2
3	B	403	EDO	O1-C1-C2-O2
2	B	401	ONV	C18-C17-C20-O5
2	A	401	ONV	C1-C3-O2-C4
2	A	401	ONV	O1-C1-C3-O2
2	B	401	ONV	C16-C17-C20-O5
2	B	401	ONV	N2-C13-C21-O6
3	A	402	EDO	O1-C1-C2-O2
2	B	401	ONV	C2-C1-C3-O2

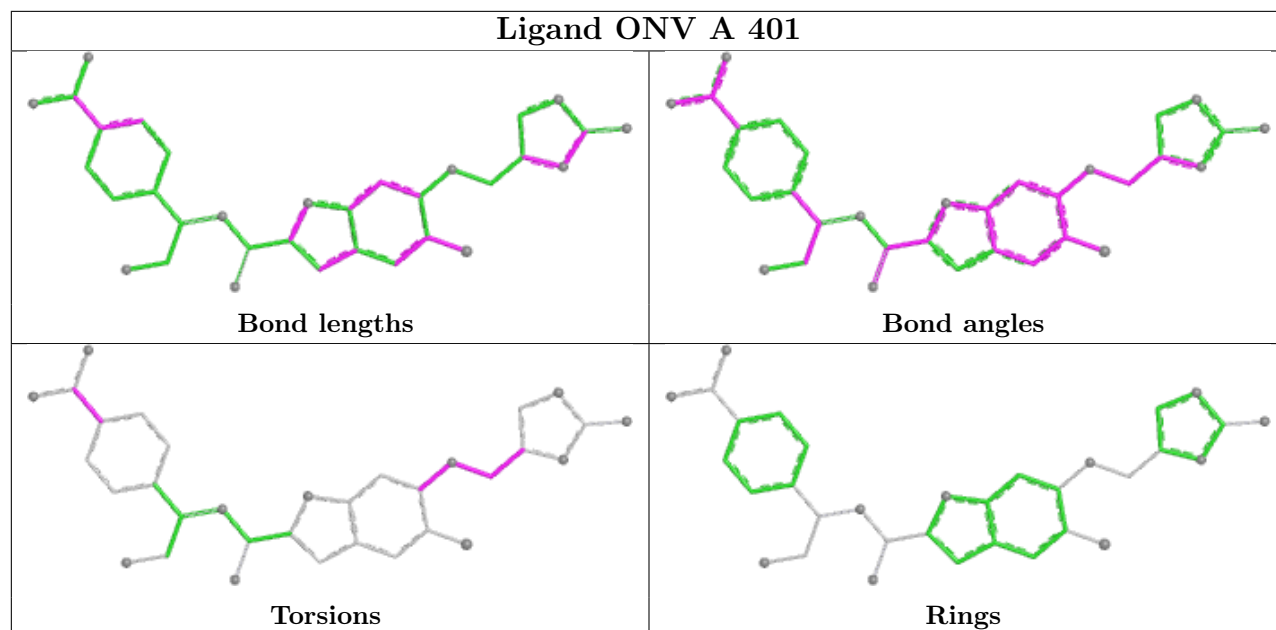
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	EDO	2	0
2	B	401	ONV	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/314 (97%)	0.87	55 (18%) 3 3	9, 31, 93, 107	7 (2%)
1	B	292/314 (92%)	1.16	80 (27%) 1 1	11, 30, 104, 139	5 (1%)
All	All	597/628 (95%)	1.01	135 (22%) 2 2	9, 30, 100, 139	12 (2%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	VAL	6.8
1	B	63	VAL	6.8
1	B	11	ILE	6.2
1	B	61	ALA	5.8
1	B	42	ILE	5.7
1	B	31	VAL	5.3
1	B	52	ILE	5.3
1	B	30	VAL	5.3
1	B	299	ILE	5.3
1	B	28	LEU	5.2
1	B	41	LEU	5.2
1	B	76	ALA	5.2
1	B	304	VAL	5.0
1	B	36	LEU	4.9
1	B	83	VAL	4.9
1	B	15	LEU	4.9
1	B	56	ALA	4.8
1	B	64	ILE	4.7
1	B	10	LEU	4.3
1	B	73	VAL	4.3
1	B	45	LEU	4.3
1	A	41	LEU	4.2
1	B	80	VAL	4.2
1	B	19	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	4.2
1	B	22	ILE	4.2
1	A	43	ALA	4.1
1	A	28	LEU	4.1
1	B	23	LEU	4.0
1	B	13	ASP	4.0
1	B	53	VAL	3.9
1	B	99	PRO	3.9
1	B	43	ALA	3.9
1	A	18	CYS	3.9
1	A	31	VAL	3.9
1	B	18	CYS	3.9
1	A	307	VAL	3.7
1	B	85	LEU	3.7
1	B	305	ASP	3.7
1	A	42	ILE	3.6
1	B	50	GLY	3.6
1	B	51	LEU	3.6
1	A	19	CYS	3.6
1	B	81	ASP	3.6
1	B	301	VAL	3.5
1	B	72	VAL	3.5
1	A	6	LEU	3.5
1	B	303	PHE	3.4
1	A	70	LEU	3.4
1	B	27	GLY	3.4
1	B	138	PHE	3.4
1	B	79	GLY	3.3
1	A	83	VAL	3.3
1	A	78	THR	3.3
1	B	17	PRO	3.2
1	A	304	VAL	3.2
1	A	48	CYS	3.2
1	A	303	PHE	3.2
1	A	80	VAL	3.2
1	B	306	MET	3.2
1	A	94	LEU	3.2
1	B	21	LYS	3.1
1	B	48	CYS	3.1
1	B	62	ASP	3.0
1	B	26	GLY	3.0
1	B	155[A]	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	56	ALA	3.0
1	B	67	ALA	3.0
1	B	88	ALA	3.0
1	A	22	ILE	3.0
1	A	64	ILE	3.0
1	A	85	LEU	3.0
1	B	70	LEU	3.0
1	A	26	GLY	3.0
1	A	67	ALA	2.9
1	B	29	GLN	2.9
1	A	61	ALA	2.9
1	B	302	GLN	2.9
1	B	12	SER	2.9
1	B	34	GLN	2.8
1	A	63	VAL	2.8
1	A	66	ALA	2.8
1	B	47	ASP	2.7
1	A	23	LEU	2.7
1	B	82	ASN	2.6
1	A	15	LEU	2.6
1	A	95	VAL	2.6
1	A	299	ILE	2.6
1	A	93	ILE	2.6
1	B	91	LYS	2.6
1	A	99	PRO	2.6
1	B	77	GLY	2.5
1	A	10	LEU	2.5
1	A	174	TYR	2.5
1	A	301	VAL	2.5
1	A	87	ALA	2.5
1	B	300	ALA	2.5
1	B	78	THR	2.5
1	B	66	ALA	2.5
1	B	87	ALA	2.5
1	A	27	GLY	2.5
1	A	72	VAL	2.5
1	A	36	LEU	2.4
1	A	90	ARG	2.4
1	B	8	LYS	2.4
1	B	35	ASN	2.4
1	B	298	GLU	2.4
1	B	7	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	5	ASN	2.4
1	B	46	GLN	2.3
1	A	55[A]	SER	2.3
1	A	45	LEU	2.3
1	A	60	THR	2.3
1	A	89	THR	2.3
1	A	59	VAL	2.3
1	A	52	ILE	2.3
1	B	49	GLU	2.3
1	A	11	ILE	2.3
1	B	296	GLY	2.3
1	B	74	GLY	2.2
1	B	33	LYS	2.2
1	A	51	LEU	2.2
1	A	96	MET	2.2
1	B	95	VAL	2.2
1	B	295	CYS	2.2
1	A	79	GLY	2.2
1	A	33	LYS	2.1
1	A	17	PRO	2.1
1	B	96	MET	2.1
1	B	54	ARG	2.1
1	B	93	ILE	2.1
1	A	74	GLY	2.1
1	A	73	VAL	2.1
1	B	100	ASN	2.0
1	B	92	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

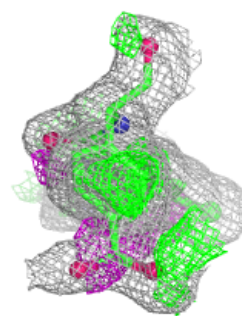
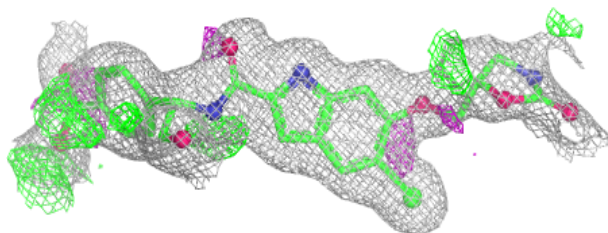
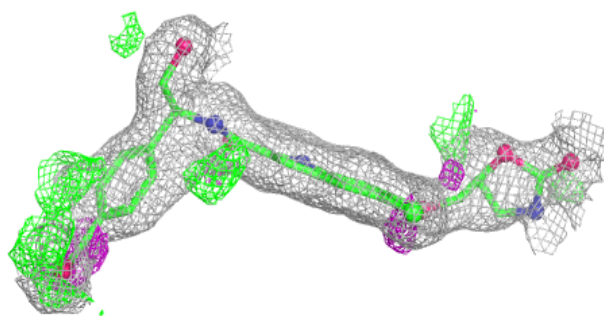
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

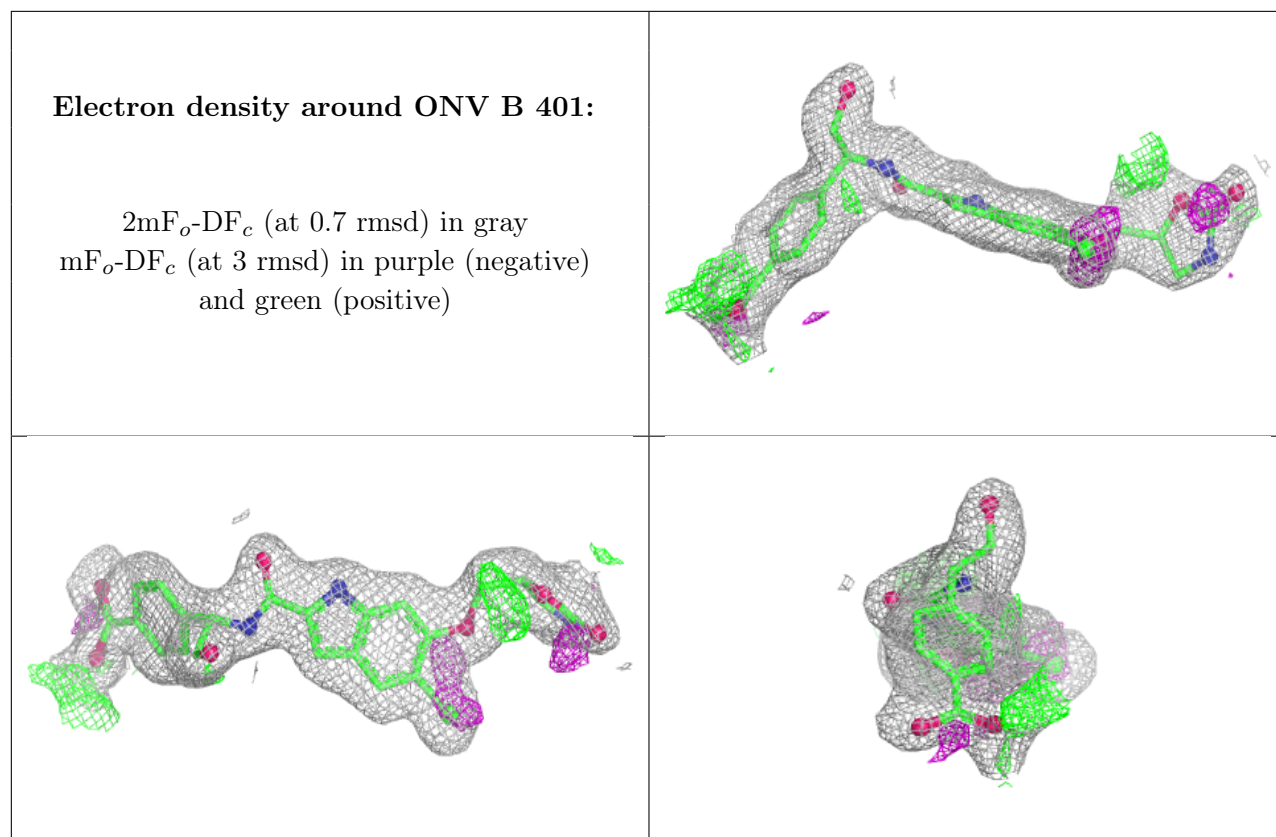
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ONV	A	401	33/33	0.88	0.13	24,36,76,81	0
2	ONV	B	401	33/33	0.89	0.11	31,38,47,49	0
3	EDO	A	404	4/4	0.89	0.12	38,41,42,42	0
3	EDO	B	403	4/4	0.89	0.13	39,40,41,52	0
3	EDO	B	402	4/4	0.95	0.08	30,30,32,35	0
3	EDO	A	402	4/4	0.95	0.13	27,30,32,33	0
3	EDO	A	403	4/4	0.97	0.06	23,23,24,26	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 ONV A 401:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.