



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:06 PM UTC

PDB ID : 6HAX / pdb_00006hax
Title : Crystal structure of PROTAC 2 in complex with the bromodomain of human SMARCA2 and pVHL:ElonginC:ElonginB
Authors : Roy, M.; Bader, G.; Diers, E.; Trainor, N.; Farnaby, W.; Ciulli, A.
Deposited on : 2018-08-09
Resolution : 2.35 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

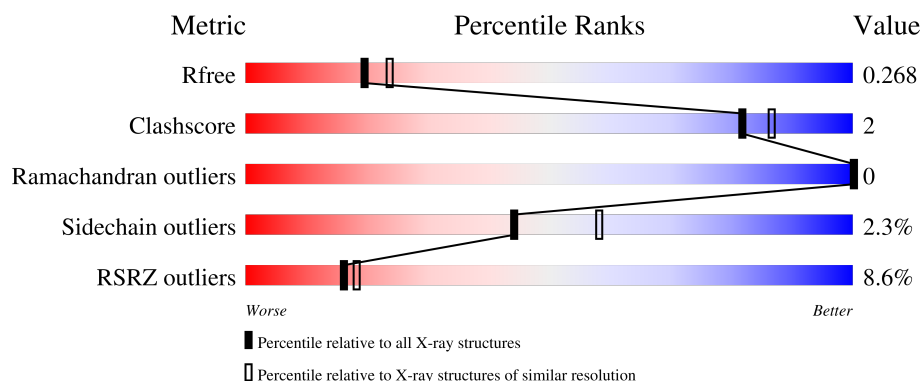
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



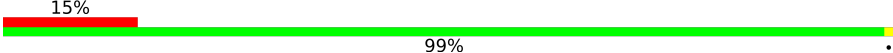
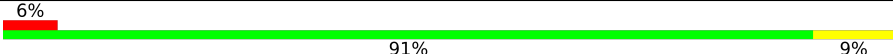
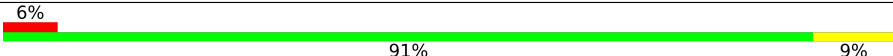
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	123	5% 85% 8% 7%
1	E	123	12% 92% 7% .
2	B	162	7% 79% 13% 8%
2	F	162	6% 78% 14% 8%
3	C	97	11% 81% 9% 9%

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Mol	Chain	Length	Quality of chain
3	G	97	 15%99%
4	D	104	 6%91%9%
4	H	104	 6%91%9%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7780 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 Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			915	581	159	172	3			
1	E	121	Total	C	N	O	S	0	0	0
			964	612	168	180	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1371	SER	-	expression tag	UNP P51531
A	1372	MET	-	expression tag	UNP P51531
E	1371	SER	-	expression tag	UNP P51531
E	1372	MET	-	expression tag	UNP P51531

- Molecule 2 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1201	762	220	217	2			
2	F	149	Total	C	N	O	S	0	0	0
			1201	763	217	219	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	GLY	-	expression tag	UNP P40337
B	53	SER	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	88	Total	C	N	O	S	0	0	0
			696	449	109	131	7			
3	G	97	Total	C	N	O	S	0	0	0
			748	479	119	143	7			

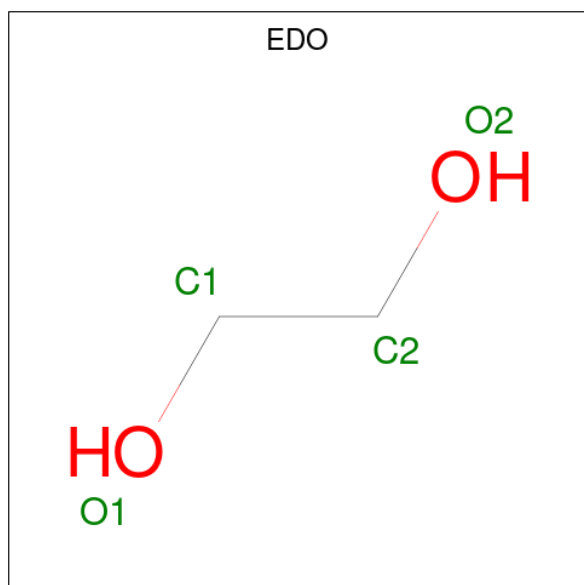
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369
G	16	MET	-	initiating methionine	UNP Q15369

- Molecule 4 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	104	Total	C	N	O	S	0	0	0
			820	518	138	160	4			
4	H	104	Total	C	N	O	S	0	0	0
			819	518	138	158	5			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



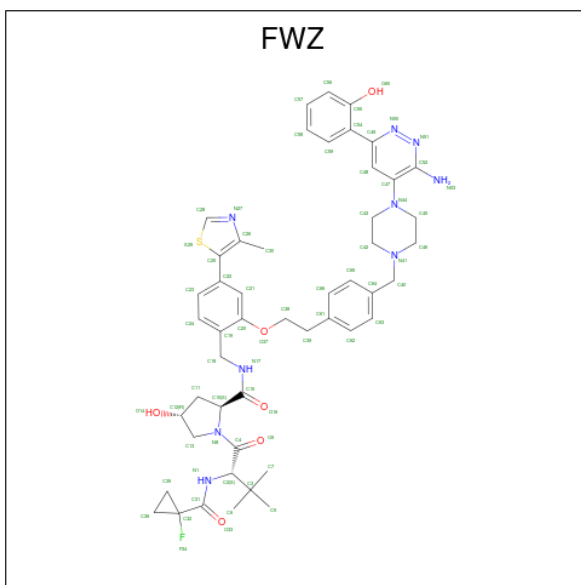
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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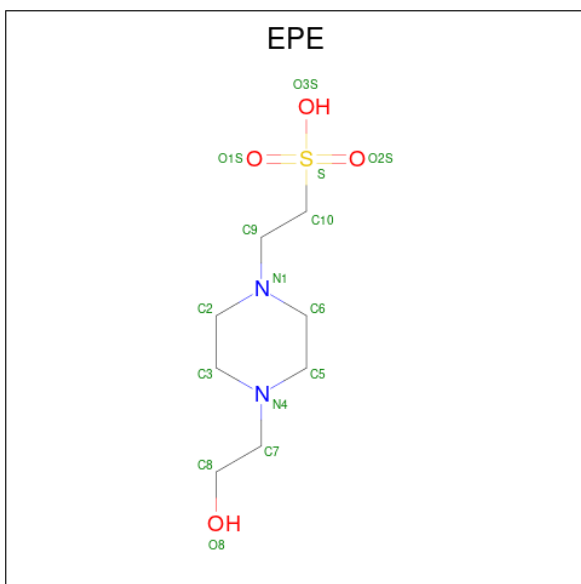
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (2 {S},4 {R})- {N}-[[2-[2-[4-[[4-[3-azanyl-6-(2-hydroxyphenyl)pyridazin-4-yl]piperazin-1-yl)methyl]phenyl]ethoxy]-4-(4-methyl-1,3-thiazol-5-yl)phenyl)methyl]-1-[(2 {S})-2-[(1-fluoranylcyclopropyl)carbonylamino]-3,3-dimethyl-butanoyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: FWZ) (formula: C₄₉H₅₈FN₉O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 66	C 49	F 1	N 9	O 6	S 1	0	0
6	F	1	Total 66	C 49	F 1	N 9	O 6	S 1	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

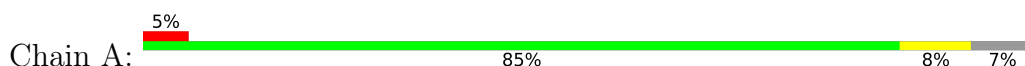
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total 16	O 16	0	0
8	B	42	Total 42	O 42	0	0
8	C	23	Total 23	O 23	0	0
8	D	26	Total 26	O 26	0	0
8	E	13	Total 13	O 13	0	0
8	F	45	Total 45	O 45	0	0
8	G	17	Total 17	O 17	0	0
8	H	31	Total 31	O 31	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.

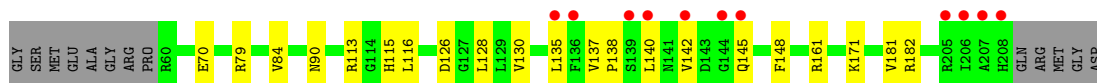
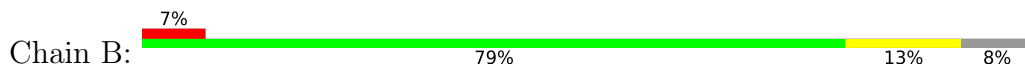
- Molecule 1: Probable global transcription activator SNF2L2



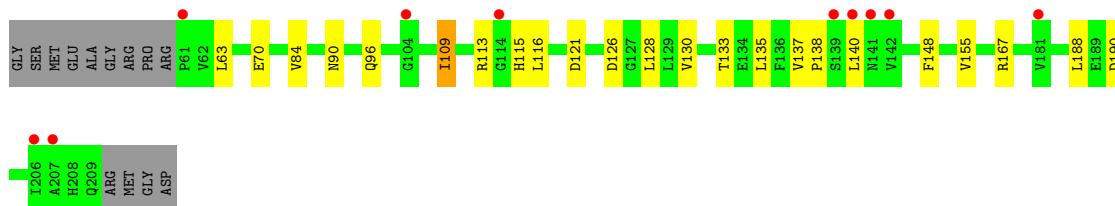
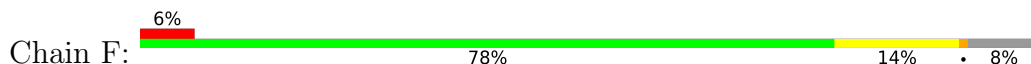
- Molecule 1: Probable global transcription activator SNF2L2



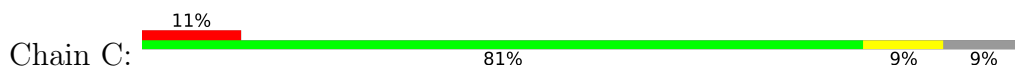
- Molecule 2: von Hippel-Lindau disease tumor suppressor

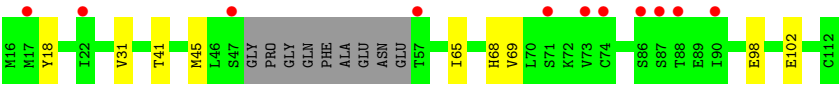


- Molecule 2: von Hippel-Lindau disease tumor suppressor

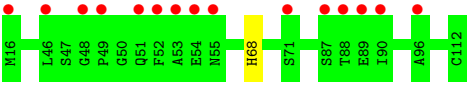


- Molecule 3: Elongin-C

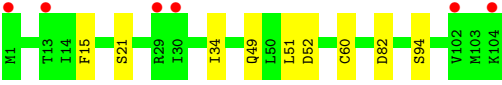
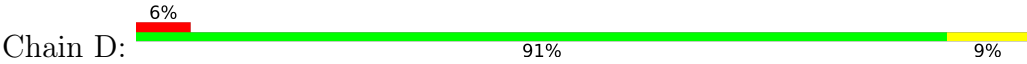




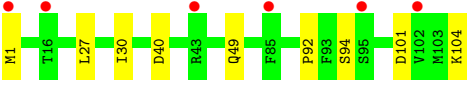
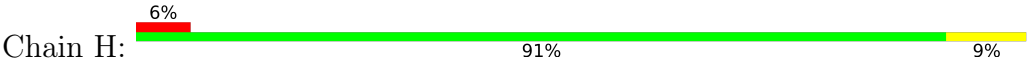
● Molecule 3: Elongin-C



● Molecule 4: Elongin-B



● Molecule 4: Elongin-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.51Å 116.24Å 120.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.41 – 2.35 34.41 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.41-2.35) 99.9 (34.41-2.35)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.232 , 0.268 0.233 , 0.268	Depositor DCC
R_{free} test set	2398 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.57% 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: FWZ, EDO, EPE

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	0.88	0/931	1.49	9/1259 (0.7%)
1	E	0.94	0/980	1.51	2/1321 (0.2%)
2	B	0.90	0/1232	1.28	2/1684 (0.1%)
2	F	0.90	0/1233	1.30	5/1687 (0.3%)
3	C	0.94	0/710	1.29	0/958
3	G	0.93	0/764	1.27	0/1034
4	D	0.89	0/836	1.22	3/1129 (0.3%)
4	H	0.91	0/835	1.23	0/1127
All	All	0.91	0/7521	1.33	21/10199 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1438	ILE	CA-C-N	6.68	129.53	120.38
1	A	1438	ILE	C-N-CA	6.68	129.53	120.38
1	E	1438	ILE	CA-C-N	6.63	129.47	120.38
1	E	1438	ILE	C-N-CA	6.63	129.47	120.38
1	A	1478	GLN	CA-C-N	6.38	128.82	120.28
1	A	1478	GLN	C-N-CA	6.38	128.82	120.28
2	F	90	ASN	CA-CB-CG	6.27	118.87	112.60
2	B	90	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	1425	ILE	CA-C-N	5.62	128.27	120.29
1	A	1425	ILE	C-N-CA	5.62	128.27	120.29
4	D	82	ASP	CA-CB-CG	5.48	118.08	112.60
2	F	155	VAL	N-CA-CB	5.34	117.75	111.66
2	B	126	ASP	CA-CB-CG	5.14	117.74	112.60
2	F	126	ASP	CA-CB-CG	5.13	117.73	112.60
2	F	190	ASP	CA-CB-CG	5.10	117.70	112.60
2	F	121	ASP	N-CA-C	-5.08	101.48	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1446	LEU	CA-C-N	5.03	125.54	120.00
1	A	1446	LEU	C-N-CA	5.03	125.54	120.00
1	A	1472	GLU	CB-CG-CD	5.02	121.13	112.60
4	D	52	ASP	CA-C-N	5.00	127.23	120.38
4	D	52	ASP	C-N-CA	5.00	127.23	120.38

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	915	0	904	1	0
1	E	964	0	963	2	0
2	B	1201	0	1182	14	0
2	F	1201	0	1176	11	0
3	C	696	0	693	6	0
3	G	748	0	730	1	0
4	D	820	0	817	4	0
4	H	819	0	820	4	0
5	A	8	0	12	0	0
5	B	12	0	18	1	0
5	C	4	0	6	1	0
5	D	8	0	12	0	0
5	E	4	0	6	0	0
5	F	4	0	6	1	0
5	G	4	0	6	0	0
5	H	12	0	18	1	0
6	B	66	0	0	0	0
6	F	66	0	0	1	0
7	B	15	0	17	4	0
8	A	16	0	0	0	0
8	B	42	0	0	1	0
8	C	23	0	0	0	0
8	D	26	0	0	0	0
8	E	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	45	0	0	0	0
8	G	17	0	0	0	0
8	H	31	0	0	0	0
All	All	7780	0	7386	37	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 2.

All (37) 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)
2:B:145:GLN:HG2	2:F:133:THR:HG21	1.64	0.79
2:B:182:ARG:HE	7:B:305:EPE:H62	1.58	0.68
3:C:41:THR:HG22	3:C:45:MET:HE2	1.79	0.65
2:F:109:ILE:HG13	6:F:301:FWZ:C23	2.27	0.64
2:B:161:ARG:HH12	5:B:303:EDO:H22	1.64	0.63
2:B:181:VAL:HG13	7:B:305:EPE:H101	1.79	0.63
3:C:65:ILE:HG12	5:C:201:EDO:H22	1.83	0.61
2:B:70:GLU:HB3	2:B:140:LEU:HD21	1.84	0.59
2:F:96:GLN:HB3	5:F:302:EDO:H11	1.87	0.55
2:F:70:GLU:HB3	2:F:140:LEU:HD21	1.88	0.55
3:G:68:HIS:HB3	4:H:94:SER:O	2.09	0.51
2:B:116:LEU:HD13	2:B:137:VAL:HG22	1.94	0.49
4:H:101:ASP:HA	4:H:104:LYS:HD2	1.94	0.48
3:C:68:HIS:HB3	4:D:94:SER:O	2.14	0.48
4:H:27:LEU:HA	4:H:30:ILE:HD12	1.96	0.48
2:F:113:ARG:HG3	2:F:140:LEU:HG	1.97	0.47
2:F:116:LEU:HD13	2:F:137:VAL:HG22	1.97	0.47
4:H:92:PRO:HA	5:H:202:EDO:H21	1.98	0.46
3:C:31:VAL:HG12	4:D:15:PHE:HB2	1.96	0.46
2:B:113:ARG:HG3	2:B:140:LEU:HG	1.98	0.45
1:E:1373:ALA:HA	1:E:1376:LEU:HD12	1.99	0.45
2:B:116:LEU:HD11	2:B:135:LEU:HB3	1.99	0.45
2:F:115:HIS:O	2:F:138:PRO:HD2	2.18	0.44
4:D:51:LEU:HD22	4:D:60:CYS:SG	2.58	0.43
2:B:84:VAL:HG22	2:B:128:LEU:CD1	2.49	0.43
2:F:84:VAL:HG22	2:F:128:LEU:CD1	2.49	0.43
2:F:116:LEU:HD11	2:F:135:LEU:HB3	1.99	0.43
3:C:69:VAL:HG21	3:C:102:GLU:HB3	2.02	0.42
1:A:1484:ALA:O	1:A:1488:ILE:HG12	2.20	0.42
3:C:18:TYR:CZ	4:D:34:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:HIS:O	2:B:138:PRO:HD2	2.19	0.42
2:F:167:ARG:HD3	2:F:188:LEU:O	2.20	0.41
2:B:148:PHE:HB3	2:F:148:PHE:HB3	2.01	0.41
2:B:182:ARG:NE	7:B:305:EPE:H62	2.29	0.41
2:B:181:VAL:HA	7:B:305:EPE:H61	2.01	0.41
1:E:1391:ILE:HD12	1:E:1391:ILE:HA	2.00	0.41
2:B:142:VAL:HG12	8:B:411:HOH:O	2.22	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	113/123 (92%)	110 (97%)	3 (3%)	0	100	100
1	E	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
2	B	147/162 (91%)	145 (99%)	2 (1%)	0	100	100
2	F	147/162 (91%)	144 (98%)	3 (2%)	0	100	100
3	C	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
3	G	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
4	D	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
4	H	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
All	All	909/972 (94%)	888 (98%)	21 (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	100/115 (87%)	97 (97%)	3 (3%)	36	48
1	E	105/115 (91%)	101 (96%)	4 (4%)	29	39
2	B	134/148 (90%)	131 (98%)	3 (2%)	45	59
2	F	135/148 (91%)	132 (98%)	3 (2%)	45	59
3	C	79/86 (92%)	78 (99%)	1 (1%)	61	76
3	G	82/86 (95%)	82 (100%)	0	100	100
4	D	91/92 (99%)	89 (98%)	2 (2%)	45	59
4	H	91/92 (99%)	88 (97%)	3 (3%)	33	44
All	All	817/882 (93%)	798 (98%)	19 (2%)	44	58

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1382	LYS
1	A	1424	LEU
1	A	1432	LYS
2	B	79	ARG
2	B	130	VAL
2	B	171	LYS
3	C	98	GLU
4	D	21	SER
4	D	49	GLN
1	E	1382	LYS
1	E	1424	LEU
1	E	1452	ASP
1	E	1488	ILE
2	F	63	LEU
2	F	109	ILE
2	F	130	VAL
4	H	1	MET
4	H	40	ASP
4	H	49	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1464	ASN
3	C	108	ASN
1	E	1464	ASN
2	F	174	ASN
2	F	203	GLN
3	G	108	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](#)

17 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	$\# Z > 2$
5	EDO	H	202	-	3,3,3	0.54	0	2,2,2	0.22	0
5	EDO	F	302	-	3,3,3	0.58	0	2,2,2	0.40	0
5	EDO	G	201	-	3,3,3	0.52	0	2,2,2	0.34	0
7	EPE	B	305	-	15,15,15	1.00	1 (6%)	19,20,20	0.51	0
5	EDO	B	303	-	3,3,3	0.56	0	2,2,2	0.33	0
5	EDO	C	201	-	3,3,3	0.61	0	2,2,2	0.13	0
5	EDO	D	201	-	3,3,3	0.45	0	2,2,2	0.45	0
5	EDO	H	203	-	3,3,3	0.60	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FWZ	F	301	-	71,73,73	0.39	0	97,107,107	0.76	2 (2%)
6	FWZ	B	301	-	71,73,73	0.32	0	97,107,107	0.74	2 (2%)
5	EDO	H	201	-	3,3,3	0.50	0	2,2,2	0.44	0
5	EDO	E	1501	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	B	302	-	3,3,3	0.59	0	2,2,2	0.45	0
5	EDO	D	202	-	3,3,3	0.52	0	2,2,2	0.37	0
5	EDO	A	1502	-	3,3,3	0.43	0	2,2,2	0.50	0
5	EDO	A	1501	-	3,3,3	0.50	0	2,2,2	0.42	0
5	EDO	B	304	-	3,3,3	0.44	0	2,2,2	0.50	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
5	EDO	H	202	-	-	1/1/1/1	-
5	EDO	F	302	-	-	1/1/1/1	-
5	EDO	G	201	-	-	0/1/1/1	-
7	EPE	B	305	-	-	3/9/19/19	0/1/1/1
5	EDO	B	303	-	-	1/1/1/1	-
5	EDO	C	201	-	-	0/1/1/1	-
5	EDO	D	201	-	-	1/1/1/1	-
5	EDO	H	203	-	-	0/1/1/1	-
6	FWZ	F	301	-	-	3/53/81/81	0/8/8/8
6	FWZ	B	301	-	-	2/53/81/81	0/8/8/8
5	EDO	H	201	-	-	0/1/1/1	-
5	EDO	E	1501	-	-	1/1/1/1	-
5	EDO	B	302	-	-	0/1/1/1	-
5	EDO	D	202	-	-	0/1/1/1	-
5	EDO	A	1502	-	-	0/1/1/1	-
5	EDO	A	1501	-	-	0/1/1/1	-
5	EDO	B	304	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	305	EPE	C10-S	-3.69	1.72	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	FWZ	C36-C32-C31	4.19	124.75	116.20
6	F	301	FWZ	C36-C32-C31	4.18	124.74	116.20
6	B	301	FWZ	C35-C32-C31	3.55	123.44	116.20
6	F	301	FWZ	C35-C32-C31	3.08	122.48	116.20

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	301	FWZ	C64-C40-N41-C46
6	B	301	FWZ	C64-C40-N41-C46
6	F	301	FWZ	C64-C40-N41-C42
6	B	301	FWZ	C64-C40-N41-C42
5	D	201	EDO	O1-C1-C2-O2
5	H	202	EDO	O1-C1-C2-O2
7	B	305	EPE	C8-C7-N4-C5
7	B	305	EPE	S-C10-C9-N1
5	F	302	EDO	O1-C1-C2-O2
7	B	305	EPE	C8-C7-N4-C3
5	E	1501	EDO	O1-C1-C2-O2
5	B	303	EDO	O1-C1-C2-O2
6	F	301	FWZ	O33-C31-C32-C35

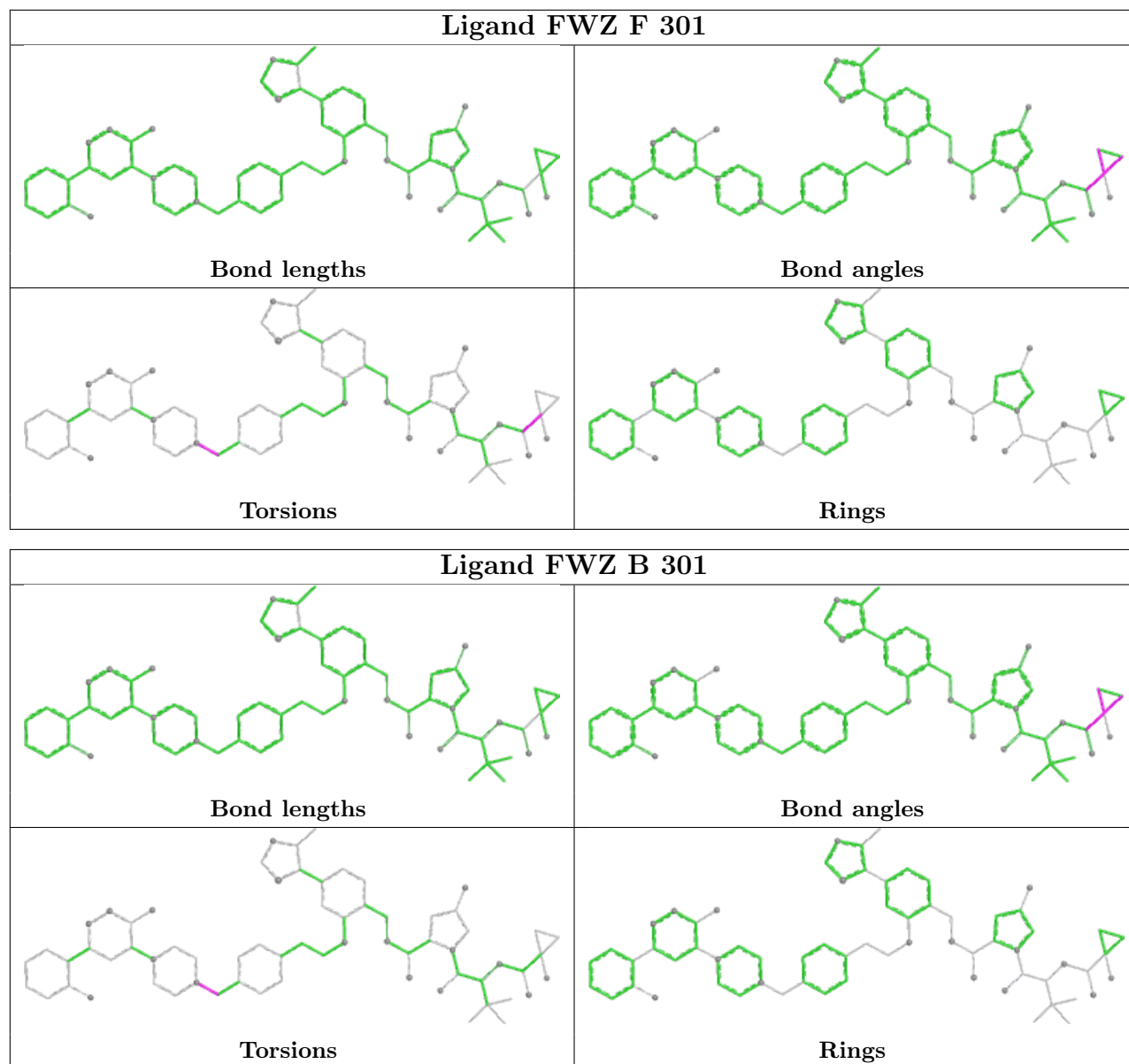
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	202	EDO	1	0
5	F	302	EDO	1	0
7	B	305	EPE	4	0
5	B	303	EDO	1	0
5	C	201	EDO	1	0
6	F	301	FWZ	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 ⓘ

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, 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	115/123 (93%)	0.95	6 (5%) 33 38	36, 53, 86, 105	0
1	E	121/123 (98%)	1.07	15 (12%) 8 9	39, 54, 74, 103	0
2	B	149/162 (91%)	0.76	11 (7%) 20 23	34, 47, 79, 128	0
2	F	149/162 (91%)	0.72	10 (6%) 24 27	28, 46, 79, 103	0
3	C	88/97 (90%)	0.93	11 (12%) 8 9	36, 47, 73, 97	0
3	G	97/97 (100%)	1.15	15 (15%) 5 5	33, 47, 84, 94	0
4	D	104/104 (100%)	0.77	6 (5%) 29 33	35, 47, 66, 95	0
4	H	104/104 (100%)	0.78	6 (5%) 29 33	33, 45, 68, 97	0
All	All	927/972 (95%)	0.88	80 (8%) 16 18	28, 49, 79, 128	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	208	HIS	5.9
1	A	1376	LEU	5.9
3	G	88	THR	4.9
3	G	52	PHE	4.7
2	F	142	VAL	4.0
2	B	144	GLY	3.9
2	B	139	SER	3.6
1	A	1490	LYS	3.6
2	B	140	LEU	3.6
3	C	73	VAL	3.5
3	C	88	THR	3.4
3	G	49	PRO	3.4
2	B	142	VAL	3.4
2	F	139	SER	3.4
2	F	140	LEU	3.3
3	C	87	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	16	MET	3.2
4	H	85	PHE	3.2
3	G	53	ALA	3.2
1	E	1402	GLY	3.1
4	D	102	VAL	3.1
2	B	206	ILE	3.0
1	E	1373	ALA	2.9
1	E	1372	MET	2.9
2	F	61	PRO	2.9
1	A	1410	ILE	2.9
3	G	71	SER	2.8
4	H	1	MET	2.8
1	A	1488	ILE	2.8
3	C	74	CYS	2.8
2	B	135	LEU	2.8
3	G	51	GLN	2.7
4	D	1	MET	2.7
2	F	181	VAL	2.7
2	F	206	ILE	2.7
3	G	89	GLU	2.7
1	A	1377	SER	2.7
4	H	102	VAL	2.7
2	F	207	ALA	2.6
3	G	54	GLU	2.6
3	G	87	SER	2.6
1	E	1449	LEU	2.6
3	G	90	ILE	2.6
4	H	95	SER	2.6
1	A	1402	GLY	2.5
3	C	71	SER	2.5
3	G	96	ALA	2.5
2	B	136	PHE	2.5
4	H	43	ARG	2.5
3	C	90	ILE	2.5
3	C	57	THR	2.4
1	E	1384	THR	2.4
3	G	46	LEU	2.4
2	B	207	ALA	2.4
1	E	1451	LYS	2.4
3	G	48	GLY	2.3
1	E	1374	GLU	2.3
1	E	1421	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	30	ILE	2.3
2	B	145	GLN	2.3
2	F	104	GLY	2.3
3	C	86	SER	2.3
1	E	1382	LYS	2.3
1	E	1418	LEU	2.3
1	E	1392	ASP	2.3
1	E	1424	LEU	2.2
1	E	1431	PHE	2.2
4	D	29	ARG	2.2
1	E	1409	PHE	2.2
2	F	141	ASN	2.2
3	C	47	SER	2.2
2	B	205	ARG	2.1
3	C	17	MET	2.1
2	F	114	GLY	2.1
1	E	1393	THR	2.1
4	H	16	THR	2.1
3	C	22	ILE	2.1
4	D	13	THR	2.0
3	G	55	ASN	2.0
4	D	104	LYS	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($\text{\AA}^2$)	Q<0.9
5	EDO	B	303	4/4	0.66	0.21	65,67,68,68	0

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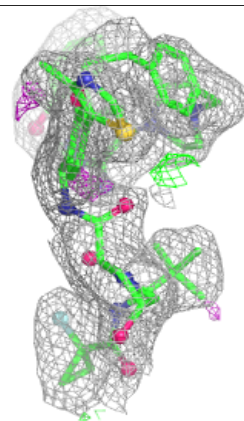
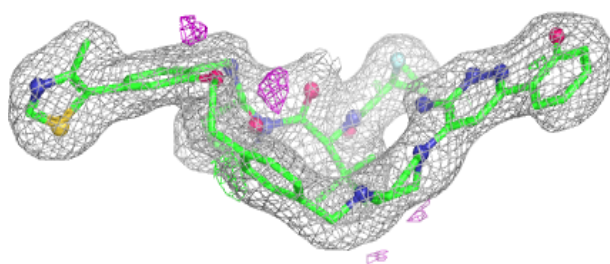
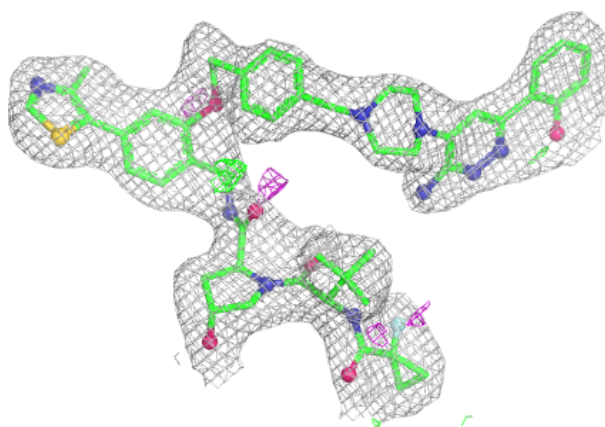
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	304	4/4	0.67	0.21	53,56,59,62	0
7	EPE	B	305	15/15	0.67	0.22	74,79,96,98	0
5	EDO	A	1501	4/4	0.76	0.17	64,65,66,67	0
5	EDO	D	201	4/4	0.77	0.14	59,59,59,61	0
5	EDO	H	203	4/4	0.80	0.16	52,55,58,60	0
5	EDO	B	302	4/4	0.80	0.16	55,56,57,58	0
5	EDO	H	201	4/4	0.81	0.17	65,65,67,69	0
5	EDO	G	201	4/4	0.82	0.20	52,55,56,57	0
5	EDO	D	202	4/4	0.83	0.16	61,61,62,62	0
5	EDO	E	1501	4/4	0.83	0.24	55,55,57,59	0
5	EDO	H	202	4/4	0.86	0.16	54,55,55,56	0
5	EDO	C	201	4/4	0.87	0.17	54,54,54,55	0
5	EDO	F	302	4/4	0.88	0.15	57,57,59,59	0
6	FWZ	F	301	66/66	0.90	0.10	29,37,45,47	0
6	FWZ	B	301	66/66	0.91	0.10	26,35,44,46	0
5	EDO	A	1502	4/4	0.93	0.14	54,54,56,59	0

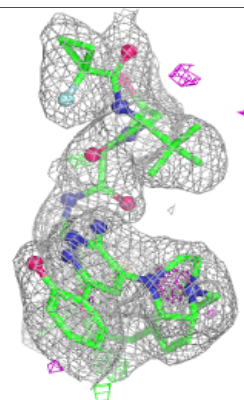
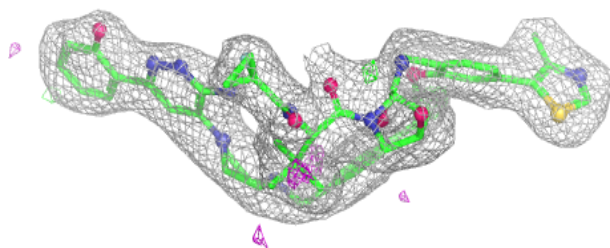
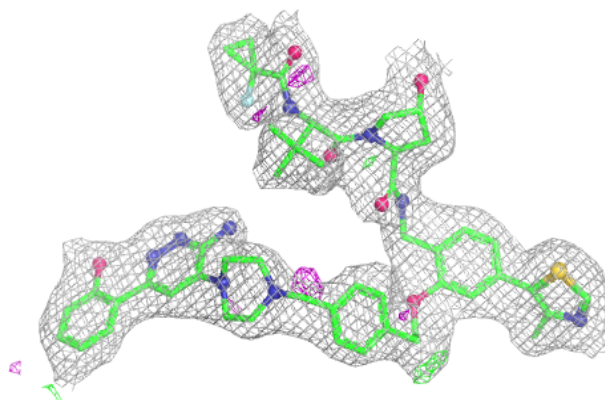
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FWZ F 301:

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

**Electron density around FWZ B 301:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.