



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:19 am BST

PDB ID : 5ZRF
Title : Crystal structure of human topoisomerase II beta in complex with 5-iodouridine-containing-DNA and etoposide in space group p21
Authors : Chen, S.F.; Wang, Y.R.; Wu, C.C.; Chan, N.L.
Deposited on : 2018-04-24
Resolution : 2.30 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 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 : 2.11
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) : 2.11

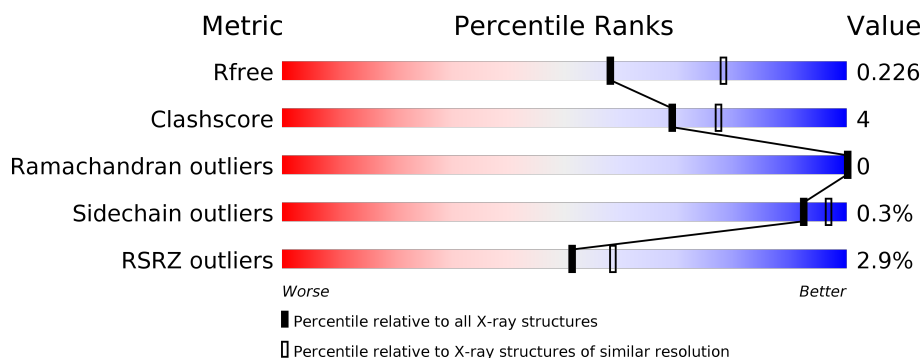
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	803	<div> <div>2%</div> <div>76% 7% 17%</div> </div>
1	B	803	<div> <div>3%</div> <div>78% 6% 16%</div> </div>
2	C	8	<div> <div>13%</div> <div>75% 25%</div> </div>
2	E	8	<div> <div>13%</div> <div>88% 13%</div> </div>
3	D	12	<div> <div>75% 25%</div> </div>
3	F	12	<div> <div>75% 17% 8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	1302	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11909 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 DNA topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	669	Total	C	N	O	S	0	9	0
			5218	3343	884	968	23			
1	B	671	Total	C	N	O	S	0	3	0
			5255	3352	894	986	23			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	expression tag	UNP Q02880
A	420	ALA	-	expression tag	UNP Q02880
A	421	SER	-	expression tag	UNP Q02880
A	422	TRP	-	expression tag	UNP Q02880
A	423	SER	-	expression tag	UNP Q02880
A	424	HIS	-	expression tag	UNP Q02880
A	425	PRO	-	expression tag	UNP Q02880
A	426	GLN	-	expression tag	UNP Q02880
A	427	PHE	-	expression tag	UNP Q02880
A	428	GLU	-	expression tag	UNP Q02880
A	429	LYS	-	expression tag	UNP Q02880
A	430	GLY	-	expression tag	UNP Q02880
A	431	ALA	-	expression tag	UNP Q02880
A	432	ASP	-	expression tag	UNP Q02880
A	433	ASP	-	expression tag	UNP Q02880
A	434	ASP	-	expression tag	UNP Q02880
A	435	ASP	-	expression tag	UNP Q02880
A	436	LYS	-	expression tag	UNP Q02880
A	437	VAL	-	expression tag	UNP Q02880
A	438	PRO	-	expression tag	UNP Q02880
A	439	ASP	-	expression tag	UNP Q02880
A	440	PRO	-	expression tag	UNP Q02880
A	441	THR	-	expression tag	UNP Q02880
A	442	SER	-	expression tag	UNP Q02880
A	443	VAL	-	expression tag	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASP	-	expression tag	UNP Q02880
A	1202	GLY	-	expression tag	UNP Q02880
A	1203	ALA	-	expression tag	UNP Q02880
A	1204	PRO	-	expression tag	UNP Q02880
A	1205	GLY	-	expression tag	UNP Q02880
A	1206	PHE	-	expression tag	UNP Q02880
A	1207	SER	-	expression tag	UNP Q02880
A	1208	SER	-	expression tag	UNP Q02880
A	1209	ILE	-	expression tag	UNP Q02880
A	1210	SER	-	expression tag	UNP Q02880
A	1211	ALA	-	expression tag	UNP Q02880
A	1212	HIS	-	expression tag	UNP Q02880
A	1213	HIS	-	expression tag	UNP Q02880
A	1214	HIS	-	expression tag	UNP Q02880
A	1215	HIS	-	expression tag	UNP Q02880
A	1216	HIS	-	expression tag	UNP Q02880
A	1217	HIS	-	expression tag	UNP Q02880
A	1218	HIS	-	expression tag	UNP Q02880
A	1219	HIS	-	expression tag	UNP Q02880
A	1220	HIS	-	expression tag	UNP Q02880
A	1221	HIS	-	expression tag	UNP Q02880
B	419	MET	-	expression tag	UNP Q02880
B	420	ALA	-	expression tag	UNP Q02880
B	421	SER	-	expression tag	UNP Q02880
B	422	TRP	-	expression tag	UNP Q02880
B	423	SER	-	expression tag	UNP Q02880
B	424	HIS	-	expression tag	UNP Q02880
B	425	PRO	-	expression tag	UNP Q02880
B	426	GLN	-	expression tag	UNP Q02880
B	427	PHE	-	expression tag	UNP Q02880
B	428	GLU	-	expression tag	UNP Q02880
B	429	LYS	-	expression tag	UNP Q02880
B	430	GLY	-	expression tag	UNP Q02880
B	431	ALA	-	expression tag	UNP Q02880
B	432	ASP	-	expression tag	UNP Q02880
B	433	ASP	-	expression tag	UNP Q02880
B	434	ASP	-	expression tag	UNP Q02880
B	435	ASP	-	expression tag	UNP Q02880
B	436	LYS	-	expression tag	UNP Q02880
B	437	VAL	-	expression tag	UNP Q02880
B	438	PRO	-	expression tag	UNP Q02880
B	439	ASP	-	expression tag	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	expression tag	UNP Q02880
B	441	THR	-	expression tag	UNP Q02880
B	442	SER	-	expression tag	UNP Q02880
B	443	VAL	-	expression tag	UNP Q02880
B	444	ASP	-	expression tag	UNP Q02880
B	1202	GLY	-	expression tag	UNP Q02880
B	1203	ALA	-	expression tag	UNP Q02880
B	1204	PRO	-	expression tag	UNP Q02880
B	1205	GLY	-	expression tag	UNP Q02880
B	1206	PHE	-	expression tag	UNP Q02880
B	1207	SER	-	expression tag	UNP Q02880
B	1208	SER	-	expression tag	UNP Q02880
B	1209	ILE	-	expression tag	UNP Q02880
B	1210	SER	-	expression tag	UNP Q02880
B	1211	ALA	-	expression tag	UNP Q02880
B	1212	HIS	-	expression tag	UNP Q02880
B	1213	HIS	-	expression tag	UNP Q02880
B	1214	HIS	-	expression tag	UNP Q02880
B	1215	HIS	-	expression tag	UNP Q02880
B	1216	HIS	-	expression tag	UNP Q02880
B	1217	HIS	-	expression tag	UNP Q02880
B	1218	HIS	-	expression tag	UNP Q02880
B	1219	HIS	-	expression tag	UNP Q02880
B	1220	HIS	-	expression tag	UNP Q02880
B	1221	HIS	-	expression tag	UNP Q02880

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			
2	E	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			

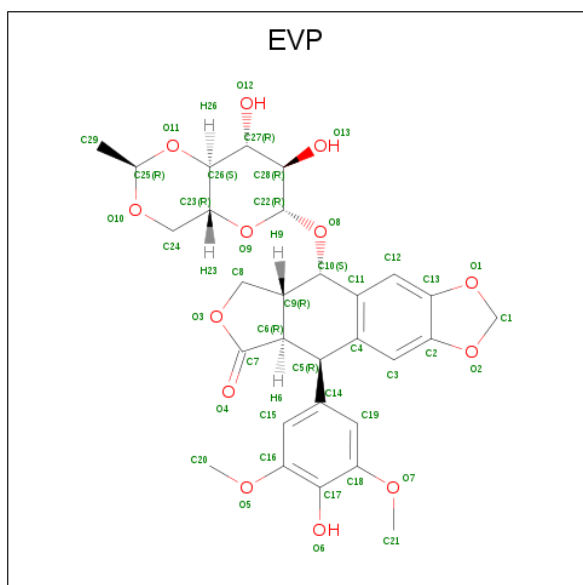
- Molecule 3 is DNA/RNA hybrid called DNA/RNA (5'-R(P*(IU))-D(P*GP*CP*AP*GP*C)-R(P*(IU))-D(P*CP*GP*GP*C)-R(P*(IU))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	I	N	O	P	0	0
			245	113	3	43	74	12		
3	F	12	Total	C	I	N	O	P	0	0
			247	113	3	43	76	12		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	D	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is (5S,5aR,8aR,9R)-9-(4-hydroxy-3,5-dimethoxyphenyl)-8-oxo-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-5-yl 4,6-O-[(1R)-ethylidene]-beta-D-glucopyranoside (three-letter code: EVP) (formula: C₂₉H₃₂O₁₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			42	29	13		
5	F	1	Total	C	O	0	0
			42	29	13		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total	O	0	0
			213	213		
6	B	240	Total	O	0	0
			240	240		

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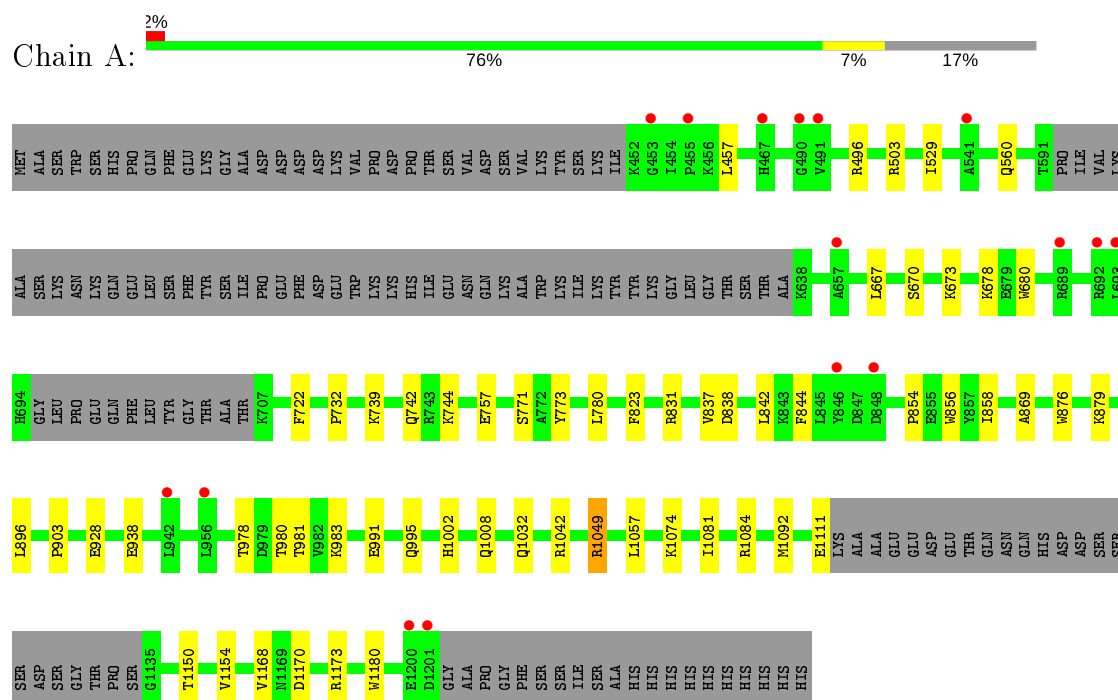
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	20	Total 20	O 20	0	0
6	D	15	Total 15	O 15	0	0
6	E	15	Total 15	O 15	0	0
6	F	21	Total 21	O 21	0	0

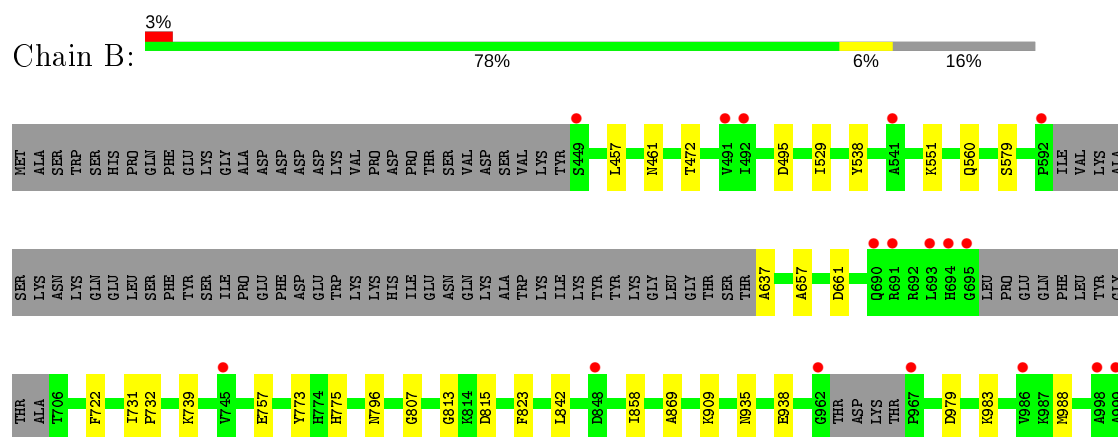
3 Residue-property plots [i](#)

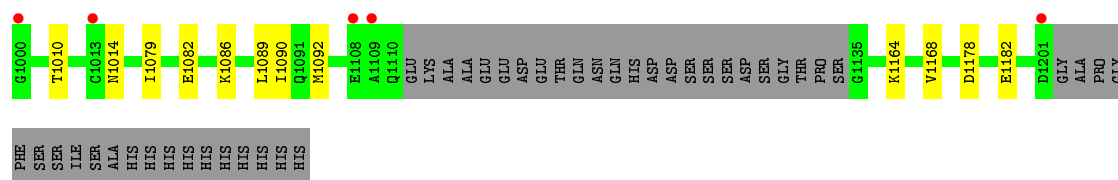
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA topoisomerase 2-beta

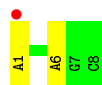
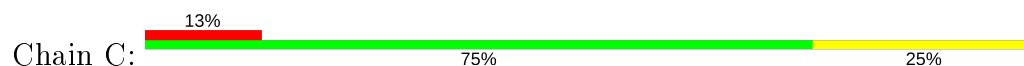


• Molecule 1: DNA topoisomerase 2-beta

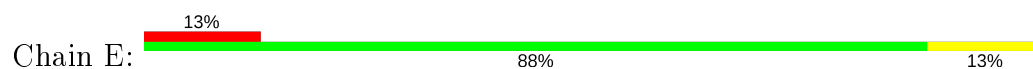




- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')



- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')



- Molecule 3: DNA/RNA (5'-R(P*(IU))-D(P*GP*CP*AP*GP*C)-R(P*(IU))-D(P*CP*GP*GP*C)-R(P*(IU))-3')



- Molecule 3: DNA/RNA (5'-R(P*(IU))-D(P*GP*CP*AP*GP*C)-R(P*(IU))-D(P*CP*GP*GP*C)-R(P*(IU))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.15Å 176.27Å 94.33Å 90.00° 111.44° 90.00°	Depositor
Resolution (Å)	19.87 – 2.30 19.87 – 2.29	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.87-2.30) 92.0 (19.87-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.189 , 0.227 0.189 , 0.226	Depositor DCC
R_{free} test set	1989 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11909	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EVP, MG, IU

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	0.32	0/5343	0.51	0/7231
1	B	0.32	0/5365	0.51	0/7254
2	C	0.84	0/185	0.81	0/283
2	E	0.83	0/185	0.83	0/283
3	D	0.80	0/208	0.85	0/321
3	F	0.76	0/208	0.86	1/321 (0.3%)
All	All	0.37	0/11494	0.54	1/15693 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	19	DC	C1'-O4'-C4'	-5.13	104.97	110.10

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	5218	0	5058	39	0
1	B	5255	0	5112	29	0
2	C	165	0	89	3	0
2	E	165	0	89	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	245	0	121	4	0
3	F	247	0	125	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	D	42	0	31	3	0
5	F	42	0	31	5	0
6	A	213	0	0	2	0
6	B	240	0	0	1	0
6	C	20	0	0	0	0
6	D	15	0	0	2	0
6	E	15	0	0	0	0
6	F	21	0	0	0	0
All	All	11909	0	10656	80	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 (80) 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)
5:D:101:EVP:C6	5:D:101:EVP:C9	1.78	1.26
5:F:1301:EVP:C9	5:F:1301:EVP:C6	1.78	1.23
1:A:739:LYS:H	1:A:742:GLN:HE21	1.26	0.81
1:A:1111:GLU:N	1:A:1111:GLU:OE1	2.18	0.75
1:A:879:LYS:NZ	3:F:20:IU:OP1	2.25	0.69
1:A:732:PRO:HG2	1:A:869:ALA:HB1	1.75	0.69
1:B:732:PRO:HG2	1:B:869:ALA:HB1	1.75	0.69
5:F:1301:EVP:C10	5:F:1301:EVP:C6	2.71	0.66
5:D:101:EVP:C10	5:D:101:EVP:C6	2.71	0.66
1:A:744:LYS:HG2	1:A:771:SER:HB2	1.78	0.65
5:D:101:EVP:C5	5:D:101:EVP:C9	2.71	0.64
1:A:457:LEU:HD22	1:A:529:ILE:HG12	1.79	0.64
5:F:1301:EVP:C9	5:F:1301:EVP:C5	2.73	0.64
1:B:938:GLU:OE2	1:B:983:LYS:HE3	1.99	0.63
1:B:637:ALA:N	6:B:1404:HOH:O	2.32	0.62
1:A:739:LYS:H	1:A:742:GLN:NE2	1.98	0.62
3:D:15:IU:I5	6:D:513:HOH:O	2.86	0.59
1:A:1081:ILE:HA	1:A:1084:ARG:HD2	1.85	0.58
1:A:1170:ASP:OD1	1:A:1173:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:LEU:HD22	1:B:529:ILE:HG12	1.85	0.57
1:A:1002:HIS:HB3	1:A:1008:GLN:HG3	1.87	0.57
1:B:1010:THR:HG23	3:D:20:IU:H5'	1.87	0.56
1:B:1014:ASN:HB2	3:D:19:DC:OP1	2.07	0.55
1:A:858:ILE:HG13	1:A:1042:ARG:HD2	1.89	0.54
1:A:1032[A]:GLN:HG2	6:A:1583:HOH:O	2.06	0.54
1:B:1079:ILE:HD11	1:B:1092:MET:CE	2.38	0.53
1:B:472:THR:HG23	1:B:551:LYS:HG3	1.91	0.53
1:B:796:ASN:ND2	1:B:909:LYS:H	2.07	0.52
1:A:744:LYS:HG2	1:A:771:SER:CB	2.40	0.52
1:A:757:GLU:HB2	1:A:823:PHE:HB3	1.92	0.51
1:A:739:LYS:HD2	2:C:6:DA:H5''	1.91	0.51
1:A:1074:LYS:NZ	1:B:1082:GLU:OE2	2.43	0.51
1:A:670:SER:HB3	1:A:673:LYS:HG2	1.92	0.51
1:B:773:TYR:CZ	1:B:775:HIS:HB2	2.47	0.49
1:A:678:LYS:HE3	1:A:876:TRP:CD1	2.46	0.49
1:B:1086:LYS:O	1:B:1090:ILE:HG12	2.12	0.49
1:A:560:GLN:HB3	1:A:722:PHE:HA	1.94	0.49
3:F:19:DC:H4'	3:F:20:IU:OP1	2.12	0.48
3:D:19:DC:O5'	6:D:501:HOH:O	2.20	0.47
1:B:757:GLU:HB2	1:B:823:PHE:HB3	1.96	0.47
1:A:938:GLU:OE2	1:A:983:LYS:HE3	2.15	0.47
1:A:903:PRO:HA	1:A:1032[A]:GLN:HE21	1.80	0.47
1:B:1178:ASP:O	1:B:1182:GLU:HG3	2.15	0.46
1:A:1092:MET:HB3	1:A:1092:MET:HE2	1.71	0.46
1:A:773:TYR:CE2	1:A:780:LEU:HG	2.50	0.46
1:B:538:TYR:O	1:B:579:SER:HB2	2.16	0.46
1:B:1079:ILE:HD11	1:B:1092:MET:HE1	1.98	0.45
1:A:837:VAL:HG13	1:A:1049:ARG:HD2	1.97	0.45
2:C:1:DA:H2	3:F:20:IU:O2	1.99	0.45
3:F:19:DC:H2'	3:F:20:IU:I5	2.86	0.45
1:A:978:THR:HG23	1:A:980:THR:H	1.82	0.44
2:C:1:DA:H8	2:C:1:DA:P	2.41	0.44
1:A:844:PHE:HA	1:A:854:PRO:HA	2.00	0.44
1:A:1150:THR:O	1:A:1154:VAL:HG23	2.18	0.43
1:A:991:GLU:O	1:A:995:GLN:HG3	2.18	0.43
1:A:928:GLU:HG2	6:A:1567:HOH:O	2.17	0.43
1:B:739:LYS:NZ	2:E:6:DA:OP1	2.49	0.42
1:B:935:ASN:HA	1:B:988:MET:O	2.20	0.42
1:A:496:ARG:HA	1:A:496:ARG:HD3	1.93	0.42
1:A:978:THR:HG22	1:A:981:THR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASN:HB2	1:B:495:ASP:HA	2.01	0.42
1:B:815:ASP:N	1:B:815:ASP:OD1	2.49	0.42
1:B:842:LEU:HD21	1:B:858:ILE:HG22	2.02	0.42
1:A:1057:LEU:HB3	1:A:1168:VAL:HG22	2.02	0.42
1:B:560:GLN:HB3	1:B:722:PHE:HA	2.01	0.42
1:B:807:GLY:HA3	1:B:813:GLY:HA2	2.02	0.42
1:A:896:LEU:HD21	1:A:1180:TRP:CE3	2.55	0.41
1:A:503[A]:ARG:HB3	5:F:1301:EVP:H3	2.02	0.41
3:F:15:IU:H6	3:F:15:IU:O5'	2.21	0.41
1:A:667:LEU:HD21	1:A:680:TRP:CG	2.56	0.41
1:A:838:ASP:OD1	1:A:1049:ARG:HD3	2.21	0.41
1:B:657:ALA:N	1:B:661:ASP:OD2	2.45	0.41
1:A:842:LEU:HD21	1:A:858:ILE:HG22	2.02	0.41
1:B:731:ILE:HA	1:B:732:PRO:HD3	1.94	0.41
1:A:831:ARG:HD3	1:A:831:ARG:HA	1.99	0.40
1:B:551:LYS:HB3	1:B:551:LYS:HE2	1.94	0.40
1:B:1089:LEU:HD12	1:B:1092:MET:HE2	2.03	0.40
1:B:1164:LYS:O	1:B:1168:VAL:HG12	2.21	0.40
1:A:503[B]:ARG:HB3	5:F:1301:EVP:H3	2.03	0.40
1:B:472:THR:OG1	1:B:551:LYS:HD2	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	670/803 (83%)	655 (98%)	15 (2%)	0	100	100
1	B	664/803 (83%)	649 (98%)	15 (2%)	0	100	100
All	All	1334/1606 (83%)	1304 (98%)	30 (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	531/704 (75%)	529 (100%)	2 (0%)	91	96
1	B	545/704 (77%)	544 (100%)	1 (0%)	93	97
All	All	1076/1408 (76%)	1073 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	856	TRP
1	A	1049	ARG
1	B	979	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	GLN
1	A	742	GLN
1	B	796	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](#)

6 non-standard protein/DNA/RNA residues 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	IU	D	9	1,3	14,21,23	5.41	9 (64%)	16,30,35	1.90	4 (25%)
3	IU	F	15	3,2	14,22,23	3.56	3 (21%)	16,32,35	2.02	3 (18%)
3	IU	D	15	3,2	14,21,23	5.40	9 (64%)	16,30,35	1.86	2 (12%)
3	IU	F	20	3,2	14,22,23	3.92	4 (28%)	16,32,35	2.03	3 (18%)
3	IU	F	9	1,3	14,21,23	5.28	9 (64%)	16,30,35	1.95	3 (18%)
3	IU	D	20	3,2	14,21,23	5.82	8 (57%)	16,30,35	2.37	5 (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
3	IU	D	9	1,3	-	1/4/21/26	0/2/2/2
3	IU	F	15	3,2	-	2/5/25/26	0/2/2/2
3	IU	D	15	3,2	-	1/4/21/26	0/2/2/2
3	IU	F	20	3,2	-	0/5/25/26	0/2/2/2
3	IU	F	9	1,3	-	1/4/21/26	0/2/2/2
3	IU	D	20	3,2	-	2/4/21/26	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	20	IU	C6-C5	11.81	1.51	1.38
3	F	20	IU	C6-C5	10.35	1.50	1.38
3	D	9	IU	C6-C5	10.00	1.49	1.38
3	F	15	IU	C6-C5	9.62	1.49	1.38
3	D	15	IU	C6-C5	9.58	1.49	1.38
3	F	9	IU	C6-C5	9.22	1.48	1.38
3	D	20	IU	C3'-C4'	-8.96	1.28	1.53
3	F	9	IU	C2'-C1'	-8.65	1.28	1.52
3	D	15	IU	C2'-C1'	-8.64	1.28	1.52
3	D	15	IU	C3'-C4'	-8.63	1.29	1.53
3	D	9	IU	C2'-C1'	-8.60	1.28	1.52
3	D	20	IU	C2'-C1'	-8.45	1.28	1.52
3	D	9	IU	C3'-C4'	-8.40	1.29	1.53
3	F	9	IU	C3'-C4'	-8.35	1.30	1.53
3	F	20	IU	C4-N3	7.57	1.46	1.33
3	D	20	IU	C4-N3	7.53	1.46	1.33
3	D	15	IU	C4-N3	6.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	9	IU	C4-N3	6.99	1.45	1.33
3	F	15	IU	C4-N3	6.69	1.44	1.33
3	D	9	IU	C4-N3	6.65	1.44	1.33
3	F	20	IU	C2-N3	6.57	1.51	1.38
3	D	20	IU	C2-N3	6.31	1.50	1.38
3	D	9	IU	O4'-C1'	5.96	1.55	1.42
3	D	15	IU	C2-N3	5.94	1.49	1.38
3	D	20	IU	O4'-C1'	5.89	1.55	1.42
3	F	15	IU	C2-N3	5.79	1.49	1.38
3	F	9	IU	C2-N3	5.62	1.49	1.38
3	F	9	IU	O4'-C1'	5.60	1.54	1.42
3	D	15	IU	O4'-C1'	5.58	1.54	1.42
3	D	9	IU	C2-N3	5.53	1.49	1.38
3	F	9	IU	C2'-C3'	4.86	1.65	1.52
3	D	9	IU	C2'-C3'	4.84	1.65	1.52
3	D	20	IU	C2'-C3'	4.73	1.65	1.52
3	D	15	IU	C2'-C3'	4.51	1.64	1.52
3	D	15	IU	O4'-C4'	4.48	1.55	1.45
3	D	20	IU	O4'-C4'	4.19	1.54	1.45
3	D	9	IU	O4'-C4'	4.10	1.54	1.45
3	F	9	IU	O4'-C4'	3.69	1.53	1.45
3	D	9	IU	O4-C4	-2.29	1.18	1.24
3	D	15	IU	O4-C4	-2.11	1.19	1.24
3	F	9	IU	O4-C4	-2.08	1.19	1.24
3	F	20	IU	O4-C4	-2.05	1.19	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	15	IU	C4-N3-C2	6.87	120.94	115.14
3	F	20	IU	C4-N3-C2	6.84	120.91	115.14
3	D	20	IU	C4-N3-C2	6.00	120.21	115.14
3	F	9	IU	C4-N3-C2	5.53	119.81	115.14
3	D	15	IU	C4-N3-C2	5.49	119.78	115.14
3	D	9	IU	C4-N3-C2	5.45	119.75	115.14
3	D	20	IU	C6-C5-I5	4.54	122.21	118.52
3	D	20	IU	C6-N1-C1'	3.46	127.00	119.24
3	F	9	IU	C4'-O4'-C1'	-3.05	102.08	109.45
3	F	15	IU	C5-C4-N3	-3.01	119.24	123.27
3	F	20	IU	C5-C4-N3	-2.75	119.59	123.27
3	D	9	IU	C4'-O4'-C1'	-2.71	102.91	109.45
3	F	9	IU	C5-C4-N3	-2.51	119.91	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	20	IU	C2'-C3'-C4'	2.45	107.87	102.76
3	F	15	IU	C6-C5-I5	2.33	120.41	118.52
3	F	20	IU	C5-C6-N1	2.26	121.97	120.70
3	D	9	IU	C2'-C3'-C4'	2.24	107.43	102.76
3	D	15	IU	C5-C4-N3	-2.13	120.42	123.27
3	D	9	IU	C5-C4-N3	-2.12	120.44	123.27
3	D	20	IU	C3'-C2'-C1'	2.03	107.63	102.54

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	9	IU	O4'-C1'-N1-C6
3	F	15	IU	O4'-C1'-N1-C6
3	F	15	IU	C2'-C1'-N1-C6
3	D	15	IU	O4'-C1'-N1-C6
3	F	9	IU	O4'-C1'-N1-C6
3	D	20	IU	O4'-C1'-N1-C6
3	D	20	IU	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	15	IU	1	0
3	D	15	IU	1	0
3	F	20	IU	4	0
3	D	20	IU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 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
5	EVP	F	1301	-	48,48,48	5.62	26 (54%)	72,73,73	1.76	15 (20%)
5	EVP	D	101	-	48,48,48	5.60	26 (54%)	72,73,73	1.78	14 (19%)

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	EVP	F	1301	-	-	0/12/76/76	0/7/7/7
5	EVP	D	101	-	-	0/12/76/76	0/7/7/7

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1301	EVP	C6-C7	-20.79	1.24	1.51
5	D	101	EVP	C6-C7	-20.37	1.25	1.51
5	F	1301	EVP	C11-C4	12.74	1.62	1.40
5	F	1301	EVP	C8-C9	-12.65	1.30	1.53
5	D	101	EVP	C11-C4	12.62	1.62	1.40
5	D	101	EVP	C8-C9	-12.44	1.30	1.53
5	F	1301	EVP	C6-C9	12.01	1.78	1.54
5	D	101	EVP	O3-C7	12.00	1.61	1.35
5	D	101	EVP	C6-C9	11.99	1.78	1.54
5	F	1301	EVP	O3-C7	11.62	1.60	1.35
5	D	101	EVP	C4-C5	11.23	1.67	1.51
5	F	1301	EVP	C4-C5	11.04	1.67	1.51
5	F	1301	EVP	C11-C10	9.17	1.68	1.50
5	D	101	EVP	C11-C10	8.77	1.67	1.50
5	D	101	EVP	O3-C8	6.27	1.58	1.45
5	F	1301	EVP	O11-C25	6.19	1.50	1.42
5	F	1301	EVP	O3-C8	6.07	1.58	1.45
5	D	101	EVP	O11-C25	5.95	1.50	1.42
5	D	101	EVP	C14-C5	4.40	1.58	1.52
5	D	101	EVP	O7-C18	4.30	1.44	1.37
5	D	101	EVP	C12-C13	4.29	1.46	1.38
5	D	101	EVP	C3-C2	4.29	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1301	EVP	C12-C11	-4.23	1.32	1.39
5	F	1301	EVP	O7-C18	4.16	1.43	1.37
5	D	101	EVP	C12-C11	-4.07	1.32	1.39
5	F	1301	EVP	C3-C2	4.00	1.46	1.38
5	F	1301	EVP	C3-C4	-3.96	1.33	1.39
5	F	1301	EVP	C12-C13	3.85	1.45	1.38
5	F	1301	EVP	C9-C10	-3.53	1.47	1.53
5	D	101	EVP	O10-C25	3.51	1.49	1.41
5	F	1301	EVP	C14-C5	3.47	1.57	1.52
5	D	101	EVP	C3-C4	-3.32	1.34	1.39
5	F	1301	EVP	O10-C25	3.29	1.48	1.41
5	D	101	EVP	O9-C23	3.29	1.52	1.44
5	F	1301	EVP	O9-C22	3.27	1.50	1.41
5	D	101	EVP	C9-C10	-3.24	1.48	1.53
5	F	1301	EVP	O9-C23	3.20	1.52	1.44
5	F	1301	EVP	C13-C2	2.98	1.46	1.39
5	D	101	EVP	O9-C22	2.95	1.49	1.41
5	D	101	EVP	C24-C23	-2.93	1.46	1.51
5	D	101	EVP	C13-C2	2.86	1.46	1.39
5	F	1301	EVP	C24-C23	-2.74	1.47	1.51
5	F	1301	EVP	O10-C24	2.74	1.48	1.43
5	D	101	EVP	O10-C24	2.68	1.48	1.43
5	D	101	EVP	O5-C16	2.40	1.41	1.37
5	D	101	EVP	C6-C5	-2.33	1.51	1.56
5	F	1301	EVP	C6-C5	-2.29	1.51	1.56
5	D	101	EVP	C29-C25	-2.25	1.43	1.50
5	F	1301	EVP	C29-C25	-2.14	1.44	1.50
5	F	1301	EVP	O5-C16	2.08	1.40	1.37
5	D	101	EVP	C15-C16	2.07	1.42	1.38
5	F	1301	EVP	O8-C10	-2.02	1.40	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	101	EVP	C4-C5-C6	5.97	116.61	106.58
5	F	1301	EVP	C4-C5-C6	5.48	115.80	106.58
5	F	1301	EVP	O7-C18-C17	5.42	120.01	114.54
5	D	101	EVP	O7-C18-C17	5.31	119.90	114.54
5	F	1301	EVP	C8-O3-C7	-4.46	106.21	110.28
5	D	101	EVP	C14-C5-C4	-4.43	106.18	112.86
5	F	1301	EVP	C14-C5-C4	-3.91	106.97	112.86
5	D	101	EVP	C8-O3-C7	-3.78	106.83	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	101	EVP	C11-C10-C9	3.78	116.12	111.51
5	F	1301	EVP	C11-C10-C9	3.33	115.57	111.51
5	D	101	EVP	O2-C2-C3	3.19	132.12	127.85
5	D	101	EVP	O1-C13-C12	3.16	132.08	127.85
5	F	1301	EVP	C22-O8-C10	-3.04	110.05	114.99
5	F	1301	EVP	O5-C16-C17	3.02	117.59	114.54
5	D	101	EVP	O8-C10-C11	-2.91	101.88	108.96
5	F	1301	EVP	O2-C2-C3	2.80	131.59	127.85
5	F	1301	EVP	C24-C23-C26	2.78	113.55	109.40
5	F	1301	EVP	C9-C6-C7	2.76	106.77	103.07
5	F	1301	EVP	O1-C13-C12	2.67	131.42	127.85
5	D	101	EVP	C8-C9-C6	2.65	105.61	101.79
5	D	101	EVP	O7-C18-C19	-2.58	119.68	124.12
5	D	101	EVP	O2-C1-O1	-2.55	104.01	108.08
5	F	1301	EVP	O7-C18-C19	-2.53	119.76	124.12
5	D	101	EVP	O2-C2-C13	-2.40	107.05	109.78
5	D	101	EVP	C9-C6-C7	2.27	106.11	103.07
5	F	1301	EVP	O11-C26-C23	2.24	112.28	108.88
5	F	1301	EVP	O2-C1-O1	-2.13	104.67	108.08
5	F	1301	EVP	O3-C7-O4	2.11	123.60	121.42
5	D	101	EVP	O1-C13-C2	-2.02	107.48	109.78

There are no chirality outliers.

There are no torsion outliers.

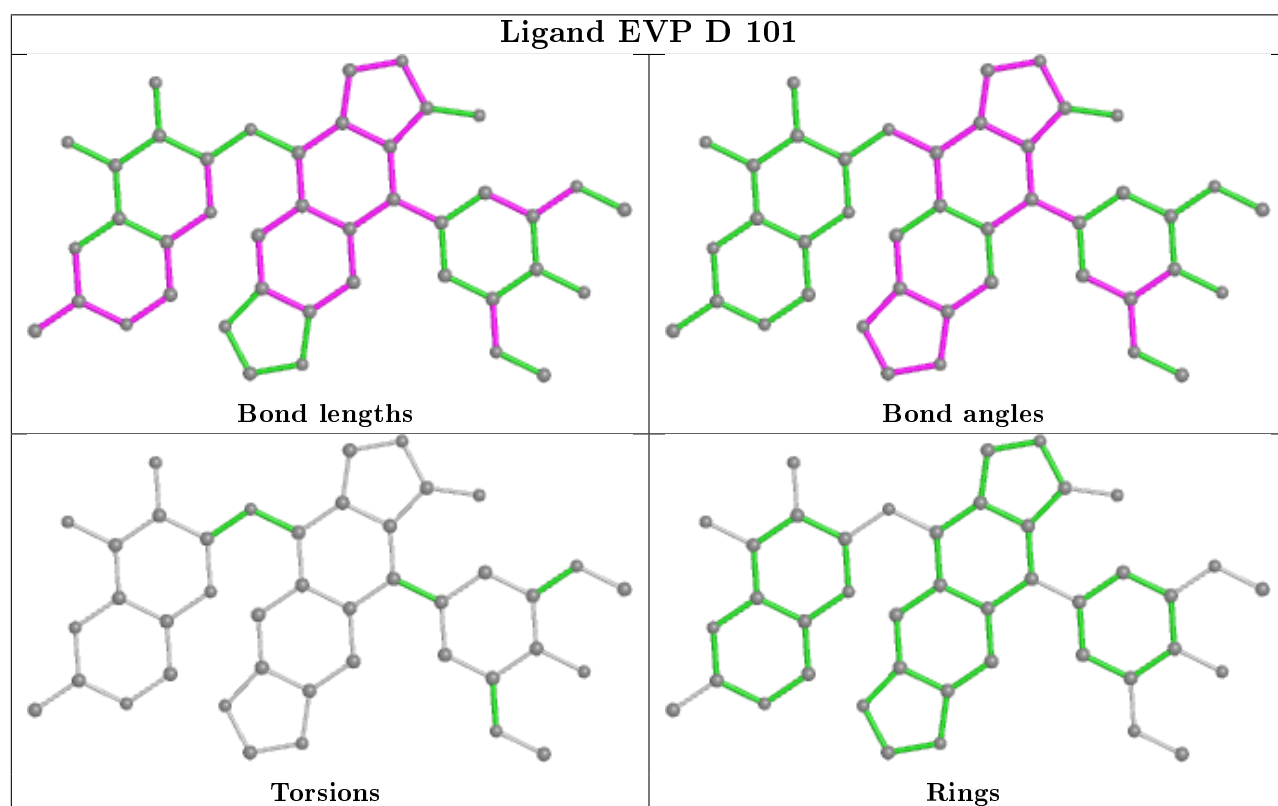
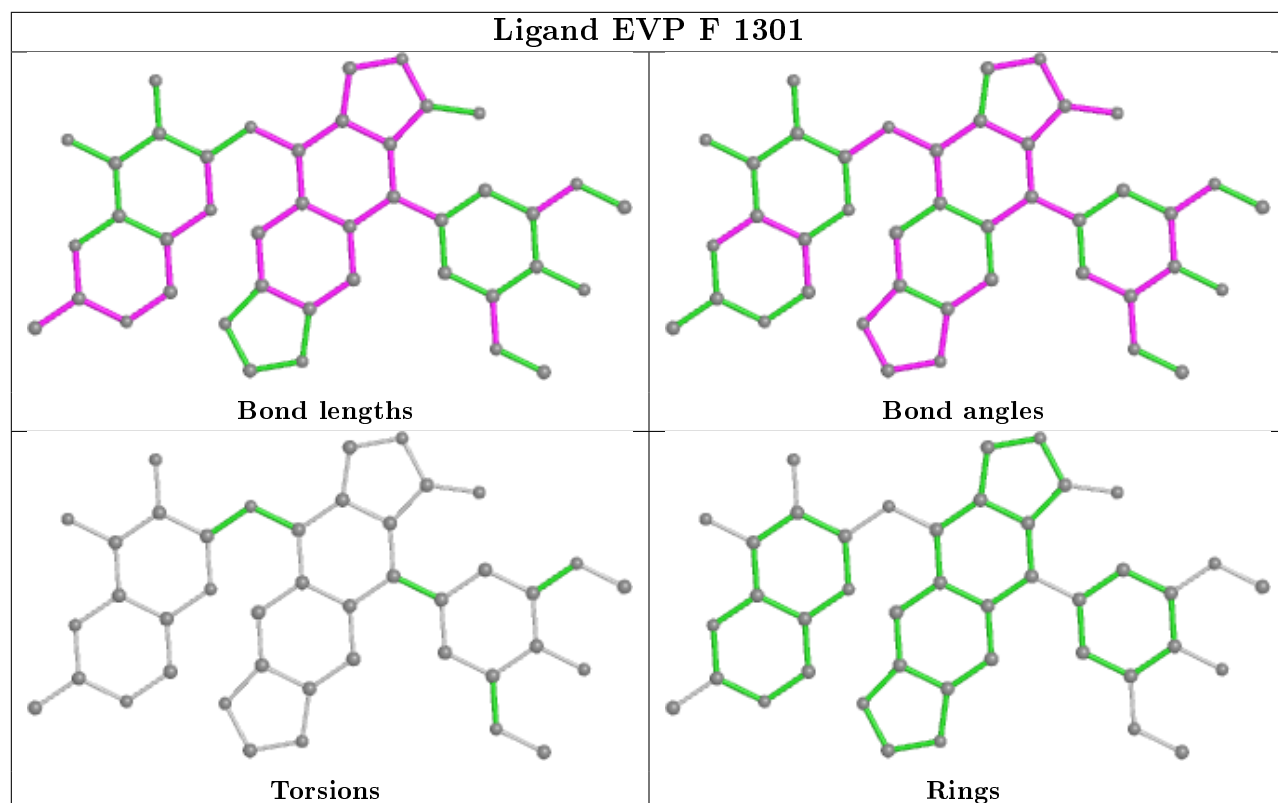
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1301	EVP	5	0
5	D	101	EVP	3	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	669/803 (83%)	-0.13	16 (2%) 59 66	27, 44, 76, 104	0
1	B	671/803 (83%)	-0.13	22 (3%) 46 53	28, 43, 72, 100	0
2	C	8/8 (100%)	-0.25	1 (12%) 3 5	31, 34, 61, 94	0
2	E	8/8 (100%)	-0.41	1 (12%) 3 5	32, 34, 61, 90	0
3	D	9/12 (75%)	-0.74	0 100 100	32, 38, 45, 55	0
3	F	9/12 (75%)	-0.65	0 100 100	35, 41, 49, 62	0
All	All	1374/1646 (83%)	-0.14	40 (2%) 51 58	27, 43, 75, 104	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	693	LEU	4.3
1	A	693	LEU	4.0
1	A	657	ALA	3.7
1	A	455	PRO	3.6
1	A	467	HIS	3.5
1	B	449	SER	3.3
1	B	1000	GLY	3.3
1	B	694	HIS	3.2
1	A	1201	ASP	3.1
1	A	453	GLY	3.1
1	B	1201	ASP	3.1
1	B	1013	CYS	3.1
1	B	848	ASP	3.0
1	A	541	ALA	3.0
1	A	490	GLY	3.0
1	B	998	ALA	3.0
1	A	692	ARG	2.9
2	C	1	DA	2.8
1	B	690	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1109	ALA	2.7
1	A	942	LEU	2.7
1	A	491	VAL	2.6
1	A	956	LEU	2.5
1	B	695	GLY	2.5
1	B	541	ALA	2.4
1	A	1200	GLU	2.4
1	B	492	ILE	2.4
1	B	592	PRO	2.4
1	B	967	PRO	2.3
1	B	745	VAL	2.3
1	A	846	TYR	2.2
1	B	691	ARG	2.2
2	E	1	DA	2.2
1	A	848	ASP	2.2
1	B	986	VAL	2.2
1	A	689	ARG	2.2
1	B	491	VAL	2.1
1	B	1108	GLU	2.1
1	B	962	GLY	2.1
1	B	999	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
3	IU	F	20	21/22	0.86	0.24	54,73,82,125	0
3	IU	D	9	20/22	0.95	0.12	36,45,69,85	0
3	IU	D	20	20/22	0.95	0.12	30,48,71,82	0
3	IU	F	9	20/22	0.96	0.11	31,39,62,86	0
3	IU	D	15	20/22	0.97	0.14	28,33,60,68	0
3	IU	F	15	21/22	0.98	0.11	32,38,44,64	0

6.3 Carbohydrates [i](#)

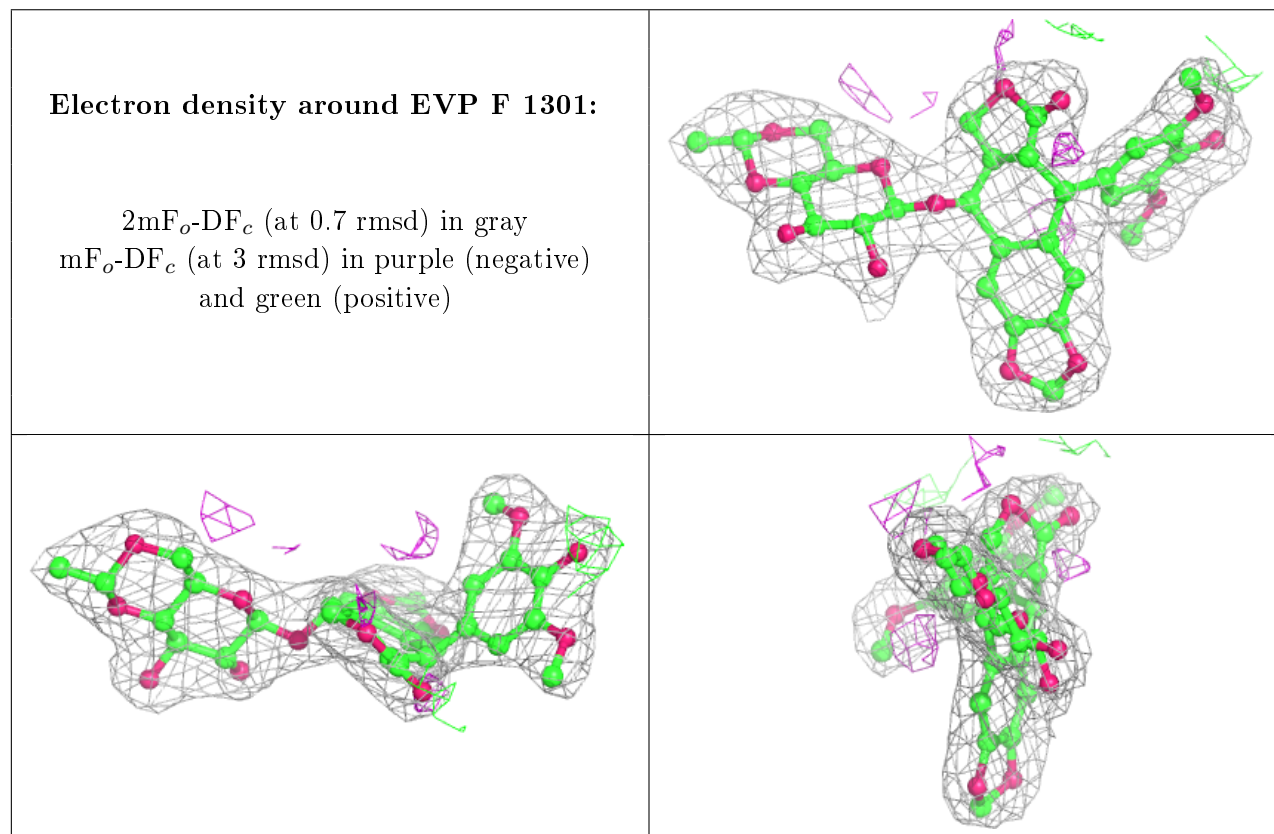
There are no carbohydrates in this entry.

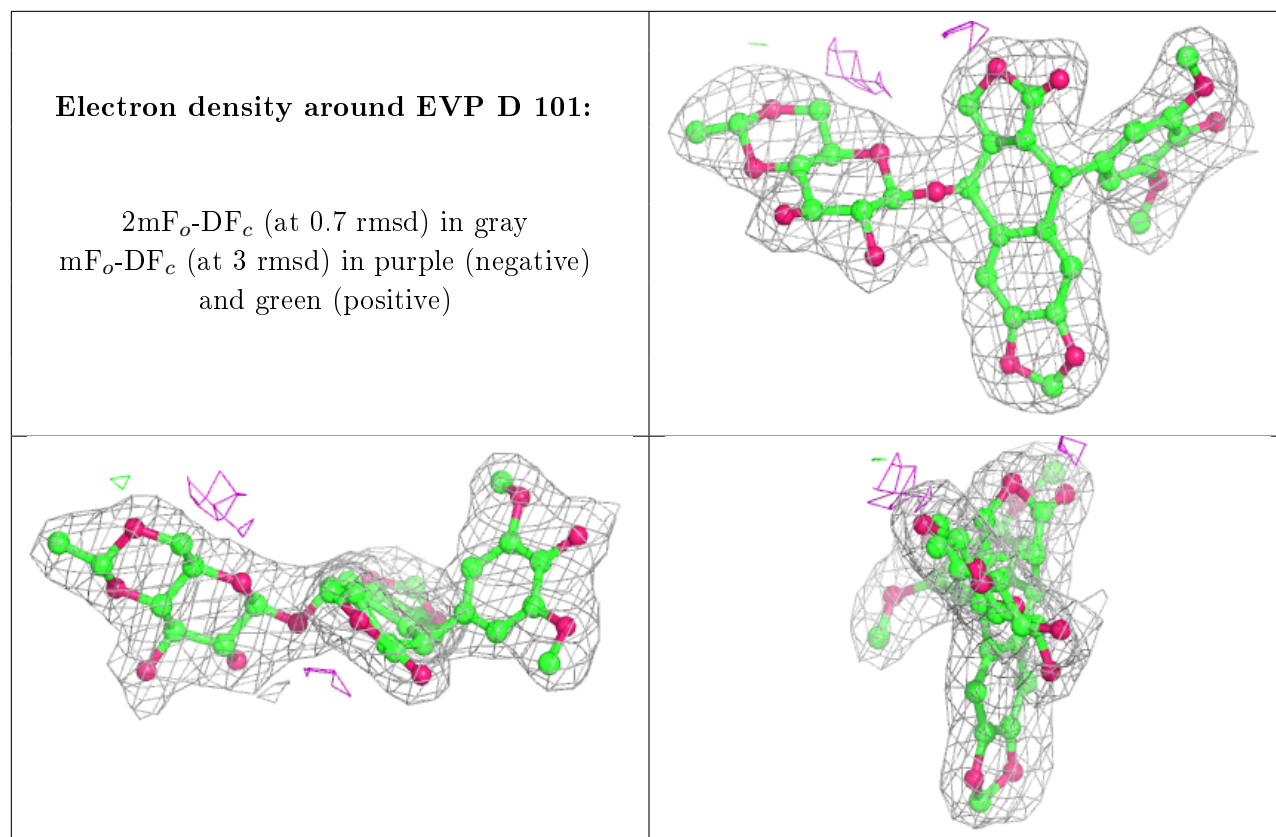
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	1302	1/1	0.18	0.46	73,73,73,73	0
4	MG	B	1301	1/1	0.88	0.27	64,64,64,64	0
4	MG	F	1302	1/1	0.94	0.12	54,54,54,54	0
4	MG	D	102	1/1	0.95	0.48	63,63,63,63	0
5	EVP	F	1301	42/42	0.96	0.11	31,38,41,43	0
5	EVP	D	101	42/42	0.97	0.12	27,34,40,43	0
4	MG	B	1302	1/1	0.98	0.03	36,36,36,36	0
4	MG	A	1301	1/1	0.98	0.04	27,27,27,27	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.