



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:52 pm BST

PDB ID : 6EO0  
Title : Zebrafish Sirt5 in complex with stalled peptidylimide and bicyclic intermediate of inhibitory compound 29  
Authors : Pannek, M.; Steegborn, C.  
Deposited on : 2017-10-08  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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

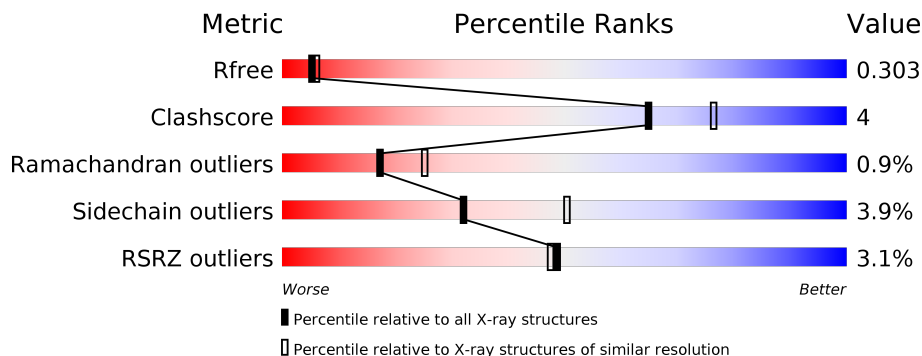
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	277	 87% 10% ...
1	B	277	 86% 12% ..
1	C	277	 86% 12% ..
1	D	277	 88% 10% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	302	-	-	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 9175 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 NAD-dependent protein deacylase sirtuin-5, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2138	1351	384	387	16	0	1	0
1	B	275	2147	1354	386	391	16	0	1	0
1	C	274	2147	1358	385	388	16	0	2	0
1	D	275	2147	1355	387	389	16	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q6DHI5
A	23	ILE	-	expression tag	UNP Q6DHI5
A	24	ASP	-	expression tag	UNP Q6DHI5
A	25	PRO	-	expression tag	UNP Q6DHI5
A	26	PHE	-	expression tag	UNP Q6DHI5
A	27	THR	-	expression tag	UNP Q6DHI5
B	22	GLY	-	expression tag	UNP Q6DHI5
B	23	ILE	-	expression tag	UNP Q6DHI5
B	24	ASP	-	expression tag	UNP Q6DHI5
B	25	PRO	-	expression tag	UNP Q6DHI5
B	26	PHE	-	expression tag	UNP Q6DHI5
B	27	THR	-	expression tag	UNP Q6DHI5
C	22	GLY	-	expression tag	UNP Q6DHI5
C	23	ILE	-	expression tag	UNP Q6DHI5
C	24	ASP	-	expression tag	UNP Q6DHI5
C	25	PRO	-	expression tag	UNP Q6DHI5
C	26	PHE	-	expression tag	UNP Q6DHI5
C	27	THR	-	expression tag	UNP Q6DHI5
D	22	GLY	-	expression tag	UNP Q6DHI5
D	23	ILE	-	expression tag	UNP Q6DHI5
D	24	ASP	-	expression tag	UNP Q6DHI5

*Continued on next page...*

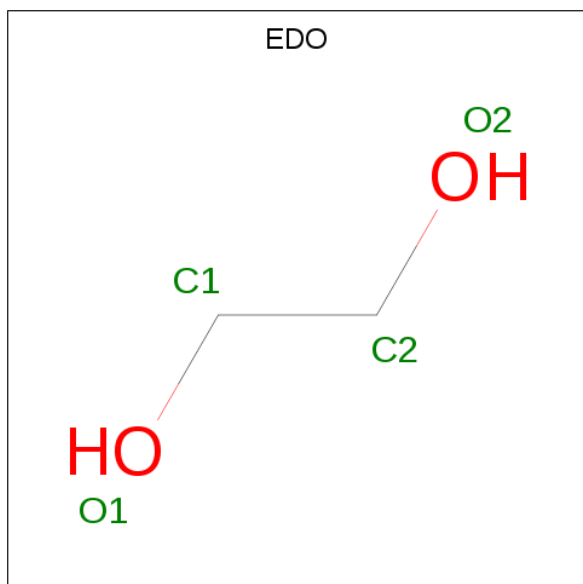
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	25	PRO	-	expression tag	UNP Q6DHI5
D	26	PHE	-	expression tag	UNP Q6DHI5
D	27	THR	-	expression tag	UNP Q6DHI5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

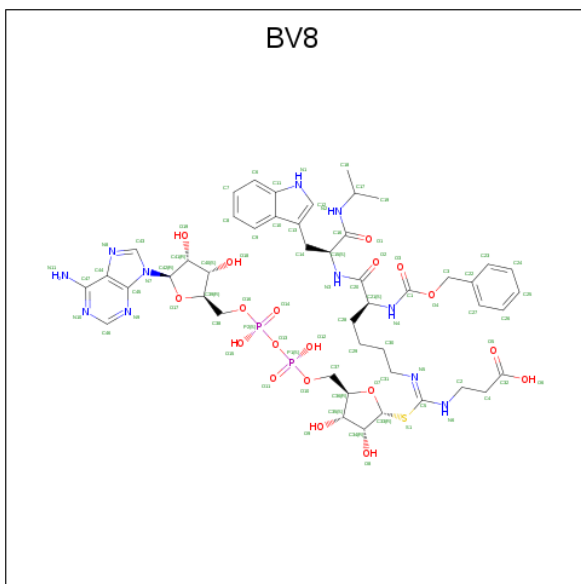
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



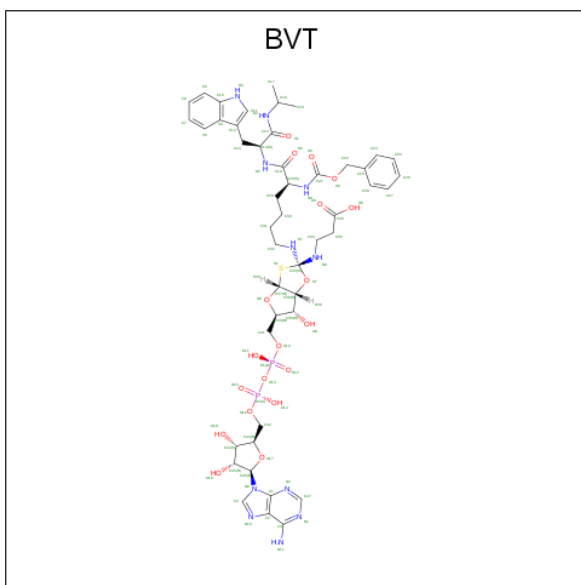
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is 3-[[[ (Z) - {C} - [(2 {R}, 3 {R}, 4 {S}, 5 {R}) - 5 - [[[(2 {R}, 3 {S}, 4 {R}, 5 {R}) - 5 - (6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-3,4-bis(oxidanyl)oxolan-2-yl]sulfanyl- {N} - [(5 {S}) - 6 - [(2 {S}) - 3 - (1 {H} - indol-3-yl) - 1-oxidanylidene-1-(propan-2-ylamino)propan-2-yl]amino] - 6-oxidanylidene-5-(phenylmethoxycarbonylamino)hexyl]carbonimidoyl]amino]propanoic acid (three-letter code: BV8) (formula: C<sub>47</sub>H<sub>63</sub>N<sub>11</sub>O<sub>19</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	80	47	11	19	2	1	0	1

- Molecule 5 is 3-[[[(2 {S}, 3 {a} {R}, 5 {R}, 6 {R}, 6 {a} {R}) - 5 - [[[(2 {R}, 3 {S}, 4 {R}, 5 {R}) - 5 - (6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-2-[[[(5 {S}) - 6 - [(2 {S}) - 3 - (1 {H} - indol-3-yl) - 1-oxidanylidene-1-(propan-2-ylamino)propan-2-yl]amino] - 6-oxidanylidene-5-(phenylmethoxycarbonylamino)hexyl]amino] - 6-oxidanyl-3 {a}, 5, 6, 6 {a} - tetrahydrofuro[2,3-d][1,3]oxathiol-2-yl]amino]propanoic acid (three-letter code: BVT) (formula: C<sub>47</sub>H<sub>63</sub>N<sub>11</sub>O<sub>19</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	A	1	Total 80	C 47	N 11	O 19	P 2	S 1	0	1
5	B	1	Total 80	C 47	N 11	O 19	P 2	S 1	0	1
5	C	1	Total 80	C 47	N 11	O 19	P 2	S 1	0	0
5	D	1	Total 80	C 47	N 11	O 19	P 2	S 1	0	0


- Molecule 6 is water.

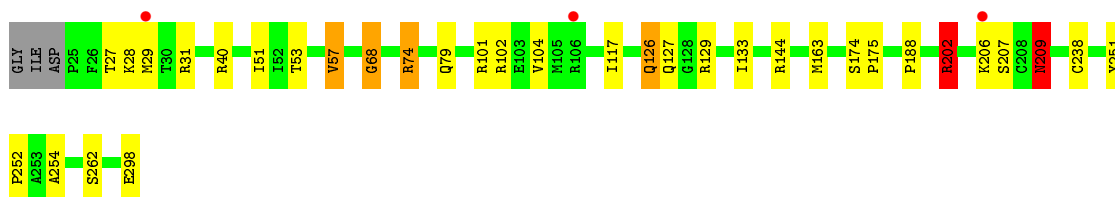
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total 36	O 36	0	0
6	B	40	Total 40	O 40	0	0
6	C	50	Total 50	O 50	0	0
6	D	50	Total 50	O 50	0	0

### 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.

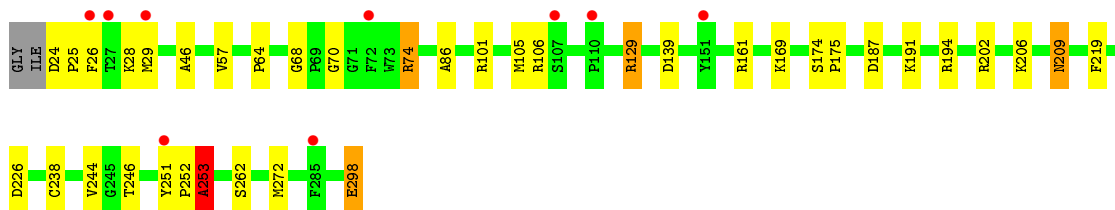
- Molecule 1: NAD-dependent protein deacylase sirtuin-5, mitochondrial

Chain A: 




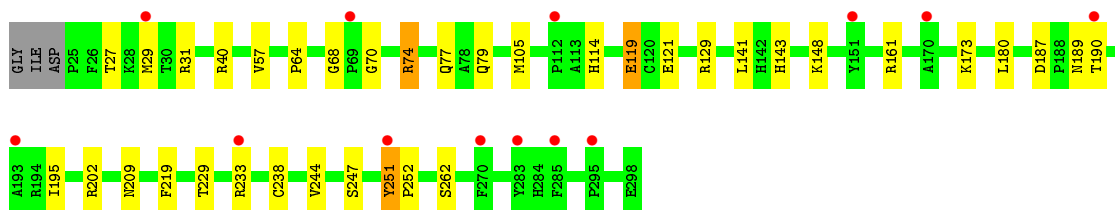
- Molecule 1: NAD-dependent protein deacylase sirtuin-5, mitochondrial

Chain B: 




- Molecule 1: NAD-dependent protein deacylase sirtuin-5, mitochondrial

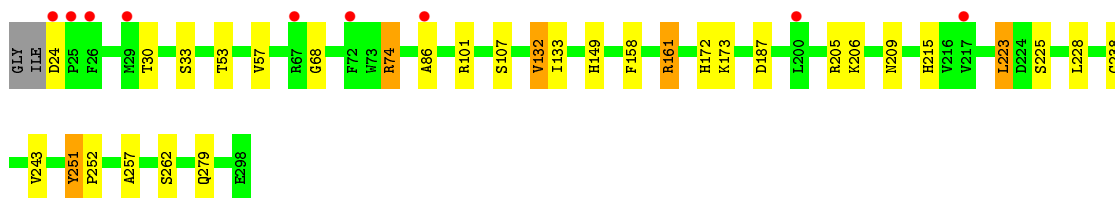
Chain C: 



- Molecule 1: NAD-dependent protein deacylase sirtuin-5, mitochondrial

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.93Å 113.59Å 72.31Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	48.41 – 2.40 48.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (48.41-2.40) 96.3 (48.41-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.253 , 0.305 0.257 , 0.303	Depositor DCC
$R_{free}$ test set	1923 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9175	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BV8, EDO, BVT

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	0.68	0/2200	0.91	5/2983 (0.2%)
1	B	0.69	0/2205	0.97	10/2990 (0.3%)
1	C	0.65	0/2212	0.89	7/2999 (0.2%)
1	D	0.69	1/2209 (0.0%)	0.91	6/2995 (0.2%)
All	All	0.68	1/8826 (0.0%)	0.92	28/11967 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	33	SER	CB-OG	-5.34	1.35	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NE-CZ-NH1	-12.12	114.24	120.30
1	A	202	ARG	CG-CD-NE	11.83	136.65	111.80
1	D	161	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	D	161	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	B	161	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	161	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	163	MET	CG-SD-CE	6.96	111.33	100.20
1	A	129	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	101	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	D	74	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	C	161	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	101	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	74	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	253	ALA	N-CA-CB	6.21	118.80	110.10
1	D	223	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	74	ARG	NE-CZ-NH2	-5.83	117.39	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	40	ARG	CG-CD-NE	5.60	123.57	111.80
1	C	74	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	161	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	129	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	169	LYS	CD-CE-NZ	-5.43	99.21	111.70
1	B	226	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	202	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	129	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	144	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	202	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	205	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2138	0	2100	24	0
1	B	2147	0	2110	15	0
1	C	2147	0	2118	19	0
1	D	2147	0	2111	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	80	0	0	3	0
5	A	80	0	0	2	0
5	B	80	0	0	2	0
5	C	80	0	0	2	0
5	D	80	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	36	0	0	1	0
6	B	40	0	0	1	0
6	C	50	0	0	2	0
6	D	50	0	0	2	0
All	All	9175	0	8463	71	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 (71) 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:D:223:LEU:HD12	1:D:228:LEU:HD13	1.52	0.89
1:A:117:ILE:CG2	1:A:133:ILE:HD11	2.10	0.81
1:A:102:ARG:NH1	6:A:401:HOH:O	2.14	0.81
1:C:74:ARG:HD3	1:C:190:THR:HB	1.63	0.81
1:A:27:THR:HG21	1:B:86:ALA:HB2	1.63	0.81
1:A:53:THR:HG21	1:A:57:VAL:HG11	1.64	0.80
1:C:121:GLU:OE2	1:C:148:LYS:HG3	1.82	0.79
1:B:246:THR:HA	5:B:303[A]:BVT:O12	1.90	0.72
1:B:64:PRO:HB2	1:B:70:GLY:HA3	1.73	0.70
1:A:117:ILE:HG21	1:A:133:ILE:HD11	1.73	0.70
1:A:31:ARG:NH1	1:B:74:ARG:O	2.25	0.69
4:A:303[B]:BV8:C29	4:A:303[B]:BV8:O2	2.45	0.64
1:C:57:VAL:HG12	1:C:114:HIS:CE1	2.33	0.63
1:C:31:ARG:NH1	1:D:74:ARG:O	2.31	0.63
1:C:74:ARG:HD3	1:C:190:THR:CB	2.28	0.62
1:A:202:ARG:NH1	1:A:209:ASN:O	2.32	0.62
1:D:53:THR:HG23	1:D:57:VAL:CG2	2.30	0.62
1:D:187:ASP:HB3	6:D:416:HOH:O	2.00	0.61
1:D:30:THR:HB	1:D:279:GLN:HE21	1.65	0.61
1:A:51:ILE:HB	1:A:133:ILE:HD13	1.84	0.60
1:D:107:SER:O	6:D:401:HOH:O	2.16	0.60
1:A:117:ILE:HG23	1:A:133:ILE:HD11	1.83	0.59
1:A:53:THR:CG2	1:A:57:VAL:HG11	2.32	0.59
1:D:53:THR:HG23	1:D:57:VAL:HG21	1.85	0.58
1:A:117:ILE:HG21	1:A:133:ILE:CD1	2.34	0.57
4:A:303[B]:BV8:C9	4:A:303[B]:BV8:C15	2.83	0.56
1:C:64:PRO:HB2	1:C:70:GLY:HA3	1.88	0.56
1:A:101:ARG:HA	1:A:104:VAL:HG22	1.88	0.55
1:A:251[A]:TYR:CD1	1:A:254:ALA:HB3	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:304[A]:BVT:C14	5:A:304[A]:BVT:C8	2.84	0.55
1:C:119:GLU:HA	1:C:119:GLU:OE1	2.06	0.55
1:A:74:ARG:HA	1:A:188:PRO:HA	1.89	0.54
1:B:46:ALA:O	1:B:129:ARG:NH1	2.38	0.54
1:C:189:ASN:ND2	6:C:402:HOH:O	2.42	0.53
1:A:27:THR:HG21	1:B:86:ALA:CB	2.37	0.52
1:C:180:LEU:HD12	1:C:195:ILE:CD1	2.39	0.51
1:A:40:ARG:NH1	1:A:298:GLU:OXT	2.44	0.50
1:C:247:SER:OG	5:C:303:BVT:O14	2.27	0.49
1:D:161:ARG:HD3	1:D:215:HIS:ND1	2.28	0.49
1:B:25:PRO:O	1:B:26:PHE:HB2	2.15	0.47
1:C:143:HIS:N	6:C:403:HOH:O	2.45	0.47
1:C:229:THR:HG23	1:C:233:ARG:NH1	2.31	0.46
1:B:46:ALA:O	1:B:129:ARG:HD2	2.16	0.45
1:A:53:THR:CG2	1:A:57:VAL:CG1	2.94	0.45
1:A:68:GLY:HA2	6:B:428:HOH:O	2.16	0.45
1:B:298:GLU:HA	1:B:298:GLU:OE1	2.17	0.44
1:C:251[A]:TYR:CD2	1:C:252:PRO:HA	2.53	0.44
1:D:251:TYR:CD2	1:D:252:PRO:HA	2.53	0.43
1:C:27:THR:HG22	1:D:86:ALA:HA	2.01	0.43
1:B:106:ARG:CZ	1:B:174:SER:HB2	2.48	0.43
1:C:74:ARG:NH1	1:C:190:THR:OG1	2.52	0.43
1:C:77:GLN:HB3	1:C:79[B]:GLN:HE21	1.84	0.43
1:C:57:VAL:HG22	1:C:244:VAL:HG12	2.00	0.42
1:D:133:ILE:HD12	1:D:133:ILE:N	2.34	0.42
1:B:219:PHE:CZ	5:B:303[A]:BVT:S1	3.12	0.42
1:D:243:VAL:HG21	1:D:257:ALA:CB	2.49	0.42
1:D:132:VAL:HG13	1:D:149:HIS:CE1	2.54	0.42
1:A:174:SER:HA	1:A:175:PRO:HA	1.84	0.42
1:C:219:PHE:CZ	5:C:303:BVT:S1	3.13	0.42
1:A:251[B]:TYR:CD2	1:A:252:PRO:HA	2.54	0.41
1:B:252:PRO:O	1:B:253:ALA:HB2	2.20	0.41
1:A:101:ARG:NH2	5:A:304[A]:BVT:O6	2.51	0.41
1:B:57:VAL:HG22	1:B:244:VAL:HG12	2.01	0.41
1:A:206:LYS:O	1:A:207:SER:CB	2.69	0.41
1:A:206:LYS:O	1:A:207:SER:HB2	2.21	0.41
1:B:105:MET:SD	1:B:139:ASP:HB2	2.62	0.41
1:C:105:MET:HE1	1:C:141:LEU:HD11	2.02	0.40
1:A:126:GLN:HE21	1:A:127:GLN:NE2	2.19	0.40
1:B:174:SER:HA	1:B:175:PRO:HA	1.87	0.40
4:A:303[B]:BV8:C13	4:A:303[B]:BV8:N2	2.82	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:PHE:HB3	1:D:172:HIS:CD2	2.57	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	273/277 (99%)	259 (95%)	12 (4%)	2 (1%)	22	32
1	B	274/277 (99%)	260 (95%)	10 (4%)	4 (2%)	10	14
1	C	274/277 (99%)	258 (94%)	14 (5%)	2 (1%)	22	32
1	D	274/277 (99%)	262 (96%)	10 (4%)	2 (1%)	22	32
All	All	1095/1108 (99%)	1039 (95%)	46 (4%)	10 (1%)	17	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	ALA
1	A	209	ASN
1	B	209	ASN
1	C	209	ASN
1	D	209	ASN
1	C	68	GLY
1	B	206	LYS
1	B	68	GLY
1	D	68	GLY
1	A	68	GLY

### 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	229/231 (99%)	220 (96%)	9 (4%)	32	50
1	B	231/231 (100%)	219 (95%)	12 (5%)	23	38
1	C	231/231 (100%)	223 (96%)	8 (4%)	36	55
1	D	231/231 (100%)	223 (96%)	8 (4%)	36	55
All	All	922/924 (100%)	885 (96%)	37 (4%)	32	49

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	29	MET
1	A	57	VAL
1	A	79	GLN
1	A	126	GLN
1	A	202	ARG
1	A	209	ASN
1	A	238	CYS
1	A	262	SER
1	B	24	ASP
1	B	28	LYS
1	B	29	MET
1	B	187	ASP
1	B	191	LYS
1	B	194	ARG
1	B	209	ASN
1	B	238	CYS
1	B	251	TYR
1	B	262	SER
1	B	272	MET
1	B	298	GLU
1	C	29	MET
1	C	119	GLU
1	C	173	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	187	ASP
1	C	238	CYS
1	C	251[A]	TYR
1	C	251[B]	TYR
1	C	262	SER
1	D	24	ASP
1	D	132	VAL
1	D	173	LYS
1	D	206	LYS
1	D	225	SER
1	D	238	CYS
1	D	251	TYR
1	D	262	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	127	GLN
1	A	259	GLN
1	B	189	ASN
1	B	259	GLN
1	C	172	HIS
1	D	172	HIS
1	D	259	GLN
1	D	279	GLN
1	D	284	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	BVT	C	303	-	73,87,87	1.61	11 (15%)	84,126,126	1.88	18 (21%)
4	BV8	A	303[B]	-	77,86,86	1.70	14 (18%)	87,122,122	1.70	17 (19%)
3	EDO	B	302	-	3,3,3	0.56	0	2,2,2	0.08	0
5	BVT	B	303[A]	-	73,87,87	1.71	13 (17%)	84,126,126	1.64	14 (16%)
5	BVT	D	303	-	73,87,87	1.71	12 (16%)	84,126,126	1.74	16 (19%)
5	BVT	A	304[A]	-	73,87,87	1.63	11 (15%)	84,126,126	1.71	16 (19%)
3	EDO	C	302	-	3,3,3	0.55	0	2,2,2	0.18	0
3	EDO	D	302	-	3,3,3	0.53	0	2,2,2	0.15	0
3	EDO	A	302	-	3,3,3	0.54	0	2,2,2	0.25	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	BVT	C	303	-	-	11/54/109/109	0/8/8/8
4	BV8	A	303[B]	-	-	20/56/101/101	0/7/7/7
3	EDO	B	302	-	-	1/1/1/1	-
5	BVT	B	303[A]	-	-	14/54/109/109	0/8/8/8
5	BVT	D	303	-	-	7/54/109/109	0/8/8/8
5	BVT	A	304[A]	-	-	19/54/109/109	0/8/8/8
3	EDO	C	302	-	-	1/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	303	BVT	O7-C38	5.86	1.52	1.43
5	B	303[A]	BVT	O7-C38	5.55	1.52	1.43
5	C	303	BVT	C47-N2	5.04	1.40	1.32
5	B	303[A]	BVT	C5-C10	-4.98	1.33	1.41
5	C	303	BVT	O7-C38	4.95	1.51	1.43
5	A	304[A]	BVT	C5-C10	-4.87	1.33	1.41
5	B	303[A]	BVT	C22-C23	-4.85	1.39	1.50
4	A	303[B]	BV8	C6-C11	-4.84	1.33	1.41
5	A	304[A]	BVT	C22-C23	-4.81	1.39	1.50
5	D	303	BVT	C47-N2	4.69	1.39	1.32
4	A	303[B]	BV8	C3-C22	-4.61	1.39	1.50
5	D	303	BVT	C5-C10	-4.56	1.33	1.41
4	A	303[B]	BV8	C46-N9	4.29	1.39	1.32
4	A	303[B]	BV8	C9-C10	-4.28	1.33	1.42
5	A	304[A]	BVT	C8-C9	-4.28	1.33	1.42
5	A	304[A]	BVT	C47-N2	4.27	1.39	1.32
5	C	303	BVT	C5-C10	-4.14	1.34	1.41
5	D	303	BVT	C47-N1	4.13	1.41	1.33
4	A	303[B]	BV8	C33-S1	-4.05	1.76	1.81
5	D	303	BVT	C8-C9	-4.01	1.34	1.42
5	A	304[A]	BVT	O7-C38	3.91	1.49	1.43
4	A	303[B]	BV8	O17-C42	3.89	1.46	1.41
5	B	303[A]	BVT	C37-S1	-3.82	1.75	1.82
5	B	303[A]	BVT	C47-N2	3.81	1.38	1.32
5	C	303	BVT	C22-C23	-3.80	1.41	1.50
4	A	303[B]	BV8	C5-N5	3.78	1.35	1.26
5	D	303	BVT	C37-S1	-3.76	1.75	1.82
5	D	303	BVT	C22-C23	-3.65	1.42	1.50
5	A	304[A]	BVT	O17-C46	3.39	1.45	1.41
5	B	303[A]	BVT	C8-C9	-3.33	1.35	1.42
4	A	303[B]	BV8	C46-N10	3.28	1.40	1.33
5	C	303	BVT	C37-S1	-3.26	1.76	1.82
5	B	303[A]	BVT	C32-N7	3.25	1.50	1.46
5	A	304[A]	BVT	C47-N1	3.24	1.39	1.33
5	C	303	BVT	C8-C9	-3.24	1.35	1.42
5	A	304[A]	BVT	C9-C10	-3.06	1.34	1.42
4	A	303[B]	BV8	C10-C11	-3.04	1.34	1.42
5	A	304[A]	BVT	C37-S1	-3.04	1.76	1.82
5	A	304[A]	BVT	C2-C1	-2.99	1.33	1.40
5	D	303	BVT	C9-C10	-2.96	1.34	1.42
4	A	303[B]	BV8	C44-C45	-2.95	1.33	1.40
5	B	303[A]	BVT	C47-N1	2.86	1.39	1.33
5	C	303	BVT	C47-N1	2.84	1.39	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	303	BVT	C32-N7	2.81	1.50	1.46
5	B	303[A]	BVT	C9-C10	-2.80	1.35	1.42
5	B	303[A]	BVT	C3-C2	-2.68	1.33	1.43
5	C	303	BVT	C32-N7	2.65	1.50	1.46
5	C	303	BVT	C9-C10	-2.63	1.35	1.42
5	C	303	BVT	C2-C1	-2.62	1.34	1.40
5	A	304[A]	BVT	C3-C2	-2.58	1.33	1.43
4	A	303[B]	BV8	P2-O14	2.56	1.60	1.50
4	A	303[B]	BV8	C47-C44	-2.55	1.33	1.43
5	D	303	BVT	C3-C2	-2.50	1.34	1.43
4	A	303[B]	BV8	P1-O11	2.40	1.59	1.50
5	B	303[A]	BVT	C2-C1	-2.32	1.34	1.40
5	D	303	BVT	C2-C1	-2.32	1.34	1.40
5	B	303[A]	BVT	C29-C20	-2.31	1.48	1.53
5	B	303[A]	BVT	O17-C46	2.11	1.44	1.41
4	A	303[B]	BV8	C33-C34	-2.10	1.48	1.52
5	D	303	BVT	O17-C46	2.04	1.43	1.41
5	C	303	BVT	C6-C5	2.01	1.41	1.36

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	303[A]	BVT	N2-C47-N1	-6.92	117.86	128.68
5	C	303	BVT	N2-C47-N1	-6.90	117.90	128.68
5	D	303	BVT	N2-C47-N1	-6.74	118.14	128.68
4	A	303[B]	BV8	N9-C46-N10	-6.29	118.85	128.68
5	A	304[A]	BVT	N2-C47-N1	-6.28	118.86	128.68
5	C	303	BVT	C13-C12-C11	-5.67	120.97	127.97
5	C	303	BVT	O4-C21-N6	5.47	121.63	110.50
5	B	303[A]	BVT	C31-C30-C29	-4.84	96.50	113.62
5	D	303	BVT	O4-C21-N6	4.69	120.03	110.50
5	C	303	BVT	P2-O13-P1	-4.69	116.75	132.83
5	A	304[A]	BVT	O4-C21-N6	4.17	118.98	110.50
5	B	303[A]	BVT	C29-C20-N6	-4.17	102.44	110.88
5	A	304[A]	BVT	C13-C12-C11	-4.12	122.87	127.97
4	A	303[B]	BV8	C13-C14-C15	-4.11	105.40	113.45
4	A	303[B]	BV8	O4-C1-N4	4.11	118.85	110.50
5	A	304[A]	BVT	C12-C13-C14	-4.06	105.50	113.45
4	A	303[B]	BV8	C14-C13-C12	-4.05	122.97	127.97
4	A	303[B]	BV8	P2-O13-P1	-4.02	119.04	132.83
5	C	303	BVT	C31-C30-C29	-4.02	99.42	113.62
5	A	304[A]	BVT	C46-N9-C1	-3.96	119.68	126.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	303	BVT	O3-C21-N6	-3.89	118.47	124.85
5	A	304[A]	BVT	C31-C30-C29	-3.86	99.95	113.62
4	A	303[B]	BV8	C42-N7-C45	-3.83	119.91	126.64
5	A	304[A]	BVT	P2-O13-P1	-3.81	119.75	132.83
5	D	303	BVT	C31-C30-C29	-3.81	100.15	113.62
5	B	303[A]	BVT	O7-C38-C39	3.77	117.94	110.17
5	C	303	BVT	O3-C21-N6	-3.75	118.70	124.85
5	D	303	BVT	O7-C38-C37	3.72	108.04	103.79
5	B	303[A]	BVT	C46-N9-C1	-3.59	120.33	126.64
5	D	303	BVT	P2-O13-P1	-3.41	121.12	132.83
4	A	303[B]	BV8	C2-C4-C32	-3.36	100.99	112.65
5	A	304[A]	BVT	C34-C35-C36	-3.35	101.05	112.65
5	B	303[A]	BVT	O4-C21-N6	3.33	117.28	110.50
4	A	303[B]	BV8	C28-C21-N4	-3.25	104.30	110.88
5	D	303	BVT	C46-N9-C1	-3.19	121.03	126.64
5	B	303[A]	BVT	C22-O4-C21	-3.17	108.85	115.93
5	D	303	BVT	C13-C14-N5	-3.12	104.23	110.79
5	A	304[A]	BVT	C29-C20-N6	-3.10	104.62	110.88
4	A	303[B]	BV8	O3-C1-N4	-2.94	120.02	124.85
4	A	303[B]	BV8	C30-C29-C28	-2.91	103.31	113.62
5	C	303	BVT	C46-N9-C1	-2.91	121.53	126.64
5	B	303[A]	BVT	O4-C21-O3	-2.85	118.78	124.25
5	A	304[A]	BVT	O3-C21-N6	-2.85	120.18	124.85
5	A	304[A]	BVT	C22-O4-C21	-2.80	109.67	115.93
5	C	303	BVT	O8-C40-C39	2.77	110.61	105.11
5	A	304[A]	BVT	C35-C34-N8	-2.71	105.51	111.53
5	D	303	BVT	C22-O4-C21	2.69	121.93	115.93
5	B	303[A]	BVT	O8-C40-C41	-2.67	100.58	109.37
5	D	303	BVT	O8-C40-C41	-2.63	100.73	109.37
5	D	303	BVT	C12-C13-C14	-2.58	108.40	113.45
5	B	303[A]	BVT	C34-C35-C36	-2.57	103.75	112.65
5	C	303	BVT	O7-C38-C37	2.55	106.70	103.79
5	C	303	BVT	C1-C2-N10	-2.47	106.83	109.40
5	D	303	BVT	C8-C9-C10	2.46	121.43	118.17
4	A	303[B]	BV8	C14-C15-C16	-2.43	103.94	110.25
5	D	303	BVT	O17-C43-C42	-2.42	101.40	109.37
5	C	303	BVT	O4-C22-C23	2.42	115.20	109.39
4	A	303[B]	BV8	C29-C30-C31	-2.40	105.22	113.57
5	C	303	BVT	O4-C21-O3	-2.39	119.66	124.25
4	A	303[B]	BV8	O7-C36-C37	-2.37	101.56	109.37
4	A	303[B]	BV8	O15-P2-O16	2.36	118.72	107.75
5	D	303	BVT	O17-C46-C45	-2.34	103.50	106.93

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	303	BVT	C8-C9-C10	2.32	121.25	118.17
5	B	303[A]	BVT	O17-C46-C45	-2.30	103.57	106.93
4	A	303[B]	BV8	C4-C2-N6	-2.22	105.29	111.99
5	A	304[A]	BVT	O7-C38-C37	2.19	106.30	103.79
5	B	303[A]	BVT	C1-C2-N10	-2.16	107.15	109.40
5	C	303	BVT	C2-C3-N11	-2.15	117.08	120.35
5	A	304[A]	BVT	C2-C3-N11	-2.14	117.09	120.35
5	C	303	BVT	C44-C45-C46	2.14	104.20	100.98
5	C	303	BVT	C13-C14-N5	-2.12	106.33	110.79
5	C	303	BVT	C14-N5-C19	2.12	126.21	121.67
5	B	303[A]	BVT	C20-N6-C21	2.11	126.06	120.90
4	A	303[B]	BV8	C44-C47-N11	-2.10	117.16	120.35
5	C	303	BVT	C6-C7-C8	-2.10	117.50	120.44
5	D	303	BVT	C2-C3-N11	-2.08	117.20	120.35
5	B	303[A]	BVT	C6-C7-C8	-2.07	117.54	120.44
5	D	303	BVT	C13-C12-C11	-2.05	125.43	127.97
5	A	304[A]	BVT	C13-C14-C15	-2.04	104.97	110.25
4	A	303[B]	BV8	C45-C44-N8	-2.02	107.29	109.40
5	A	304[A]	BVT	C8-C9-C10	2.01	120.83	118.17

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304[A]	BVT	C40-C41-O10-P1
5	A	304[A]	BVT	C41-O10-P1-O12
5	A	304[A]	BVT	C42-O16-P2-O15
5	B	303[A]	BVT	N6-C21-O4-C22
5	B	303[A]	BVT	O3-C21-O4-C22
5	B	303[A]	BVT	N8-C34-C35-C36
5	B	303[A]	BVT	C39-C40-C41-O10
5	B	303[A]	BVT	C42-O16-P2-O15
4	A	303[B]	BV8	C37-O10-P1-O11
4	A	303[B]	BV8	C37-O10-P1-O12
5	D	303	BVT	O8-C40-C41-O10
5	D	303	BVT	C39-C40-C41-O10
4	A	303[B]	BV8	C14-C15-C16-N2
5	A	304[A]	BVT	C18-C16-N4-C15
5	A	304[A]	BVT	C13-C14-C15-N4
5	A	304[A]	BVT	C13-C14-C15-O1
4	A	303[B]	BV8	C14-C15-C16-O1
5	C	303	BVT	O8-C40-C41-O10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	303	BVT	C39-C40-C41-O10
5	A	304[A]	BVT	O8-C40-C41-O10
5	A	304[A]	BVT	C39-C40-C41-O10
5	B	303[A]	BVT	O8-C40-C41-O10
4	A	303[B]	BV8	C19-C17-N2-C16
5	C	303	BVT	C12-C13-C14-C15
5	C	303	BVT	C12-C13-C14-N5
5	D	303	BVT	C31-C32-N7-C33
4	A	303[B]	BV8	C13-C14-C15-N3
5	A	304[A]	BVT	N8-C34-C35-C36
5	C	303	BVT	O16-C42-C43-O17
5	C	303	BVT	O16-C42-C43-C44
4	A	303[B]	BV8	C13-C14-C15-C16
3	B	302	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2
5	D	303	BVT	C35-C34-N8-C33
5	A	304[A]	BVT	C12-C13-C14-C15
5	A	304[A]	BVT	C12-C13-C14-N5
4	A	303[B]	BV8	N6-C2-C4-C32
4	A	303[B]	BV8	C36-C37-O10-P1
5	C	303	BVT	C31-C32-N7-C33
4	A	303[B]	BV8	O2-C20-C21-N4
4	A	303[B]	BV8	C20-C21-C28-C29
4	A	303[B]	BV8	N3-C20-C21-N4
5	C	303	BVT	N5-C14-C15-N4
3	C	302	EDO	O1-C1-C2-O2
4	A	303[B]	BV8	N4-C21-C28-C29
5	A	304[A]	BVT	C11-C12-C13-C14
5	A	304[A]	BVT	P2-O13-P1-O10
4	A	303[B]	BV8	C12-C13-C14-C15
4	A	303[B]	BV8	P2-O13-P1-O10
5	A	304[A]	BVT	C42-O16-P2-O13
5	B	303[A]	BVT	C42-O16-P2-O13
5	A	304[A]	BVT	C41-O10-P1-O11
5	A	304[A]	BVT	C42-O16-P2-O14
5	C	303	BVT	N5-C14-C15-O1
5	B	303[A]	BVT	C40-C41-O10-P1
5	B	303[A]	BVT	C30-C31-C32-N7
5	D	303	BVT	C19-C20-C29-C30
5	C	303	BVT	C23-C22-O4-C21
5	B	303[A]	BVT	N5-C14-C15-O1
5	B	303[A]	BVT	O16-C42-C43-O17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	303[B]	BV8	O16-C38-C39-O17
5	B	303[A]	BVT	P1-O13-P2-O16
5	C	303	BVT	N6-C20-C29-C30
5	A	304[A]	BVT	C19-C20-C29-C30
5	A	304[A]	BVT	C41-O10-P1-O13
4	A	303[B]	BV8	C37-O10-P1-O13
5	D	303	BVT	C23-C22-O4-C21
5	A	304[A]	BVT	O16-C42-C43-O17
4	A	303[B]	BV8	O2-C20-C21-C28
5	B	303[A]	BVT	C23-C22-O4-C21
4	A	303[B]	BV8	O7-C36-C37-O10
5	D	303	BVT	O16-C42-C43-O17
4	A	303[B]	BV8	N3-C20-C21-C28
5	B	303[A]	BVT	N5-C14-C15-N4

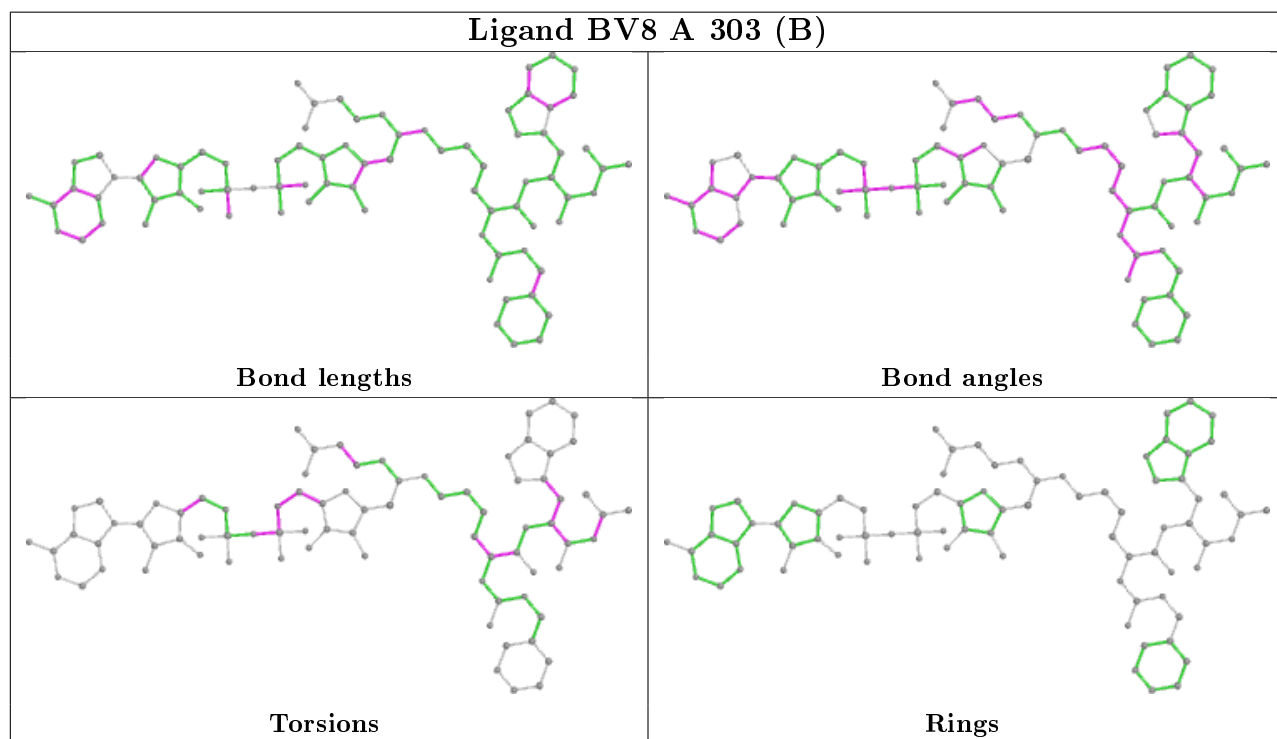
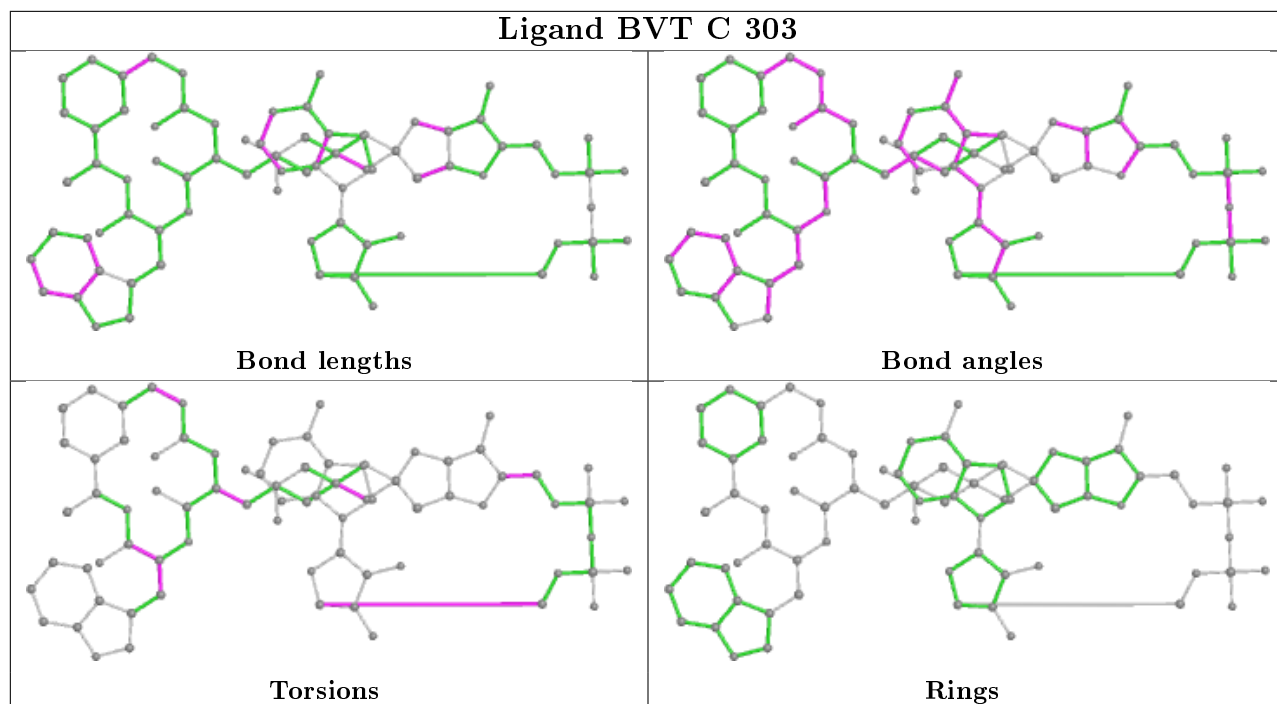
There are no ring outliers.

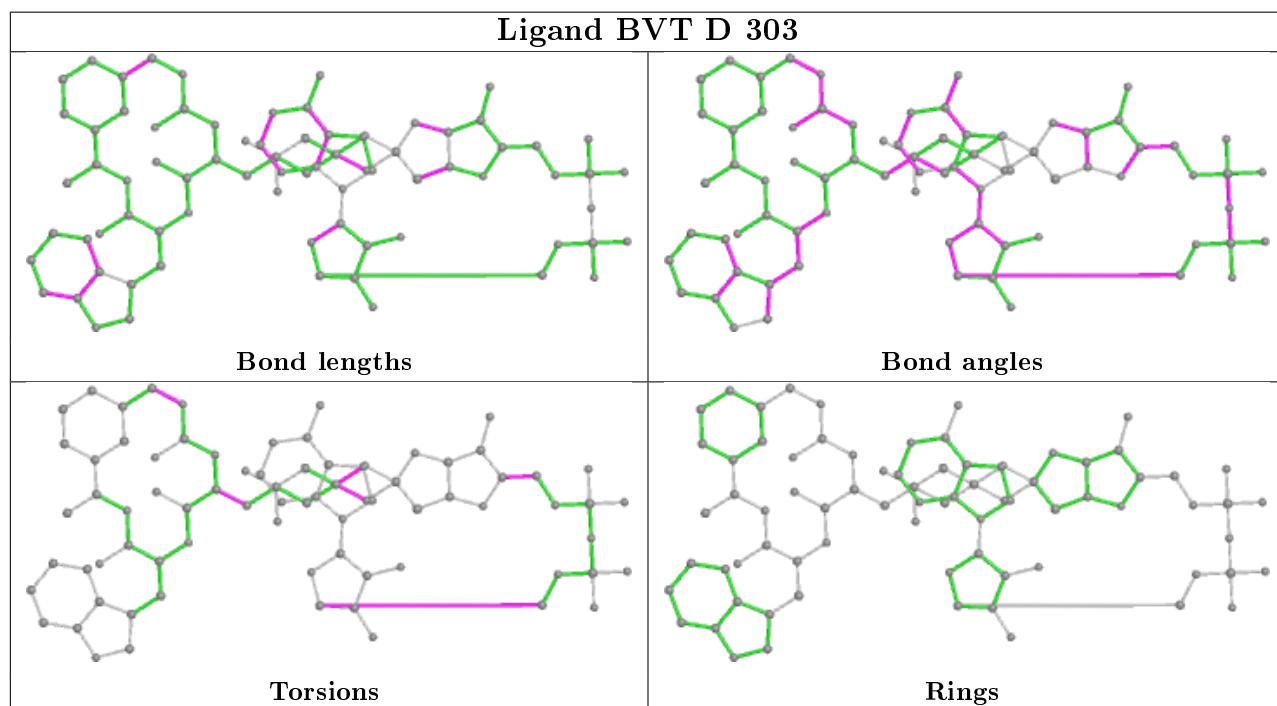
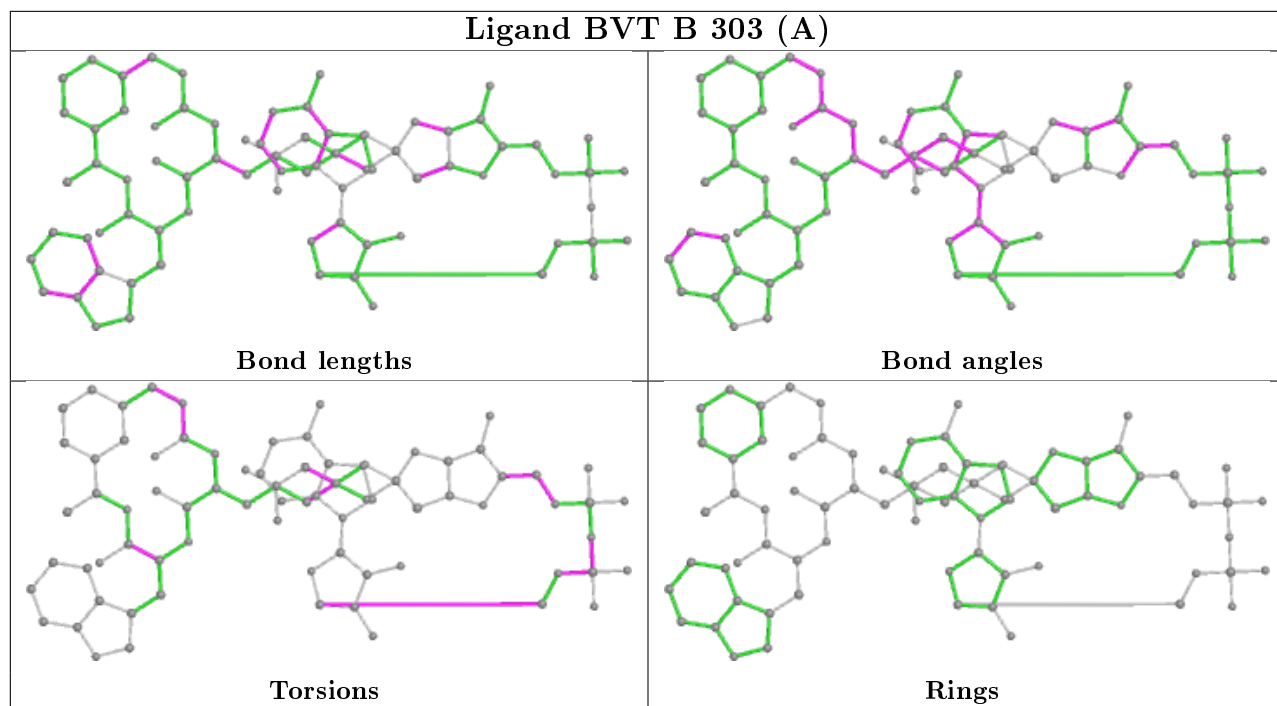
4 monomers are involved in 9 short contacts:

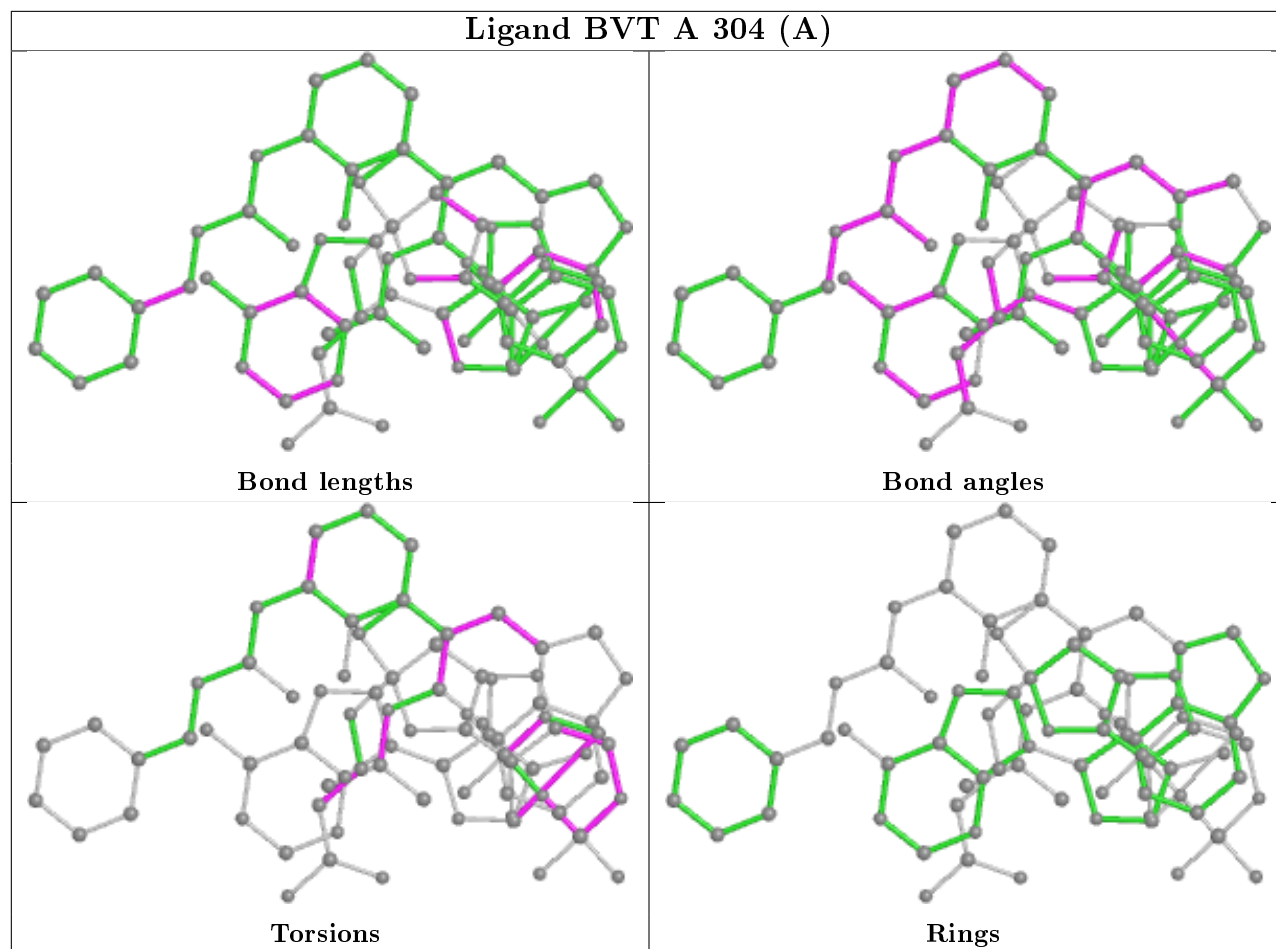
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	303	BVT	2	0
4	A	303[B]	BV8	3	0
5	B	303[A]	BVT	2	0
5	A	304[A]	BVT	2	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	274/277 (98%)	0.19	3 (1%) 80 79	34, 49, 66, 107	0
1	B	275/277 (99%)	0.33	9 (3%) 46 45	37, 50, 70, 87	0
1	C	274/277 (98%)	0.42	13 (4%) 31 30	38, 53, 82, 111	0
1	D	275/277 (99%)	0.32	9 (3%) 46 45	40, 52, 73, 130	0
All	All	1098/1108 (99%)	0.31	34 (3%) 49 47	34, 51, 72, 130	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	THR	5.2
1	D	29	MET	3.2
1	C	170	ALA	3.2
1	C	193	ALA	3.1
1	C	233	ARG	3.1
1	C	69	PRO	3.1
1	A	106	ARG	3.1
1	A	29	MET	3.0
1	D	72	PHE	3.0
1	C	295	PRO	3.0
1	D	24	ASP	2.8
1	B	107	SER	2.8
1	C	251[A]	TYR	2.8
1	C	283	TYR	2.8
1	C	112	PRO	2.7
1	B	72	PHE	2.6
1	C	151	TYR	2.6
1	B	151	TYR	2.6
1	B	26	PHE	2.4
1	C	285	PHE	2.4
1	D	25	PRO	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	110	PRO	2.2
1	B	251	TYR	2.2
1	D	217	VAL	2.2
1	D	200	LEU	2.2
1	B	27	THR	2.1
1	C	29	MET	2.1
1	D	67	ARG	2.1
1	B	29	MET	2.1
1	D	86	ALA	2.1
1	B	285	PHE	2.1
1	A	206	LYS	2.0
1	C	270	PHE	2.0
1	D	26	PHE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

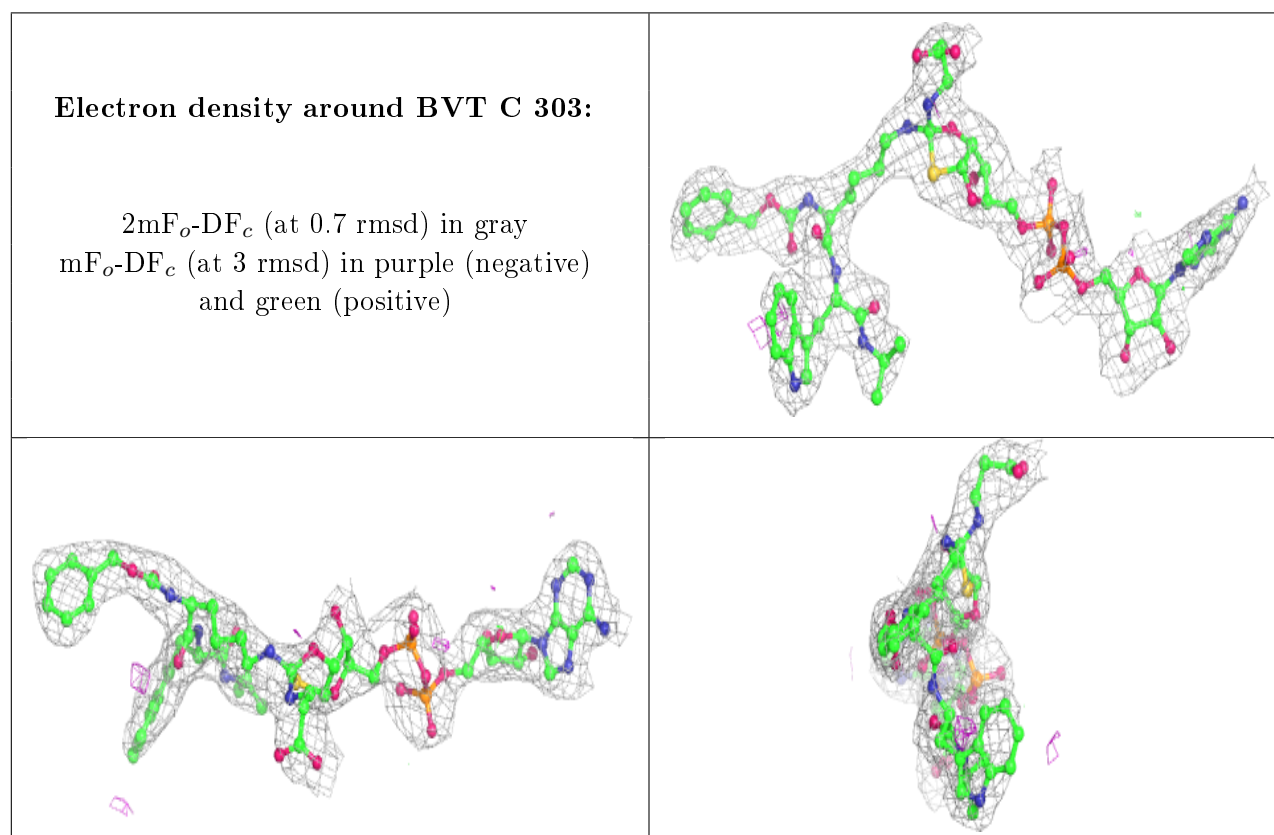
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	302	4/4	0.52	0.41	71,74,76,77	0
3	EDO	D	302	4/4	0.80	0.20	44,45,46,47	0
3	EDO	C	302	4/4	0.85	0.23	56,56,58,58	0
5	BVT	C	303	80/80	0.89	0.17	39,50,62,69	0
5	BVT	B	303[A]	80/80	0.89	0.18	32,51,68,75	0
3	EDO	A	302	4/4	0.91	0.18	54,56,56,56	0
2	ZN	C	301	1/1	0.91	0.05	57,57,57,57	0
4	BV8	A	303[B]	80/80	0.92	0.17	33,39,64,65	80
5	BVT	A	304[A]	80/80	0.92	0.17	37,49,72,72	80
5	BVT	D	303	80/80	0.93	0.17	28,49,64,69	0

*Continued on next page...*

*Continued from previous page...*

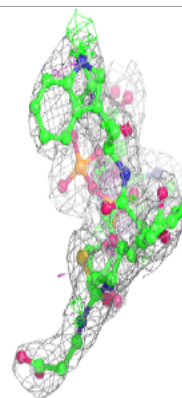
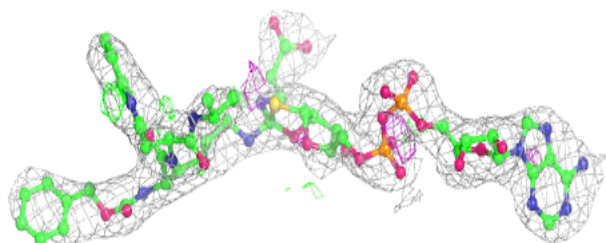
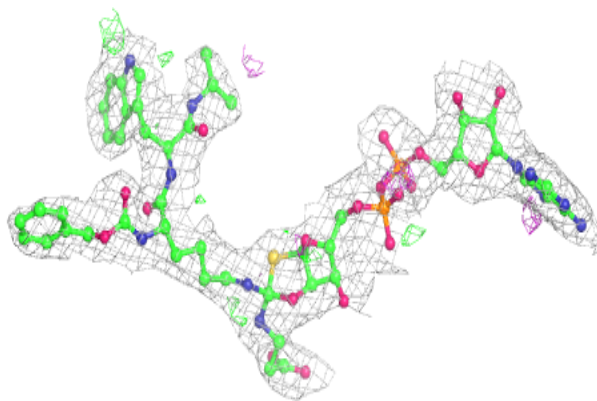
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	B	301	1/1	0.94	0.07	50,50,50,50	0
2	ZN	D	301	1/1	0.96	0.05	48,48,48,48	0
2	ZN	A	301	1/1	0.96	0.06	50,50,50,50	0

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.

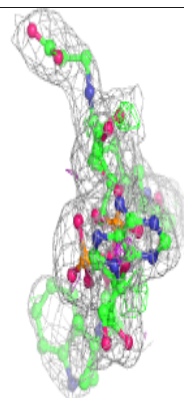
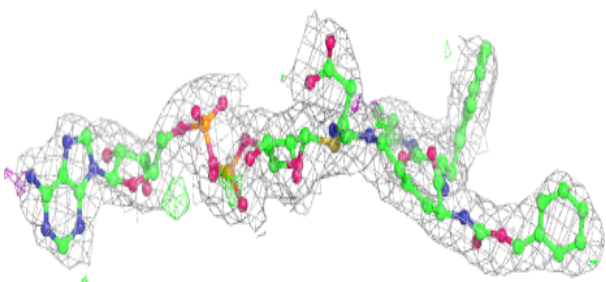
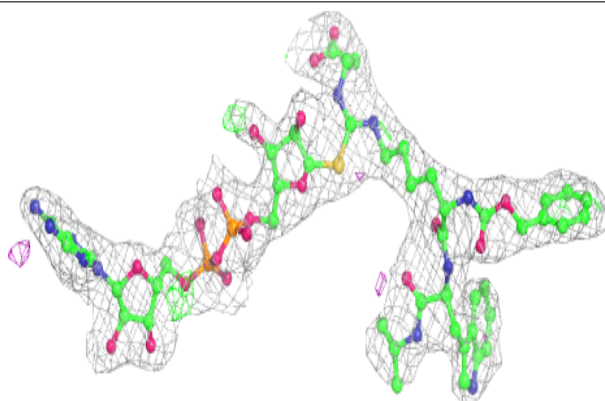


**Electron density around BVT B 303 (A):**

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

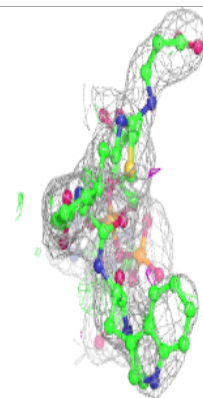
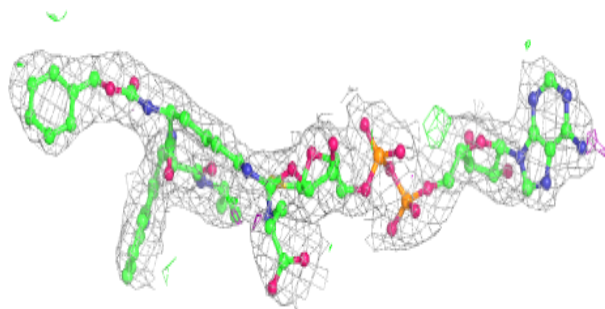
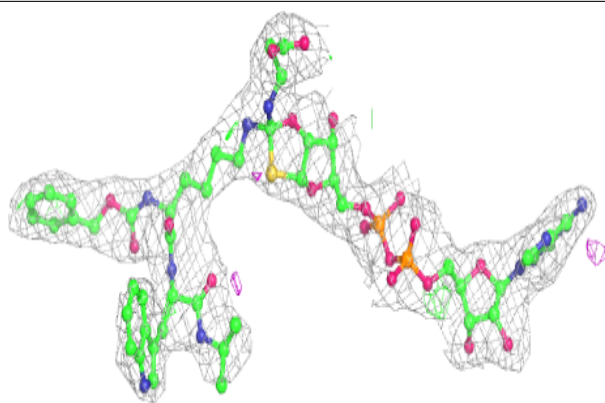
**Electron density around BV8 A 303 (B):**

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

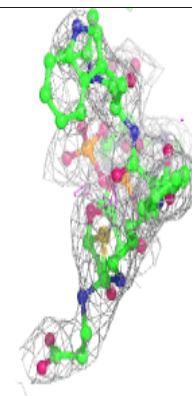
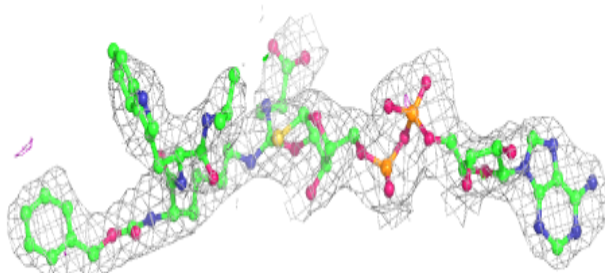
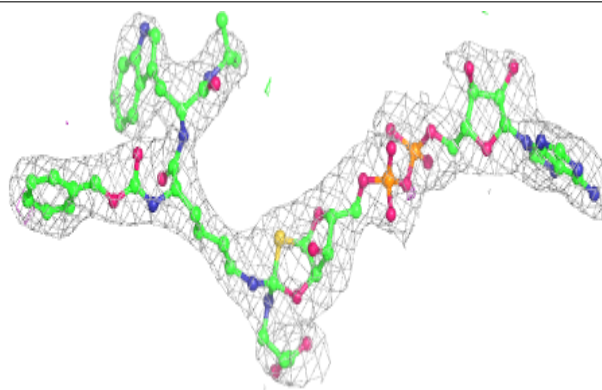


**Electron density around BVT A 304 (A):**

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

**Electron density around BVT D 303:**

$2mF_o-DF_c$  (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.