



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 PM UTC

PDB ID : 6EO0 / pdb_00006eo0
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

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

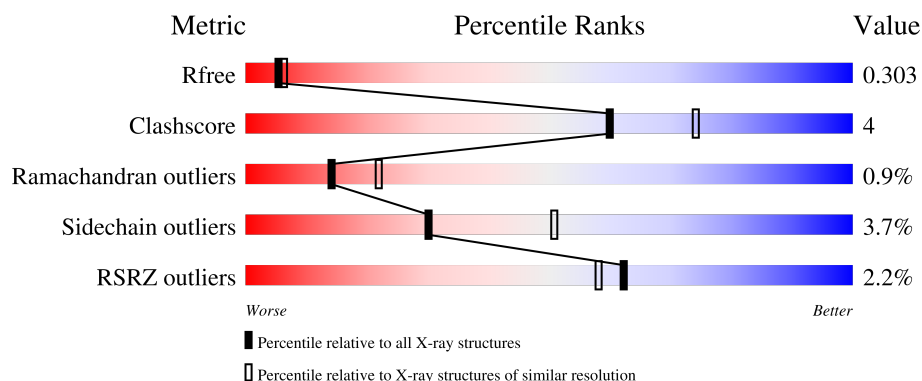
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	277	0% 87% 9% ...
1	B	277	2% 87% 11% ..
1	C	277	4% 85% 13% ..
1	D	277	2% 88% 9% ..

2 Entry composition

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
1	A	274	Total	C	N	O	S	0	1	0
			2138	1351	384	387	16			
1	B	275	Total	C	N	O	S	0	1	0
			2147	1354	386	391	16			
1	C	274	Total	C	N	O	S	0	2	0
			2147	1358	385	388	16			
1	D	275	Total	C	N	O	S	0	1	0
			2147	1355	387	389	16			

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

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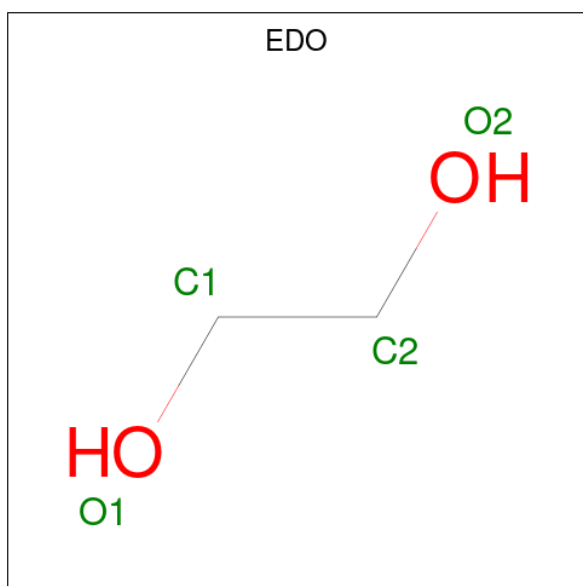
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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	PRO	-	expression tag	UNP Q6DHI5
D	26	PHE	-	expression tag	UNP Q6DHI5
D	27	THR	-	expression tag	UNP Q6DHI5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

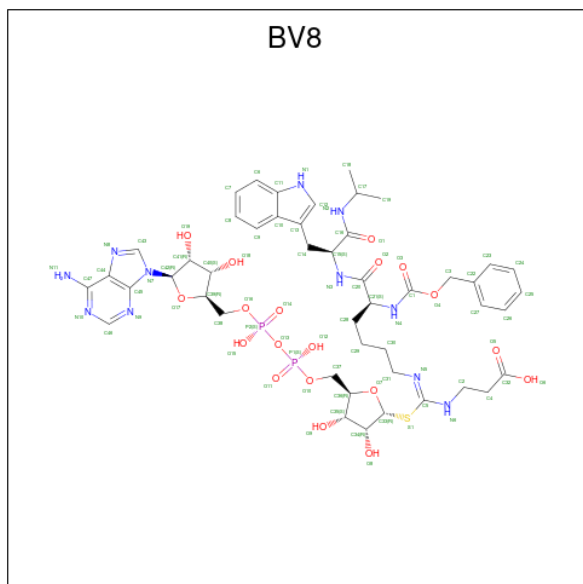
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



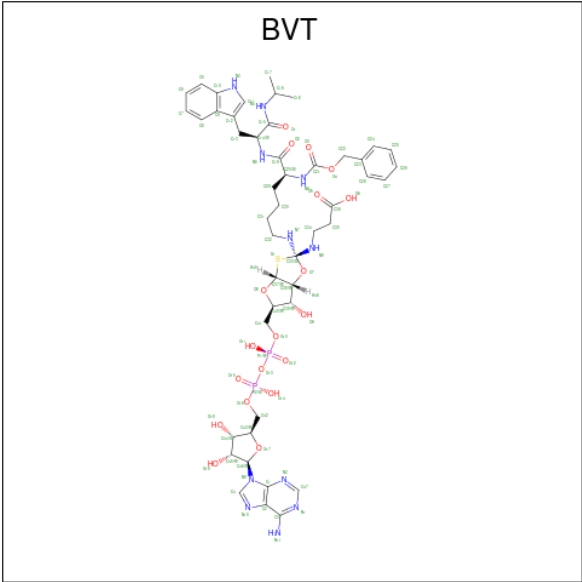
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- 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 (CCD ID: BV8) (formula: C₄₇H₆₃N₁₁O₁₉P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	1
			80	47	11	19	2	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 (CCD ID: BVT) (formula: C₄₇H₆₃N₁₁O₁₉P₂S).



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

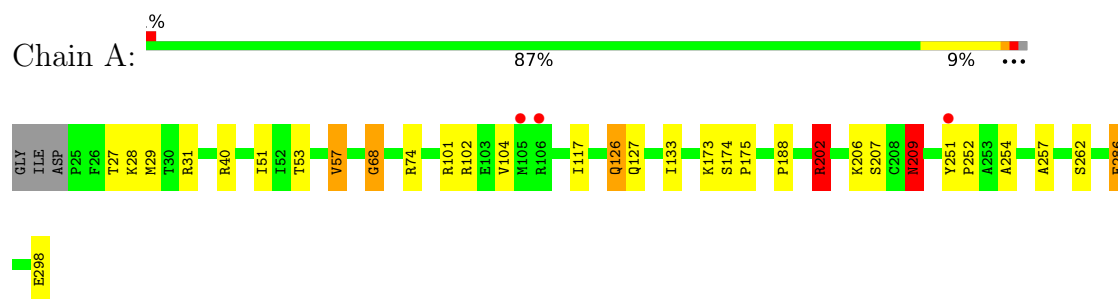
- Molecule 6 is water.

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

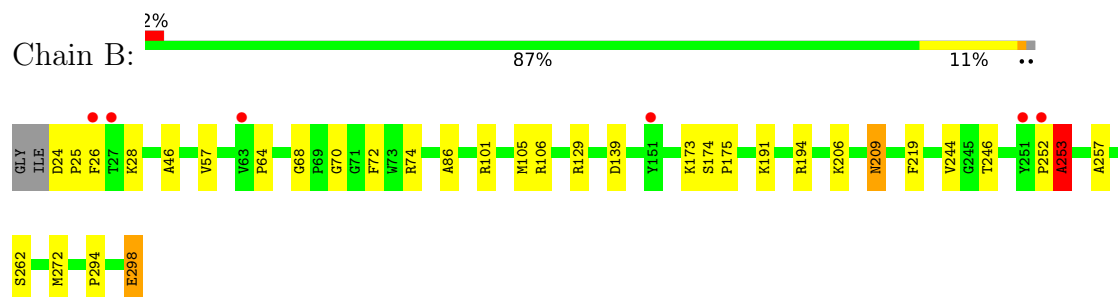
3 Residue-property plots [i](#)

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.

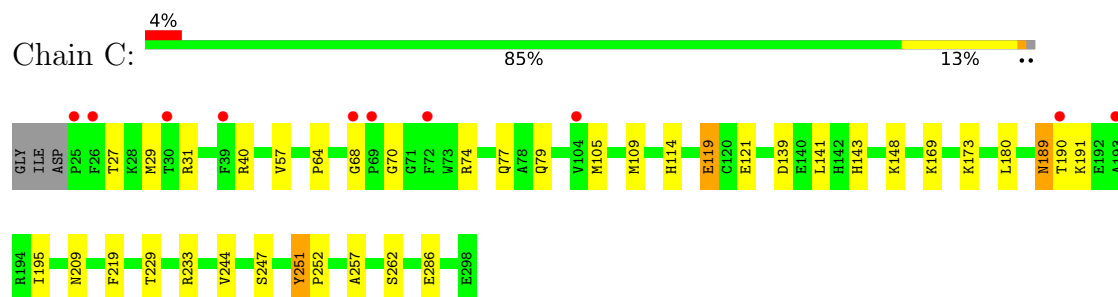
- Molecule 1: NAD-dependent protein deacetylase sirtuin-5, mitochondrial



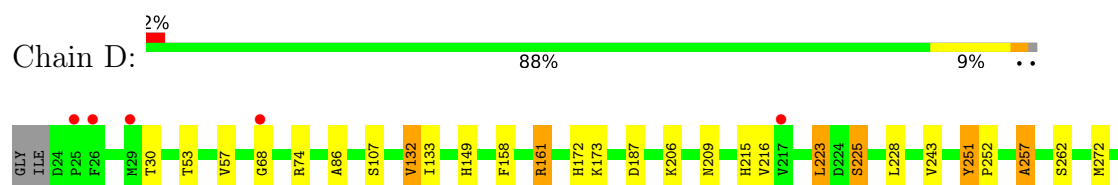
- Molecule 1: NAD-dependent protein deacetylase sirtuin-5, mitochondrial



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.39Å)	Xtriage
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 ²)	43.8	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9175	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, BV8, ZN, 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	0.86	0/2200	1.05	3/2983 (0.1%)
1	B	0.90	1/2205 (0.0%)	1.10	5/2990 (0.2%)
1	C	0.84	0/2212	1.04	5/2999 (0.2%)
1	D	0.86	0/2209	1.05	6/2995 (0.2%)
All	All	0.87	1/8826 (0.0%)	1.06	19/11967 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ALA	C-O	-5.18	1.17	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ARG	CG-CD-NE	11.21	136.65	112.00
1	B	101	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	D	161	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	B	253	ALA	N-CA-C	-6.12	97.76	110.80
1	C	189	ASN	N-CA-C	-6.00	103.89	110.91
1	D	257	ALA	CA-C-N	-5.73	113.28	119.24
1	D	257	ALA	C-N-CA	-5.73	113.28	119.24
1	A	257	ALA	CA-C-N	-5.71	113.30	119.24
1	A	257	ALA	C-N-CA	-5.71	113.30	119.24
1	C	257	ALA	CA-C-N	-5.71	113.30	119.24
1	C	257	ALA	C-N-CA	-5.71	113.30	119.24
1	C	191	LYS	N-CA-C	-5.67	98.69	108.56
1	B	257	ALA	CA-C-N	-5.65	113.36	119.24
1	B	257	ALA	C-N-CA	-5.65	113.36	119.24
1	D	161	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	C	40	ARG	CG-CD-NE	5.26	123.57	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	SER	N-CA-C	5.24	117.67	111.33
1	B	294	PRO	N-CA-C	5.15	116.99	110.70
1	D	225	SER	CA-CB-OG	5.15	121.40	111.10

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	25	0
1	B	2147	0	2110	16	0
1	C	2147	0	2118	21	0
1	D	2147	0	2111	15	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	1	0
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	75	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 (75) 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:O2	4:A:303[B]:BV8:C29	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:30:THR:HB	1:D:279:GLN:HE21	1.65	0.61
1:D:187:ASP:HB3	6:D:416:HOH:O	2.00	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
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:272:MET:HE2	5:D:303:BVT:N11	2.27	0.49
1:D:161:ARG:HD3	1:D:215:HIS:ND1	2.28	0.49
1:C:143:HIS:N	6:C:403:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PRO:O	1:B:26:PHE:HB2	2.15	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:OE1	1:B:298:GLU:HA	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:109:MET:HA	1:C:109:MET:HE2	1.99	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:C:105:MET:HE1	1:C:141:LEU:HD11	2.01	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:A:286:GLU:CD	1:B:72:PHE:CE2	2.97	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:C:105:MET:HE2	1:C:139:ASP:HB2	2.02	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: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
1:D:158:PHE:HB3	1:D:172:HIS:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	18	28
1	B	274/277 (99%)	260 (95%)	10 (4%)	4 (2%)	8	12
1	C	274/277 (99%)	258 (94%)	14 (5%)	2 (1%)	18	28
1	D	274/277 (99%)	262 (96%)	10 (4%)	2 (1%)	18	28
All	All	1095/1108 (99%)	1039 (95%)	46 (4%)	10 (1%)	14	22

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

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%)	28	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	231/231 (100%)	222 (96%)	9 (4%)	28	48
1	C	231/231 (100%)	223 (96%)	8 (4%)	32	53
1	D	231/231 (100%)	222 (96%)	9 (4%)	28	48
All	All	922/924 (100%)	887 (96%)	35 (4%)	30	49

All (35) 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	126	GLN
1	A	173	LYS
1	A	202	ARG
1	A	209	ASN
1	A	262	SER
1	A	286	GLU
1	B	24	ASP
1	B	28	LYS
1	B	173	LYS
1	B	191	LYS
1	B	194	ARG
1	B	209	ASN
1	B	262	SER
1	B	272	MET
1	B	298	GLU
1	C	29	MET
1	C	119	GLU
1	C	169	LYS
1	C	173	LYS
1	C	251[A]	TYR
1	C	251[B]	TYR
1	C	262	SER
1	C	286	GLU
1	D	132	VAL
1	D	173	LYS
1	D	206	LYS
1	D	216	VAL
1	D	223	LEU
1	D	225	SER
1	D	251	TYR

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Mol	Chain	Res	Type
1	D	262	SER
1	D	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

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

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](#)

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
3	EDO	C	302	-	3,3,3	0.51	0	2,2,2	0.22	0
5	BVT	B	303[A]	-	82,87,87	1.88	18 (21%)	107,126,126	1.92	28 (26%)
5	BVT	A	304[A]	-	82,87,87	1.81	18 (21%)	107,126,126	1.82	26 (24%)
4	BV8	A	303[B]	-	85,86,86	1.82	19 (22%)	110,122,122	1.83	27 (24%)
5	BVT	D	303	-	82,87,87	1.97	20 (24%)	107,126,126	1.84	26 (24%)
3	EDO	B	302	-	3,3,3	0.53	0	2,2,2	0.04	0
3	EDO	D	302	-	3,3,3	0.49	0	2,2,2	0.17	0
5	BVT	C	303	-	82,87,87	1.84	18 (21%)	107,126,126	1.97	31 (28%)
3	EDO	A	302	-	3,3,3	0.51	0	2,2,2	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	302	-	-	1/1/1/1	-
5	BVT	B	303[A]	-	-	16/61/109/109	0/8/8/8
5	BVT	A	304[A]	-	-	24/61/109/109	0/8/8/8
4	BV8	A	303[B]	-	-	21/63/101/101	0/7/7/7
5	BVT	D	303	-	-	8/61/109/109	0/8/8/8
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
5	BVT	C	303	-	-	14/61/109/109	0/8/8/8
3	EDO	A	302	-	-	1/1/1/1	-

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	303	BVT	C9-C12	-6.91	1.32	1.44
5	B	303[A]	BVT	C9-C12	-6.29	1.33	1.44
4	A	303[B]	BV8	C10-C13	-6.24	1.33	1.44
5	A	304[A]	BVT	C9-C12	-6.23	1.33	1.44
5	C	303	BVT	C9-C12	-6.16	1.33	1.44
5	D	303	BVT	O7-C38	5.72	1.52	1.43
5	A	304[A]	BVT	C9-C10	-5.62	1.34	1.41
4	A	303[B]	BV8	C10-C11	-5.56	1.34	1.41
5	B	303[A]	BVT	O7-C38	5.42	1.52	1.43
5	D	303	BVT	C9-C10	-5.41	1.34	1.41
5	C	303	BVT	P2-O13	5.34	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	303[A]	BVT	C9-C10	-5.04	1.35	1.41
5	B	303[A]	BVT	C22-C23	-4.90	1.39	1.50
5	D	303	BVT	P2-O13	4.88	1.64	1.59
5	A	304[A]	BVT	C22-C23	-4.85	1.39	1.50
5	C	303	BVT	O7-C38	4.83	1.51	1.43
5	C	303	BVT	C9-C10	-4.68	1.35	1.41
4	A	303[B]	BV8	C3-C22	-4.65	1.39	1.50
5	D	303	BVT	C47-N1	4.31	1.41	1.33
4	A	303[B]	BV8	C9-C10	-4.26	1.33	1.39
5	A	304[A]	BVT	C8-C9	-4.26	1.33	1.39
5	B	303[A]	BVT	C5-C10	-4.01	1.33	1.39
5	A	304[A]	BVT	C5-C10	-3.90	1.33	1.39
5	D	303	BVT	C8-C9	-3.90	1.34	1.39
4	A	303[B]	BV8	C6-C11	-3.87	1.33	1.39
5	C	303	BVT	C22-C23	-3.84	1.41	1.50
5	B	303[A]	BVT	C37-S1	-3.82	1.75	1.82
5	A	304[A]	BVT	O7-C38	3.81	1.49	1.43
5	D	303	BVT	C37-S1	-3.76	1.75	1.82
4	A	303[B]	BV8	C33-S1	-3.76	1.76	1.81
5	D	303	BVT	C22-C23	-3.69	1.42	1.50
5	D	303	BVT	C5-C10	-3.57	1.33	1.39
5	C	303	BVT	C47-N2	3.54	1.40	1.33
4	A	303[B]	BV8	C46-N10	3.42	1.40	1.33
5	A	304[A]	BVT	C2-C1	-3.39	1.33	1.39
5	B	303[A]	BVT	C2-N10	-3.39	1.32	1.39
5	A	304[A]	BVT	C47-N1	3.38	1.39	1.33
4	A	303[B]	BV8	C44-C45	-3.34	1.33	1.39
5	B	303[A]	BVT	C32-N7	3.34	1.50	1.46
5	B	303[A]	BVT	C10-N3	-3.29	1.32	1.37
5	C	303	BVT	C37-S1	-3.26	1.76	1.82
5	D	303	BVT	C47-N2	3.23	1.39	1.33
5	B	303[A]	BVT	C4-N9	-3.17	1.32	1.37
5	C	303	BVT	C5-C10	-3.12	1.34	1.39
5	A	304[A]	BVT	C37-S1	-3.04	1.76	1.82
5	D	303	BVT	C10-N3	-3.00	1.33	1.37
5	B	303[A]	BVT	C8-C9	-2.98	1.35	1.39
5	B	303[A]	BVT	C47-N1	2.98	1.39	1.33
5	C	303	BVT	C47-N1	2.96	1.39	1.33
5	D	303	BVT	C2-N10	-2.92	1.33	1.39
5	D	303	BVT	C32-N7	2.89	1.50	1.46
4	A	303[B]	BV8	C44-N8	-2.89	1.33	1.39
5	C	303	BVT	C2-C1	-2.86	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303[B]	BV8	C46-N9	2.86	1.39	1.33
5	A	304[A]	BVT	C2-N10	-2.86	1.33	1.39
5	C	303	BVT	C8-C9	-2.85	1.35	1.39
5	A	304[A]	BVT	C4-N9	-2.85	1.32	1.37
5	A	304[A]	BVT	C47-N2	2.84	1.39	1.33
4	A	303[B]	BV8	C43-N7	-2.83	1.32	1.37
5	D	303	BVT	C4-N9	-2.81	1.32	1.37
5	D	303	BVT	C11-C12	-2.80	1.32	1.36
5	A	304[A]	BVT	C1-N9	-2.79	1.31	1.37
5	B	303[A]	BVT	C2-C3	-2.74	1.33	1.41
5	C	303	BVT	C32-N7	2.72	1.50	1.46
4	A	303[B]	BV8	C45-N7	-2.71	1.32	1.37
5	C	303	BVT	P1-O13	2.70	1.62	1.59
5	C	303	BVT	C4-N9	-2.69	1.33	1.37
4	A	303[B]	BV8	P2-O14	2.64	1.60	1.50
5	A	304[A]	BVT	C2-C3	-2.61	1.33	1.41
5	A	304[A]	BVT	C10-N3	-2.59	1.33	1.37
4	A	303[B]	BV8	C44-C47	-2.58	1.33	1.41
4	A	303[B]	BV8	C11-N1	-2.56	1.33	1.37
5	D	303	BVT	C2-C3	-2.51	1.34	1.41
4	A	303[B]	BV8	P1-O11	2.48	1.59	1.50
5	B	303[A]	BVT	C47-N2	2.43	1.38	1.33
5	B	303[A]	BVT	C2-C1	-2.41	1.34	1.39
5	D	303	BVT	C2-C1	-2.41	1.34	1.39
4	A	303[B]	BV8	C12-N1	-2.40	1.33	1.37
5	A	304[A]	BVT	C11-N3	-2.40	1.33	1.37
5	D	303	BVT	C11-N3	-2.39	1.33	1.37
5	D	303	BVT	C1-N9	-2.39	1.32	1.37
5	C	303	BVT	C2-N10	-2.35	1.34	1.39
5	B	303[A]	BVT	C29-C20	-2.33	1.48	1.53
5	A	304[A]	BVT	P2-O13	2.31	1.62	1.59
5	C	303	BVT	C10-N3	-2.28	1.34	1.37
5	A	304[A]	BVT	C11-C12	-2.27	1.33	1.36
5	C	303	BVT	C11-N3	-2.22	1.33	1.37
5	C	303	BVT	C11-C12	-2.19	1.33	1.36
4	A	303[B]	BV8	C33-C34	-2.17	1.48	1.52
4	A	303[B]	BV8	C12-C13	-2.15	1.33	1.36
5	D	303	BVT	O6-C36	-2.12	1.23	1.30
5	B	303[A]	BVT	C11-C12	-2.09	1.33	1.36
5	B	303[A]	BVT	C11-N3	-2.04	1.33	1.37

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	303[A]	BVT	N2-C47-N1	-7.08	117.86	128.58
5	C	303	BVT	N2-C47-N1	-7.06	117.90	128.58
5	D	303	BVT	N2-C47-N1	-6.90	118.14	128.58
4	A	303[B]	BV8	N10-C46-N9	-6.43	118.85	128.58
5	A	304[A]	BVT	N2-C47-N1	-6.42	118.86	128.58
4	A	303[B]	BV8	C2-C4-C32	-5.54	100.99	112.98
5	A	304[A]	BVT	C34-C35-C36	-5.51	101.05	112.98
5	C	303	BVT	O4-C21-N6	5.23	121.63	110.45
5	B	303[A]	BVT	O17-C46-N9	-5.17	98.15	108.09
5	C	303	BVT	C2-C1-N2	-5.09	119.70	126.72
5	B	303[A]	BVT	C2-C1-N2	-4.57	120.42	126.72
5	B	303[A]	BVT	C31-C30-C29	-4.54	96.50	113.62
5	A	304[A]	BVT	N9-C4-N10	-4.52	107.53	113.94
5	D	303	BVT	O4-C21-N6	4.48	120.03	110.45
4	A	303[B]	BV8	N7-C43-N8	-4.45	107.63	113.94
5	C	303	BVT	C9-C12-C11	4.37	110.63	106.16
5	B	303[A]	BVT	C29-C20-N6	-4.28	102.44	110.91
5	B	303[A]	BVT	C34-C35-C36	-4.26	103.75	112.98
4	A	303[B]	BV8	C15-C14-C13	-4.25	105.40	113.44
5	A	304[A]	BVT	C14-C13-C12	-4.19	105.50	113.44
5	C	303	BVT	N9-C4-N10	-4.17	108.03	113.94
5	D	303	BVT	N9-C4-N10	-4.02	108.23	113.94
5	A	304[A]	BVT	O4-C21-N6	3.99	118.98	110.45
5	C	303	BVT	C47-N2-C1	3.93	121.43	111.83
4	A	303[B]	BV8	O4-C1-N4	3.93	118.85	110.45
5	D	303	BVT	O3-C21-N6	-3.90	118.47	124.86
4	A	303[B]	BV8	C44-C45-N9	-3.86	121.40	126.72
5	B	303[A]	BVT	O7-C38-C39	3.82	117.94	110.20
5	C	303	BVT	C31-C30-C29	-3.77	99.42	113.62
5	C	303	BVT	O3-C21-N6	-3.76	118.70	124.86
5	A	304[A]	BVT	C2-C1-N2	-3.75	121.55	126.72
5	D	303	BVT	C9-C12-C11	3.72	109.97	106.16
5	D	303	BVT	O7-C38-C37	3.70	108.04	103.80
5	B	303[A]	BVT	N9-C4-N10	-3.64	108.77	113.94
5	A	304[A]	BVT	C31-C30-C29	-3.63	99.95	113.62
5	D	303	BVT	C2-C1-N2	-3.61	121.74	126.72
5	D	303	BVT	C31-C30-C29	-3.57	100.15	113.62
5	B	303[A]	BVT	C47-N2-C1	3.42	120.17	111.83
5	D	303	BVT	C13-C14-N5	-3.36	104.23	110.64
4	A	303[B]	BV8	C28-C21-N4	-3.34	104.30	110.91
5	C	303	BVT	C1-C2-N10	-3.28	106.83	110.58
5	C	303	BVT	C2-N10-C4	3.24	108.54	103.45
5	B	303[A]	BVT	O14-P2-O13	-3.20	98.63	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	303[A]	BVT	O4-C21-N6	3.19	117.28	110.45
5	C	303	BVT	C12-C11-N3	-3.19	106.81	110.31
5	A	304[A]	BVT	C29-C20-N6	-3.18	104.62	110.91
4	A	303[B]	BV8	C4-C2-N6	-3.15	105.29	112.00
5	B	303[A]	BVT	C22-O4-C21	-3.14	108.85	115.93
5	D	303	BVT	C34-C35-C36	-3.14	106.18	112.98
5	A	304[A]	BVT	C9-C12-C11	3.09	109.32	106.16
5	C	303	BVT	C13-C12-C11	-3.08	120.97	126.97
5	D	303	BVT	C12-C11-N3	-3.03	106.99	110.31
5	B	303[A]	BVT	C1-C2-N10	-3.00	107.15	110.58
4	A	303[B]	BV8	C46-N9-C45	3.00	119.15	111.83
4	A	303[B]	BV8	C10-C13-C12	2.98	109.20	106.16
5	A	304[A]	BVT	C1-N9-C46	-2.97	119.68	126.63
5	A	304[A]	BVT	C47-N2-C1	2.96	119.05	111.83
4	A	303[B]	BV8	O3-C1-N4	-2.95	120.02	124.86
4	A	303[B]	BV8	C44-N8-C43	2.94	108.07	103.45
5	B	303[A]	BVT	C2-N10-C4	2.92	108.04	103.45
5	A	304[A]	BVT	C2-N10-C4	2.91	108.03	103.45
5	D	303	BVT	C2-N10-C4	2.91	108.03	103.45
5	B	303[A]	BVT	C43-O17-C46	-2.91	103.04	109.47
4	A	303[B]	BV8	C45-C44-N8	-2.88	107.29	110.58
4	A	303[B]	BV8	C45-N7-C42	-2.87	119.91	126.63
5	B	303[A]	BVT	O4-C21-O3	-2.86	118.78	124.26
5	A	304[A]	BVT	O3-C21-N6	-2.86	120.18	124.86
5	A	304[A]	BVT	C1-C2-N10	-2.84	107.33	110.58
5	D	303	BVT	C47-N2-C1	2.84	118.77	111.83
5	A	304[A]	BVT	O14-P2-O13	-2.83	99.62	107.27
5	A	304[A]	BVT	C12-C11-N3	-2.83	107.20	110.31
4	A	303[B]	BV8	C14-C15-C16	-2.81	103.94	110.57
5	C	303	BVT	C34-C35-C36	-2.80	106.91	112.98
5	A	304[A]	BVT	C22-O4-C21	-2.78	109.67	115.93
5	B	303[A]	BVT	C2-C1-N9	2.77	108.83	105.81
5	C	303	BVT	O8-C40-C39	2.75	110.61	105.15
4	A	303[B]	BV8	C13-C12-N1	-2.74	107.30	110.31
4	A	303[B]	BV8	C30-C29-C28	-2.74	103.31	113.62
5	B	303[A]	BVT	O8-C40-C41	-2.73	100.58	109.33
5	A	304[A]	BVT	C1-N9-C4	2.72	108.60	105.74
5	D	303	BVT	C1-N9-C4	2.71	108.58	105.74
5	B	303[A]	BVT	C1-N9-C46	-2.69	120.33	126.63
5	D	303	BVT	O8-C40-C41	-2.69	100.73	109.33
5	C	303	BVT	C2-C1-N9	2.67	108.72	105.81
5	D	303	BVT	C22-O4-C21	2.67	121.93	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	303	BVT	C14-C13-C12	-2.66	108.40	113.44
5	D	303	BVT	C1-C2-N10	-2.65	107.55	110.58
5	B	303[A]	BVT	O11-P1-O13	2.62	114.36	107.27
5	C	303	BVT	N2-C1-N9	2.59	131.57	127.17
4	A	303[B]	BV8	C45-N7-C43	2.58	108.44	105.74
5	C	303	BVT	C31-C32-N7	-2.55	104.81	110.98
5	D	303	BVT	C31-C32-N7	-2.55	104.82	110.98
4	A	303[B]	BV8	C47-C44-C45	2.54	120.64	117.18
5	C	303	BVT	O7-C38-C37	2.53	106.70	103.80
4	A	303[B]	BV8	C44-C45-N7	2.53	108.57	105.81
5	C	303	BVT	C2-C3-N11	-2.51	117.08	123.29
5	A	304[A]	BVT	C2-C3-N11	-2.50	117.09	123.29
5	D	303	BVT	C8-C9-C10	2.50	121.43	118.84
5	A	304[A]	BVT	C2-C1-N9	2.48	108.51	105.81
5	D	303	BVT	O17-C43-C42	-2.48	101.40	109.33
4	A	303[B]	BV8	C44-C47-N11	-2.47	117.16	123.29
5	D	303	BVT	C3-C2-C1	2.47	120.55	117.18
5	A	304[A]	BVT	C3-C2-C1	2.46	120.54	117.18
4	A	303[B]	BV8	O15-P2-O16	2.46	118.72	107.57
5	D	303	BVT	C2-C3-N11	-2.46	117.20	123.29
4	A	303[B]	BV8	O7-C36-C37	-2.43	101.56	109.33
5	C	303	BVT	O4-C21-O3	-2.40	119.66	124.26
4	A	303[B]	BV8	O12-P1-O13	2.40	113.75	107.27
5	D	303	BVT	C1-N9-C46	-2.40	121.03	126.63
5	C	303	BVT	O4-C22-C23	2.39	115.20	109.40
5	A	304[A]	BVT	C13-C14-C15	-2.38	104.97	110.57
5	B	303[A]	BVT	C46-N9-C4	2.37	132.36	127.09
4	A	303[B]	BV8	C29-C30-C31	-2.34	105.22	113.38
5	C	303	BVT	C8-C9-C10	2.32	121.25	118.84
5	C	303	BVT	O5-C36-C35	-2.31	115.76	123.09
5	C	303	BVT	C13-C14-N5	-2.26	106.33	110.64
5	C	303	BVT	C6-C7-C8	-2.22	117.50	120.24
5	B	303[A]	BVT	C2-C3-N11	-2.21	117.82	123.29
5	D	303	BVT	C43-O17-C46	-2.20	104.61	109.47
5	B	303[A]	BVT	C6-C7-C8	-2.19	117.54	120.24
5	C	303	BVT	C1-N9-C46	-2.18	121.53	126.63
5	A	304[A]	BVT	O7-C38-C37	2.18	106.30	103.80
5	A	304[A]	BVT	C31-C32-N7	-2.18	105.72	110.98
5	C	303	BVT	C3-C2-C1	2.17	120.15	117.18
5	B	303[A]	BVT	C45-C46-N9	2.17	118.70	113.30
5	B	303[A]	BVT	C3-C2-C1	2.12	120.08	117.18
5	C	303	BVT	C14-N5-C19	2.12	126.21	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	303[A]	BVT	N2-C1-N9	2.10	130.74	127.17
5	A	304[A]	BVT	C13-C12-C11	-2.10	122.87	126.97
5	A	304[A]	BVT	C46-N9-C4	2.08	131.72	127.09
5	C	303	BVT	O13-P1-O12	2.07	116.94	110.70
5	B	303[A]	BVT	C20-N6-C21	2.06	126.06	120.93
5	D	303	BVT	N2-C1-N9	2.05	130.66	127.17
5	C	303	BVT	C1-N9-C4	2.05	107.89	105.74
4	A	303[B]	BV8	C14-C13-C12	-2.05	122.97	126.97
4	A	303[B]	BV8	C42-N7-C43	2.05	131.64	127.09
5	C	303	BVT	C20-C19-N5	-2.02	112.32	116.63
5	B	303[A]	BVT	O5-C36-C35	-2.00	116.74	123.09

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303[B]	BV8	C37-O10-P1-O11
4	A	303[B]	BV8	C37-O10-P1-O12
4	A	303[B]	BV8	C37-O10-P1-O13
5	A	304[A]	BVT	C40-C41-O10-P1
5	A	304[A]	BVT	C41-O10-P1-O12
5	A	304[A]	BVT	C41-O10-P1-O13
5	A	304[A]	BVT	C42-O16-P2-O13
5	A	304[A]	BVT	C42-O16-P2-O15
5	B	303[A]	BVT	C42-O16-P2-O15
5	D	303	BVT	O8-C40-C41-O10
5	D	303	BVT	C39-C40-C41-O10
5	B	303[A]	BVT	O3-C21-O4-C22
5	B	303[A]	BVT	N6-C21-O4-C22
4	A	303[B]	BV8	C14-C15-C16-N2
5	A	304[A]	BVT	C13-C14-C15-N4
4	A	303[B]	BV8	C14-C15-C16-O1
5	A	304[A]	BVT	C13-C14-C15-O1
5	B	303[A]	BVT	C39-C40-C41-O10
4	A	303[B]	BV8	C12-C13-C14-C15
5	A	304[A]	BVT	C11-C12-C13-C14
5	C	303	BVT	C12-C13-C14-N5
5	B	303[A]	BVT	O8-C40-C41-O10
5	C	303	BVT	O8-C40-C41-O10
5	A	304[A]	BVT	C18-C16-N4-C15
5	D	303	BVT	C31-C32-N7-C33
5	D	303	BVT	C34-C35-C36-O5

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Mol	Chain	Res	Type	Atoms
5	D	303	BVT	C34-C35-C36-O6
4	A	303[B]	BV8	C10-C13-C14-C15
5	A	304[A]	BVT	C9-C12-C13-C14
5	A	304[A]	BVT	C39-C40-C41-O10
5	C	303	BVT	C39-C40-C41-O10
4	A	303[B]	BV8	C19-C17-N2-C16
5	C	303	BVT	C12-C13-C14-C15
3	A	302	EDO	O1-C1-C2-O2
3	B	302	EDO	O1-C1-C2-O2
5	D	303	BVT	C35-C34-N8-C33
5	C	303	BVT	C34-C35-C36-O5
5	B	303[A]	BVT	N8-C34-C35-C36
4	A	303[B]	BV8	C36-C37-O10-P1
4	A	303[B]	BV8	C13-C14-C15-N3
5	A	304[A]	BVT	C12-C13-C14-N5
5	A	304[A]	BVT	O8-C40-C41-O10
5	C	303	BVT	C31-C32-N7-C33
5	A	304[A]	BVT	N8-C34-C35-C36
5	C	303	BVT	O16-C42-C43-C44
4	A	303[B]	BV8	O2-C20-C21-N4
4	A	303[B]	BV8	C20-C21-C28-C29
4	A	303[B]	BV8	N4-C21-C28-C29
5	B	303[A]	BVT	C34-C35-C36-O5
5	C	303	BVT	N5-C14-C15-N4
4	A	303[B]	BV8	N3-C20-C21-N4
5	C	303	BVT	O16-C42-C43-O17
4	A	303[B]	BV8	P2-O13-P1-O10
5	A	304[A]	BVT	P2-O13-P1-O10
5	B	303[A]	BVT	C34-C35-C36-O6
5	C	303	BVT	C34-C35-C36-O6
3	C	302	EDO	O1-C1-C2-O2
4	A	303[B]	BV8	C41-C42-N7-C43
5	A	304[A]	BVT	C45-C46-N9-C4
4	A	303[B]	BV8	C13-C14-C15-C16
5	A	304[A]	BVT	C12-C13-C14-C15
5	A	304[A]	BVT	C34-C35-C36-O5
5	A	304[A]	BVT	C41-O10-P1-O11
5	A	304[A]	BVT	C42-O16-P2-O14
5	B	303[A]	BVT	C42-O16-P2-O13
5	C	303	BVT	N5-C14-C15-O1
5	A	304[A]	BVT	C34-C35-C36-O6
5	B	303[A]	BVT	C40-C41-O10-P1

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Mol	Chain	Res	Type	Atoms
5	D	303	BVT	C19-C20-C29-C30
5	B	303[A]	BVT	C30-C31-C32-N7
5	C	303	BVT	C23-C22-O4-C21
5	B	303[A]	BVT	P1-O13-P2-O16
5	B	303[A]	BVT	N5-C14-C15-O1
5	C	303	BVT	N6-C20-C29-C30
5	A	304[A]	BVT	C19-C20-C29-C30
5	D	303	BVT	C23-C22-O4-C21
4	A	303[B]	BV8	O2-C20-C21-C28
4	A	303[B]	BV8	O16-C38-C39-O17
5	B	303[A]	BVT	O16-C42-C43-O17
5	C	303	BVT	C9-C12-C13-C14
5	B	303[A]	BVT	C23-C22-O4-C21
5	A	304[A]	BVT	C35-C34-N8-C33
4	A	303[B]	BV8	O17-C42-N7-C43
5	A	304[A]	BVT	O17-C46-N9-C4
4	A	303[B]	BV8	N3-C20-C21-C28
5	B	303[A]	BVT	P1-O13-P2-O14

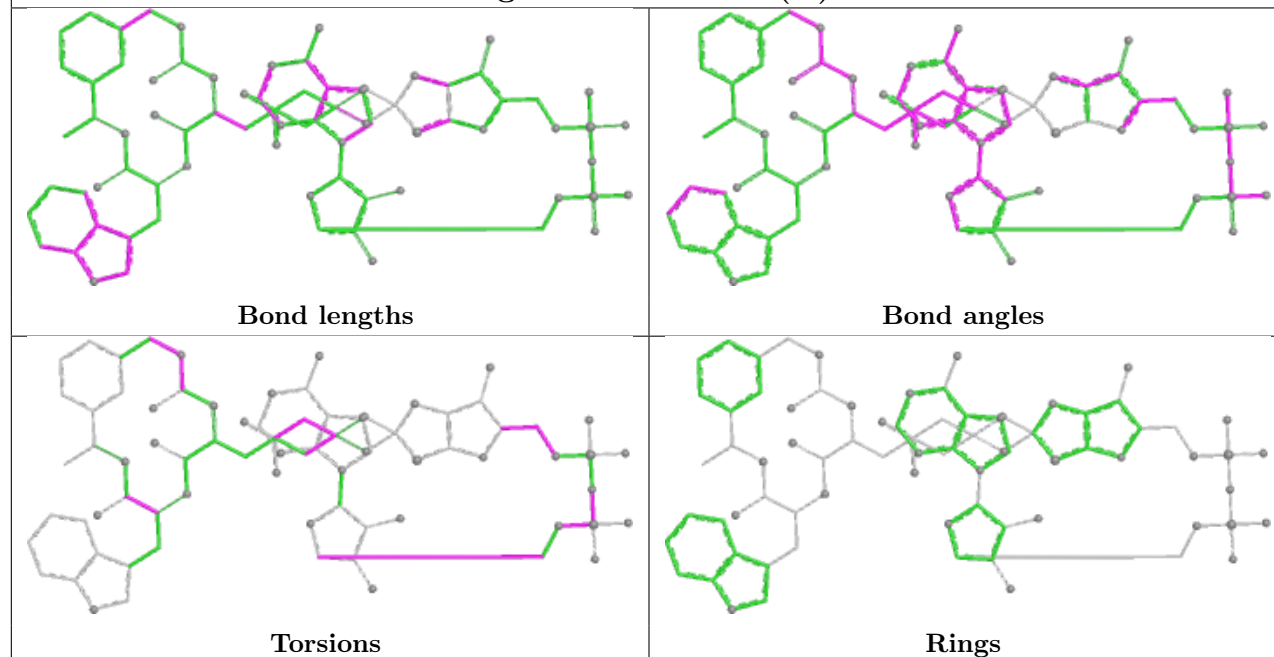
There are no ring outliers.

5 monomers are involved in 10 short contacts:

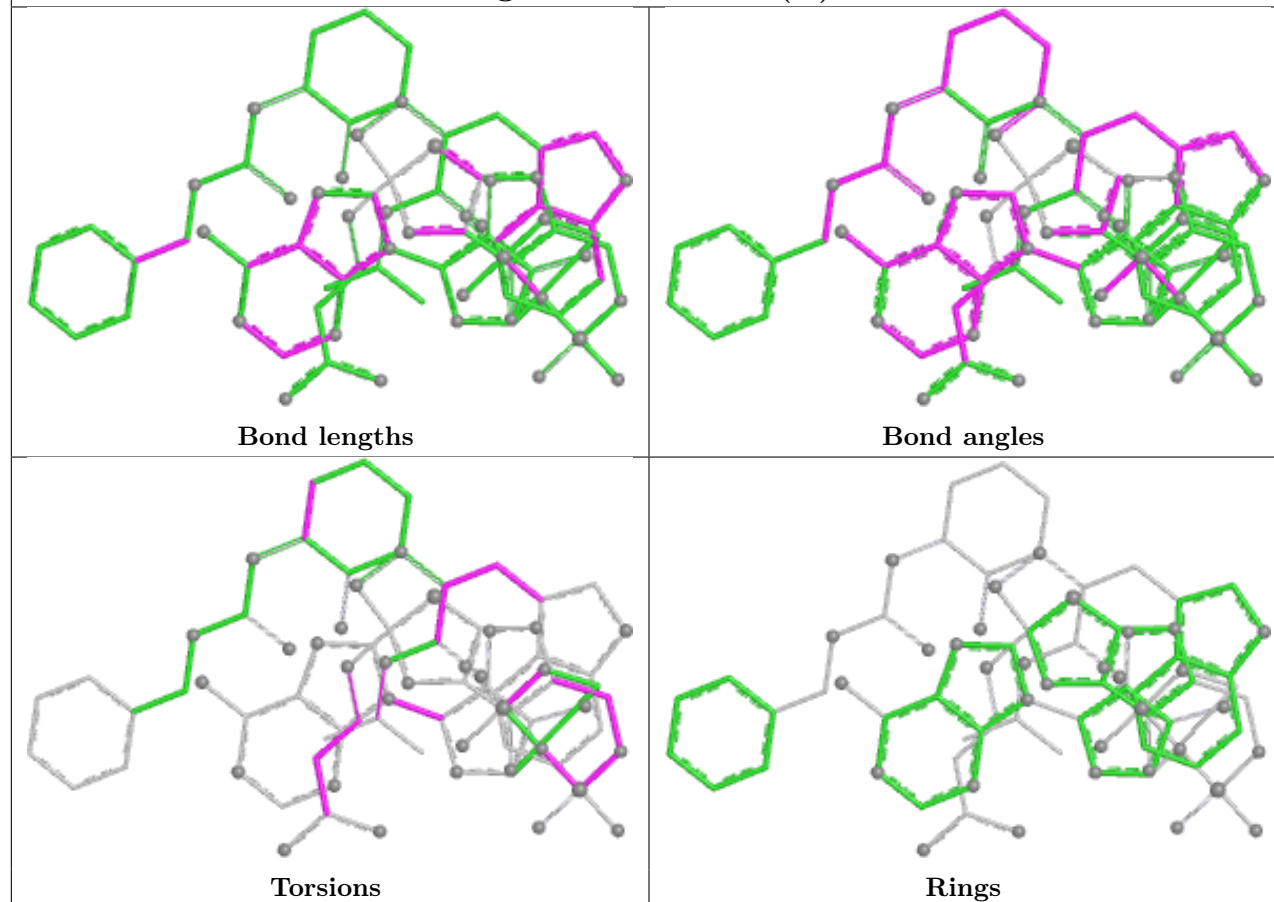
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	303[A]	BVT	2	0
5	A	304[A]	BVT	2	0
4	A	303[B]	BV8	3	0
5	D	303	BVT	1	0
5	C	303	BVT	2	0

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.

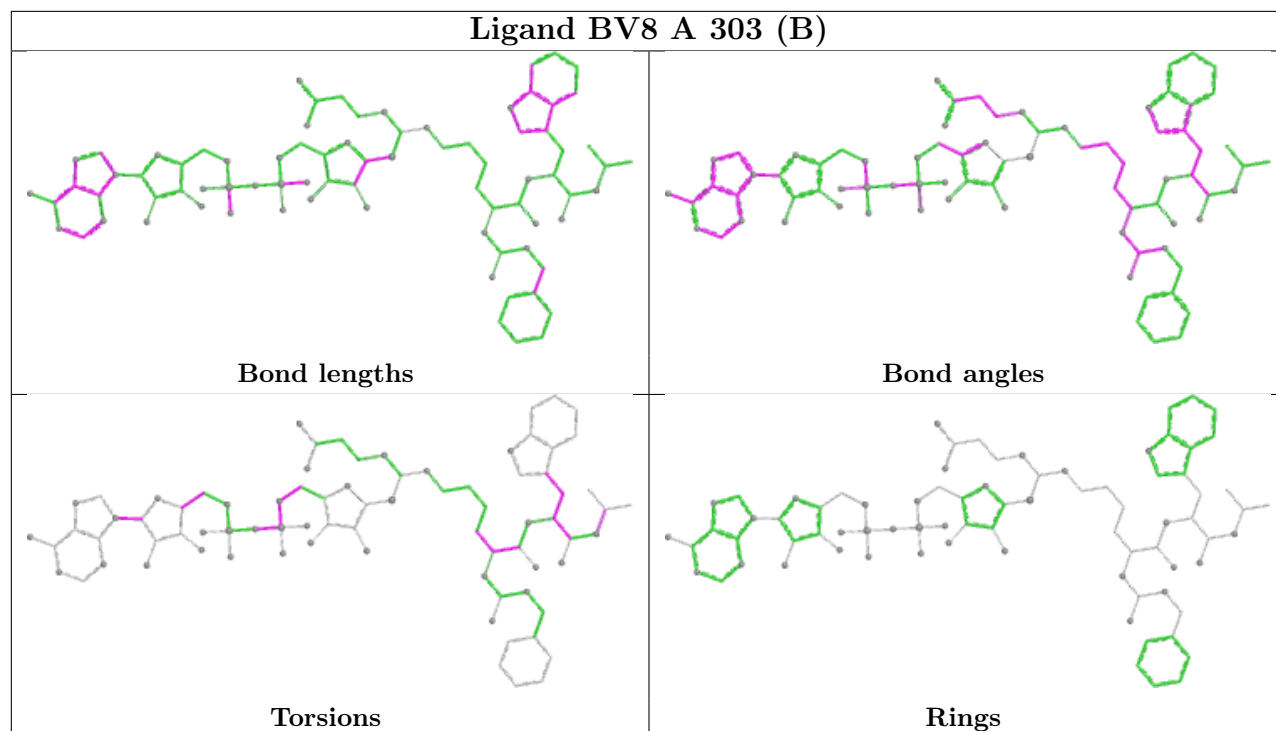
Ligand BVT B 303 (A)



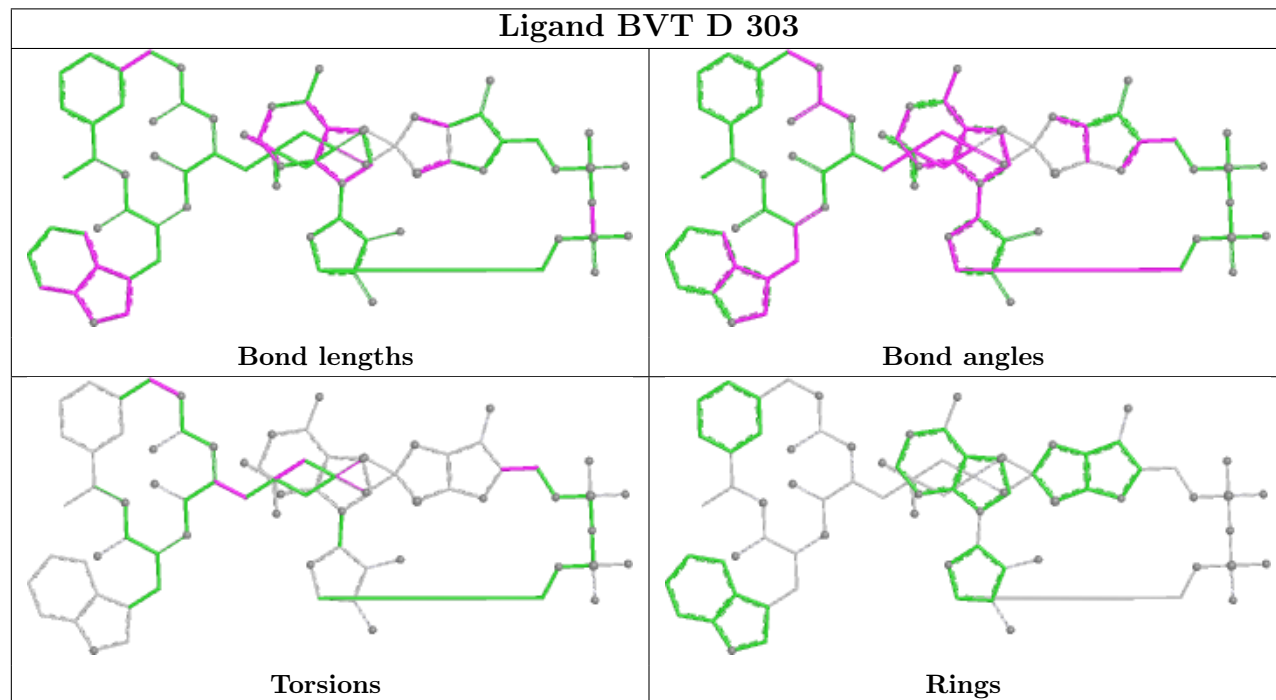
Ligand BVT A 304 (A)

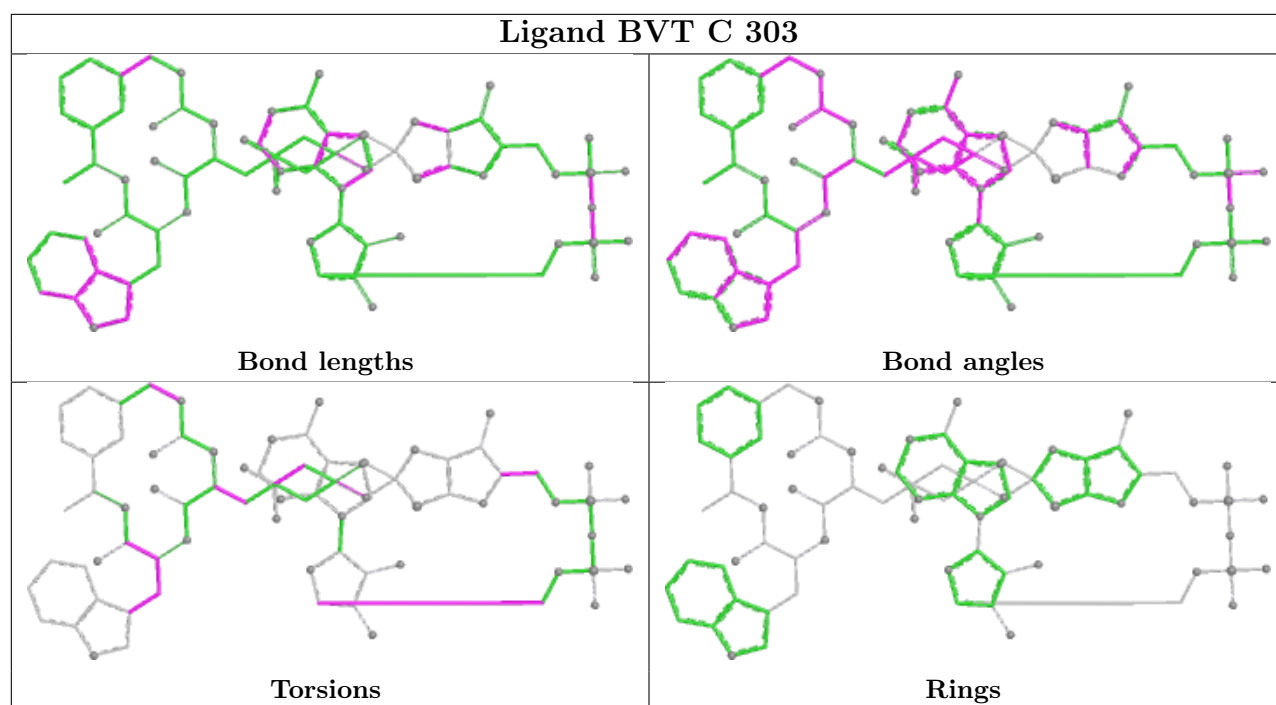


Ligand BV8 A 303 (B)



Ligand BVT D 303





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	274/277 (98%)	0.31	3 (1%) 78 74	24, 49, 66, 107	1 (0%)
1	B	275/277 (99%)	0.38	6 (2%) 62 58	37, 50, 70, 87	1 (0%)
1	C	274/277 (98%)	0.48	10 (3%) 46 42	30, 53, 82, 111	2 (0%)
1	D	275/277 (99%)	0.40	5 (1%) 67 63	30, 52, 73, 130	1 (0%)
All	All	1098/1108 (99%)	0.39	24 (2%) 62 58	24, 51, 72, 130	5 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	THR	3.7
1	A	251[A]	TYR	3.1
1	D	26	PHE	3.0
1	C	26	PHE	2.9
1	B	251	TYR	2.7
1	B	26	PHE	2.7
1	C	72	PHE	2.5
1	C	193	ALA	2.5
1	D	29	MET	2.5
1	A	106	ARG	2.4
1	B	252	PRO	2.3
1	D	25	PRO	2.3
1	D	68	GLY	2.3
1	D	217	VAL	2.3
1	C	25	PRO	2.3
1	C	39	PHE	2.3
1	B	63	VAL	2.2
1	C	69	PRO	2.2
1	C	104	VAL	2.1
1	A	105	MET	2.1
1	C	30	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	68	GLY	2.1
1	B	27	THR	2.1
1	B	151	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

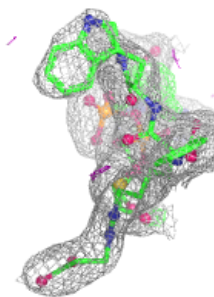
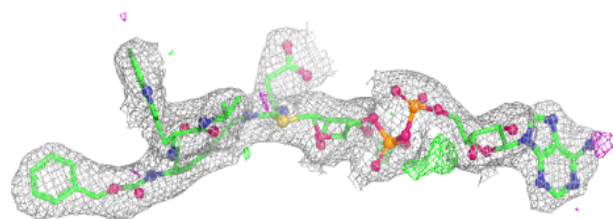
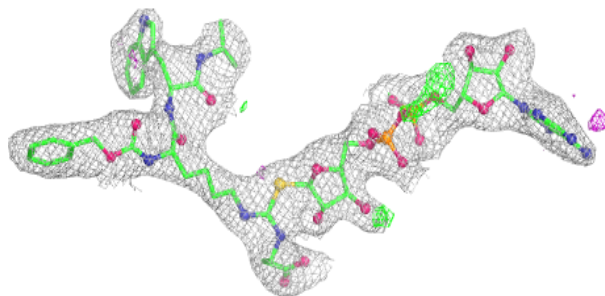
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	302	4/4	0.78	0.13	54,56,56,56	0
3	EDO	B	302	4/4	0.78	0.16	71,74,76,77	0
3	EDO	C	302	4/4	0.78	0.20	56,56,58,58	0
3	EDO	D	302	4/4	0.85	0.12	44,45,46,47	0
4	BV8	A	303[B]	80/80	0.88	0.11	33,39,64,65	80
5	BVT	A	304[A]	80/80	0.88	0.12	37,49,72,72	80
5	BVT	B	303[A]	80/80	0.88	0.11	32,51,68,75	0
5	BVT	C	303	80/80	0.88	0.11	39,50,62,69	0
5	BVT	D	303	80/80	0.92	0.10	28,49,64,69	0
2	ZN	B	301	1/1	0.94	0.07	50,50,50,50	0
2	ZN	C	301	1/1	0.97	0.06	57,57,57,57	0
2	ZN	A	301	1/1	0.97	0.04	50,50,50,50	0
2	ZN	D	301	1/1	0.98	0.04	48,48,48,48	0

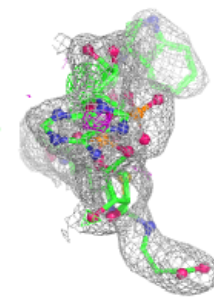
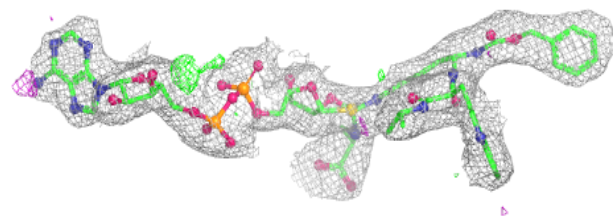
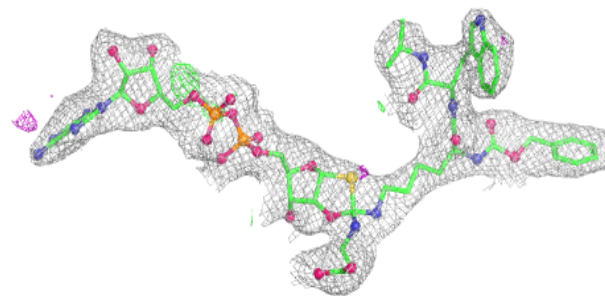
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

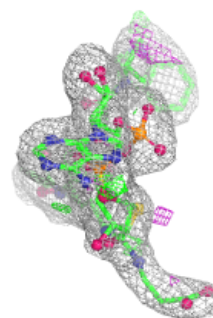
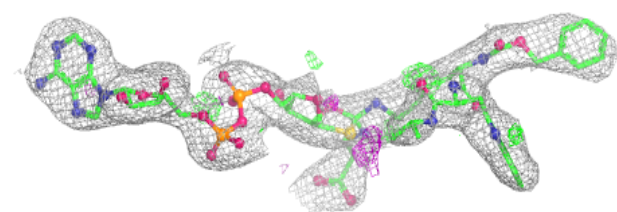
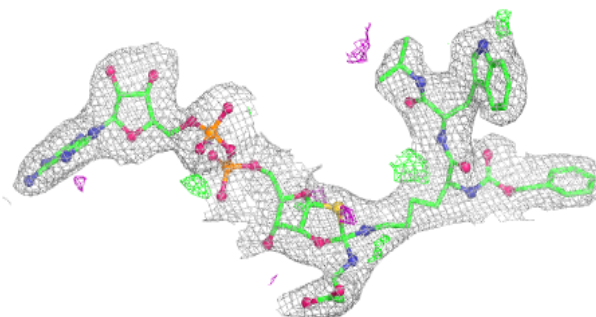
**Electron density around BVT A 304 (A):**

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

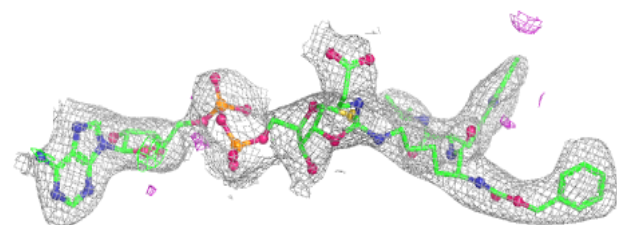
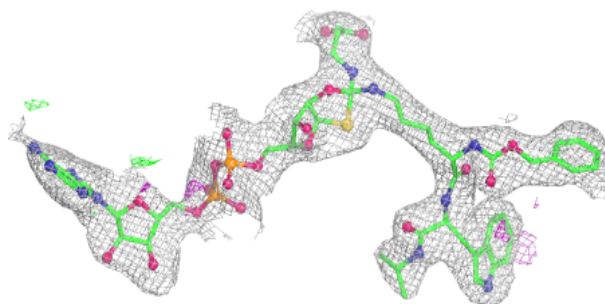


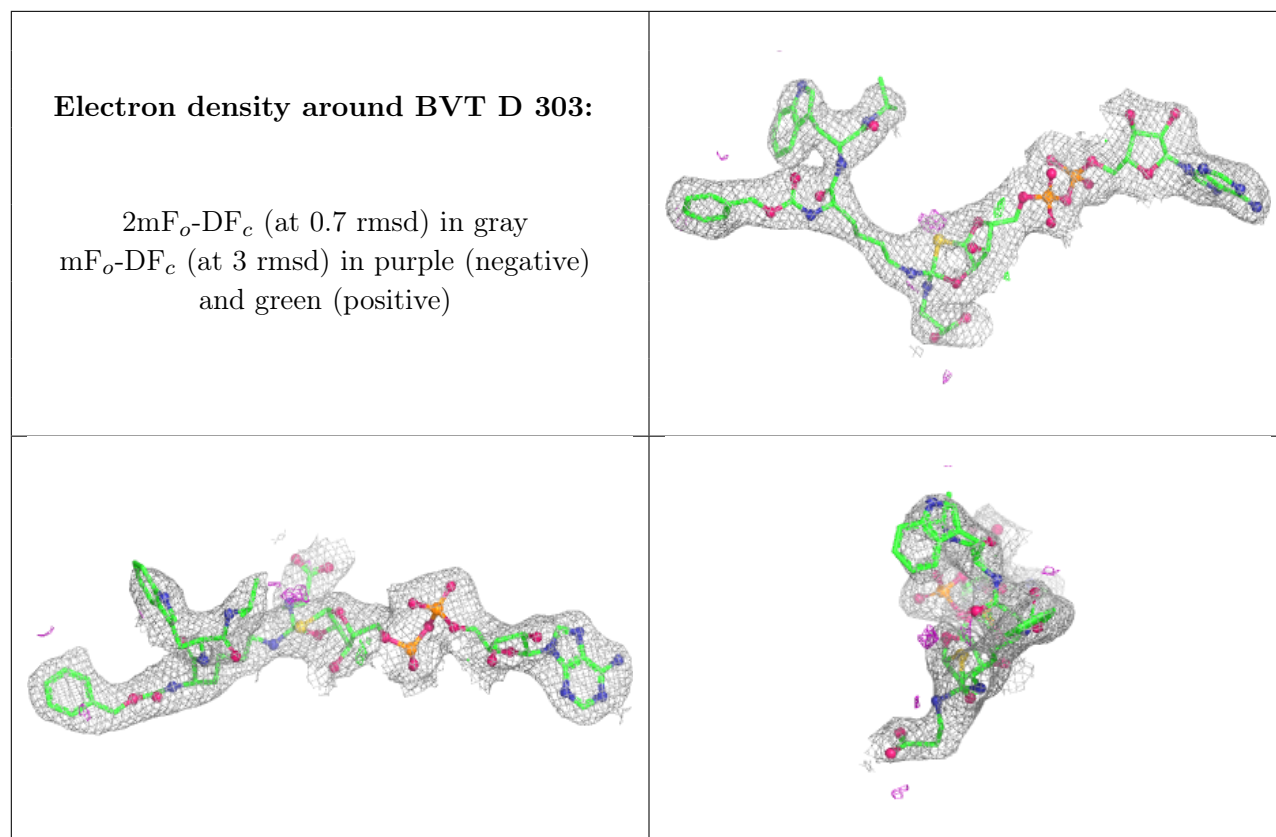
Electron density around BVT B 303 (A):

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

**Electron density around BVT C 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 [i](#)

There are no such residues in this entry.