



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:44 am BST

PDB ID : 6EQS  
Title : Human Sirt5 in complex with stalled peptidylimide intermediate of inhibitory compound 29  
Authors : Pannek, M.; Steegborn, C.  
Deposited on : 2017-10-15  
Resolution : 1.32 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.

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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

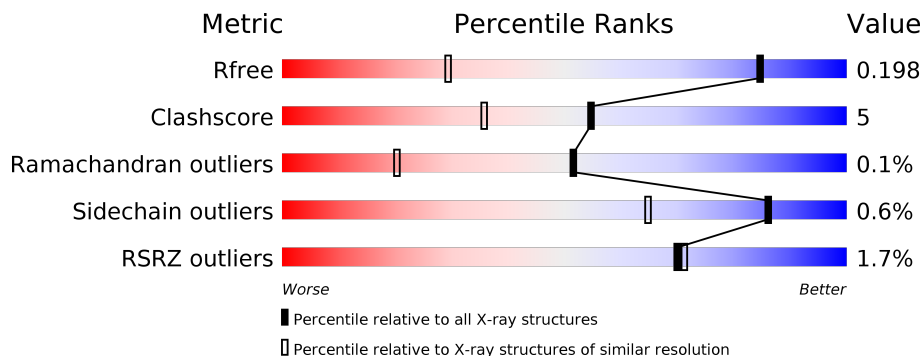
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.32 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	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

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  $\geq 3$ , 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	275	 3% 79% 17% ...
1	B	275	 82% 13% ..
1	C	275	 3% 83% 16% .
1	D	275	 3% 83% 15% .

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
4	EDO	B	406	-	-	X	-
4	EDO	C	404	-	-	X	-
5	BU2	A	408	-	-	X	-
5	BU2	B	408[A]	-	-	X	-
5	BU2	B	410	-	-	X	-
5	BU2	D	405	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 10389 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	269	2113	1334	387	377	15	0	9	0
1	B	268	2107	1333	384	376	14	0	10	0
1	C	274	2136	1351	388	384	13	0	6	0
1	D	275	2145	1356	389	387	13	0	7	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	expression tag	UNP Q9NXA8
A	29	ILE	-	expression tag	UNP Q9NXA8
A	30	ASP	-	expression tag	UNP Q9NXA8
A	31	PRO	-	expression tag	UNP Q9NXA8
A	32	PHE	-	expression tag	UNP Q9NXA8
A	33	THR	-	expression tag	UNP Q9NXA8
B	28	GLY	-	expression tag	UNP Q9NXA8
B	29	ILE	-	expression tag	UNP Q9NXA8
B	30	ASP	-	expression tag	UNP Q9NXA8
B	31	PRO	-	expression tag	UNP Q9NXA8
B	32	PHE	-	expression tag	UNP Q9NXA8
B	33	THR	-	expression tag	UNP Q9NXA8
C	28	GLY	-	expression tag	UNP Q9NXA8
C	29	ILE	-	expression tag	UNP Q9NXA8
C	30	ASP	-	expression tag	UNP Q9NXA8
C	31	PRO	-	expression tag	UNP Q9NXA8
C	32	PHE	-	expression tag	UNP Q9NXA8
C	33	THR	-	expression tag	UNP Q9NXA8
D	28	GLY	-	expression tag	UNP Q9NXA8
D	29	ILE	-	expression tag	UNP Q9NXA8
D	30	ASP	-	expression tag	UNP Q9NXA8

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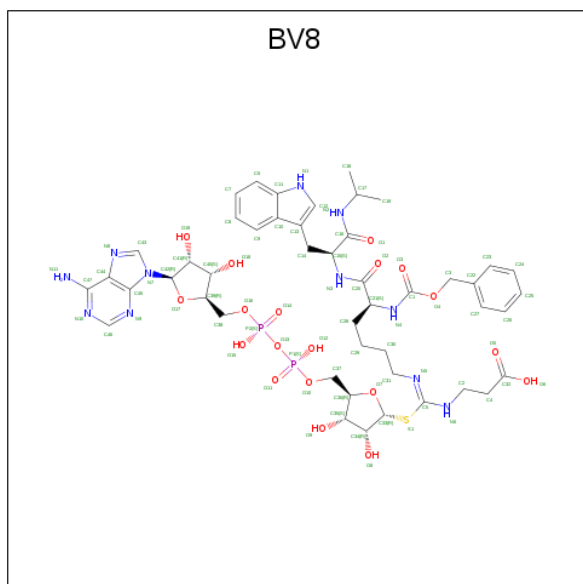
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Chain	Residue	Modelled	Actual	Comment	Reference
D	31	PRO	-	expression tag	UNP Q9NXA8
D	32	PHE	-	expression tag	UNP Q9NXA8
D	33	THR	-	expression tag	UNP Q9NXA8

- 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 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).



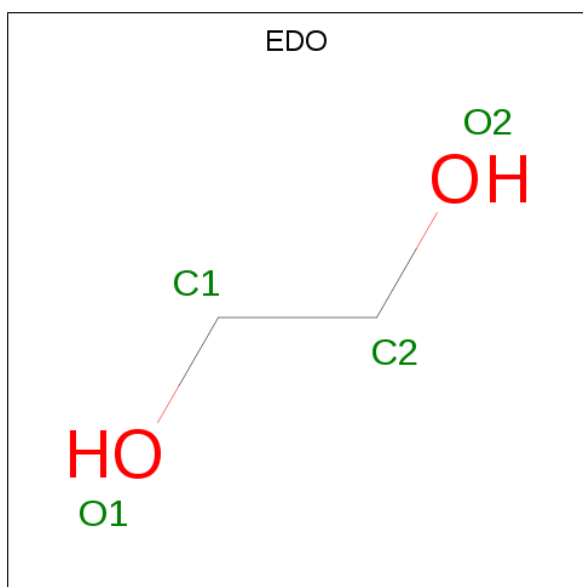
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 160 94 22 38 4 2	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	B	1	Total	C	N	O	P	S	0	1
			160	94	22	38	4	2		
3	C	1	Total	C	N	O	P	S	0	1
			160	94	22	38	4	2		
3	D	1	Total	C	N	O	P	S	0	1
			160	94	22	38	4	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



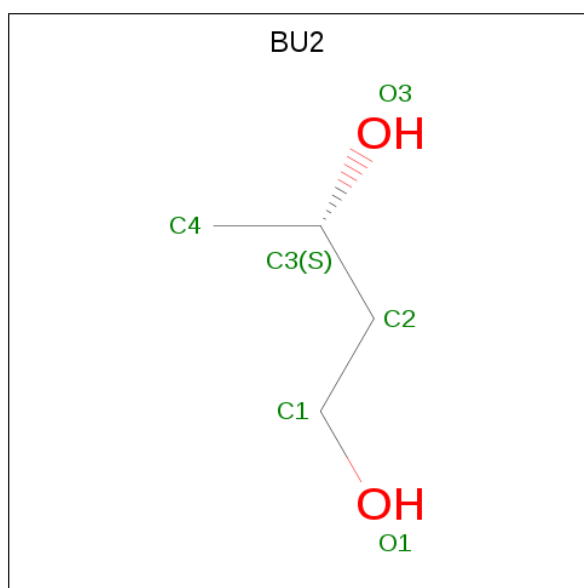
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	1
			8	4 4		
4	A	1	Total	C O	0	1
			8	4 4		
4	A	1	Total	C O	0	1
			8	4 4		
4	A	1	Total	C O	0	0
			4	2 2		
4	A	1	Total	C O	0	0
			4	2 2		
4	B	1	Total	C O	0	1
			8	4 4		
4	B	1	Total	C O	0	1
			8	4 4		
4	B	1	Total	C O	0	1
			8	4 4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 8 4 4	0	1
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 8 4 4	0	1
4	D	1	Total C O 8 4 4	0	1

- Molecule 5 is 1,3-BUTANEDIOL (three-letter code: BU2) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



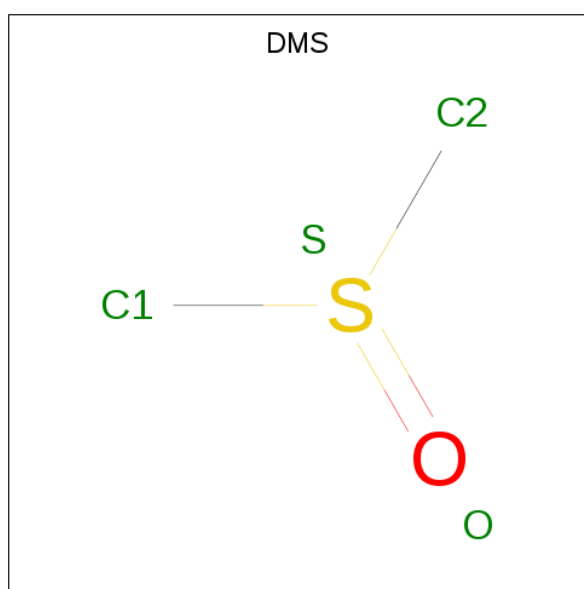
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 4 2	0	0
5	A	1	Total C O 6 4 2	0	0
5	B	1	Total C O 12 8 4	0	1
5	B	1	Total C O 6 4 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 4 2	0	0
5	C	1	Total C O 6 4 2	0	0
5	D	1	Total C O 6 4 2	0	0
5	D	1	Total C O 6 4 2	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	294	Total O 294 294	0	0
7	B	288	Total O 288 288	0	0
7	C	255	Total O 255 255	0	0

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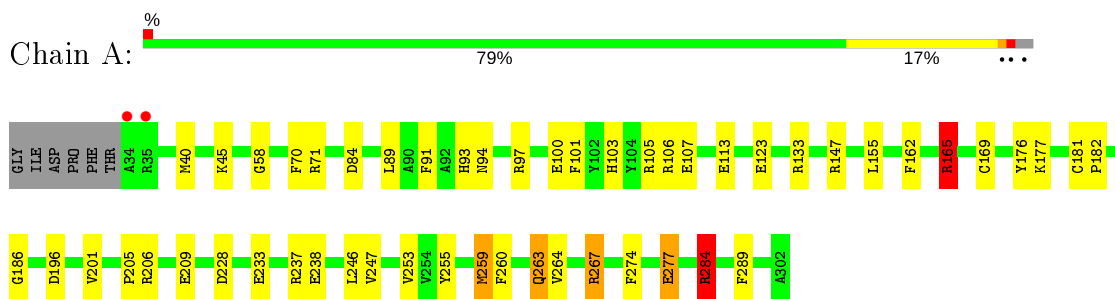
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	D	249	Total 249	O 249	0	0

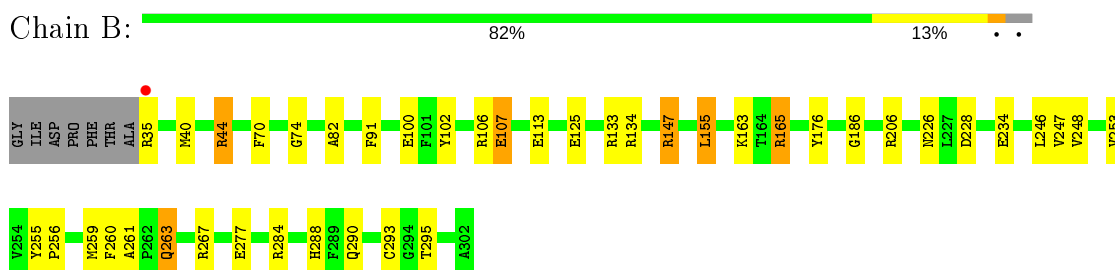
### 3 Residue-property plots [i](#)

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.

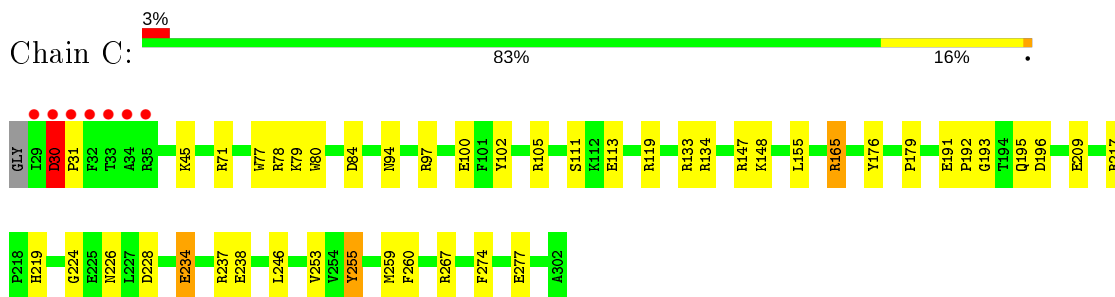
- Molecule 1: NAD-dependent protein deacylase sirtuin-5, mitochondrial



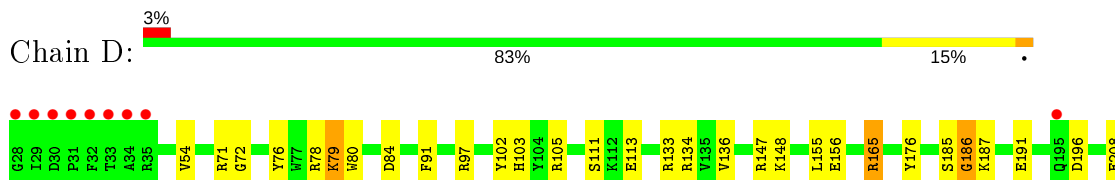
- Molecule 1: NAD-dependent protein deacylase sirtuin-5, mitochondrial

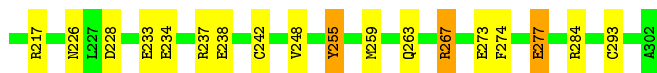


- Molecule 1: NAD-dependent protein deacylase sirtuin-5, mitochondrial



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





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.33Å 55.97Å 123.03Å 97.39° 99.29° 90.52°	Depositor
Resolution (Å)	43.77 – 1.32 43.77 – 1.32	Depositor EDS
% Data completeness (in resolution range)	91.9 (43.77-1.32) 91.9 (43.77-1.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.32Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.160 , 0.209 0.159 , 0.198	Depositor DCC
$R_{free}$ test set	2388 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10389	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 91.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3245e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: BU2, ZN, BV8, DMS, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.58	17/2187 (0.8%)	1.59	37/2964 (1.2%)
1	B	1.52	19/2187 (0.9%)	1.52	27/2965 (0.9%)
1	C	1.60	21/2203 (1.0%)	1.44	29/2990 (1.0%)
1	D	1.69	23/2218 (1.0%)	1.43	25/3009 (0.8%)
All	All	1.60	80/8795 (0.9%)	1.50	118/11928 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	6

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	234	GLU	CD-OE2	30.55	1.59	1.25
1	C	234	GLU	CD-OE2	18.00	1.45	1.25
1	D	234	GLU	CD-OE1	13.73	1.40	1.25
1	A	238	GLU	CD-OE1	-11.62	1.12	1.25
1	C	165	ARG	CZ-NH1	-9.30	1.21	1.33
1	C	234	GLU	CG-CD	9.06	1.65	1.51
1	C	111	SER	CB-OG	8.88	1.53	1.42
1	D	156	GLU	CD-OE2	-8.70	1.16	1.25
1	D	277	GLU	CB-CG	-8.63	1.35	1.52
1	D	111	SER	CB-OG	8.15	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	GLU	CD-OE2	-7.99	1.16	1.25
1	D	238	GLU	CD-OE1	-7.87	1.17	1.25
1	B	165	ARG	CZ-NH1	-7.87	1.22	1.33
1	A	165	ARG	CZ-NH1	-7.76	1.23	1.33
1	D	78	ARG	CZ-NH1	7.70	1.43	1.33
1	B	277	GLU	CB-CG	-7.70	1.37	1.52
1	C	238	GLU	CD-OE1	-7.69	1.17	1.25
1	C	255	TYR	CE2-CZ	7.40	1.48	1.38
1	B	263	GLN	CB-CG	-7.32	1.32	1.52
1	B	100	GLU	CD-OE1	-7.04	1.18	1.25
1	C	78	ARG	CZ-NH1	7.02	1.42	1.33
1	A	113	GLU	CD-OE1	-6.97	1.18	1.25
1	C	255	TYR	CE1-CZ	-6.73	1.29	1.38
1	C	195	GLN	CD-OE1	6.72	1.38	1.24
1	D	217	ARG	CZ-NH2	-6.58	1.24	1.33
1	A	100	GLU	CD-OE2	6.58	1.32	1.25
1	C	30	ASP	CG-OD1	6.56	1.40	1.25
1	A	263	GLN	CB-CG	-6.51	1.34	1.52
1	B	125	GLU	CD-OE1	-6.50	1.18	1.25
1	B	100	GLU	CD-OE2	6.32	1.32	1.25
1	D	233	GLU	CD-OE2	6.29	1.32	1.25
1	C	100	GLU	CD-OE2	6.27	1.32	1.25
1	A	147	ARG	CG-CD	6.19	1.67	1.51
1	D	72	GLY	C-O	-6.19	1.13	1.23
1	A	247	VAL	CB-CG1	-6.17	1.39	1.52
1	C	195	GLN	CD-NE2	6.10	1.48	1.32
1	A	277	GLU	CB-CG	-6.09	1.40	1.52
1	A	58	GLY	N-CA	-6.08	1.36	1.46
1	D	134	ARG	CZ-NH1	5.98	1.40	1.33
1	D	113	GLU	CG-CD	5.97	1.60	1.51
1	B	155	LEU	CB-CG	-5.96	1.35	1.52
1	A	201	VAL	CB-CG2	-5.95	1.40	1.52
1	D	191	GLU	CD-OE1	5.91	1.32	1.25
1	B	44	ARG	CG-CD	-5.86	1.37	1.51
1	D	226	ASN	CB-CG	-5.85	1.37	1.51
1	D	208	GLU	CG-CD	-5.84	1.43	1.51
1	A	107	GLU	CD-OE2	-5.82	1.19	1.25
1	B	255	TYR	CE1-CZ	-5.79	1.31	1.38
1	D	208	GLU	CB-CG	-5.77	1.41	1.52
1	D	165	ARG	CD-NE	-5.74	1.36	1.46
1	B	253	VAL	CB-CG2	-5.71	1.40	1.52
1	C	192	PRO	C-O	5.60	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284[A]	ARG	CZ-NH2	5.60	1.40	1.33
1	B	284[B]	ARG	CZ-NH2	5.60	1.40	1.33
1	C	209	GLU	CB-CG	-5.59	1.41	1.52
1	C	102	TYR	CE2-CZ	-5.50	1.31	1.38
1	D	255	TYR	CG-CD1	5.50	1.46	1.39
1	C	277	GLU	CD-OE2	5.49	1.31	1.25
1	D	234	GLU	CG-CD	5.47	1.60	1.51
1	A	253	VAL	CB-CG1	-5.45	1.41	1.52
1	C	267	ARG	CD-NE	-5.41	1.37	1.46
1	D	273	GLU	CD-OE1	5.40	1.31	1.25
1	B	147	ARG	CZ-NH2	5.40	1.40	1.33
1	C	77	TRP	CZ3-CH2	-5.40	1.31	1.40
1	D	165	ARG	NE-CZ	5.38	1.40	1.33
1	D	111	SER	CA-CB	5.37	1.61	1.52
1	B	74	GLY	C-O	-5.35	1.15	1.23
1	B	277	GLU	CA-CB	-5.30	1.42	1.53
1	B	107	GLU	CD-OE2	-5.28	1.19	1.25
1	A	176	TYR	CE1-CZ	-5.25	1.31	1.38
1	B	102	TYR	CG-CD2	-5.17	1.32	1.39
1	A	91	PHE	CG-CD2	-5.16	1.31	1.38
1	D	186	GLY	CA-C	-5.16	1.43	1.51
1	B	35	ARG	N-CA	5.16	1.56	1.46
1	B	134	ARG	CZ-NH2	-5.13	1.26	1.33
1	C	193	GLY	N-CA	5.08	1.53	1.46
1	C	191	GLU	CD-OE1	5.06	1.31	1.25
1	A	274	PHE	CB-CG	-5.05	1.42	1.51
1	A	209	GLU	C-O	5.02	1.32	1.23
1	C	179	PRO	CA-C	-5.00	1.42	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284[A]	ARG	NE-CZ-NH2	17.53	129.06	120.30
1	A	284[B]	ARG	NE-CZ-NH2	17.53	129.06	120.30
1	B	267[A]	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	B	267[B]	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	D	267	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	C	267	ARG	NE-CZ-NH1	-12.31	114.14	120.30
1	C	133	ARG	NE-CZ-NH1	11.29	125.94	120.30
1	A	267[A]	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	267[B]	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	D	84	ASP	CB-CG-OD2	-11.06	108.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ASP	CB-CG-OD2	-10.92	108.47	118.30
1	B	106	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	C	267	ARG	NE-CZ-NH2	10.37	125.49	120.30
1	A	106	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	D	234	GLU	OE1-CD-OE2	10.00	135.30	123.30
1	D	133	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	D	217	ARG	NE-CZ-NH1	-9.74	115.43	120.30
1	C	78	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	A	237	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	B	133	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	C	133	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	B	267[A]	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	B	267[B]	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	228	ASP	CB-CG-OD1	9.13	126.52	118.30
1	B	228	ASP	CB-CG-OD1	9.11	126.50	118.30
1	B	260	PHE	CB-CG-CD1	9.10	127.17	120.80
1	C	246	LEU	CB-CG-CD1	9.06	126.40	111.00
1	A	40	MET	CG-SD-CE	-8.67	86.32	100.20
1	B	133	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	B	102	TYR	CB-CG-CD2	8.54	126.13	121.00
1	B	255	TYR	CB-CG-CD1	8.50	126.10	121.00
1	C	148	LYS	CD-CE-NZ	-8.39	92.40	111.70
1	B	246	LEU	CB-CG-CD1	8.37	125.22	111.00
1	B	102	TYR	CB-CG-CD1	-8.35	115.99	121.00
1	A	155	LEU	CA-CB-CG	8.22	134.22	115.30
1	A	147	ARG	CG-CD-NE	-8.10	94.78	111.80
1	A	133	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	C	134	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	D	217	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	D	259	MET	CG-SD-CE	7.89	112.83	100.20
1	D	284	ARG	CG-CD-NE	-7.75	95.53	111.80
1	B	260	PHE	CB-CG-CD2	-7.71	115.40	120.80
1	B	206[A]	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	206[B]	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	C	259	MET	CG-SD-CE	7.51	112.22	100.20
1	D	228	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	196	ASP	CB-CG-OD1	7.46	125.02	118.30
1	D	148	LYS	CD-CE-NZ	-7.45	94.56	111.70
1	A	113	GLU	OE1-CD-OE2	-7.33	114.51	123.30
1	D	133	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	C	234	GLU	CG-CD-OE1	-7.19	103.91	118.30
1	C	274	PHE	CB-CG-CD1	7.18	125.83	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	TYR	CB-CG-CD2	7.18	125.31	121.00
1	C	228	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	40	MET	CG-SD-CE	-7.01	88.98	100.20
1	A	260	PHE	CB-CG-CD1	6.96	125.67	120.80
1	A	284[A]	ARG	CG-CD-NE	6.85	126.19	111.80
1	A	284[B]	ARG	CG-CD-NE	6.85	126.19	111.80
1	D	267	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	101	PHE	CB-CG-CD1	6.80	125.56	120.80
1	B	147	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	C	45	LYS	CD-CE-NZ	6.76	127.24	111.70
1	A	97	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	289	PHE	CB-CG-CD2	6.68	125.48	120.80
1	A	101	PHE	CB-CG-CD2	-6.63	116.16	120.80
1	B	253	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	A	259[A]	MET	CG-SD-CE	6.49	110.59	100.20
1	A	259[B]	MET	CG-SD-CE	6.49	110.59	100.20
1	D	78	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	C	260	PHE	CB-CG-CD1	6.43	125.30	120.80
1	D	237	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	234	GLU	CG-CD-OE1	-6.38	105.54	118.30
1	C	191	GLU	OE1-CD-OE2	-6.33	115.71	123.30
1	C	113	GLU	CG-CD-OE2	6.28	130.86	118.30
1	A	284[A]	ARG	NH1-CZ-NH2	-6.28	112.50	119.40
1	A	284[B]	ARG	NH1-CZ-NH2	-6.28	112.50	119.40
1	A	169	CYS	CA-CB-SG	-6.27	102.72	114.00
1	A	71	ARG	CG-CD-NE	-6.22	98.75	111.80
1	C	176	TYR	CB-CG-CD2	5.97	124.58	121.00
1	A	196	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	A	45	LYS	CD-CE-NZ	-5.86	98.23	111.70
1	A	84	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	237	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	D	274	PHE	CB-CG-CD1	5.77	124.84	120.80
1	B	155	LEU	CA-CB-CG	5.74	128.49	115.30
1	D	97	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	228	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	177	LYS	CD-CE-NZ	5.70	124.80	111.70
1	D	176	TYR	CB-CG-CD1	5.66	124.39	121.00
1	A	123	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	A	162	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	D	102	TYR	CZ-CE2-CD2	5.60	124.84	119.80
1	B	91	PHE	CB-CG-CD1	5.58	124.70	120.80
1	C	30	ASP	CB-CA-C	5.55	121.50	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	267[A]	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	A	267[B]	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	C	217	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	44	ARG	CG-CD-NE	5.45	123.25	111.80
1	C	105	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	113	GLU	CG-CD-OE1	-5.43	107.44	118.30
1	C	71	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	97	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	255	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	D	105	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	246	LEU	CB-CG-CD1	5.20	119.84	111.00
1	B	106	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	D	156	GLU	CG-CD-OE2	5.19	128.68	118.30
1	C	102	TYR	CB-CG-CD2	5.17	124.10	121.00
1	B	246	LEU	CB-CA-C	-5.17	100.38	110.20
1	D	91	PHE	CB-CG-CD1	5.15	124.41	120.80
1	D	267	ARG	CG-CD-NE	-5.10	101.09	111.80
1	C	119	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	D	155	LEU	CA-CB-CG	5.03	126.87	115.30
1	C	105	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	155	LEU	CA-CB-CG	5.01	126.82	115.30
1	D	267	ARG	CD-NE-CZ	5.01	130.61	123.60
1	B	165	ARG	CD-NE-CZ	5.01	130.61	123.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	B	165	ARG	Sidechain
1	C	165	ARG	Sidechain
1	C	234	GLU	Sidechain
1	D	165	ARG	Sidechain
1	D	255	TYR	Sidechain

## 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	2113	0	2106	17	0
1	B	2107	0	2110	27	1
1	C	2136	0	2118	15	0
1	D	2145	0	2127	18	1
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	160	0	0	0	0
3	B	160	0	0	9	0
3	C	160	0	0	3	0
3	D	160	0	0	2	0
4	A	32	0	47	5	0
4	B	32	0	45	4	0
4	C	16	0	23	5	0
4	D	16	0	24	0	0
5	A	12	0	19	9	0
5	B	24	0	40	13	0
5	C	6	0	9	0	0
5	D	12	0	20	4	0
6	A	8	0	12	0	0
7	A	294	0	0	8	2
7	B	288	0	0	10	2
7	C	255	0	0	3	1
7	D	249	0	0	7	2
All	All	10389	0	8700	94	5

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 5.

All (94) 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:103:HIS:NE2	5:D:405:BU2:HC11	1.73	1.01
5:B:408[B]:BU2:O1	5:B:408[B]:BU2:O3	1.63	0.98
1:B:295[B]:THR:HG23	7:B:509:HOH:O	1.70	0.92
1:B:234:GLU:OE2	7:B:501:HOH:O	1.91	0.88
3:B:402[A]:BV8:C8	7:B:728:HOH:O	2.28	0.81
4:A:403[A]:EDO:O1	4:A:404[A]:EDO:H22	1.81	0.81
1:D:248:VAL:HG13	1:D:293[B]:CYS:SG	2.20	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:OD1	7:A:501:HOH:O	1.99	0.79
1:D:103:HIS:NE2	5:D:405:BU2:C1	2.46	0.78
1:A:263:GLN:OE1	3:D:402[B]:BV8:O3	2.03	0.77
3:B:402[A]:BV8:C9	7:B:728:HOH:O	2.35	0.74
4:B:404[B]:EDO:O2	4:B:406:EDO:O1	2.04	0.74
4:A:403[A]:EDO:O1	4:A:404[A]:EDO:C2	2.39	0.69
1:C:94:ASN:OD1	7:C:501:HOH:O	2.11	0.68
1:D:76:TYR:OH	7:D:501:HOH:O	2.08	0.67
1:B:248:VAL:HG13	1:B:293[B]:CYS:SG	2.35	0.66
1:B:295[B]:THR:HG22	7:B:587:HOH:O	1.94	0.66
1:C:30:ASP:HB3	1:C:31:PRO:HD3	1.77	0.66
1:B:263:GLN:NE2	3:C:402[A]:BV8:O3	2.29	0.65
1:D:196:ASP:OD1	7:D:502:HOH:O	2.15	0.65
1:C:219:HIS:HE2	4:C:404:EDO:H21	1.65	0.61
1:D:185:SER:CB	7:D:585:HOH:O	2.49	0.61
1:D:186:GLY:HA2	5:D:405:BU2:HC22	1.82	0.61
5:B:409:BU2:HC22	1:C:253:VAL:O	2.01	0.60
1:B:155:LEU:HD21	1:B:234:GLU:CD	2.23	0.59
1:C:30:ASP:HB3	1:C:31:PRO:CD	2.33	0.58
1:B:147:ARG:HH12	1:B:163:LYS:NZ	2.00	0.58
3:B:402[A]:BV8:C8	7:B:646:HOH:O	2.51	0.58
1:D:263[B]:GLN:HG3	7:D:624:HOH:O	2.04	0.57
1:A:181:CYS:HB2	5:A:408:BU2:HC43	1.86	0.56
5:A:408:BU2:HC12	7:A:696:HOH:O	2.06	0.55
1:D:248:VAL:CG1	1:D:293[B]:CYS:SG	2.94	0.55
1:A:70:PHE:HE1	7:A:750:HOH:O	1.88	0.55
1:A:182:PRO:HD2	5:A:408:BU2:HC43	1.89	0.55
1:C:219:HIS:HE2	4:C:404:EDO:C1	2.21	0.54
1:C:219:HIS:NE2	4:C:404:EDO:H21	2.24	0.53
1:B:226:ASN:ND2	5:B:409:BU2:HC21	2.25	0.52
5:A:408:BU2:HC12	7:A:506:HOH:O	2.09	0.52
1:B:147:ARG:HH12	1:B:163:LYS:HZ3	1.55	0.52
1:B:247[B]:VAL:HG21	1:B:261:ALA:CB	2.40	0.52
1:D:79:LYS:HE3	1:D:80:TRP:CZ2	2.46	0.51
1:B:186:GLY:H	4:B:406:EDO:H11	1.76	0.51
3:B:402[A]:BV8:C9	7:B:646:HOH:O	2.58	0.51
5:A:408:BU2:C1	7:A:506:HOH:O	2.58	0.50
1:A:89:LEU:HD11	1:A:93:HIS:NE2	2.27	0.50
1:B:155:LEU:HD21	1:B:234:GLU:OE2	2.11	0.49
1:C:255:TYR:CE1	3:C:402[D]:BV8:C23	2.95	0.49
1:C:219:HIS:HE2	4:C:404:EDO:C2	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:HE3	1:C:80:TRP:CZ2	2.49	0.48
1:B:113:GLU:OE2	7:B:502:HOH:O	2.20	0.48
1:C:196:ASP:OD1	7:C:502:HOH:O	2.20	0.48
1:A:205:PRO:HA	5:A:408:BU2:HC21	1.97	0.47
1:D:185:SER:HB3	7:D:585:HOH:O	2.11	0.47
1:D:79:LYS:HE3	1:D:80:TRP:CE2	2.50	0.46
1:A:206[B]:ARG:H	5:A:408:BU2:C2	2.28	0.46
1:D:71:ARG:NH2	1:D:277:GLU:OE2	2.49	0.46
1:B:247[B]:VAL:CG2	1:B:261:ALA:CB	2.92	0.46
1:A:182:PRO:HD2	5:A:408:BU2:C4	2.46	0.46
1:A:277:GLU:HB2	7:A:693:HOH:O	2.16	0.46
1:A:284[B]:ARG:NH1	7:A:502:HOH:O	2.25	0.46
1:B:70:PHE:CD1	5:B:408[A]:BU2:HC41	2.51	0.46
1:B:256:PRO:O	1:B:259[B]:MET:SD	2.73	0.46
1:B:259[B]:MET:HE2	1:C:224:GLY:HA2	1.97	0.46
3:B:402[B]:BV8:O15	5:B:410:BU2:HC11	2.16	0.45
1:B:186:GLY:H	4:B:406:EDO:C1	2.29	0.45
1:A:206[A]:ARG:H	5:A:408:BU2:C2	2.29	0.44
1:D:267:ARG:HD2	7:D:713:HOH:O	2.16	0.44
1:B:247[B]:VAL:CG2	1:B:261:ALA:HB2	2.47	0.44
1:B:247[B]:VAL:HG22	1:B:261:ALA:HB2	1.99	0.44
1:B:263:GLN:HG2	1:C:226:ASN:OD1	2.18	0.44
1:B:70:PHE:HA	5:B:408[A]:BU2:HC43	1.99	0.44
3:C:402[A]:BV8:O4	3:C:402[A]:BV8:C20	2.65	0.44
1:D:147[A]:ARG:HG3	7:D:564:HOH:O	2.17	0.43
1:A:105:ARG:HE	4:A:403[B]:EDO:H11	1.82	0.43
1:B:82:ALA:HB2	5:B:408[A]:BU2:HC12	1.99	0.43
1:B:288:HIS:HB2	7:B:652:HOH:O	2.18	0.43
3:B:402[A]:BV8:O15	5:B:410:BU2:HC11	2.19	0.43
3:B:402[B]:BV8:O15	5:B:410:BU2:C1	2.67	0.43
1:B:107:GLU:CD	4:B:406:EDO:H21	2.39	0.42
1:A:264:VAL:HA	1:A:267[B]:ARG:HH21	1.85	0.42
3:B:402[A]:BV8:C20	3:B:402[A]:BV8:O3	2.67	0.42
1:C:219:HIS:HE2	4:C:404:EDO:H11	1.83	0.42
1:B:70:PHE:CE1	5:B:408[A]:BU2:HC41	2.55	0.42
1:A:165:ARG:HD2	7:A:537:HOH:O	2.20	0.42
1:B:226:ASN:HD22	5:B:409:BU2:HC21	1.83	0.41
3:D:402[B]:BV8:O4	3:D:402[B]:BV8:C20	2.68	0.41
1:C:147[A]:ARG:HG3	7:C:680:HOH:O	2.20	0.41
1:D:54:VAL:HG22	1:D:136[A]:VAL:CG1	2.50	0.41
5:B:408[B]:BU2:HC12	7:B:524:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:402[A]:BV8:O15	5:B:410:BU2:C1	2.68	0.41
1:A:103:HIS:NE2	4:A:406:EDO:H12	2.36	0.40
1:A:186:GLY:H	4:A:406:EDO:C1	2.33	0.40
1:D:187:LYS:O	5:D:405:BU2:HC21	2.20	0.40
1:D:54:VAL:HG23	1:D:242:CYS:HB3	2.03	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:547:HOH:O	7:D:729:HOH:O[1_455]	1.75	0.45
7:A:608:HOH:O	7:C:696:HOH:O[1_444]	1.76	0.44
7:A:580:HOH:O	7:A:768:HOH:O[1_455]	1.87	0.33
1:B:234:GLU:OE1	7:B:785:HOH:O[1_655]	2.11	0.09
1:D:147[A]:ARG:NH2	7:D:748:HOH:O[1_655]	2.12	0.08

## 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	276/275 (100%)	273 (99%)	3 (1%)	0	100	100
1	B	276/275 (100%)	273 (99%)	3 (1%)	0	100	100
1	C	278/275 (101%)	274 (99%)	3 (1%)	1 (0%)	34	10
1	D	280/275 (102%)	277 (99%)	3 (1%)	0	100	100
All	All	1110/1100 (101%)	1097 (99%)	12 (1%)	1 (0%)	51	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	30	ASP

### 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	223/219 (102%)	219 (98%)	4 (2%)	59	22
1	B	224/219 (102%)	222 (99%)	2 (1%)	78	51
1	C	225/219 (103%)	225 (100%)	0	100	100
1	D	226/219 (103%)	225 (100%)	1 (0%)	91	76
All	All	898/876 (102%)	891 (99%)	7 (1%)	86	57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259[A]	MET
1	A	259[B]	MET
1	A	284[A]	ARG
1	A	284[B]	ARG
1	B	44	ARG
1	B	290	GLN
1	D	79	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 4 are monoatomic - leaving 43 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	BU2	A	408	-	5,5,5	0.99	0	5,5,5	3.56	1 (20%)
4	EDO	D	403[A]	-	3,3,3	0.77	0	2,2,2	0.56	0
4	EDO	D	403[B]	-	3,3,3	0.94	0	2,2,2	0.62	0
4	EDO	A	404[A]	-	3,3,3	0.42	0	2,2,2	0.99	0
4	EDO	B	403[B]	-	3,3,3	0.89	0	2,2,2	0.33	0
4	EDO	A	406	-	3,3,3	1.30	0	2,2,2	1.20	0
4	EDO	B	403[A]	-	3,3,3	1.28	0	2,2,2	0.60	0
5	BU2	B	408[B]	-	5,5,5	0.51	0	5,5,5	2.66	2 (40%)
5	BU2	A	409	-	5,5,5	1.45	1 (20%)	5,5,5	1.62	1 (20%)
5	BU2	B	408[A]	-	5,5,5	0.44	0	5,5,5	1.13	1 (20%)
5	BU2	C	406	-	5,5,5	0.87	0	5,5,5	1.64	1 (20%)
4	EDO	A	403[A]	-	3,3,3	1.23	1 (33%)	2,2,2	0.67	0
3	BV8	D	402[B]	-	77,86,86	1.84	16 (20%)	87,122,122	1.63	14 (16%)
4	EDO	A	403[B]	-	3,3,3	1.17	0	2,2,2	0.57	0
3	BV8	D	402[C]	-	77,86,86	1.88	18 (23%)	87,122,122	1.79	19 (21%)
4	EDO	B	404[A]	-	3,3,3	0.36	0	2,2,2	0.48	0
4	EDO	B	404[B]	-	3,3,3	0.40	0	2,2,2	0.56	0
4	EDO	C	405	-	3,3,3	0.81	0	2,2,2	0.37	0
5	BU2	D	406	-	5,5,5	0.63	0	5,5,5	2.02	2 (40%)
4	EDO	C	404	-	3,3,3	0.96	0	2,2,2	0.41	0
6	DMS	A	410	-	3,3,3	0.49	0	3,3,3	1.69	1 (33%)
5	BU2	D	405	-	5,5,5	1.37	0	5,5,5	2.45	2 (40%)
3	BV8	A	402[B]	-	77,86,86	2.18	16 (20%)	87,122,122	1.76	19 (21%)
3	BV8	A	402[A]	-	77,86,86	2.03	14 (18%)	87,122,122	1.68	15 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	D	404[B]	-	3,3,3	0.47	0	2,2,2	1.35	0
4	EDO	B	405[A]	-	3,3,3	0.70	0	2,2,2	0.10	0
4	EDO	D	404[A]	-	3,3,3	0.86	0	2,2,2	0.28	0
4	EDO	A	407	-	3,3,3	0.79	0	2,2,2	0.76	0
3	BV8	B	402[A]	-	77,86,86	1.62	10 (12%)	87,122,122	1.97	16 (18%)
4	EDO	A	405[B]	-	3,3,3	0.37	0	2,2,2	0.69	0
3	BV8	B	402[B]	-	77,86,86	1.52	15 (19%)	87,122,122	1.66	16 (18%)
6	DMS	A	411	-	3,3,3	0.36	0	3,3,3	1.92	1 (33%)
4	EDO	B	405[B]	-	3,3,3	0.85	0	2,2,2	0.98	0
5	BU2	B	410	-	5,5,5	0.85	0	5,5,5	0.88	0
4	EDO	A	405[A]	-	3,3,3	0.91	0	2,2,2	0.17	0
4	EDO	C	403[B]	-	3,3,3	0.86	0	2,2,2	0.48	0
4	EDO	B	407	-	3,3,3	0.51	0	2,2,2	0.76	0
4	EDO	C	403[A]	-	3,3,3	1.61	1 (33%)	2,2,2	1.07	0
3	BV8	C	402[D]	-	77,86,86	1.50	12 (15%)	87,122,122	1.65	14 (16%)
5	BU2	B	409	-	5,5,5	0.62	0	5,5,5	1.29	0
3	BV8	C	402[A]	-	77,86,86	1.48	11 (14%)	87,122,122	1.42	12 (13%)
4	EDO	B	406	-	3,3,3	1.37	0	2,2,2	0.71	0
4	EDO	A	404[B]	-	3,3,3	0.85	0	2,2,2	2.11	1 (50%)

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	BU2	A	408	-	-	1/3/3/3	-
4	EDO	D	403[A]	-	-	0/1/1/1	-
4	EDO	D	403[B]	-	-	0/1/1/1	-
4	EDO	A	404[A]	-	-	1/1/1/1	-
4	EDO	B	403[B]	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	B	403[A]	-	-	0/1/1/1	-
5	BU2	B	408[B]	-	-	2/3/3/3	-
5	BU2	A	409	-	-	0/3/3/3	-
5	BU2	B	408[A]	-	-	1/3/3/3	-
5	BU2	C	406	-	-	3/3/3/3	-
4	EDO	A	403[A]	-	-	0/1/1/1	-
3	BV8	D	402[B]	-	-	7/56/101/101	0/7/7/7
4	EDO	A	403[B]	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BV8	D	402[C]	-	-	6/56/101/101	0/7/7/7
4	EDO	B	404[A]	-	-	0/1/1/1	-
4	EDO	B	404[B]	-	-	1/1/1/1	-
4	EDO	C	405	-	-	1/1/1/1	-
5	BU2	D	406	-	-	2/3/3/3	-
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	D	404[B]	-	-	1/1/1/1	-
5	BU2	D	405	-	-	0/3/3/3	-
3	BV8	A	402[B]	-	-	2/56/101/101	0/7/7/7
3	BV8	A	402[A]	-	-	2/56/101/101	0/7/7/7
4	EDO	A	404[B]	-	-	0/1/1/1	-
4	EDO	B	405[A]	-	-	0/1/1/1	-
4	EDO	D	404[A]	-	-	0/1/1/1	-
4	EDO	A	407	-	-	1/1/1/1	-
3	BV8	B	402[A]	-	-	5/56/101/101	0/7/7/7
4	EDO	A	405[B]	-	-	0/1/1/1	-
3	BV8	B	402[B]	-	-	5/56/101/101	0/7/7/7
5	BU2	B	409	-	-	1/3/3/3	-
4	EDO	B	405[B]	-	-	0/1/1/1	-
5	BU2	B	410	-	-	3/3/3/3	-
4	EDO	A	405[A]	-	-	1/1/1/1	-
4	EDO	C	403[B]	-	-	0/1/1/1	-
4	EDO	B	407	-	-	1/1/1/1	-
4	EDO	C	403[A]	-	-	0/1/1/1	-
3	BV8	C	402[D]	-	-	5/56/101/101	0/7/7/7
3	BV8	C	402[A]	-	-	8/56/101/101	0/7/7/7
4	EDO	B	406	-	-	0/1/1/1	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[B]	BV8	O17-C42	10.57	1.55	1.41
3	A	402[A]	BV8	O17-C42	10.17	1.55	1.41
3	B	402[A]	BV8	C6-C11	-6.22	1.31	1.41
3	A	402[B]	BV8	C6-C11	-6.13	1.31	1.41
3	D	402[B]	BV8	C41-C42	-5.79	1.45	1.53
3	A	402[B]	BV8	C41-C42	-5.76	1.45	1.53
3	D	402[C]	BV8	C41-C42	-5.41	1.45	1.53
3	A	402[A]	BV8	C41-C42	-5.28	1.45	1.53
3	D	402[C]	BV8	C5-S1	-5.17	1.65	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[B]	BV8	C9-C10	-4.93	1.32	1.42
3	D	402[B]	BV8	C6-C11	-4.73	1.33	1.41
3	D	402[C]	BV8	C6-C11	-4.57	1.33	1.41
3	B	402[A]	BV8	C10-C11	-4.52	1.30	1.42
3	D	402[B]	BV8	O17-C39	-4.50	1.35	1.45
3	A	402[A]	BV8	C46-N9	4.47	1.39	1.32
3	A	402[B]	BV8	C10-C11	-4.45	1.30	1.42
3	D	402[C]	BV8	O17-C42	4.43	1.47	1.41
3	C	402[A]	BV8	C6-C11	-4.41	1.34	1.41
3	C	402[D]	BV8	C6-C11	-4.27	1.34	1.41
3	B	402[A]	BV8	C9-C10	-4.24	1.33	1.42
3	D	402[B]	BV8	C3-C22	-4.21	1.40	1.50
3	B	402[A]	BV8	C46-N9	4.20	1.38	1.32
3	B	402[B]	BV8	C6-C11	-4.19	1.34	1.41
3	A	402[A]	BV8	C33-S1	-4.19	1.76	1.81
3	C	402[D]	BV8	C46-N9	4.10	1.38	1.32
3	D	402[C]	BV8	O8-C34	4.05	1.52	1.43
3	D	402[B]	BV8	O17-C42	4.02	1.46	1.41
3	A	402[B]	BV8	C45-N9	-3.92	1.30	1.35
3	A	402[A]	BV8	C8-C9	3.82	1.45	1.36
3	A	402[A]	BV8	C6-C11	-3.81	1.35	1.41
3	C	402[D]	BV8	C9-C10	-3.72	1.34	1.42
3	D	402[C]	BV8	C46-N9	3.70	1.38	1.32
3	D	402[C]	BV8	C33-C34	3.61	1.59	1.52
3	B	402[B]	BV8	C46-N9	3.53	1.37	1.32
3	D	402[B]	BV8	P1-O12	-3.51	1.38	1.55
3	A	402[A]	BV8	C28-C21	3.46	1.61	1.53
3	D	402[B]	BV8	C46-N9	3.42	1.37	1.32
3	B	402[B]	BV8	C9-C10	-3.40	1.35	1.42
3	C	402[A]	BV8	C10-C11	-3.37	1.33	1.42
3	D	402[B]	BV8	O3-C1	3.34	1.27	1.21
3	C	402[D]	BV8	C46-N10	3.30	1.40	1.33
3	A	402[A]	BV8	C9-C10	-3.28	1.35	1.42
3	D	402[C]	BV8	O17-C39	-3.28	1.37	1.45
3	D	402[B]	BV8	C10-C11	-3.23	1.34	1.42
3	A	402[B]	BV8	C46-N9	3.15	1.37	1.32
3	C	402[A]	BV8	C28-C21	3.15	1.60	1.53
3	C	402[A]	BV8	C9-C10	-3.15	1.35	1.42
3	A	402[A]	BV8	C46-N10	3.15	1.39	1.33
3	C	402[D]	BV8	C28-C21	3.11	1.60	1.53
3	D	402[C]	BV8	C9-C10	-3.09	1.35	1.42
5	A	409	BU2	C4-C3	3.05	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402[B]	BV8	P1-O11	-3.04	1.40	1.50
3	C	402[A]	BV8	C47-C44	-3.03	1.32	1.43
3	D	402[C]	BV8	O7-C33	3.01	1.48	1.43
3	C	402[D]	BV8	C10-C11	-2.99	1.34	1.42
3	B	402[B]	BV8	O8-C34	-2.98	1.36	1.43
3	D	402[C]	BV8	C10-C11	-2.90	1.34	1.42
3	D	402[B]	BV8	C45-N9	-2.89	1.31	1.35
3	A	402[A]	BV8	C5-S1	-2.86	1.69	1.75
3	B	402[B]	BV8	O7-C33	-2.85	1.39	1.43
3	D	402[B]	BV8	C9-C10	-2.79	1.36	1.42
3	C	402[A]	BV8	C46-N9	2.77	1.36	1.32
3	C	402[A]	BV8	C11-N1	-2.72	1.30	1.38
3	B	402[A]	BV8	O4-C3	-2.68	1.40	1.45
3	A	402[A]	BV8	P1-O12	-2.67	1.42	1.55
3	A	402[B]	BV8	C28-C21	2.67	1.59	1.53
3	D	402[C]	BV8	O3-C1	2.67	1.26	1.21
3	D	402[C]	BV8	P1-O11	-2.66	1.41	1.50
3	A	402[B]	BV8	O7-C33	-2.58	1.39	1.43
3	A	402[B]	BV8	C33-S1	-2.58	1.78	1.81
4	C	403[A]	EDO	O2-C2	-2.54	1.29	1.42
3	B	402[B]	BV8	C15-C16	-2.54	1.46	1.52
3	C	402[D]	BV8	C21-N4	2.53	1.51	1.45
3	B	402[B]	BV8	C12-N1	-2.51	1.31	1.36
3	C	402[D]	BV8	C5-S1	-2.49	1.70	1.75
3	A	402[A]	BV8	C3-C22	-2.46	1.44	1.50
3	C	402[D]	BV8	C11-N1	-2.44	1.31	1.38
3	C	402[D]	BV8	C47-C44	-2.44	1.34	1.43
3	A	402[A]	BV8	C45-N9	-2.44	1.32	1.35
3	B	402[B]	BV8	O1-C16	-2.43	1.18	1.23
3	C	402[A]	BV8	C3-C22	-2.43	1.44	1.50
3	B	402[B]	BV8	O17-C42	-2.43	1.37	1.41
3	B	402[A]	BV8	O8-C34	-2.42	1.37	1.43
3	B	402[B]	BV8	C10-C11	-2.42	1.36	1.42
3	D	402[C]	BV8	C3-C22	-2.41	1.44	1.50
3	A	402[B]	BV8	P2-O15	-2.40	1.44	1.55
3	C	402[D]	BV8	C5-N5	2.40	1.32	1.26
3	C	402[A]	BV8	P1-O12	-2.37	1.44	1.55
3	B	402[B]	BV8	C45-N9	-2.33	1.32	1.35
3	A	402[B]	BV8	C3-C22	-2.33	1.45	1.50
3	C	402[D]	BV8	C3-C22	-2.30	1.45	1.50
3	D	402[C]	BV8	O7-C36	2.28	1.50	1.45
3	D	402[B]	BV8	O7-C33	-2.27	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[B]	BV8	C14-C13	-2.26	1.45	1.51
3	B	402[B]	BV8	C3-C22	-2.25	1.45	1.50
3	D	402[C]	BV8	C5-N5	2.23	1.32	1.26
3	B	402[B]	BV8	C28-C21	2.20	1.58	1.53
3	D	402[C]	BV8	P1-O12	-2.17	1.45	1.55
3	D	402[B]	BV8	C24-C23	-2.16	1.34	1.38
3	B	402[A]	BV8	C46-N10	2.16	1.37	1.33
3	B	402[A]	BV8	C28-C21	2.15	1.58	1.53
3	B	402[B]	BV8	P2-O15	-2.15	1.45	1.55
3	B	402[A]	BV8	C15-C16	-2.14	1.47	1.52
3	D	402[B]	BV8	C11-N1	-2.11	1.32	1.38
4	A	403[A]	EDO	O2-C2	2.11	1.53	1.42
3	A	402[B]	BV8	C11-N1	-2.10	1.32	1.38
3	C	402[A]	BV8	C47-N10	-2.07	1.28	1.37
3	C	402[A]	BV8	O8-C34	-2.06	1.38	1.43
3	B	402[A]	BV8	C3-C22	-2.06	1.45	1.50
3	A	402[B]	BV8	O3-C1	2.06	1.25	1.21
3	D	402[B]	BV8	P2-O15	-2.05	1.45	1.55
3	D	402[C]	BV8	C47-N11	2.04	1.41	1.34
3	A	402[B]	BV8	C46-N10	2.04	1.37	1.33
3	A	402[A]	BV8	C14-C15	2.02	1.59	1.54
3	B	402[B]	BV8	C16-N2	-2.01	1.29	1.34

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402[A]	BV8	C14-C13-C10	-8.49	113.03	126.25
5	A	408	BU2	C1-C2-C3	7.63	134.98	114.04
3	A	402[A]	BV8	C14-C13-C12	-7.32	118.93	127.97
3	A	402[B]	BV8	N9-C46-N10	-7.09	117.60	128.68
3	A	402[B]	BV8	C14-C13-C10	-6.80	115.66	126.25
3	B	402[A]	BV8	N9-C46-N10	-6.76	118.11	128.68
3	B	402[B]	BV8	N9-C46-N10	-6.72	118.18	128.68
3	A	402[A]	BV8	N9-C46-N10	-6.65	118.29	128.68
3	D	402[C]	BV8	C14-C13-C12	-6.02	120.53	127.97
3	D	402[B]	BV8	C14-C13-C12	-5.80	120.81	127.97
3	D	402[B]	BV8	N9-C46-N10	-5.45	120.17	128.68
5	B	408[B]	BU2	O1-C1-C2	-5.43	92.28	111.31
3	B	402[B]	BV8	C14-C13-C12	-5.25	121.48	127.97
3	C	402[D]	BV8	C14-C13-C12	-5.24	121.49	127.97
3	C	402[D]	BV8	O4-C1-N4	5.22	121.11	110.50
3	B	402[A]	BV8	C9-C10-C11	5.20	125.06	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402[C]	BV8	N9-C46-N10	-5.04	120.80	128.68
3	D	402[C]	BV8	C24-C23-C22	4.86	128.09	120.63
3	B	402[A]	BV8	C14-C13-C12	4.80	133.89	127.97
3	D	402[B]	BV8	O4-C1-N4	4.65	119.95	110.50
3	C	402[A]	BV8	N9-C46-N10	-4.53	121.60	128.68
3	A	402[B]	BV8	C14-C13-C12	4.50	133.53	127.97
3	C	402[D]	BV8	C24-C23-C22	4.25	127.15	120.63
5	D	405	BU2	O1-C1-C2	4.23	126.14	111.31
3	D	402[B]	BV8	O4-C1-O3	-4.17	116.25	124.25
3	C	402[D]	BV8	C27-C22-C23	-4.04	111.82	118.17
3	C	402[D]	BV8	N9-C46-N10	-4.02	122.40	128.68
3	D	402[C]	BV8	O4-C3-C22	3.96	118.91	109.39
3	D	402[C]	BV8	O4-C1-N4	3.95	118.54	110.50
3	B	402[A]	BV8	C42-N7-C45	-3.87	119.84	126.64
3	A	402[A]	BV8	C31-N5-C5	3.83	124.09	117.84
3	C	402[A]	BV8	C31-N5-C5	3.81	124.05	117.84
3	A	402[B]	BV8	C31-N5-C5	3.78	124.00	117.84
3	B	402[B]	BV8	C28-C21-N4	-3.77	103.26	110.88
3	C	402[D]	BV8	C17-N2-C16	-3.72	118.84	123.18
3	C	402[A]	BV8	C28-C21-N4	-3.64	103.53	110.88
3	D	402[C]	BV8	O12-P1-O11	3.61	130.09	112.24
3	B	402[B]	BV8	C42-N7-C45	-3.59	120.34	126.64
3	C	402[D]	BV8	C31-N5-C5	3.55	123.64	117.84
3	B	402[A]	BV8	C28-C21-N4	-3.55	103.70	110.88
3	C	402[D]	BV8	O4-C1-O3	-3.46	117.60	124.25
3	C	402[A]	BV8	C8-C7-C6	-3.45	115.60	120.44
3	C	402[A]	BV8	O17-C42-C41	-3.34	102.05	106.93
3	B	402[A]	BV8	C14-C15-N3	-3.33	103.77	110.79
3	A	402[A]	BV8	C18-C17-N2	3.32	116.49	109.79
3	B	402[B]	BV8	C46-N10-C47	3.26	124.34	118.75
5	D	405	BU2	C1-C2-C3	3.24	122.94	114.04
3	B	402[A]	BV8	O3-C1-N4	-3.23	119.55	124.85
6	A	411	DMS	O-S-C2	3.22	122.95	106.54
3	D	402[B]	BV8	O12-P1-O11	3.20	128.05	112.24
3	A	402[A]	BV8	C14-C13-C10	3.18	131.20	126.25
3	B	402[B]	BV8	C19-C17-C18	3.18	118.66	111.58
3	D	402[B]	BV8	C14-C13-C10	3.18	131.19	126.25
3	D	402[C]	BV8	C14-C13-C10	3.11	131.09	126.25
3	A	402[B]	BV8	O17-C42-C41	-3.11	102.38	106.93
3	A	402[B]	BV8	C40-C41-C42	3.11	105.66	100.98
3	D	402[C]	BV8	C25-C26-C27	3.10	124.91	120.19
3	A	402[A]	BV8	C40-C41-C42	3.09	105.63	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	406	BU2	C1-C2-C3	-3.05	105.68	114.04
3	B	402[A]	BV8	C46-N10-C47	2.96	123.82	118.75
4	A	404[B]	EDO	O2-C2-C1	-2.92	90.87	111.91
3	A	402[B]	BV8	C14-C15-N3	-2.88	104.72	110.79
3	B	402[A]	BV8	C3-O4-C1	2.87	122.35	115.93
3	C	402[D]	BV8	C25-C26-C27	2.87	124.56	120.19
3	D	402[B]	BV8	C31-N5-C5	2.84	122.47	117.84
3	C	402[D]	BV8	C14-C13-C10	2.82	130.63	126.25
3	A	402[A]	BV8	C19-C17-N2	-2.81	104.13	109.79
3	D	402[C]	BV8	C21-C20-N3	-2.80	110.55	116.70
3	D	402[B]	BV8	C24-C23-C22	2.80	124.92	120.63
3	C	402[A]	BV8	O4-C1-N4	2.78	116.15	110.50
5	A	409	BU2	C1-C2-C3	-2.76	106.47	114.04
6	A	410	DMS	O-S-C2	2.74	120.53	106.54
3	C	402[D]	BV8	C8-C7-C6	-2.72	116.63	120.44
3	D	402[C]	BV8	C31-N5-C5	2.71	122.26	117.84
3	D	402[C]	BV8	C27-C22-C23	-2.71	113.91	118.17
3	B	402[A]	BV8	C9-C10-C13	-2.70	129.47	134.42
3	B	402[B]	BV8	C14-C15-N3	-2.69	105.12	110.79
3	A	402[B]	BV8	C46-N10-C47	2.68	123.34	118.75
5	C	406	BU2	O3-C3-C4	-2.68	97.79	109.38
3	C	402[A]	BV8	O4-C3-C22	2.66	115.79	109.39
3	C	402[A]	BV8	C17-N2-C16	-2.65	120.09	123.18
3	C	402[D]	BV8	O17-C42-C41	-2.64	103.07	106.93
3	A	402[A]	BV8	O3-C1-N4	-2.61	120.57	124.85
3	C	402[A]	BV8	C19-C17-N2	-2.58	104.59	109.79
3	D	402[B]	BV8	C28-C21-N4	-2.57	105.68	110.88
3	B	402[A]	BV8	C45-C44-N8	-2.56	106.73	109.40
5	D	406	BU2	O3-C3-C4	-2.56	98.28	109.38
3	B	402[A]	BV8	C8-C9-C10	-2.55	117.36	120.89
3	A	402[A]	BV8	O17-C42-C41	-2.55	103.20	106.93
3	B	402[B]	BV8	C3-O4-C1	2.55	121.61	115.93
3	D	402[B]	BV8	C21-N4-C1	2.53	127.08	120.90
3	A	402[A]	BV8	O15-P2-O14	2.51	124.66	112.24
3	D	402[B]	BV8	C20-C21-N4	-2.51	104.34	111.16
3	A	402[B]	BV8	O15-P2-O14	2.47	124.46	112.24
3	D	402[C]	BV8	C44-C47-N11	2.45	124.08	120.35
3	D	402[B]	BV8	O17-C42-C41	-2.45	103.34	106.93
3	A	402[A]	BV8	C9-C10-C11	2.44	121.41	118.17
3	A	402[B]	BV8	C9-C10-C11	2.44	121.40	118.17
3	C	402[A]	BV8	C14-C13-C10	2.43	130.03	126.25
3	A	402[B]	BV8	O2-C20-N3	-2.42	118.44	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[B]	BV8	C17-N2-C16	-2.41	120.37	123.18
3	D	402[C]	BV8	O3-C1-N4	-2.40	120.91	124.85
3	D	402[B]	BV8	C8-C7-C6	-2.40	117.08	120.44
3	C	402[A]	BV8	C45-C44-N8	-2.37	106.93	109.40
3	B	402[B]	BV8	O4-C3-C22	2.37	115.08	109.39
3	B	402[A]	BV8	O4-C1-N4	2.36	115.31	110.50
3	B	402[B]	BV8	C44-C47-N11	2.36	123.94	120.35
3	A	402[B]	BV8	C9-C10-C13	-2.36	130.08	134.42
3	A	402[A]	BV8	C46-N10-C47	2.36	122.80	118.75
3	D	402[C]	BV8	C17-N2-C16	-2.36	120.43	123.18
3	A	402[A]	BV8	O4-C1-N4	2.35	115.28	110.50
3	A	402[B]	BV8	C19-C17-N2	-2.33	105.10	109.79
3	A	402[B]	BV8	C21-N4-C1	2.32	126.56	120.90
3	D	402[C]	BV8	O2-C20-C21	2.30	125.29	120.45
3	C	402[D]	BV8	O3-C1-N4	-2.29	121.10	124.85
3	D	402[C]	BV8	C8-C7-C6	-2.28	117.25	120.44
3	B	402[B]	BV8	O4-C1-N4	2.27	115.12	110.50
3	D	402[B]	BV8	C3-O4-C1	2.23	120.92	115.93
3	B	402[B]	BV8	C3-C22-C27	2.23	125.87	120.66
3	A	402[A]	BV8	C21-N4-C1	2.22	126.33	120.90
3	B	402[B]	BV8	O1-C16-N2	2.22	127.04	122.93
3	C	402[D]	BV8	C14-C15-N3	-2.20	106.16	110.79
3	B	402[B]	BV8	C8-C7-C6	-2.18	117.39	120.44
3	B	402[A]	BV8	C44-C47-N11	2.16	123.64	120.35
3	D	402[C]	BV8	C25-C24-C23	-2.16	116.90	120.19
3	A	402[B]	BV8	C8-C7-C6	-2.11	117.48	120.44
3	B	402[A]	BV8	O4-C3-C22	2.11	114.46	109.39
5	B	408[A]	BU2	O3-C3-C2	-2.10	99.76	109.80
3	D	402[C]	BV8	C29-C28-C21	-2.09	107.46	113.92
3	A	402[B]	BV8	O3-C1-N4	-2.09	121.43	124.85
5	B	408[B]	BU2	C1-C2-C3	-2.09	108.31	114.04
3	D	402[C]	BV8	O4-C1-O3	-2.08	120.26	124.25
3	A	402[B]	BV8	C20-C21-N4	-2.08	105.51	111.16
3	B	402[B]	BV8	O7-C36-C35	2.06	109.19	105.11
3	C	402[A]	BV8	C14-C15-N3	-2.04	106.50	110.79
3	B	402[B]	BV8	C45-C44-N8	-2.01	107.30	109.40
3	A	402[B]	BV8	C8-C9-C10	-2.01	118.11	120.89
3	A	402[A]	BV8	C45-C44-N8	-2.01	107.31	109.40

There are no chirality outliers.

All (62) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
5	A	408	BU2	C1-C2-C3-C4
5	B	408[B]	BU2	O1-C1-C2-C3
5	B	408[A]	BU2	O1-C1-C2-C3
5	C	406	BU2	O1-C1-C2-C3
5	D	406	BU2	C1-C2-C3-C4
5	B	409	BU2	O1-C1-C2-C3
5	B	410	BU2	O1-C1-C2-C3
5	B	410	BU2	C1-C2-C3-C4
4	A	404[A]	EDO	O1-C1-C2-O2
3	D	402[B]	BV8	C20-C21-N4-C1
4	B	404[B]	EDO	O1-C1-C2-O2
4	A	407	EDO	O1-C1-C2-O2
4	A	405[A]	EDO	O1-C1-C2-O2
3	C	402[D]	BV8	N6-C2-C4-C32
5	C	406	BU2	C1-C2-C3-O3
5	B	410	BU2	C1-C2-C3-O3
3	C	402[A]	BV8	C13-C14-C15-C16
3	C	402[A]	BV8	N6-C2-C4-C32
4	C	405	EDO	O1-C1-C2-O2
3	B	402[B]	BV8	P2-O13-P1-O10
3	D	402[B]	BV8	C13-C14-C15-C16
3	D	402[B]	BV8	N6-C2-C4-C32
3	D	402[B]	BV8	O4-C1-N4-C21
3	D	402[C]	BV8	C13-C14-C15-C16
5	C	406	BU2	C1-C2-C3-C4
5	D	406	BU2	C1-C2-C3-O3
3	D	402[C]	BV8	N6-C2-C4-C32
3	B	402[A]	BV8	N6-C2-C4-C32
3	B	402[B]	BV8	N6-C2-C4-C32
3	C	402[D]	BV8	C28-C29-C30-C31
3	C	402[D]	BV8	C13-C14-C15-C16
3	B	402[A]	BV8	O7-C36-C37-O10
3	B	402[B]	BV8	O7-C36-C37-O10
3	A	402[A]	BV8	O16-C38-C39-O17
3	C	402[D]	BV8	O7-C36-C37-O10
3	B	402[A]	BV8	C28-C29-C30-C31
4	B	403[B]	EDO	O1-C1-C2-O2
4	B	407	EDO	O1-C1-C2-O2
3	A	402[B]	BV8	O16-C38-C39-O17
3	C	402[A]	BV8	O7-C36-C37-O10
3	B	402[A]	BV8	P2-O13-P1-O10
3	C	402[A]	BV8	O3-C1-N4-C21
3	B	402[B]	BV8	C28-C29-C30-C31

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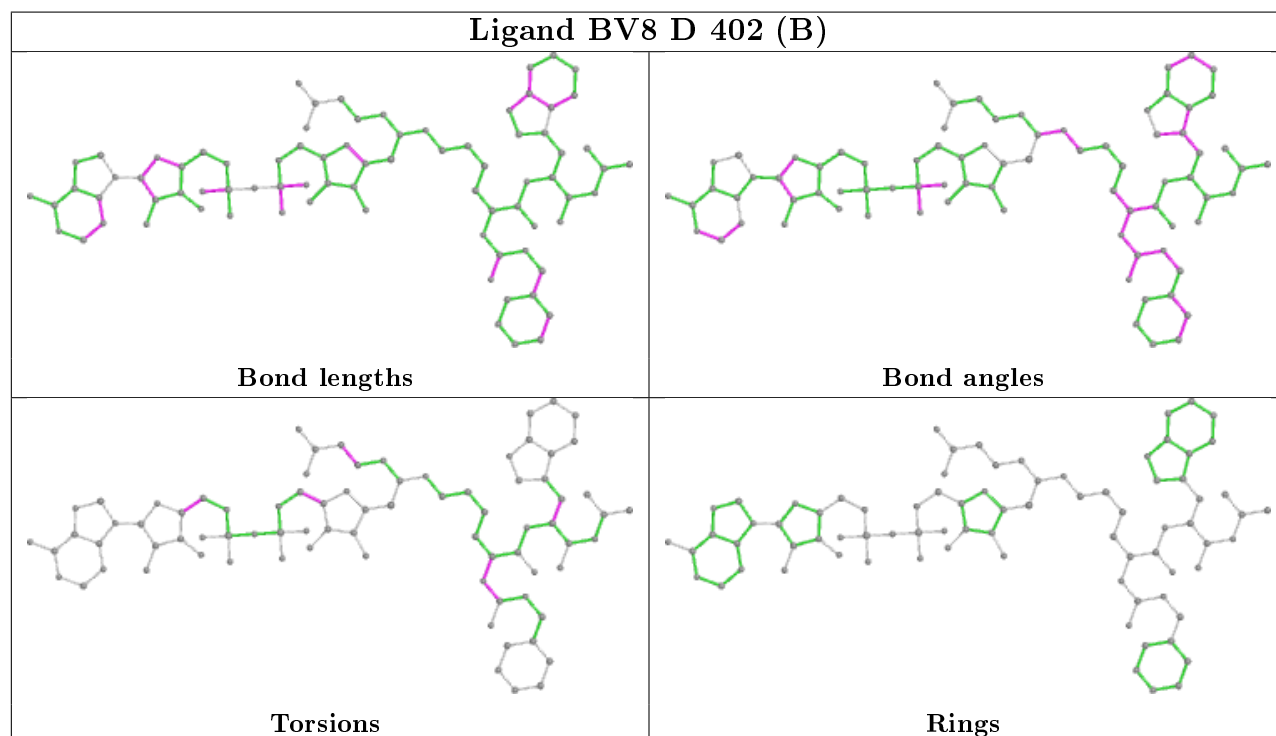
Mol	Chain	Res	Type	Atoms
3	D	402[B]	BV8	O3-C1-N4-C21
3	C	402[A]	BV8	O4-C1-N4-C21
3	D	402[C]	BV8	O7-C36-C37-O10
3	C	402[A]	BV8	C20-C21-N4-C1
5	B	408[B]	BU2	C1-C2-C3-O3
3	D	402[C]	BV8	N4-C21-C28-C29
3	C	402[A]	BV8	C28-C29-C30-C31
3	D	402[C]	BV8	C28-C29-C30-C31
3	D	402[B]	BV8	O7-C36-C37-O10
3	D	402[B]	BV8	O16-C38-C39-O17
3	D	402[C]	BV8	O16-C38-C39-O17
3	A	402[B]	BV8	O7-C36-C37-O10
3	A	402[A]	BV8	O7-C36-C37-O10
3	B	402[A]	BV8	O16-C38-C39-O17
3	B	402[B]	BV8	O16-C38-C39-O17
3	C	402[D]	BV8	O16-C38-C39-O17
3	C	402[A]	BV8	O16-C38-C39-O17
4	A	406	EDO	O1-C1-C2-O2
4	D	404[B]	EDO	O1-C1-C2-O2

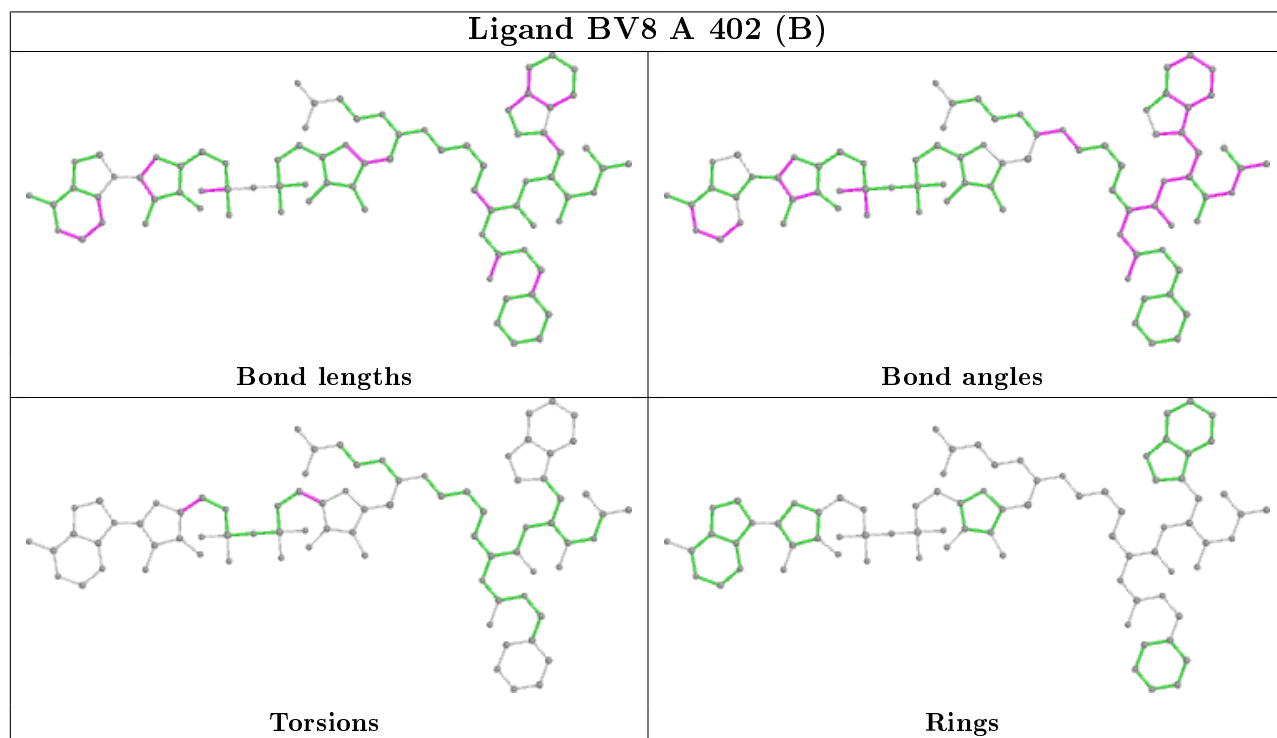
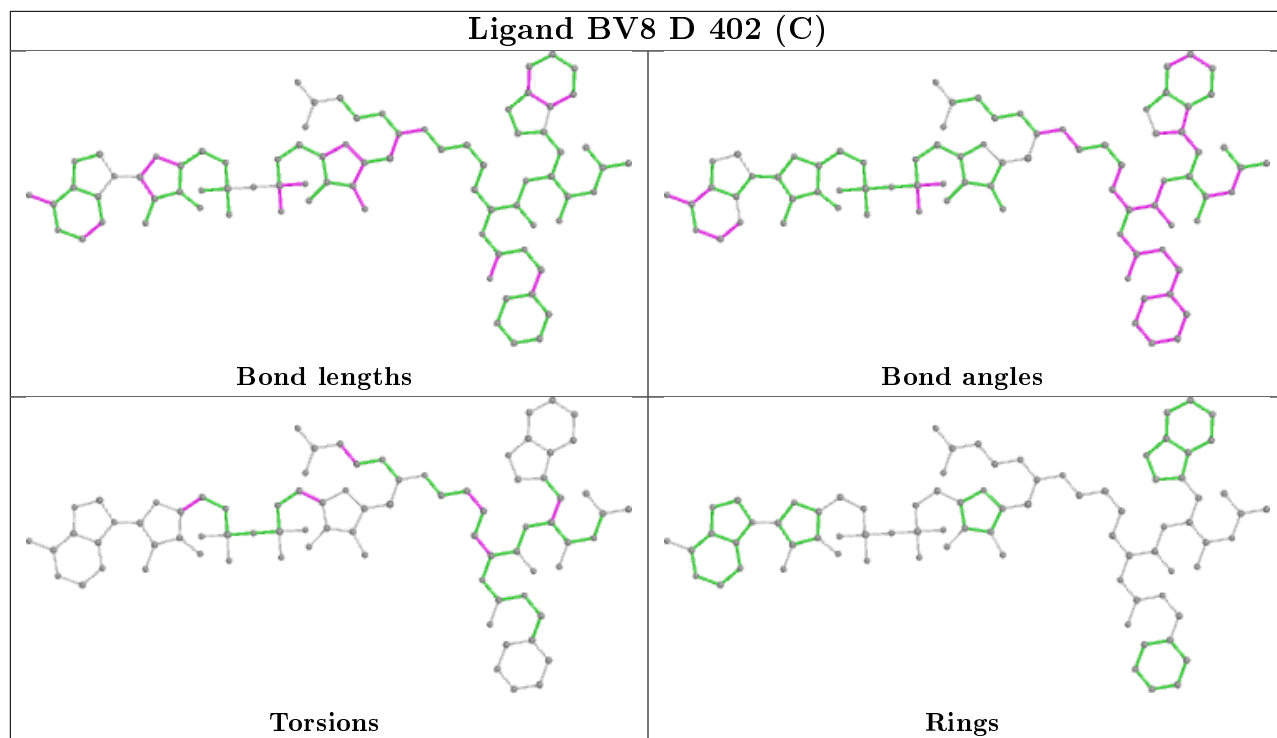
There are no ring outliers.

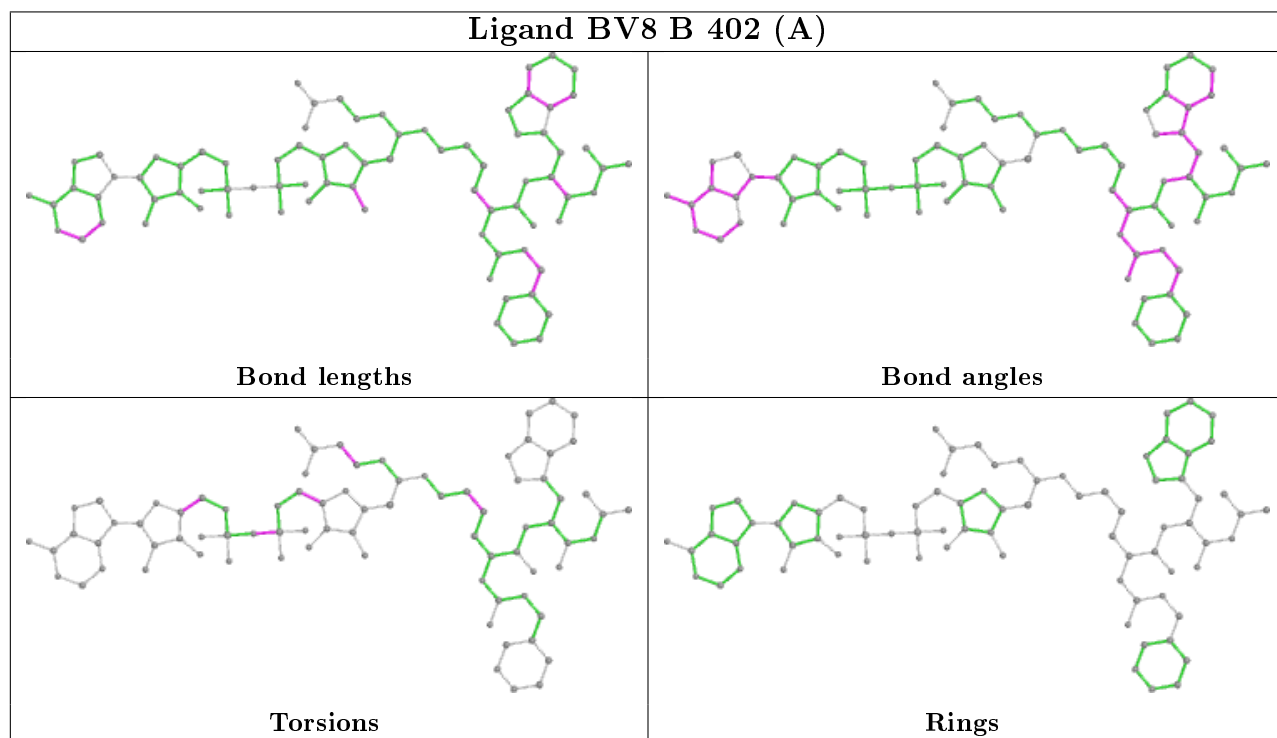
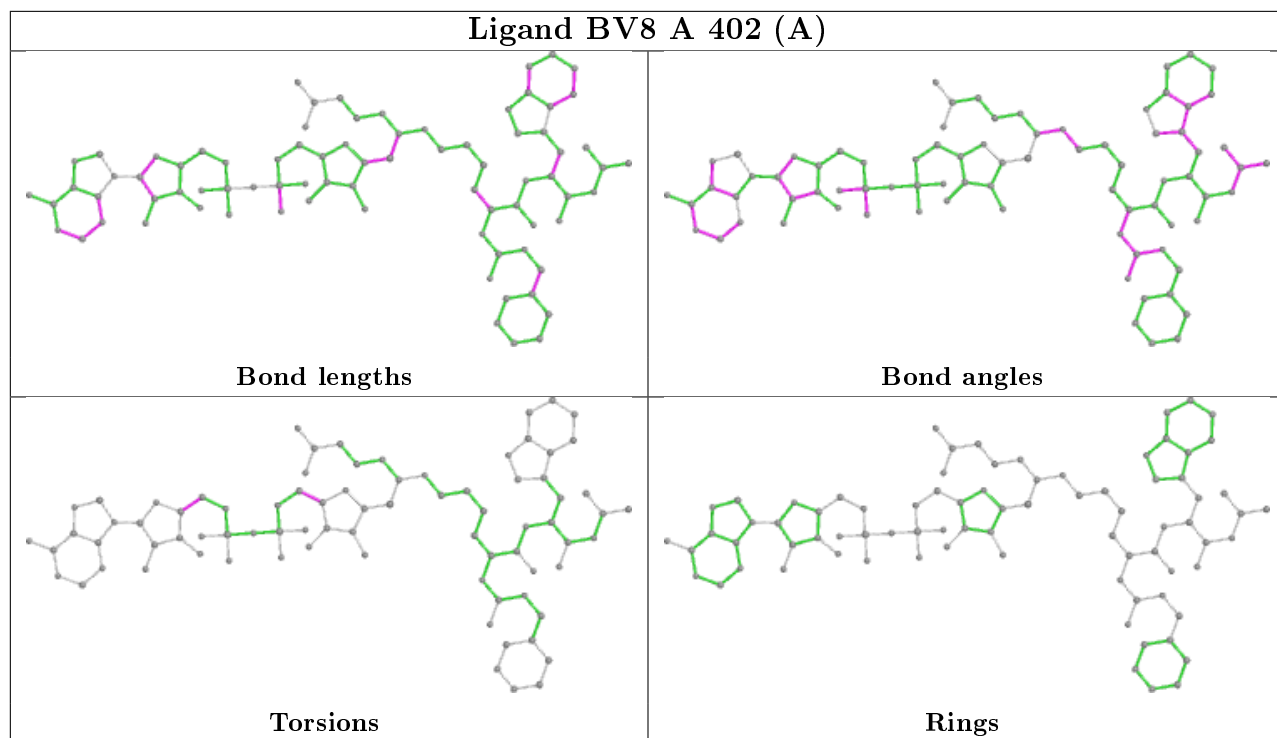
18 monomers are involved in 50 short contacts:

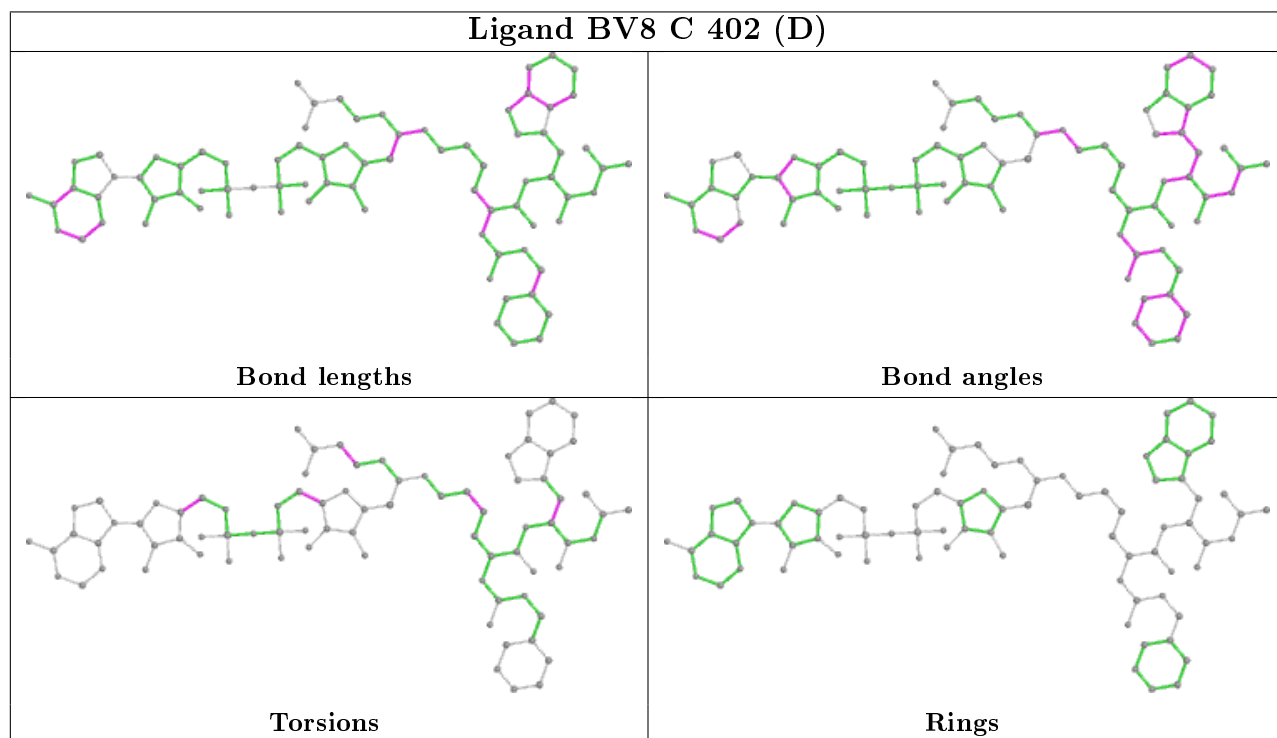
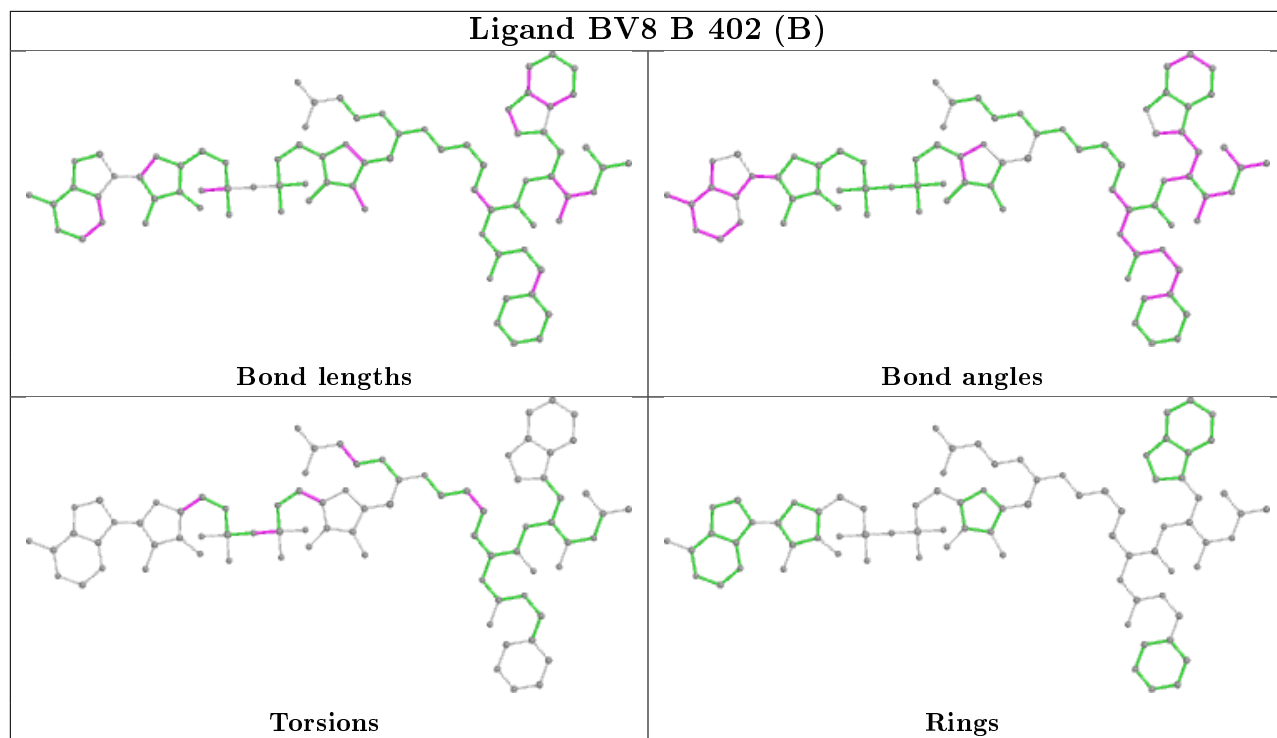
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	BU2	9	0
4	A	404[A]	EDO	2	0
4	A	406	EDO	2	0
5	B	408[B]	BU2	2	0
5	B	408[A]	BU2	4	0
4	A	403[A]	EDO	2	0
3	D	402[B]	BV8	2	0
4	A	403[B]	EDO	1	0
4	B	404[B]	EDO	1	0
4	C	404	EDO	5	0
5	D	405	BU2	4	0
3	B	402[A]	BV8	7	0
3	B	402[B]	BV8	2	0
5	B	410	BU2	4	0
3	C	402[D]	BV8	1	0
5	B	409	BU2	3	0
3	C	402[A]	BV8	2	0
4	B	406	EDO	4	0

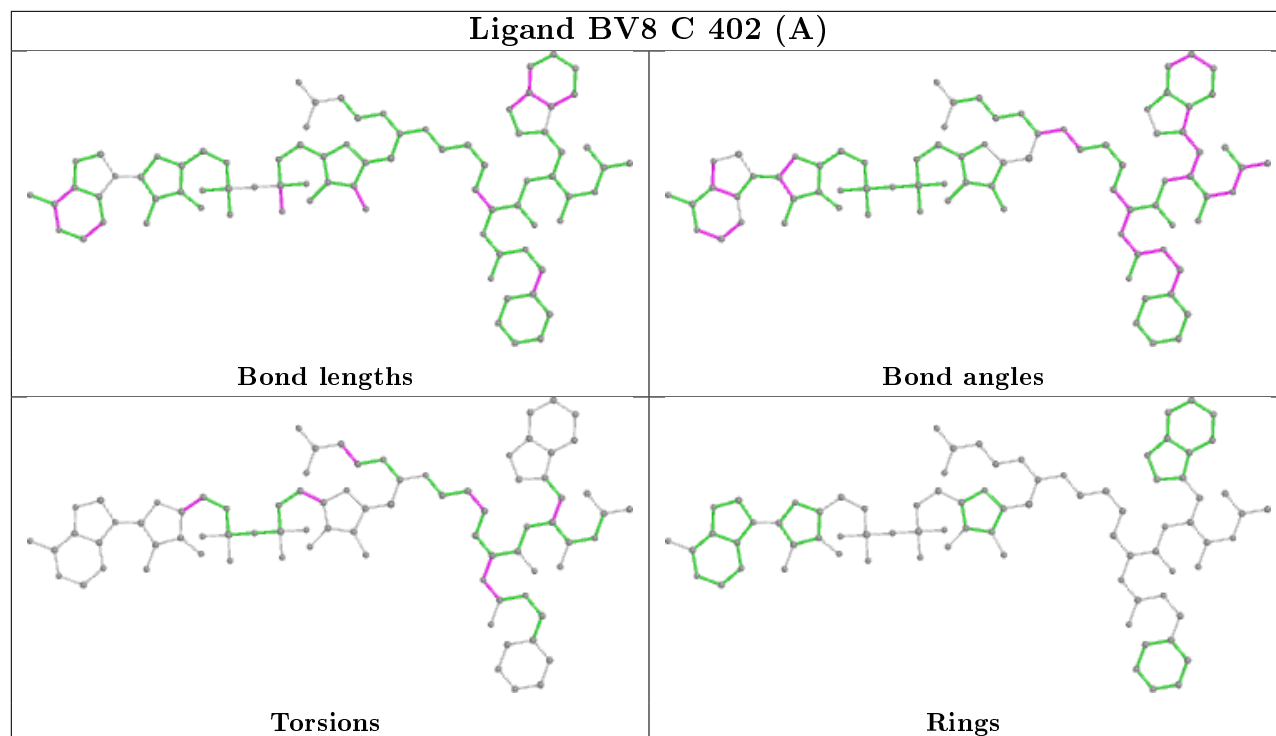
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	269/275 (97%)	-0.25	2 (0%) 87 87	8, 16, 30, 63	0
1	B	268/275 (97%)	-0.28	1 (0%) 92 91	10, 17, 31, 76	0
1	C	274/275 (99%)	-0.05	7 (2%) 56 57	10, 20, 42, 97	0
1	D	275/275 (100%)	-0.04	9 (3%) 46 47	8, 19, 41, 113	0
All	All	1086/1100 (98%)	-0.16	19 (1%) 70 71	8, 17, 37, 113	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	ILE	15.8
1	D	29	ILE	11.4
1	D	28	GLY	7.9
1	A	34	ALA	7.9
1	B	35	ARG	4.7
1	C	32	PHE	4.3
1	D	32	PHE	4.3
1	C	33	THR	4.2
1	C	35	ARG	4.1
1	A	35	ARG	4.0
1	D	33	THR	3.7
1	D	30	ASP	3.7
1	D	35	ARG	3.6
1	D	34	ALA	3.4
1	C	30	ASP	3.0
1	D	31	PRO	2.8
1	C	34	ALA	2.8
1	C	31	PRO	2.8
1	D	195	GLN	2.3



## 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(Å <sup>2</sup> )	Q<0.9
4	EDO	C	404	4/4	0.76	0.18	55,57,68,73	0
5	BU2	C	406	6/6	0.77	0.14	32,41,48,50	0
5	BU2	A	409	6/6	0.80	0.14	38,51,56,60	0
5	BU2	D	405	6/6	0.82	0.15	32,43,71,110	0
4	EDO	A	405[B]	4/4	0.83	0.16	20,27,32,34	4
4	EDO	A	405[A]	4/4	0.83	0.16	30,36,42,46	4
4	EDO	B	405[B]	4/4	0.84	0.23	27,29,41,42	4
4	EDO	B	405[A]	4/4	0.84	0.23	33,43,46,49	4
4	EDO	C	405	4/4	0.85	0.15	33,41,42,58	0
5	BU2	B	410	6/6	0.86	0.10	32,39,50,57	0
5	BU2	A	408	6/6	0.86	0.25	29,35,44,59	0
4	EDO	B	407	4/4	0.86	0.19	51,55,55,92	0
4	EDO	B	404[B]	4/4	0.90	0.13	15,22,26,29	4
4	EDO	B	404[A]	4/4	0.90	0.13	26,32,34,35	4
6	DMS	A	410	4/4	0.91	0.13	51,54,67,79	0
5	BU2	B	409	6/6	0.91	0.13	31,39,44,51	0
4	EDO	A	404[B]	4/4	0.92	0.27	16,18,20,25	4
4	EDO	A	404[A]	4/4	0.92	0.27	13,22,25,33	4
5	BU2	D	406	6/6	0.93	0.15	44,56,64,82	0
6	DMS	A	411	4/4	0.93	0.13	56,71,83,86	0
4	EDO	D	404[B]	4/4	0.93	0.12	28,29,30,34	4
4	EDO	D	404[A]	4/4	0.93	0.12	22,23,25,27	4
4	EDO	A	407	4/4	0.94	0.12	32,37,46,55	0
5	BU2	B	408[B]	6/6	0.96	0.12	25,27,28,34	6
4	EDO	A	403[B]	4/4	0.96	0.15	15,16,21,28	4
4	EDO	D	403[B]	4/4	0.96	0.16	16,19,20,22	4
5	BU2	B	408[A]	6/6	0.96	0.12	21,24,31,43	6

*Continued on next page...*

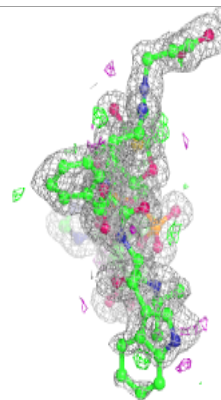
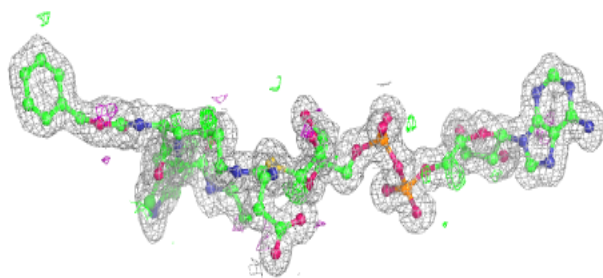
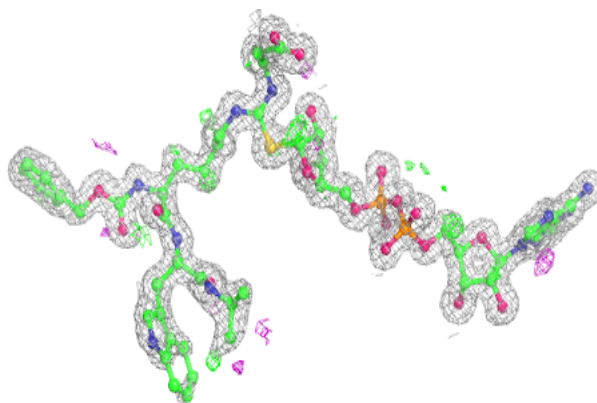
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	D	403[A]	4/4	0.96	0.16	10,10,12,13	4
4	EDO	C	403[B]	4/4	0.96	0.17	10,11,15,15	4
4	EDO	A	403[A]	4/4	0.96	0.15	6,7,9,12	4
4	EDO	C	403[A]	4/4	0.96	0.17	13,14,15,17	4
4	EDO	A	406	4/4	0.97	0.12	24,29,29,60	0
3	BV8	A	402[A]	80/80	0.98	0.07	13,19,33,39	80
3	BV8	D	402[C]	80/80	0.98	0.07	9,17,24,36	80
3	BV8	D	402[B]	80/80	0.98	0.07	8,12,19,24	80
4	EDO	B	403[A]	4/4	0.98	0.17	10,10,10,13	4
4	EDO	B	403[B]	4/4	0.98	0.17	10,12,14,20	4
3	BV8	A	402[B]	80/80	0.98	0.07	5,9,34,46	80
3	BV8	C	402[D]	80/80	0.98	0.07	7,18,24,28	80
3	BV8	C	402[A]	80/80	0.98	0.07	8,13,24,32	80
4	EDO	B	406	4/4	0.98	0.06	26,27,29,58	0
3	BV8	B	402[A]	80/80	0.99	0.07	14,19,38,51	80
3	BV8	B	402[B]	80/80	0.99	0.07	7,11,33,40	80
2	ZN	C	401	1/1	1.00	0.04	19,19,19,19	0
2	ZN	A	401	1/1	1.00	0.05	15,15,15,15	0
2	ZN	D	401	1/1	1.00	0.04	17,17,17,17	0
2	ZN	B	401	1/1	1.00	0.04	16,16,16,16	0

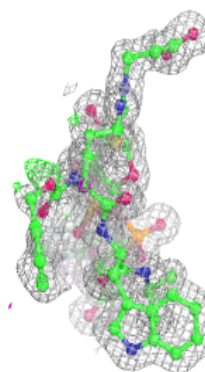
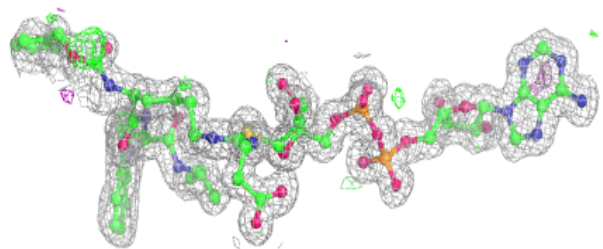
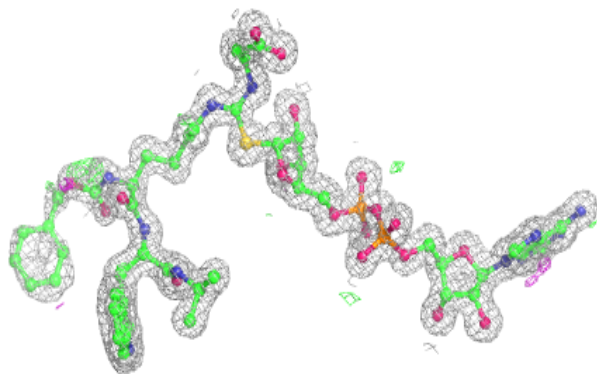
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BV8 A 402 (A):**

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

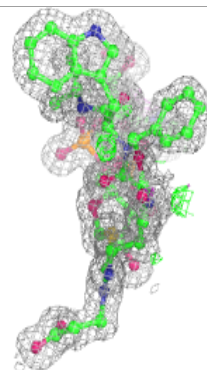
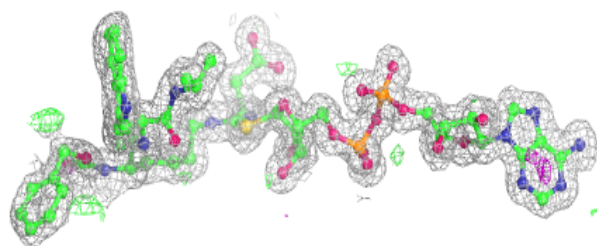
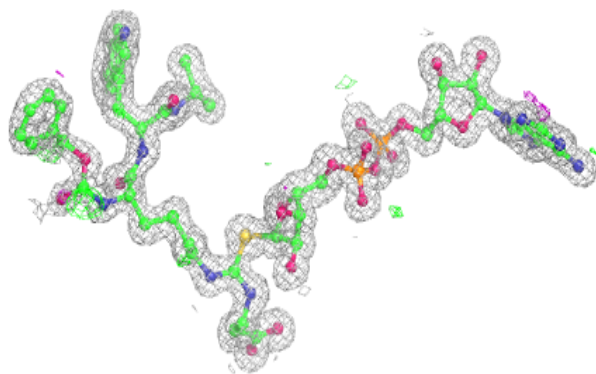
**Electron density around BV8 D 402 (C):**

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

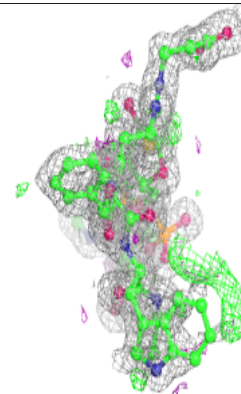
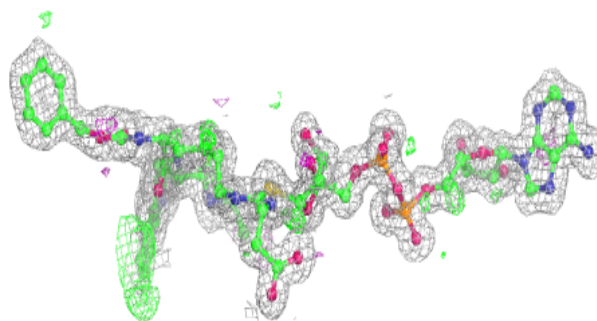
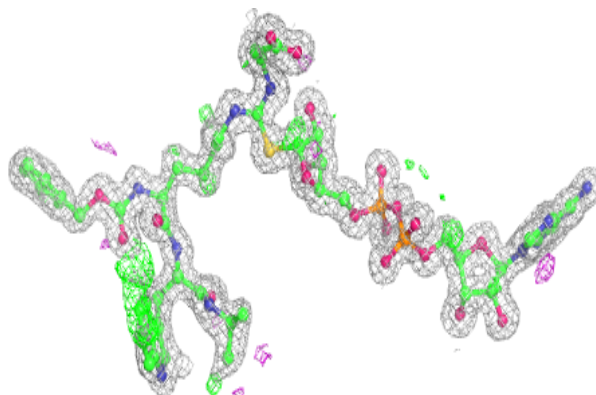


**Electron density around BV8 D 402 (B):**

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

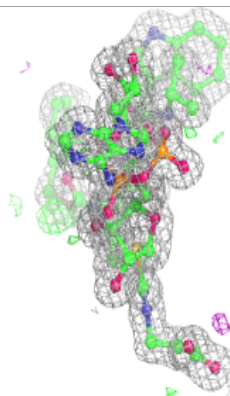
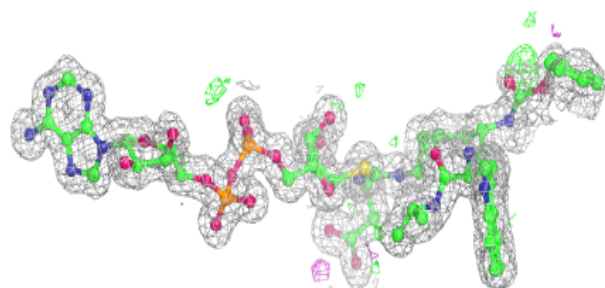
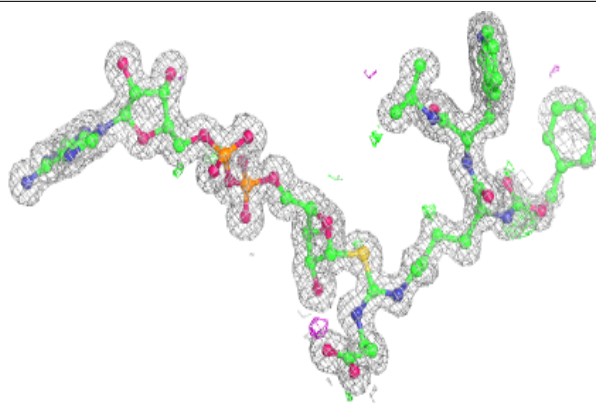
**Electron density around BV8 A 402 (B):**

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

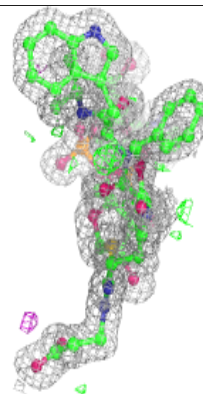
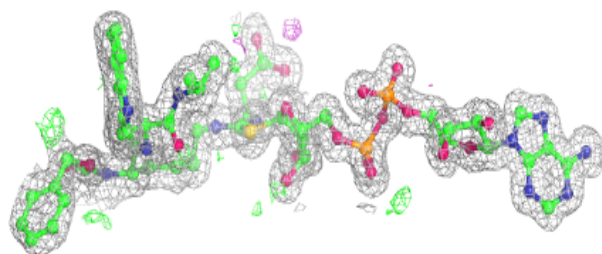
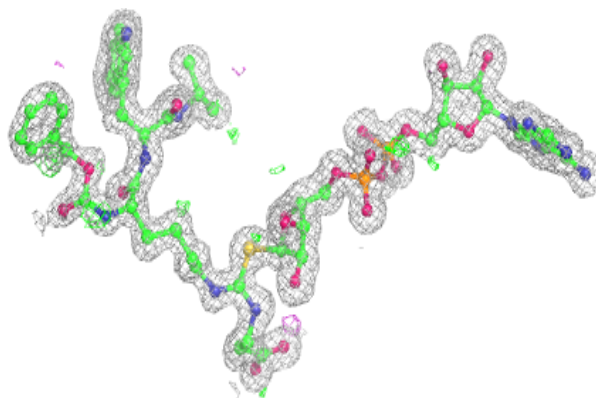


**Electron density around BV8 C 402 (D):**

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

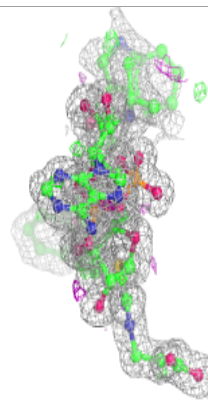
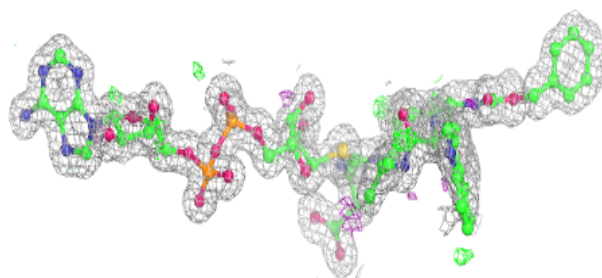
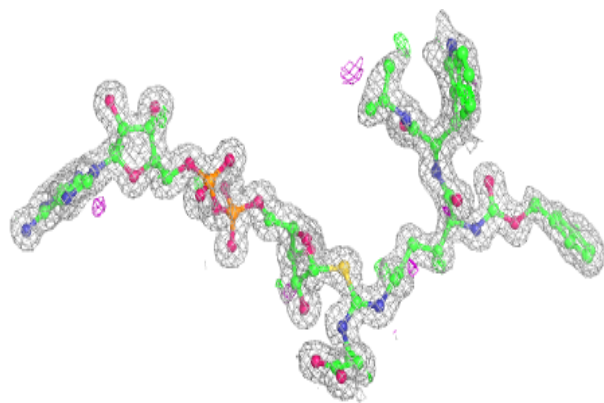
**Electron density around BV8 C 402 (A):**

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

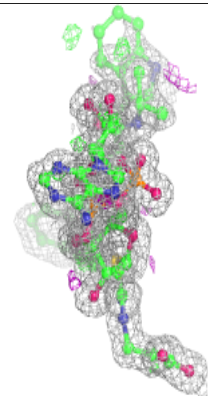
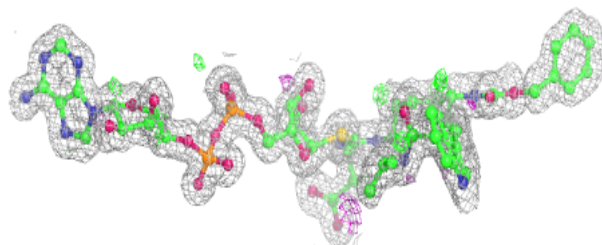
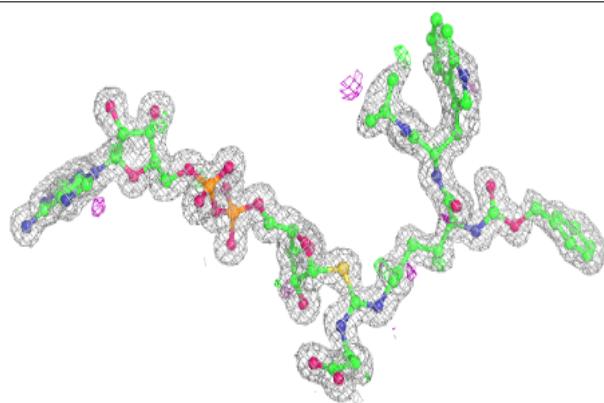


**Electron density around BV8 B 402 (A):**

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

**Electron density around BV8 B 402 (B):**

$2mF_o-DF_c$  (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.