



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 30, 2023 – 09:06 am GMT

PDB ID : 8CO7
Title : Crystal structure of human soluble adenylyl cyclase (sAC) in complex with inhibitor TDI-09066
Authors : Steegborn, C.
Deposited on : 2023-02-27
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

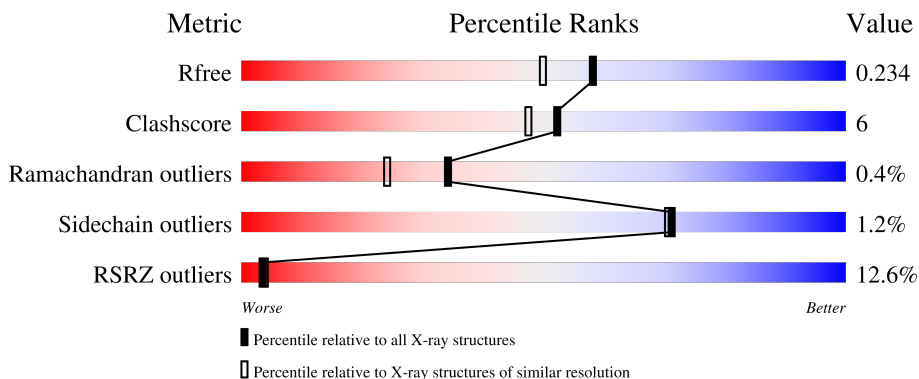
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	475	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	V9E	A	501	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PGE	A	518	-	-	-	X

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 8044 atoms, of which 3932 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.

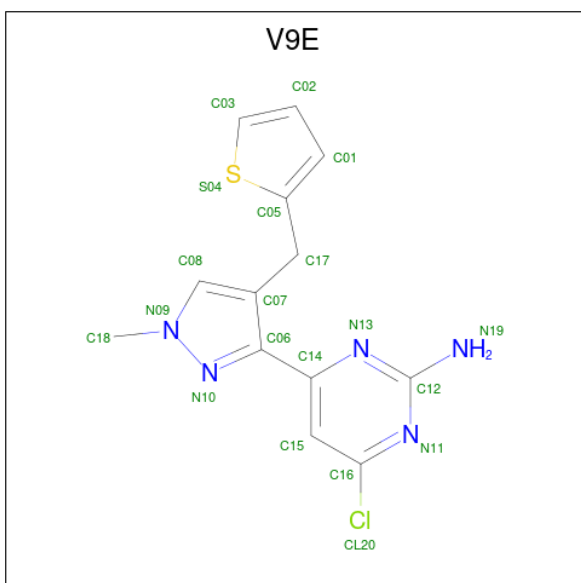
- Molecule 1 is a protein called Adenylate cyclase type 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	462	7606	2469	3813	605	681	38	0	24	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	HIS	-	expression tag	UNP Q96PN6
A	471	HIS	-	expression tag	UNP Q96PN6
A	472	HIS	-	expression tag	UNP Q96PN6
A	473	HIS	-	expression tag	UNP Q96PN6
A	474	HIS	-	expression tag	UNP Q96PN6
A	475	HIS	-	expression tag	UNP Q96PN6

- Molecule 2 is 4-chloranyl-6-[1-methyl-4-(thiophen-2-ylmethyl)pyrazol-3-yl]pyrimidin-2-amine (three-letter code: V9E) (formula: C₁₃H₁₂ClN₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	H	N			S
2	A	1	32	13	1	12	5	1	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



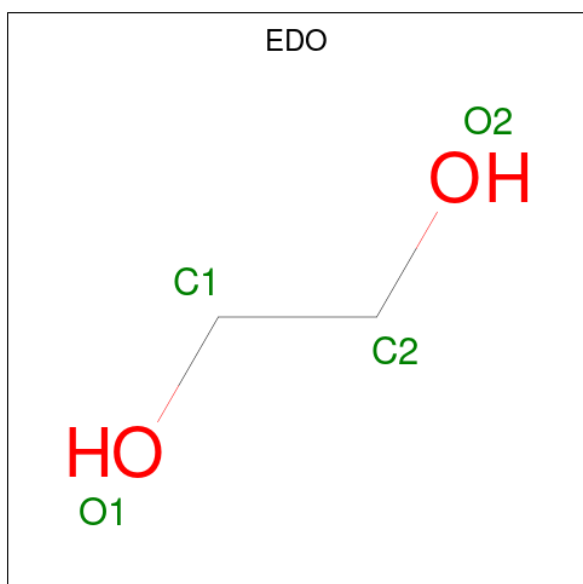
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
3	A	1	10	2	6	1	1	0	0
3	A	1	10	2	6	1	1	0	0
3	A	1	10	2	6	1	1	0	0
3	A	1	10	2	6	1	1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



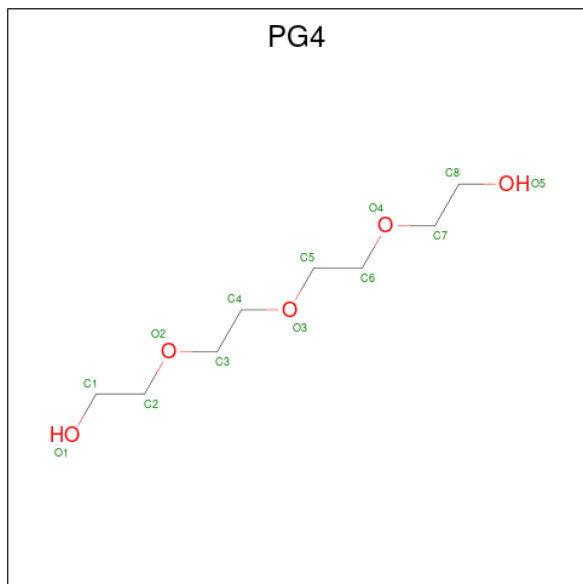
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	7	2	3	2	0	0
4	A	1	7	2	3	2	0	0
4	A	1	7	2	3	2	0	0
4	A	1	7	2	3	2	0	0
4	A	1	7	2	3	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	24	6	14	4	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	2	2	2	0	0

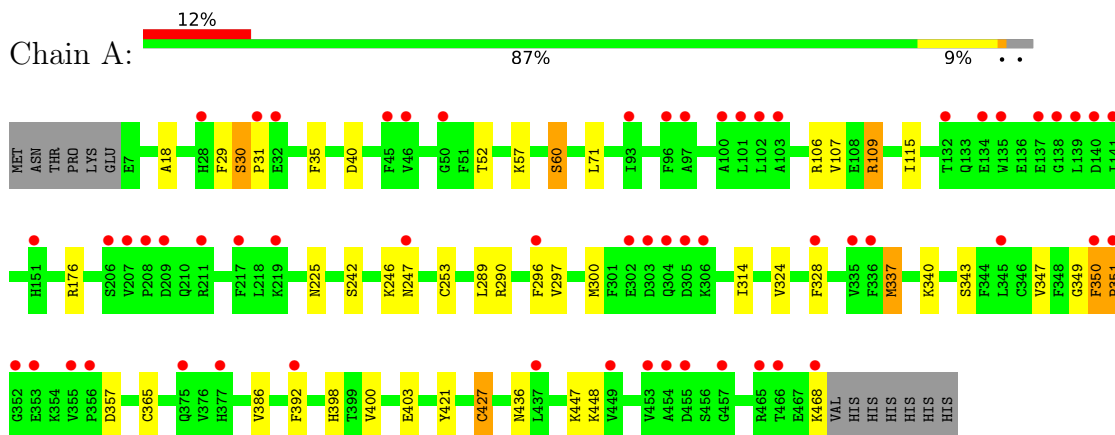
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	208	214	214	0	6

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: Adenylate cyclase type 10



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	99.29Å 99.29Å 99.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.50 – 1.90 42.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (32.50-1.90) 95.7 (42.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.191 , 0.234 0.191 , 0.234	Depositor DCC
R_{free} test set	1085 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8044	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: V9E, EDO, ACT, PGE, DMS, CME, CL, PG4

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	0.50	1/3956 (0.0%)	0.56	1/5348 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	CYS	CB-SG	-5.04	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	MET	CG-SD-CE	5.39	108.82	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3793	3813	3773	40	1
2	A	20	12	0	0	0
3	A	16	24	24	1	0
4	A	20	15	15	2	0
5	A	24	36	36	0	0
6	A	13	18	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	10	14	14	0	0
8	A	2	0	0	0	0
9	A	214	0	0	13	0
All	All	4112	3932	3880	43	1

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 6.

All (43) 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:A:347:VAL:HB	1:A:350:PHE:CE2	2.07	0.88
1:A:246:LYS:NZ	9:A:603:HOH:O	2.23	0.70
1:A:247:ASN:ND2	9:A:604:HOH:O	2.25	0.69
1:A:403:GLU:OE2	9:A:601:HOH:O	2.11	0.68
1:A:300[A]:MET:HE1	9:A:788:HOH:O	1.93	0.67
1:A:324:VAL:HG12	1:A:365:CYS:SG	2.35	0.67
1:A:350:PHE:HB2	1:A:351:PRO:HD2	1.76	0.66
1:A:347:VAL:HG11	1:A:350:PHE:HD2	1.61	0.65
1:A:289:LEU:HD21	1:A:392[A]:PHE:CZ	2.33	0.64
1:A:347:VAL:HG11	1:A:350:PHE:CD2	2.33	0.63
1:A:347:VAL:HB	1:A:350:PHE:HE2	1.64	0.60
1:A:107:VAL:HG11	1:A:115:ILE:HG13	1.86	0.58
1:A:347:VAL:CB	1:A:350:PHE:CE2	2.86	0.57
1:A:347:VAL:CG1	1:A:350:PHE:CD2	2.90	0.55
1:A:225:ASN:H	4:A:516:ACT:H2	1.70	0.55
1:A:52:THR:HG22	9:A:747:HOH:O	2.08	0.54
1:A:57:LYS:O	1:A:60:SER:HB3	2.09	0.52
1:A:289:LEU:HD21	1:A:392[A]:PHE:CE1	2.44	0.52
1:A:350:PHE:CB	1:A:351:PRO:HD2	2.39	0.51
1:A:340:LYS:HA	1:A:340:LYS:HE2	1.94	0.48
1:A:242:SER:CB	9:A:617:HOH:O	2.62	0.47
1:A:18:ALA:HB2	1:A:253:CME:OH	2.15	0.46
1:A:357:ASP:OD1	1:A:436:ASN:OD1	2.34	0.45
1:A:421:TYR:CE2	1:A:448:LYS:HE3	2.51	0.45
1:A:176:ARG:NH2	9:A:608:HOH:O	2.36	0.45
1:A:290:ARG:NE	1:A:349:GLY:O	2.38	0.45
1:A:297:VAL:O	1:A:343[A]:SER:HA	2.17	0.44
1:A:386:VAL:O	1:A:427:CYS:HA	2.18	0.44
4:A:505:ACT:O	9:A:602:HOH:O	2.21	0.44
1:A:314:ILE:HD11	1:A:337:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:508:DMS:H11	9:A:803:HOH:O	2.19	0.43
1:A:40:ASP:OD1	1:A:109:ARG:NH1	2.51	0.43
1:A:246:LYS:HE3	9:A:617:HOH:O	2.18	0.43
1:A:290:ARG:NE	1:A:350:PHE:HA	2.33	0.43
1:A:71[A]:LEU:HD23	1:A:392[A]:PHE:CD1	2.54	0.42
1:A:246:LYS:CE	9:A:617:HOH:O	2.67	0.42
1:A:328:PHE:CD2	1:A:365:CYS:HB2	2.54	0.42
1:A:297:VAL:O	1:A:343[B]:SER:HA	2.19	0.42
1:A:30:SER:CB	1:A:31:PRO:CD	2.98	0.41
1:A:29:PHE:HB3	1:A:35:PHE:CZ	2.54	0.41
6:A:512:PG4:H32	9:A:673:HOH:O	2.20	0.41
1:A:246:LYS:HD3	9:A:749:HOH:O	2.20	0.40
1:A:398:HIS:ND1	1:A:400:VAL:HG22	2.35	0.40

All (1) 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)
1:A:106:ARG:HH21	1:A:468:LYS:HZ1[5_555]	1.18	0.42

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	483/475 (102%)	468 (97%)	13 (3%)	2 (0%)	34 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	PRO
1	A	30	SER

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	426/418 (102%)	421 (99%)	5 (1%)	71 70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	109	ARG
1	A	296	PHE
1	A	350	PHE
1	A	447	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CME	A	253	1	8,9,10	1.01	0	5,9,11	0.60	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
1	CME	A	253	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	253	CME	CZ-CE-SD-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	253	CME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z > 2$
4	ACT	A	515	-	3,3,3	1.01	0	3,3,3	1.40	0
5	EDO	A	517	-	3,3,3	0.45	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PG4	A	512	-	12,12,12	0.48	0	11,11,11	0.48	0
5	EDO	A	513	-	3,3,3	0.46	0	2,2,2	0.37	0
5	EDO	A	507	-	3,3,3	0.55	0	2,2,2	0.30	0
3	DMS	A	502	-	3,3,3	0.61	0	3,3,3	0.33	0
3	DMS	A	504	-	3,3,3	0.70	0	3,3,3	0.84	0
5	EDO	A	510	-	3,3,3	0.35	0	2,2,2	0.37	0
5	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.42	0
7	PGE	A	518	-	9,9,9	0.33	0	8,8,8	0.41	0
3	DMS	A	508	-	3,3,3	0.56	0	3,3,3	0.48	0
4	ACT	A	506	-	3,3,3	0.96	0	3,3,3	1.63	1 (33%)
2	V9E	A	501	-	19,22,22	4.32	16 (84%)	18,31,31	3.69	11 (61%)
4	ACT	A	514	-	3,3,3	0.88	0	3,3,3	1.38	0
3	DMS	A	503	-	3,3,3	0.48	0	3,3,3	0.65	0
5	EDO	A	509	-	3,3,3	0.66	0	2,2,2	0.16	0
4	ACT	A	516	-	3,3,3	1.01	0	3,3,3	1.48	0
4	ACT	A	505	-	3,3,3	0.96	0	3,3,3	1.77	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	517	-	-	0/1/1/1	-
6	PG4	A	512	-	-	5/10/10/10	-
5	EDO	A	507	-	-	0/1/1/1	-
7	PGE	A	518	-	-	4/7/7/7	-
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	A	511	-	-	1/1/1/1	-
2	V9E	A	501	-	-	0/4/8/8	0/3/3/3
5	EDO	A	509	-	-	1/1/1/1	-
5	EDO	A	513	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	V9E	C05-S04	-7.99	1.57	1.73
2	A	501	V9E	C12-N11	6.68	1.47	1.35
2	A	501	V9E	C02-C01	6.33	1.60	1.39
2	A	501	V9E	C14-N13	5.96	1.44	1.34
2	A	501	V9E	C16-N11	5.18	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	V9E	C15-C16	4.67	1.46	1.38
2	A	501	V9E	C12-N13	4.62	1.43	1.35
2	A	501	V9E	C12-N19	4.49	1.42	1.33
2	A	501	V9E	C15-C14	4.37	1.46	1.39
2	A	501	V9E	C02-C03	3.45	1.45	1.34
2	A	501	V9E	C03-S04	-3.06	1.56	1.71
2	A	501	V9E	C06-C07	-3.03	1.36	1.41
2	A	501	V9E	C06-C14	2.96	1.53	1.49
2	A	501	V9E	C08-N09	-2.70	1.32	1.35
2	A	501	V9E	C01-C05	2.31	1.43	1.37
2	A	501	V9E	C06-N10	-2.13	1.33	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	V9E	C14-N13-C12	8.44	121.15	116.34
2	A	501	V9E	C02-C03-S04	-5.97	108.13	112.98
2	A	501	V9E	C06-C14-N13	5.60	123.27	116.61
2	A	501	V9E	C16-N11-C12	4.96	119.58	114.43
2	A	501	V9E	C15-C16-N11	-3.83	121.30	125.50
2	A	501	V9E	N13-C12-N11	-3.75	119.54	125.42
2	A	501	V9E	C18-N09-N10	3.10	124.15	120.50
2	A	501	V9E	N19-C12-N13	3.05	122.00	117.25
2	A	501	V9E	C15-C14-C06	-2.97	117.11	120.98
2	A	501	V9E	C07-C17-C05	-2.82	109.24	114.09
2	A	501	V9E	C15-C14-N13	-2.32	119.59	122.35
4	A	505	ACT	OXT-C-O	2.17	130.05	122.05
4	A	505	ACT	O-C-CH3	-2.16	113.94	122.33
4	A	506	ACT	O-C-CH3	-2.11	114.11	122.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	512	PG4	O2-C3-C4-O3
6	A	512	PG4	O3-C5-C6-O4
6	A	512	PG4	O1-C1-C2-O2
5	A	509	EDO	O1-C1-C2-O2
5	A	513	EDO	O1-C1-C2-O2
5	A	511	EDO	O1-C1-C2-O2
6	A	512	PG4	C3-C4-O3-C5
7	A	518	PGE	C1-C2-O2-C3

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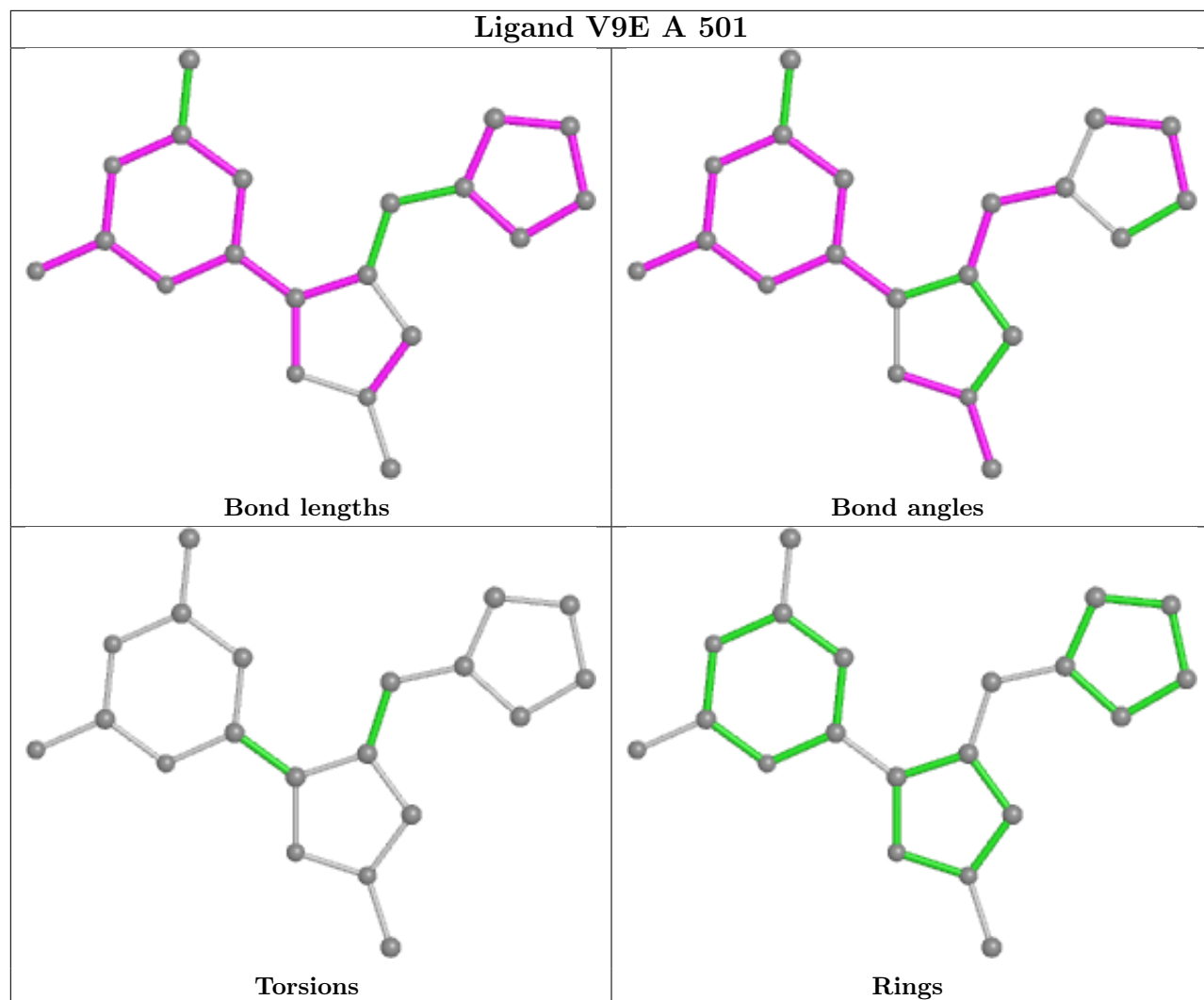
Mol	Chain	Res	Type	Atoms
7	A	518	PGE	O2-C3-C4-O3
7	A	518	PGE	C3-C4-O3-C5
6	A	512	PG4	C4-C3-O2-C2
7	A	518	PGE	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	512	PG4	1	0
3	A	508	DMS	1	0
4	A	516	ACT	1	0
4	A	505	ACT	1	0

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



5.7 Other polymers [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	461/475 (97%)	0.59	58 (12%) 3 4	22, 38, 79, 131	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	PRO	8.2
1	A	350	PHE	7.9
1	A	352	GLY	5.9
1	A	135	TRP	5.7
1	A	132	THR	5.4
1	A	355	VAL	5.2
1	A	351	PRO	5.0
1	A	336[A]	PHE	4.9
1	A	31	PRO	4.8
1	A	465	ARG	4.4
1	A	353	GLU	4.3
1	A	468	LYS	4.3
1	A	139	LEU	4.3
1	A	328	PHE	4.2
1	A	137	GLU	4.0
1	A	454	ALA	4.0
1	A	306	LYS	4.0
1	A	28	HIS	3.5
1	A	102	LEU	3.4
1	A	209	ASP	3.4
1	A	377	HIS	3.4
1	A	453	VAL	3.3
1	A	466	THR	3.3
1	A	140	ASP	3.2
1	A	45	PHE	3.2
1	A	303	ASP	3.1
1	A	304	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	208	PRO	3.1
1	A	96	PHE	3.0
1	A	101	LEU	3.0
1	A	32	GLU	2.9
1	A	449	VAL	2.9
1	A	138	GLY	2.8
1	A	335[A]	VAL	2.8
1	A	103	ALA	2.6
1	A	141	ILE	2.5
1	A	50	GLY	2.4
1	A	100	ALA	2.4
1	A	457	GLY	2.4
1	A	302	GLU	2.4
1	A	217	PHE	2.4
1	A	247	ASN	2.4
1	A	151	HIS	2.4
1	A	206	SER	2.3
1	A	97	ALA	2.3
1	A	375	GLN	2.3
1	A	219	LYS	2.2
1	A	207	VAL	2.2
1	A	437	LEU	2.2
1	A	296	PHE	2.1
1	A	46	VAL	2.1
1	A	134	GLU	2.1
1	A	211	ARG	2.1
1	A	345	LEU	2.1
1	A	93	ILE	2.1
1	A	305	ASP	2.1
1	A	392[A]	PHE	2.1
1	A	455	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
1	CME	A	253	10/11	0.95	0.09	29,46,77,81	0

6.3 Carbohydrates [i](#)

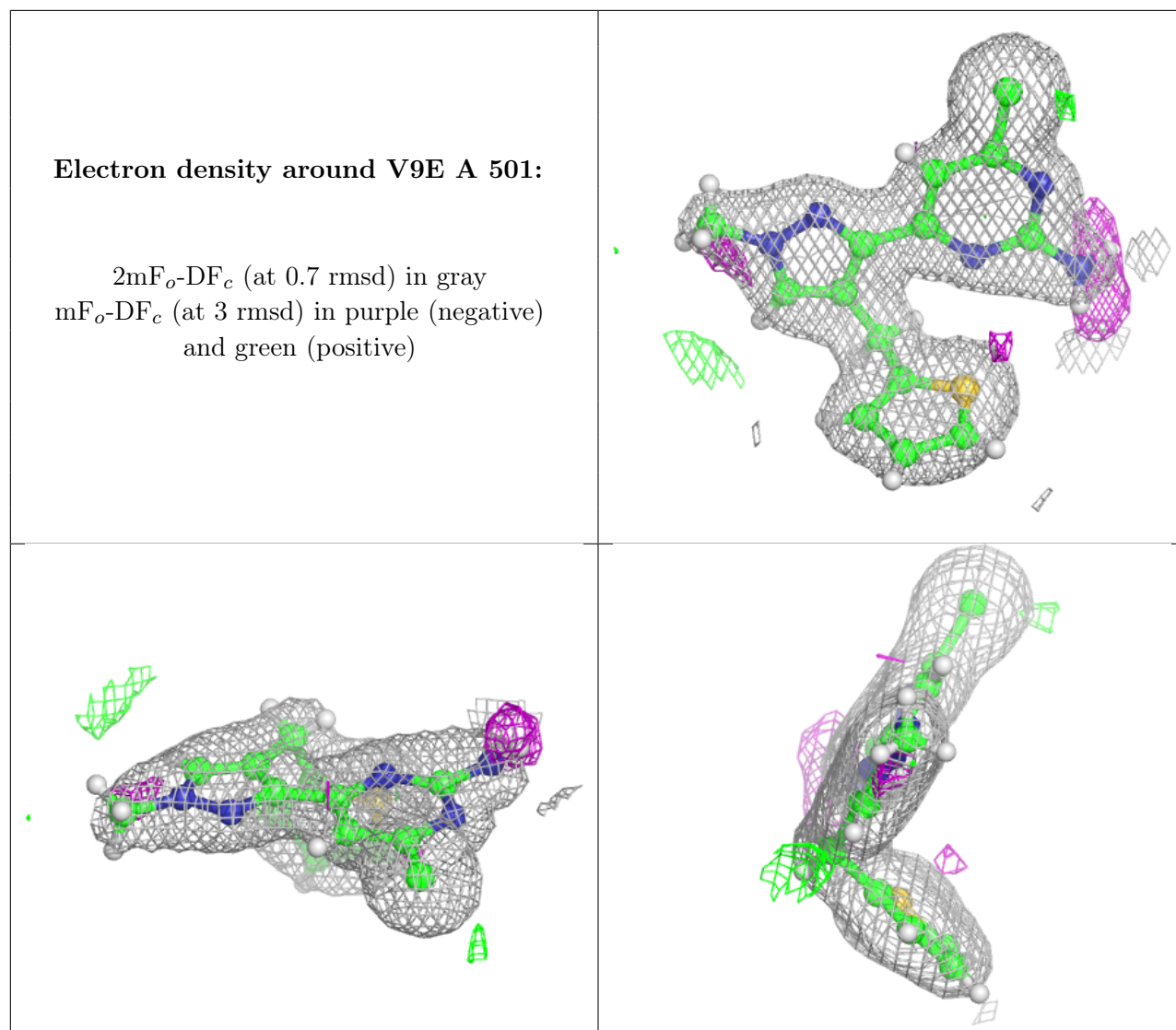
There are no monosaccharides in this entry.

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
7	PGE	A	518	10/10	0.50	0.83	90,108,117,118	0
5	EDO	A	509	4/4	0.62	0.22	54,65,66,66	0
6	PG4	A	512	13/13	0.65	0.23	63,76,85,87	0
4	ACT	A	516	4/4	0.68	0.21	71,73,85,85	0
5	EDO	A	507	4/4	0.72	0.23	53,64,65,66	0
5	EDO	A	517	4/4	0.77	0.24	71,86,87,88	0
4	ACT	A	506	4/4	0.85	0.20	59,60,71,71	0
4	ACT	A	515	4/4	0.85	0.20	65,66,78,78	0
4	ACT	A	514	4/4	0.87	0.42	70,70,84,84	0
8	CL	A	520	1/1	0.87	0.09	67,67,67,67	0
4	ACT	A	505	4/4	0.88	0.24	46,50,61,61	0
5	EDO	A	513	4/4	0.90	0.19	60,72,72,73	0
5	EDO	A	511	4/4	0.92	0.35	61,73,76,77	0
8	CL	A	519	1/1	0.94	0.17	58,58,58,58	0
3	DMS	A	503	4/4	0.95	0.13	41,50,54,54	0
5	EDO	A	510	4/4	0.96	0.14	45,54,60,62	0
3	DMS	A	504	4/4	0.96	0.15	49,63,63,63	0
3	DMS	A	508	4/4	0.97	0.13	64,77,78,78	0
2	V9E	A	501	20/20	0.97	0.19	24,30,37,40	0
3	DMS	A	502	4/4	0.98	0.10	59,71,71,71	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.