



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2026 – 12:13 PM JST

PDB ID : 26XC / pdb_000026xc
Title : Identification of AMPD2 Allosteric Inhibitors with Novel Mechanism of Action
by Fragment Merging Approach
Authors : Nomura, A.; Adachi, T.
Deposited on : 2026-05-19
Resolution : 2.50 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	:	1.8.5 (274361), CSD as541be (2020)
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

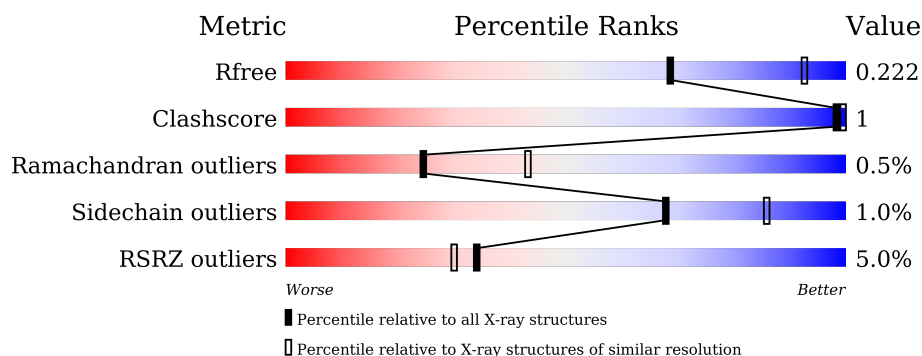
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	678	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	678	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	678	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	678	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>11%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	2005	-	X	-	-
3	PO4	B	2003	-	X	-	-
3	PO4	D	801	-	X	-	X
4	ES9	A	2004	-	-	X	-
4	ES9	B	2004	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19720 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 AMP deaminase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4901	3128	857	885	31			
1	B	601	Total	C	N	O	S	0	0	0
			4909	3130	861	887	31			
1	C	600	Total	C	N	O	S	0	0	0
			4888	3119	854	884	31			
1	D	601	Total	C	N	O	S	0	0	0
			4908	3132	859	886	31			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MET	-	initiating methionine	UNP Q01433
A	122	ASP	-	expression tag	UNP Q01433
A	123	TYR	-	expression tag	UNP Q01433
A	124	LYS	-	expression tag	UNP Q01433
A	125	ASP	-	expression tag	UNP Q01433
A	126	ASP	-	expression tag	UNP Q01433
A	127	ASP	-	expression tag	UNP Q01433
A	128	ASP	-	expression tag	UNP Q01433
A	129	LYS	-	expression tag	UNP Q01433
B	121	MET	-	initiating methionine	UNP Q01433
B	122	ASP	-	expression tag	UNP Q01433
B	123	TYR	-	expression tag	UNP Q01433
B	124	LYS	-	expression tag	UNP Q01433
B	125	ASP	-	expression tag	UNP Q01433
B	126	ASP	-	expression tag	UNP Q01433
B	127	ASP	-	expression tag	UNP Q01433
B	128	ASP	-	expression tag	UNP Q01433
B	129	LYS	-	expression tag	UNP Q01433
C	121	MET	-	initiating methionine	UNP Q01433
C	122	ASP	-	expression tag	UNP Q01433
C	123	TYR	-	expression tag	UNP Q01433

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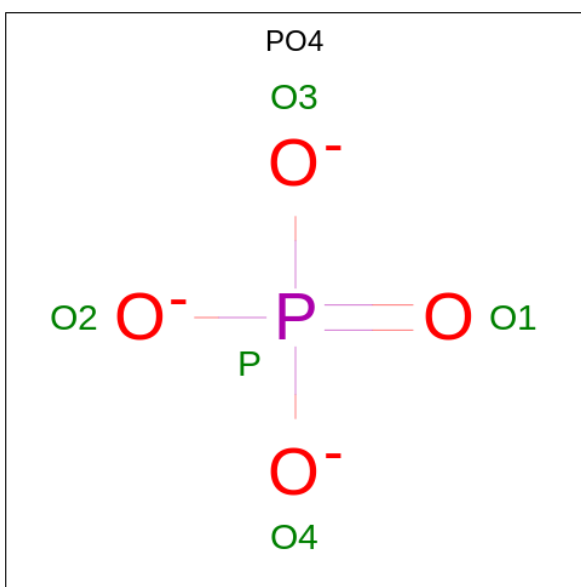
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Chain	Residue	Modelled	Actual	Comment	Reference
C	124	LYS	-	expression tag	UNP Q01433
C	125	ASP	-	expression tag	UNP Q01433
C	126	ASP	-	expression tag	UNP Q01433
C	127	ASP	-	expression tag	UNP Q01433
C	128	ASP	-	expression tag	UNP Q01433
C	129	LYS	-	expression tag	UNP Q01433
D	121	MET	-	initiating methionine	UNP Q01433
D	122	ASP	-	expression tag	UNP Q01433
D	123	TYR	-	expression tag	UNP Q01433
D	124	LYS	-	expression tag	UNP Q01433
D	125	ASP	-	expression tag	UNP Q01433
D	126	ASP	-	expression tag	UNP Q01433
D	127	ASP	-	expression tag	UNP Q01433
D	128	ASP	-	expression tag	UNP Q01433
D	129	LYS	-	expression tag	UNP Q01433

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

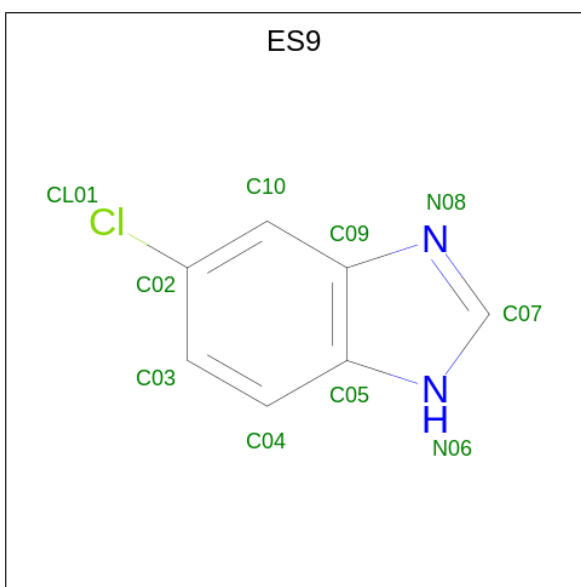
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



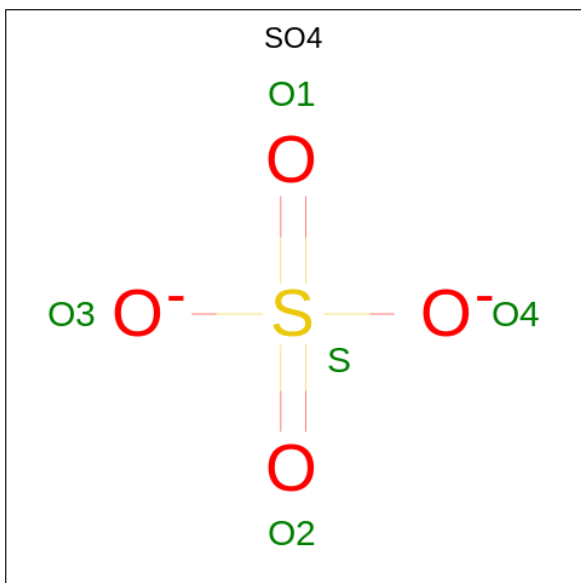
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 5-chloro-1H-benzimidazole (CCD ID: ES9) (formula: C₇H₅ClN₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			10	7	1	2		
4	B	1	Total	C	Cl	N	0	0
			10	7	1	2		
4	C	1	Total	C	Cl	N	0	0
			10	7	1	2		
4	D	1	Total	C	Cl	N	0	0
			10	7	1	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

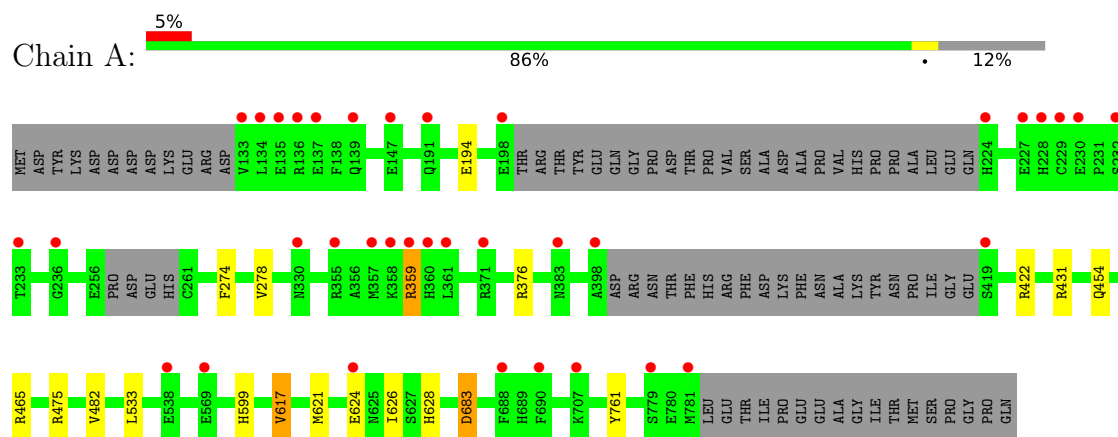


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

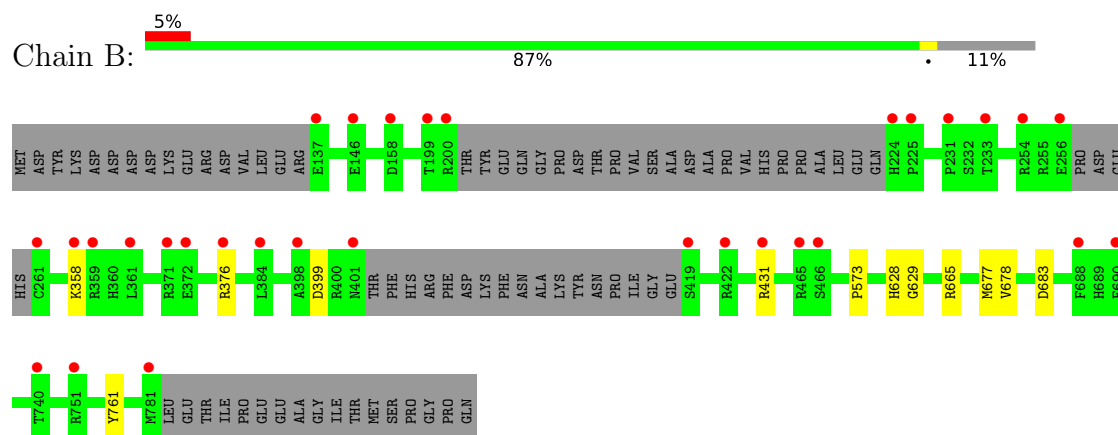
3 Residue-property plots

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.

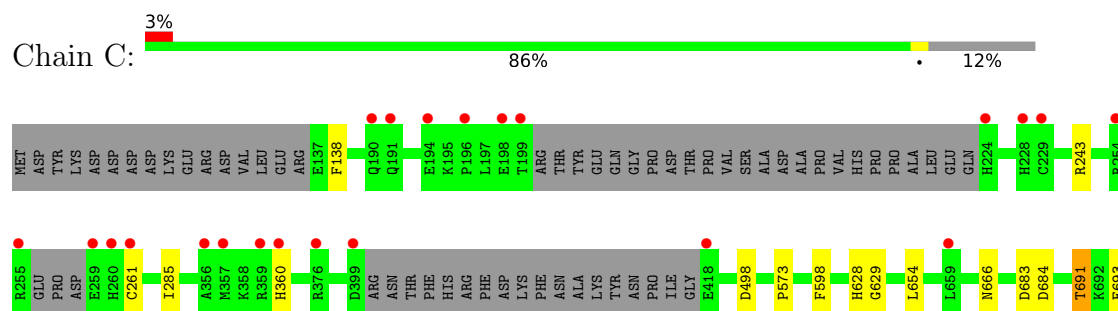
• Molecule 1: AMP deaminase 2

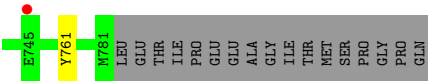


• Molecule 1: AMP deaminase 2

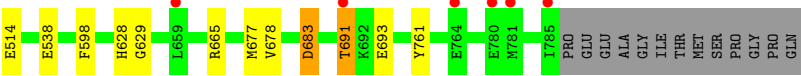
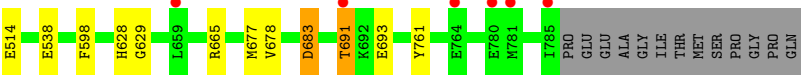
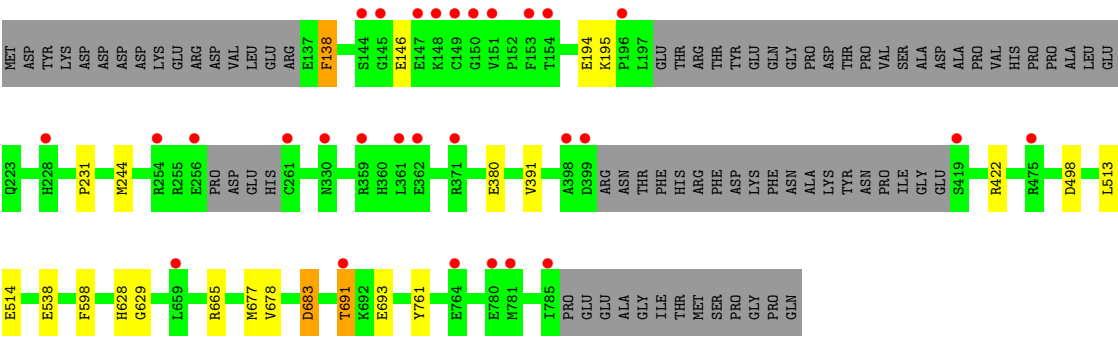
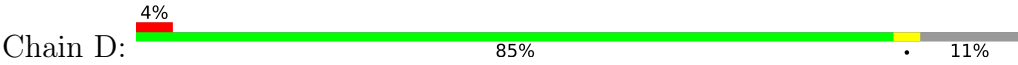


• Molecule 1: AMP deaminase 2





● Molecule 1: AMP deaminase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.44Å 162.46Å 291.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.25 – 2.50 78.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.3 (78.25-2.50) 94.3 (78.25-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.215 , 0.222 0.214 , 0.222	Depositor DCC
R_{free} test set	4803 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19720	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: PO4, SO4, ZN, ES9

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	0.77	0/5023	1.31	3/6800 (0.0%)
1	B	0.75	2/5031 (0.0%)	1.30	0/6810
1	C	0.76	2/5010 (0.0%)	1.33	8/6784 (0.1%)
1	D	0.77	2/5030 (0.0%)	1.35	4/6810 (0.1%)
All	All	0.76	6/20094 (0.0%)	1.32	15/27204 (0.1%)

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	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	677	MET	C-O	-5.93	1.17	1.23
1	D	629	GLY	C-O	-5.89	1.16	1.23
1	C	629	GLY	C-O	-5.86	1.16	1.23
1	B	629	GLY	C-O	-5.53	1.16	1.23
1	C	573	PRO	CA-C	5.37	1.54	1.51
1	B	573	PRO	CA-C	5.04	1.54	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	683	ASP	CA-CB-CG	8.57	121.17	112.60
1	D	138	PHE	CA-CB-CG	8.09	121.89	113.80
1	A	683	ASP	CA-CB-CG	7.58	120.18	112.60
1	C	629	GLY	CA-C-N	5.66	128.43	120.28
1	C	629	GLY	C-N-CA	5.66	128.43	120.28
1	A	617	VAL	N-CA-C	-5.34	105.30	110.42
1	A	626	ILE	CA-C-O	-5.31	116.25	121.67
1	D	498	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	666	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	C	598	PHE	CA-CB-CG	5.17	118.97	113.80
1	D	598	PHE	CA-CB-CG	5.16	118.96	113.80
1	C	498	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	684	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	138	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	360	HIS	CB-CG-CD2	-5.11	124.56	131.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	ARG	Sidechain
1	A	761	TYR	Sidechain
1	B	761	TYR	Sidechain
1	C	761	TYR	Sidechain
1	D	761	TYR	Sidechain

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	4901	0	4833	14	1
1	B	4909	0	4835	5	1
1	C	4888	0	4807	1	1
1	D	4908	0	4842	6	4
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	15	0	0	0	0
4	A	10	0	5	11	0
4	B	10	0	5	4	0
4	C	10	0	5	0	0
4	D	10	0	5	2	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
All	All	19720	0	19337	25	4

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 1.

All (25) 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:278:VAL:HG22	1:A:621:MET:HE1	1.45	0.96
1:B:399:ASP:CB	4:B:2004:ES9:C07	2.51	0.88
1:A:422:ARG:HD2	4:A:2004:ES9:C05	2.08	0.83
1:B:399:ASP:CB	4:B:2004:ES9:N06	2.43	0.82
1:A:422:ARG:HD2	4:A:2004:ES9:C09	2.17	0.73
1:A:422:ARG:HG2	4:A:2004:ES9:C10	2.20	0.72
1:B:399:ASP:CB	4:B:2004:ES9:H07	2.21	0.71
1:D:244:MET:HE1	1:D:513:LEU:HB2	1.74	0.69
1:B:399:ASP:CB	4:B:2004:ES9:HN06	2.06	0.68
1:A:422:ARG:HD2	4:A:2004:ES9:C07	2.34	0.57
1:A:422:ARG:HD2	4:A:2004:ES9:N06	2.20	0.57
1:A:422:ARG:CG	4:A:2004:ES9:C10	2.85	0.55
1:A:422:ARG:CD	4:A:2004:ES9:C09	2.86	0.53
1:D:244:MET:HE1	1:D:513:LEU:CB	2.37	0.53
1:A:422:ARG:HG3	4:A:2004:ES9:C03	2.40	0.52
1:B:665:ARG:HH11	1:D:665:ARG:NH1	2.08	0.51
1:A:274:PHE:O	1:A:278:VAL:HG23	2.12	0.49
1:D:691:THR:HG23	1:D:693:GLU:H	1.78	0.49
1:C:691:THR:HG23	1:C:693:GLU:H	1.79	0.47
1:D:422:ARG:HD2	4:D:805:ES9:C05	2.46	0.46
1:A:422:ARG:CG	4:A:2004:ES9:C09	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ARG:HD2	4:A:2004:ES9:N08	2.32	0.44
1:D:422:ARG:HG2	4:D:805:ES9:C10	2.48	0.43
1:A:617:VAL:HG12	1:A:621:MET:HE2	2.02	0.42
1:A:422:ARG:CD	4:A:2004:ES9:C05	2.90	0.41

All (4) 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:359:ARG:NH2	1:D:380:GLU:OE2[5_545]	1.33	0.87
1:B:358:LYS:NZ	1:D:231:PRO:CD[5_545]	1.53	0.67
1:D:146:GLU:OE2	1:D:146:GLU:OE2[3_755]	1.71	0.49
1:C:243:ARG:NH2	1:D:514:GLU:OE1[5_445]	1.77	0.43

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	592/678 (87%)	570 (96%)	19 (3%)	3 (0%)	24	43
1	B	593/678 (88%)	580 (98%)	11 (2%)	2 (0%)	36	55
1	C	592/678 (87%)	573 (97%)	16 (3%)	3 (0%)	24	43
1	D	593/678 (88%)	578 (98%)	12 (2%)	3 (0%)	24	43
All	All	2370/2712 (87%)	2301 (97%)	58 (2%)	11 (0%)	24	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	HIS
1	A	359	ARG
1	B	628	HIS

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Mol	Chain	Res	Type
1	D	628	HIS
1	D	683	ASP
1	A	683	ASP
1	C	261	CYS
1	C	628	HIS
1	C	683	ASP
1	D	138	PHE
1	B	683	ASP

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	541/612 (88%)	532 (98%)	9 (2%)	53	78
1	B	541/612 (88%)	537 (99%)	4 (1%)	76	89
1	C	538/612 (88%)	535 (99%)	3 (1%)	78	91
1	D	542/612 (89%)	536 (99%)	6 (1%)	65	84
All	All	2162/2448 (88%)	2140 (99%)	22 (1%)	68	86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	431	ARG
1	A	454	GLN
1	A	465	ARG
1	A	475	ARG
1	A	482	VAL
1	A	533	LEU
1	A	599	HIS
1	A	624	GLU
1	B	376	ARG
1	B	431	ARG
1	B	677	MET
1	B	678	VAL

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Mol	Chain	Res	Type
1	C	285	ILE
1	C	654	LEU
1	C	691	THR
1	D	194	GLU
1	D	195	LYS
1	D	391	VAL
1	D	538	GLU
1	D	678	VAL
1	D	691	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	HIS
1	A	486	ASN
1	A	526	HIS
1	A	733	HIS
1	B	299	GLN
1	B	320	GLN
1	B	486	ASN
1	B	534	HIS
1	B	558	ASN
1	B	687	GLN
1	B	747	ASN
1	C	299	GLN
1	C	320	GLN
1	C	346	GLN
1	C	360	HIS
1	C	483	HIS
1	C	510	GLN
1	C	515	ASN
1	C	628	HIS
1	D	299	GLN
1	D	320	GLN
1	D	373	GLN
1	D	439	HIS
1	D	510	GLN
1	D	526	HIS
1	D	558	ASN
1	D	595	GLN
1	D	664	HIS
1	D	747	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 4 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
3	PO4	B	2002	-	4,4,4	2.15	3 (75%)	6,6,6	0.73	0
3	PO4	D	801	-	4,4,4	2.70	4 (100%)	6,6,6	0.58	0
3	PO4	D	804	-	4,4,4	2.24	3 (75%)	6,6,6	0.94	0
4	ES9	B	2004	-	11,11,11	1.28	1 (9%)	15,15,15	1.30	1 (6%)
4	ES9	D	805	-	11,11,11	1.29	1 (9%)	15,15,15	1.29	1 (6%)
5	SO4	C	2005	-	4,4,4	0.26	0	6,6,6	0.17	0
3	PO4	A	2003	-	4,4,4	2.19	3 (75%)	6,6,6	0.80	0
3	PO4	C	2002	-	4,4,4	2.17	3 (75%)	6,6,6	0.24	0
4	ES9	A	2004	-	11,11,11	1.27	1 (9%)	15,15,15	1.30	1 (6%)
3	PO4	D	803	-	4,4,4	2.46	3 (75%)	6,6,6	0.39	0
3	PO4	A	2005	-	4,4,4	2.75	4 (100%)	6,6,6	0.54	0
4	ES9	C	2004	-	11,11,11	1.30	1 (9%)	15,15,15	1.29	1 (6%)
5	SO4	A	2006	-	4,4,4	0.30	0	6,6,6	0.13	0
3	PO4	C	2003	-	4,4,4	2.40	3 (75%)	6,6,6	0.62	0
5	SO4	B	2005	-	4,4,4	0.28	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	D	806	-	4,4,4	0.27	0	6,6,6	0.11	0
3	PO4	A	2002	-	4,4,4	2.49	3 (75%)	6,6,6	0.41	0
3	PO4	B	2003	-	4,4,4	2.18	3 (75%)	6,6,6	1.06	1 (16%)

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
4	ES9	A	2004	-	-	-	0/2/2/2
4	ES9	D	805	-	-	-	0/2/2/2
4	ES9	B	2004	-	-	-	0/2/2/2
4	ES9	C	2004	-	-	-	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2005	PO4	P-O4	-2.94	1.45	1.54
3	A	2005	PO4	P-O2	-2.90	1.45	1.54
3	D	801	PO4	P-O2	-2.87	1.46	1.54
3	D	801	PO4	P-O3	-2.83	1.46	1.54
3	D	803	PO4	P-O3	-2.80	1.46	1.54
3	A	2002	PO4	P-O4	-2.79	1.46	1.54
3	C	2003	PO4	P-O2	-2.78	1.46	1.54
3	D	801	PO4	P-O4	-2.77	1.46	1.54
3	A	2002	PO4	P-O3	-2.75	1.46	1.54
3	A	2005	PO4	P-O3	-2.69	1.46	1.54
3	D	803	PO4	P-O4	-2.66	1.46	1.54
3	C	2003	PO4	P-O4	-2.60	1.46	1.54
3	D	804	PO4	P-O2	-2.60	1.46	1.54
3	A	2002	PO4	P-O2	-2.56	1.46	1.54
3	D	803	PO4	P-O2	-2.51	1.47	1.54
3	D	804	PO4	P-O3	-2.50	1.47	1.54
3	C	2002	PO4	P-O4	-2.48	1.47	1.54
3	B	2003	PO4	P-O4	-2.45	1.47	1.54
3	A	2005	PO4	P-O1	-2.44	1.45	1.50
3	A	2003	PO4	P-O3	-2.43	1.47	1.54
3	C	2003	PO4	P-O3	-2.41	1.47	1.54
3	C	2002	PO4	P-O3	-2.39	1.47	1.54
3	D	804	PO4	P-O4	-2.37	1.47	1.54
3	A	2003	PO4	P-O2	-2.32	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	PO4	P-O3	-2.32	1.47	1.54
3	B	2003	PO4	P-O2	-2.30	1.47	1.54
3	D	801	PO4	P-O1	-2.30	1.45	1.50
4	C	2004	ES9	C05-C09	-2.30	1.37	1.40
4	D	805	ES9	C05-C09	-2.30	1.37	1.40
4	A	2004	ES9	C05-C09	-2.28	1.37	1.40
3	B	2002	PO4	P-O4	-2.27	1.47	1.54
4	B	2004	ES9	C05-C09	-2.25	1.37	1.40
3	B	2002	PO4	P-O2	-2.25	1.47	1.54
3	A	2003	PO4	P-O4	-2.20	1.48	1.54
3	C	2002	PO4	P-O2	-2.17	1.48	1.54
3	B	2003	PO4	P-O3	-2.15	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2004	ES9	N06-C07-N08	-3.02	109.20	113.90
4	B	2004	ES9	N06-C07-N08	-3.02	109.21	113.90
4	C	2004	ES9	N06-C07-N08	-3.02	109.22	113.90
4	D	805	ES9	N06-C07-N08	-3.00	109.24	113.90
3	B	2003	PO4	O3-P-O2	2.24	115.16	107.97

There are no chirality outliers.

There are no torsion outliers.

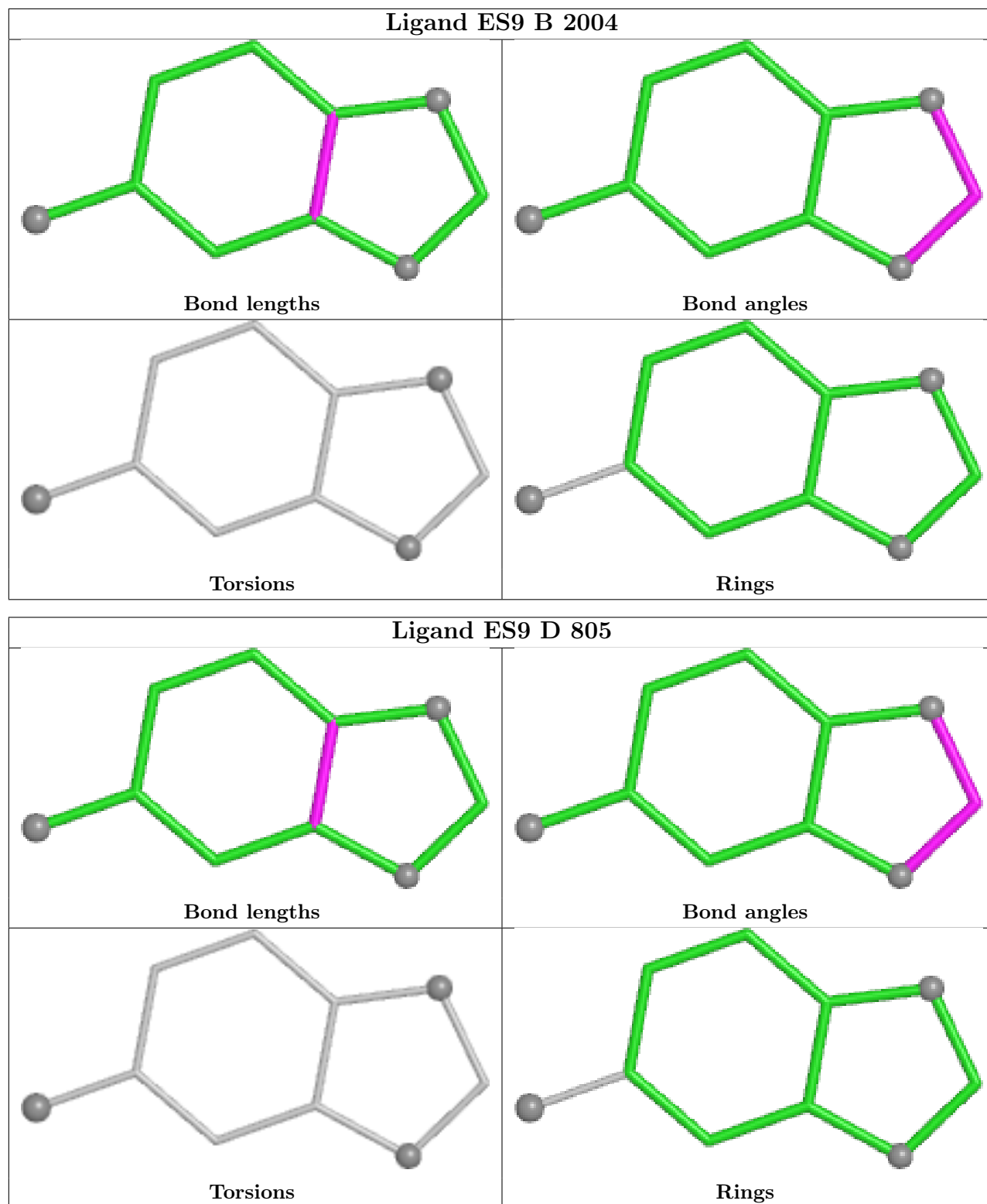
There are no ring outliers.

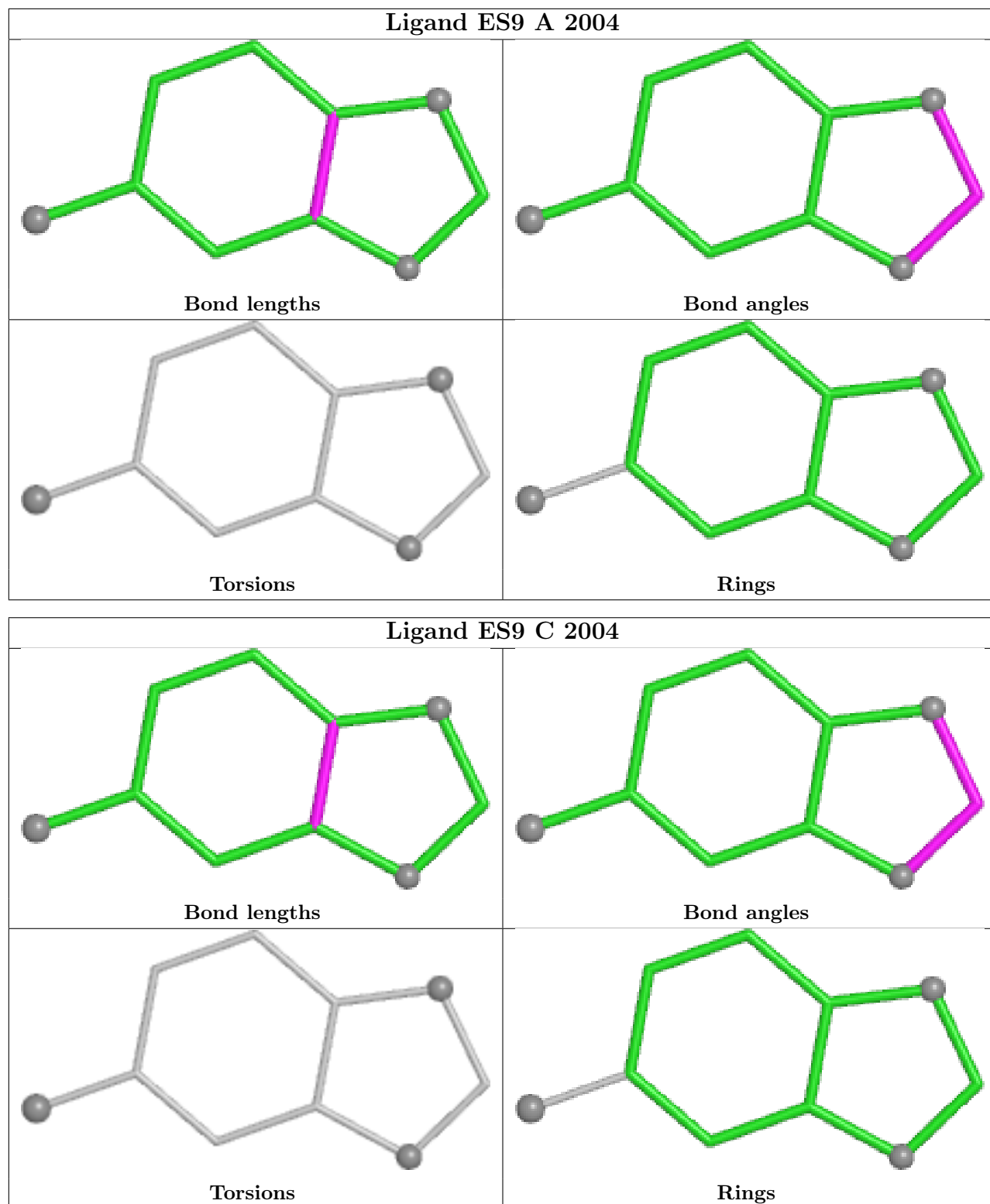
3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2004	ES9	4	0
4	D	805	ES9	2	0
4	A	2004	ES9	11	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 ⓘ

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	600/678 (88%)	0.42	36 (6%) 27 24	32, 53, 105, 192	0
1	B	601/678 (88%)	0.37	31 (5%) 33 29	32, 55, 102, 176	0
1	C	600/678 (88%)	0.17	23 (3%) 44 39	27, 47, 93, 219	0
1	D	601/678 (88%)	0.23	29 (4%) 35 31	27, 46, 102, 205	0
All	All	2402/2712 (88%)	0.29	119 (4%) 34 30	27, 50, 102, 219	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	ARG	5.1
1	C	191	GLN	5.0
1	D	362	GLU	4.9
1	A	136	ARG	4.7
1	A	361	LEU	4.6
1	C	399	ASP	4.5
1	D	785	ILE	4.4
1	D	254	ARG	4.3
1	A	360	HIS	4.3
1	B	261	CYS	4.1
1	A	230	GLU	4.0
1	C	260	HIS	4.0
1	B	690	PHE	3.8
1	C	357	MET	3.7
1	C	418	GLU	3.6
1	A	398	ALA	3.6
1	C	356	ALA	3.6
1	A	236	GLY	3.6
1	B	401	ASN	3.5
1	A	135	GLU	3.5
1	A	690	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	199	THR	3.4
1	D	196	PRO	3.4
1	A	139	GLN	3.4
1	B	422	ARG	3.3
1	B	465	ARG	3.3
1	D	256	GLU	3.3
1	B	781	MET	3.3
1	A	538	GLU	3.3
1	D	153	PHE	3.3
1	D	149	CYS	3.3
1	D	399	ASP	3.2
1	C	360	HIS	3.2
1	D	228	HIS	3.2
1	B	231	PRO	3.2
1	B	384	LEU	3.2
1	A	781	MET	3.2
1	D	145	GLY	3.2
1	C	255	ARG	3.1
1	A	357	MET	3.1
1	A	133	VAL	3.1
1	A	358	LYS	3.0
1	D	359	ARG	2.9
1	B	256	GLU	2.9
1	D	147	GLU	2.9
1	A	355	ARG	2.9
1	B	398	ALA	2.9
1	D	475	ARG	2.8
1	D	148	LYS	2.8
1	D	330	ASN	2.8
1	D	764	GLU	2.8
1	D	781	MET	2.8
1	A	224	HIS	2.8
1	C	199	THR	2.7
1	D	154	THR	2.7
1	A	228	HIS	2.7
1	B	224	HIS	2.7
1	A	134	LEU	2.7
1	B	751	ARG	2.7
1	D	361	LEU	2.7
1	D	780	GLU	2.7
1	A	191	GLN	2.7
1	D	261	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	688	PHE	2.6
1	C	259	GLU	2.6
1	A	707	LYS	2.6
1	B	254	ARG	2.6
1	D	150	GLY	2.6
1	A	419	SER	2.5
1	A	779	SER	2.5
1	D	419	SER	2.5
1	B	376	ARG	2.5
1	C	228	HIS	2.5
1	B	225	PRO	2.4
1	A	229	CYS	2.4
1	C	190	GLN	2.4
1	B	431	ARG	2.4
1	C	194	GLU	2.4
1	C	229	CYS	2.4
1	D	151	VAL	2.4
1	D	691	THR	2.4
1	C	224	HIS	2.3
1	A	147	GLU	2.3
1	C	196	PRO	2.3
1	D	398	ALA	2.3
1	A	232	SER	2.3
1	D	659	LEU	2.3
1	A	624	GLU	2.3
1	A	330	ASN	2.2
1	C	261	CYS	2.3
1	C	659	LEU	2.2
1	B	137	GLU	2.2
1	B	200	ARG	2.2
1	D	371	ARG	2.2
1	B	688	PHE	2.2
1	D	144	SER	2.2
1	A	233	THR	2.2
1	B	372	GLU	2.1
1	B	466	SER	2.1
1	B	233	THR	2.1
1	B	371	ARG	2.1
1	B	358	LYS	2.1
1	A	359	ARG	2.1
1	C	359	ARG	2.1
1	A	137	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLU	2.1
1	C	198	GLU	2.1
1	B	361	LEU	2.1
1	C	376	ARG	2.1
1	A	569	GLU	2.1
1	C	254	ARG	2.0
1	A	227	GLU	2.0
1	B	146	GLU	2.0
1	B	740	THR	2.0
1	B	419	SER	2.0
1	A	371	ARG	2.0
1	C	745	GLU	2.0
1	A	383	ASN	2.0
1	B	158	ASP	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.

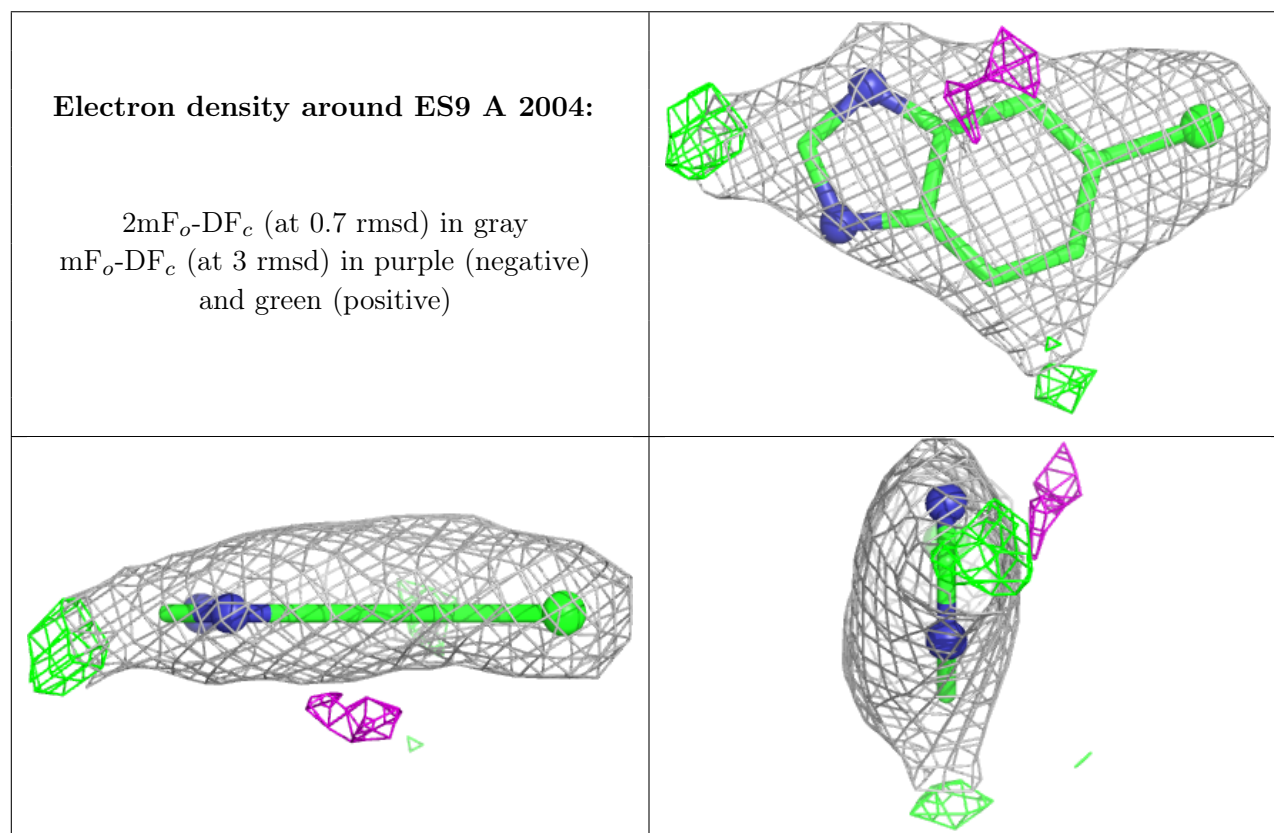
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	D	801	5/5	0.43	0.48	47,48,51,51	0
3	PO4	A	2003	5/5	0.46	0.28	41,44,49,60	0
5	SO4	C	2005	5/5	0.60	0.23	66,67,68,69	0
5	SO4	A	2006	5/5	0.64	0.25	62,63,63,67	0
5	SO4	D	806	5/5	0.64	0.29	51,51,53,53	0
5	SO4	B	2005	5/5	0.69	0.19	69,73,77,78	0
3	PO4	B	2003	5/5	0.72	0.30	43,43,45,49	0
4	ES9	A	2004	10/10	0.74	0.21	90,96,97,100	0
4	ES9	B	2004	10/10	0.76	0.24	110,116,117,120	0

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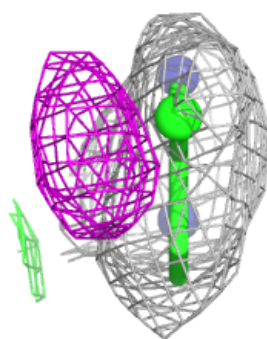
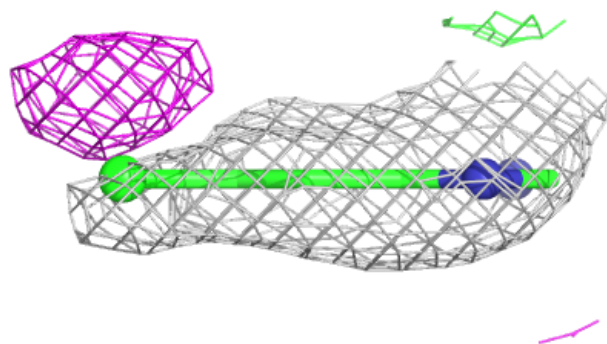
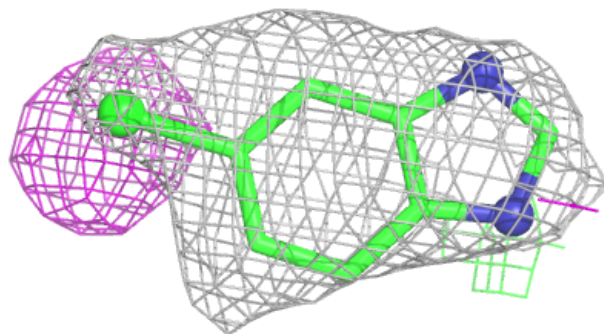
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	2005	5/5	0.80	0.32	41,42,42,43	0
3	PO4	A	2002	5/5	0.81	0.23	53,53,53,55	0
3	PO4	C	2003	5/5	0.82	0.23	39,44,51,54	0
3	PO4	D	804	5/5	0.83	0.22	36,42,44,47	0
4	ES9	D	805	10/10	0.84	0.15	78,84,86,88	0
3	PO4	B	2002	5/5	0.87	0.14	61,62,64,89	0
3	PO4	C	2002	5/5	0.89	0.20	44,44,46,49	0
4	ES9	C	2004	10/10	0.90	0.15	76,82,83,86	0
2	ZN	B	2001	1/1	0.94	0.08	32,32,32,32	0
3	PO4	D	803	5/5	0.95	0.25	37,38,39,40	0
2	ZN	A	2001	1/1	0.95	0.09	34,34,34,34	0
2	ZN	C	2001	1/1	0.96	0.08	27,27,27,27	0
2	ZN	D	802	1/1	0.97	0.07	27,27,27,27	0

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

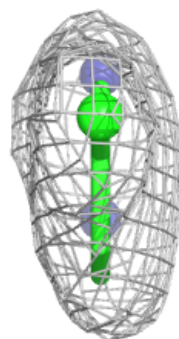
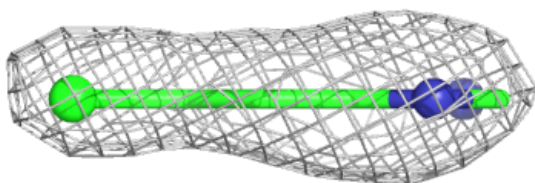
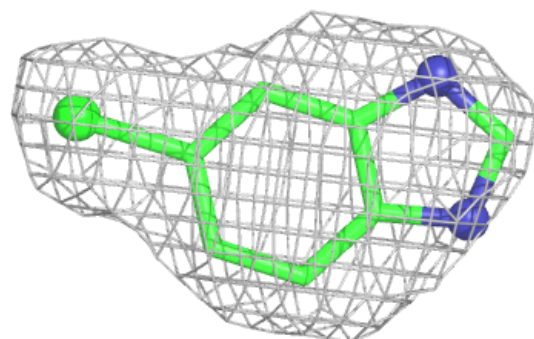


Electron density around ES9 B 2004:

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

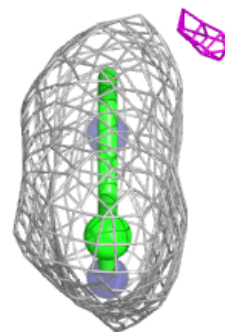
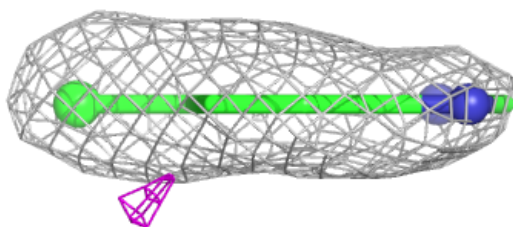
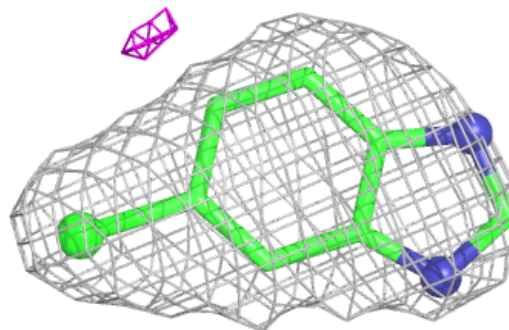
**Electron density around ES9 D 805:**

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



Electron density around ES9 C 2004:

$2mF_o - DF_c$ (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.