



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 01:27 pm BST

PDB ID : 9HL0 / pdb_00009hl0
Title : Protein Kinase CK2 and small molecule ligands
Authors : Krimm, I.; Gelin, M.; Guichou, J.F.
Deposited on : 2024-12-04
Resolution : 2.63 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

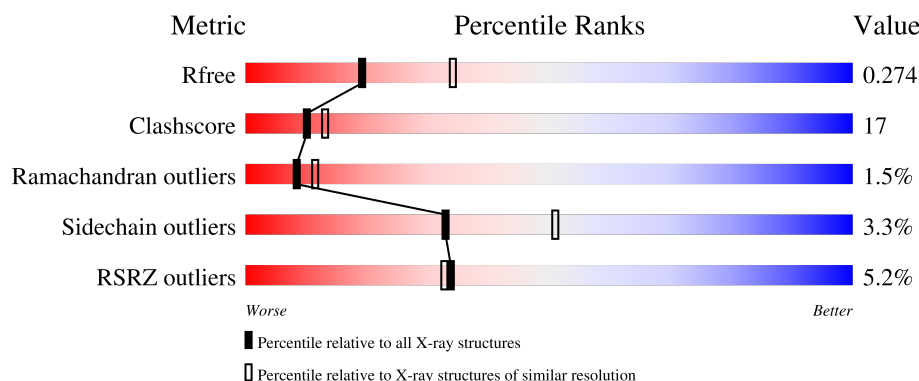
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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}	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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	359	 4% 61% 30% • 8%
1	B	359	 6% 60% 29% • 9%

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	SO4	B	402	-	-	X	-
3	PEG	B	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5633 atoms, of which 15 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2739	1756	475	497	11			
1	B	328	Total	C	N	O	S	0	1	0
			2737	1759	474	493	11			

There are 44 discrepancies between the modelled and reference sequences:

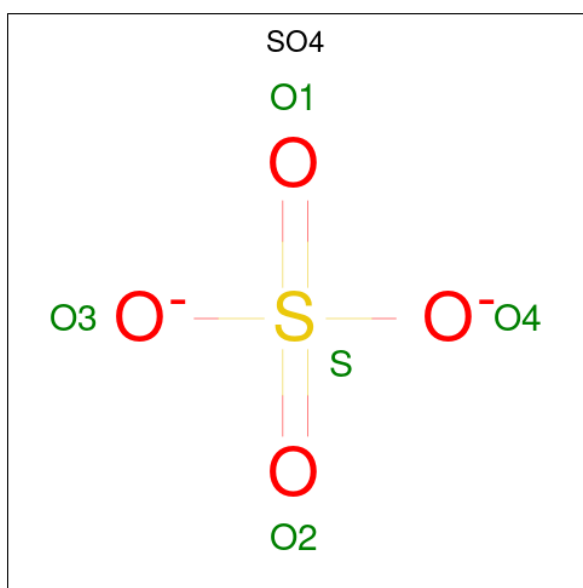
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P68400
A	-20	HIS	-	expression tag	UNP P68400
A	-19	HIS	-	expression tag	UNP P68400
A	-18	HIS	-	expression tag	UNP P68400
A	-17	HIS	-	expression tag	UNP P68400
A	-16	HIS	-	expression tag	UNP P68400
A	-15	HIS	-	expression tag	UNP P68400
A	-14	SER	-	expression tag	UNP P68400
A	-13	SER	-	expression tag	UNP P68400
A	-12	GLY	-	expression tag	UNP P68400
A	-11	VAL	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	LEU	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	THR	-	expression tag	UNP P68400
A	-6	GLU	-	expression tag	UNP P68400
A	-5	ASN	-	expression tag	UNP P68400
A	-4	LEU	-	expression tag	UNP P68400
A	-3	TYR	-	expression tag	UNP P68400
A	-2	PHE	-	expression tag	UNP P68400
A	-1	GLN	-	expression tag	UNP P68400
A	0	SER	-	expression tag	UNP P68400
B	-21	MET	-	initiating methionine	UNP P68400
B	-20	HIS	-	expression tag	UNP P68400
B	-19	HIS	-	expression tag	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP P68400
B	-17	HIS	-	expression tag	UNP P68400
B	-16	HIS	-	expression tag	UNP P68400
B	-15	HIS	-	expression tag	UNP P68400
B	-14	SER	-	expression tag	UNP P68400
B	-13	SER	-	expression tag	UNP P68400
B	-12	GLY	-	expression tag	UNP P68400
B	-11	VAL	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	LEU	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	THR	-	expression tag	UNP P68400
B	-6	GLU	-	expression tag	UNP P68400
B	-5	ASN	-	expression tag	UNP P68400
B	-4	LEU	-	expression tag	UNP P68400
B	-3	TYR	-	expression tag	UNP P68400
B	-2	PHE	-	expression tag	UNP P68400
B	-1	GLN	-	expression tag	UNP P68400
B	0	SER	-	expression tag	UNP P68400

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



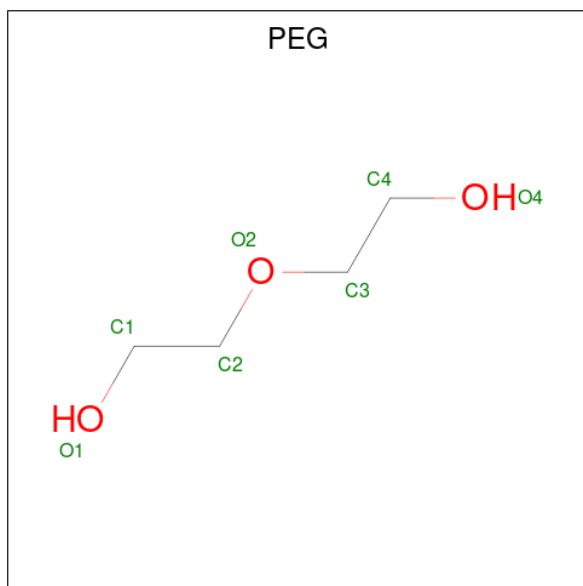
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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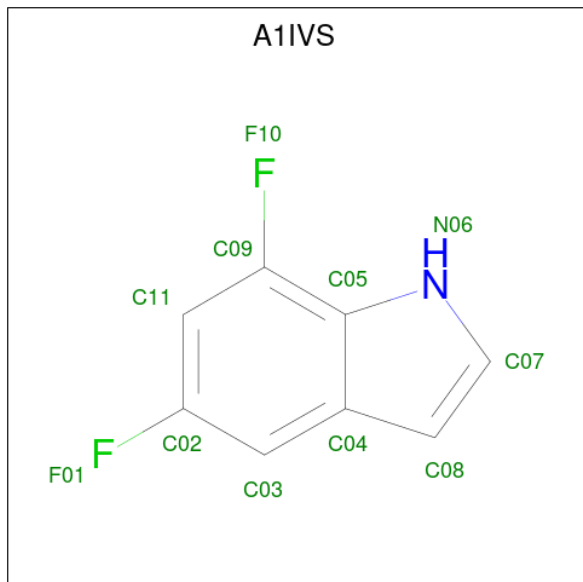
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is 5,7-bis(fluoranyl)-1 {H}-indole (CCD ID: A1IVS) (formula: $C_8H_5F_2N$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	H	N	0	0
			16	8	2	5	1		
4	B	1	Total	C	F	H	N	0	0
			16	8	2	5	1		
4	B	1	Total	C	F	H	N	0	0
			16	8	2	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	21	Total	O	0	0
			21	21		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.30Å 127.30Å 123.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.65 – 2.63 63.65 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.3 (63.65-2.63) 99.4 (63.65-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.230 , 0.280 0.229 , 0.274	Depositor DCC
R_{free} test set	2248 reflections (6.74%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5633	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.11 % 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 3.3739e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, A1IVS, SO4

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	0.39	0/2815	0.59	0/3816
1	B	0.40	0/2814	0.61	0/3811
All	All	0.39	0/5629	0.60	0/7627

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2739	0	2639	104	0
1	B	2737	0	2651	82	0
2	A	35	0	0	3	0
2	B	20	0	0	2	0
3	A	7	0	10	2	0
3	B	7	0	10	4	0
4	A	11	5	0	1	0
4	B	22	10	0	0	0
5	A	19	0	0	0	0
5	B	21	0	0	0	0
All	All	5618	15	5310	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (185) 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:B:303:LYS:HB3	1:B:313:LEU:HD13	1.54	0.90
1:A:137:MET:HE3	1:A:218:LEU:HD11	1.52	0.89
1:A:125:TYR:HA	1:A:128:LEU:HD13	1.57	0.86
1:A:276:HIS:ND1	3:A:405:PEG:H31	1.90	0.86
1:A:163:MET:HE3	1:A:163:MET:HA	1.58	0.85
1:A:118:ASN:HB2	1:A:163:MET:HE1	1.60	0.83
1:A:174:ILE:HD13	2:A:408:SO4:O1	1.82	0.78
1:A:280:ARG:HG3	2:A:407:SO4:O3	1.85	0.77
1:B:124:LEU:O	1:B:126:GLN:N	2.20	0.75
1:A:275:ARG:HH21	1:B:252:GLU:HG2	1.52	0.74
1:B:191:ARG:HD2	2:B:402:SO4:O1	1.88	0.74
1:A:70:LEU:HD12	1:A:78:ILE:HG12	1.70	0.73
1:A:118:ASN:HB2	1:A:163:MET:CE	2.19	0.72
1:B:303:LYS:HB3	1:B:313:LEU:CD1	2.19	0.72
1:A:137:MET:HE3	1:A:218:LEU:CD1	2.19	0.72
1:A:195:ARG:HH11	1:A:237:ASP:HA	1.55	0.71
1:B:293:VAL:HG12	3:B:401:PEG:H41	1.73	0.70
1:A:118:ASN:CB	1:A:163:MET:HE1	2.22	0.70
1:A:40:GLN:HG3	1:A:59:ILE:CG2	2.21	0.70
1:A:286:HIS:CE1	1:A:288:GLU:HB2	2.27	0.69
1:B:280:ARG:O	1:B:283:ARG:HG3	1.93	0.69
1:A:269:PHE:O	1:A:271:ASP:N	2.27	0.67
1:B:117:ASN:O	1:B:119:THR:N	2.27	0.67
1:B:137:MET:HE1	1:B:218:LEU:HG	1.79	0.65
1:B:189:ASN:OD1	1:B:191:ARG:N	2.27	0.65
1:B:122:LYS:HG2	1:B:159:PRO:HB2	1.78	0.64
1:A:130:ASP:O	1:A:134:ARG:HG3	1.97	0.64
1:A:300:PHE:HB2	1:A:321:HIS:CE1	2.34	0.63
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.34	0.63
1:B:324:PHE:O	1:B:328:VAL:HG23	1.98	0.63
1:A:269:PHE:C	1:A:271:ASP:H	2.06	0.63
1:A:303:LYS:NZ	3:B:401:PEG:H11	2.14	0.62
1:B:121:PHE:CD1	1:B:225:MET:HE1	2.35	0.62
1:B:122:LYS:HE3	1:B:160[A]:HIS:NE2	2.15	0.62
1:B:231:PRO:HD2	1:B:234:HIS:CD2	2.35	0.61
1:A:118:ASN:CG	1:A:163:MET:HE1	2.26	0.61
1:A:102:LYS:HD3	1:A:107:ARG:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:HE3	1:A:163:MET:CA	2.29	0.61
1:B:170:LYS:HE2	1:B:172:ARG:HH12	1.66	0.61
1:B:21:ARG:NH1	1:B:25:ASP:OD2	2.30	0.60
1:A:107:ARG:O	1:A:108:THR:C	2.45	0.60
1:B:103:ASP:OD1	1:B:104:PRO:HD2	2.02	0.60
1:A:22:GLU:H	1:A:22:GLU:CD	2.10	0.59
1:A:251:THR:HG21	1:A:274:GLY:O	2.00	0.59
1:B:221:MET:O	1:B:225:MET:HG3	2.01	0.59
1:A:216:TRP:CZ2	1:A:245:ILE:HD13	2.38	0.59
1:B:321:HIS:CG	1:B:322:PRO:HD2	2.38	0.59
1:B:254:LEU:HB2	1:B:307:TYR:CZ	2.38	0.59
1:A:58:ASN:OD1	1:A:60:THR:HB	2.04	0.58
1:B:46:GLY:C	1:B:47:ARG:HG2	2.28	0.58
1:A:224:SER:HB2	1:A:229:LYS:O	2.04	0.57
1:A:275:ARG:HH21	1:B:252:GLU:CG	2.17	0.57
1:B:286:HIS:HD2	1:B:288:GLU:H	1.50	0.57
1:B:80:ARG:NH1	1:B:180:GLU:OE2	2.30	0.57
1:A:331:GLN:O	1:A:332:ALA:HB2	2.04	0.57
1:B:137:MET:HE2	1:B:222:LEU:HB2	1.86	0.57
1:B:201:GLU:HG2	1:B:202:LEU:H	1.69	0.57
1:A:16:ASN:HD21	1:A:181:PHE:HB3	1.70	0.56
1:A:171:LEU:C	1:A:171:LEU:HD23	2.30	0.56
1:B:171:LEU:HD23	1:B:171:LEU:C	2.31	0.56
1:B:121:PHE:CE1	1:B:225:MET:HE1	2.41	0.56
1:B:64:LYS:O	1:B:65:VAL:HG23	2.06	0.56
1:B:219:GLY:HA2	1:B:304:LEU:HD12	1.88	0.55
1:A:195:ARG:HH11	1:A:237:ASP:CA	2.20	0.55
1:A:303:LYS:HZ2	3:B:401:PEG:H11	1.71	0.55
1:B:200:PRO:O	1:B:204:VAL:HG22	2.06	0.55
1:B:51:SER:HB2	1:B:69:ILE:O	2.07	0.55
1:B:71:LYS:O	1:B:73:VAL:HG22	2.08	0.53
1:A:36:GLN:NE2	1:A:102:LYS:O	2.41	0.53
1:A:134:ARG:HD3	1:A:323:TYR:O	2.08	0.53
1:A:266:ASP:OD1	1:A:267:PRO:HD2	2.08	0.53
1:A:40:GLN:HG3	1:A:59:ILE:HG21	1.90	0.53
1:B:96:THR:HB	1:B:114:GLU:HB2	1.90	0.53
1:B:201:GLU:HG2	1:B:202:LEU:N	2.23	0.53
1:A:16:ASN:ND2	1:A:181:PHE:HB3	2.24	0.53
1:A:10:ARG:HH22	1:A:317:GLU:CD	2.17	0.53
1:A:185:GLY:O	1:A:208:MET:HE2	2.08	0.53
1:B:33:TRP:CZ3	1:B:100:ILE:HG22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:TYR:CD2	1:B:58:ASN:HB3	2.44	0.52
1:A:66:VAL:HG23	1:A:115:HIS:HA	1.91	0.52
1:A:118:ASN:OD1	1:A:163:MET:HE1	2.09	0.52
1:A:190:VAL:HG11	1:A:205:ASP:HA	1.90	0.52
1:A:77:LYS:HE3	2:A:404:SO4:O3	2.09	0.52
1:B:163:MET:HE3	1:B:174:ILE:HD11	1.92	0.52
1:A:246:ALA:O	1:A:250:GLY:N	2.40	0.52
1:B:281:TRP:HB2	1:B:298:LEU:HD13	1.92	0.52
1:B:170:LYS:NZ	1:B:172:ARG:HH22	2.09	0.51
1:A:281:TRP:CB	1:A:298:LEU:HD22	2.40	0.51
1:B:190:VAL:HG11	1:B:205:ASP:HA	1.91	0.51
1:A:75:LYS:HG3	1:A:79:LYS:HE3	1.93	0.51
1:B:127:THR:O	1:B:127:THR:HG22	2.09	0.51
1:A:315:ALA:O	1:A:319:MET:HG3	2.11	0.51
1:A:321:HIS:CG	1:A:322:PRO:HD2	2.47	0.50
1:A:82:ILE:HD13	1:A:100:ILE:HD13	1.93	0.50
1:A:137:MET:CE	1:A:218:LEU:CD1	2.90	0.50
1:B:88:LEU:HB3	1:B:94:ILE:HG21	1.94	0.50
1:A:221:MET:O	1:A:225:MET:HG3	2.11	0.50
1:B:321:HIS:CE1	1:B:322:PRO:HD2	2.47	0.50
1:A:133:ILE:O	1:A:137:MET:HB2	2.12	0.49
1:A:276:HIS:CE1	3:A:405:PEG:H31	2.45	0.49
1:A:299:ASP:OD2	1:A:303:LYS:HE2	2.12	0.49
1:B:132:ASP:OD1	1:B:169:ARG:NH1	2.45	0.49
1:B:163:MET:HE3	1:B:174:ILE:CD1	2.43	0.49
1:A:114:GLU:O	1:A:114:GLU:HG3	2.13	0.49
1:A:125:TYR:CA	1:A:128:LEU:HD13	2.35	0.49
1:B:224:SER:HB2	1:B:229:LYS:O	2.12	0.49
1:A:140:ILE:HD13	1:A:221:MET:HE1	1.94	0.49
1:A:195:ARG:NH1	1:A:237:ASP:HA	2.25	0.49
1:A:269:PHE:C	1:A:271:ASP:N	2.70	0.49
1:B:321:HIS:ND1	1:B:322:PRO:HD2	2.28	0.48
1:A:74:LYS:HE2	1:A:77:LYS:HD3	1.95	0.48
1:B:191:ARG:CD	2:B:402:SO4:O1	2.60	0.48
1:A:45:LEU:HD21	1:A:55:GLU:HB2	1.96	0.48
1:A:61:ASN:N	1:A:61:ASN:OD1	2.47	0.48
1:A:69:ILE:HG12	4:A:406:A1IVS:F01	2.04	0.47
1:B:286:HIS:HD2	1:B:288:GLU:N	2.12	0.47
1:B:71:LYS:O	1:B:73:VAL:N	2.48	0.47
1:B:254:LEU:O	1:B:258:ILE:HG12	2.14	0.47
1:A:130:ASP:HB2	1:A:292:LEU:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:HG2	1:A:188:TYR:CZ	2.50	0.47
1:B:119:THR:HG23	1:B:164:ILE:O	2.14	0.47
1:B:305:LEU:O	1:B:306:ARG:HD3	2.15	0.47
1:A:190:VAL:O	1:A:192:VAL:N	2.48	0.47
1:B:286:HIS:CD2	1:B:288:GLU:H	2.31	0.47
1:B:240:ASP:O	1:B:244:ARG:HG2	2.15	0.46
1:B:299:ASP:OD2	1:B:303:LYS:HE2	2.14	0.46
1:B:153:MET:HE3	1:B:153:MET:HB2	1.79	0.46
1:A:321:HIS:CD2	1:A:322:PRO:HD2	2.50	0.46
1:B:247:LYS:HB3	1:B:247:LYS:HE3	1.65	0.46
1:A:200:PRO:HD3	1:A:216:TRP:CE2	2.51	0.46
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.58	0.46
1:A:230:GLU:HA	1:A:231:PRO:HA	1.84	0.46
1:B:27:GLU:HG2	1:B:76:LYS:HG3	1.97	0.46
1:B:103:ASP:HB3	1:B:108:THR:HB	1.97	0.46
1:A:216:TRP:HZ2	1:A:245:ILE:HD13	1.80	0.45
1:A:78:ILE:HD13	1:A:109:PRO:HG3	1.98	0.45
1:A:88:LEU:HD21	1:A:152:ILE:HD12	1.98	0.45
1:B:200:PRO:HG2	1:B:307:TYR:HA	1.98	0.45
1:B:95:ILE:HB	1:B:174:ILE:HG22	1.97	0.45
1:A:178:LEU:HD13	1:A:193:ALA:H	1.81	0.45
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.51	0.45
1:A:83:LYS:HA	1:A:83:LYS:HD2	1.84	0.44
1:A:118:ASN:CB	1:A:163:MET:CE	2.90	0.44
1:B:45:LEU:HD22	1:B:118:ASN:OD1	2.17	0.44
1:A:140:ILE:CD1	1:A:221:MET:HE1	2.48	0.44
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.81	0.44
1:A:281:TRP:HB3	1:A:298:LEU:HD22	2.00	0.44
1:A:99:ASP:OD1	1:A:100:ILE:N	2.48	0.44
1:B:105:VAL:HG12	1:B:108:THR:OG1	2.17	0.44
1:B:61:ASN:OD1	1:B:61:ASN:C	2.61	0.44
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.73	0.43
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.83	0.43
3:B:401:PEG:H22	3:B:401:PEG:H42	1.43	0.43
1:B:280:ARG:H	1:B:283:ARG:NH2	2.16	0.43
1:B:230:GLU:HA	1:B:231:PRO:HA	1.90	0.43
1:B:254:LEU:HD13	1:B:307:TYR:CE1	2.54	0.43
1:B:257:TYR:CE1	1:B:308:ASP:HA	2.54	0.43
1:B:58:ASN:C	1:B:60:THR:H	2.26	0.43
1:A:61:ASN:ND2	1:A:63:GLU:HB2	2.34	0.43
1:A:141:LEU:HD21	1:A:218:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:HD2	1:B:23:TYR:CD1	2.53	0.43
1:A:265:LEU:HD12	1:A:265:LEU:HA	1.84	0.42
1:A:15:VAL:HG12	1:A:16:ASN:N	2.35	0.42
1:A:163:MET:HA	1:A:163:MET:CE	2.41	0.42
1:A:331:GLN:O	1:A:332:ALA:CB	2.68	0.42
1:A:224:SER:HA	1:A:229:LYS:O	2.20	0.42
1:B:39:TYR:CE2	1:B:58:ASN:HB3	2.55	0.42
1:B:141:LEU:HD21	1:B:218:LEU:CD2	2.50	0.42
1:A:243:VAL:HG22	1:A:273:LEU:HD23	2.03	0.41
1:B:159:PRO:HG3	1:B:221:MET:HG2	2.02	0.41
1:A:140:ILE:CG1	1:A:171:LEU:HD11	2.50	0.41
1:A:222:LEU:HD12	1:A:222:LEU:HA	1.83	0.41
1:A:319:MET:HE2	1:A:319:MET:HB3	1.89	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.85	0.41
1:A:286:HIS:HE1	1:A:288:GLU:HB2	1.83	0.41
1:A:158:LYS:HB2	1:A:159:PRO:HD2	2.03	0.41
1:A:229:LYS:HD3	1:A:232:PHE:HA	2.02	0.41
1:B:265:LEU:HD21	1:B:269:PHE:HB3	2.01	0.41
1:A:258:ILE:HA	1:A:263:ILE:HD12	2.03	0.40
1:A:95:ILE:HD12	1:A:95:ILE:HA	1.94	0.40
1:B:131:TYR:HE1	1:B:169:ARG:HH22	1.68	0.40
1:B:107:ARG:O	1:B:108:THR:C	2.64	0.40
1:A:200:PRO:O	1:A:204:VAL:HG22	2.22	0.40
1:A:88:LEU:N	1:A:88:LEU:HD23	2.36	0.40
1:A:141:LEU:HD11	1:A:318:ALA:HB1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	330/359 (92%)	297 (90%)	29 (9%)	4 (1%)	11 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	325/359 (90%)	285 (88%)	34 (10%)	6 (2%)	7 9
All	All	655/718 (91%)	582 (89%)	63 (10%)	10 (2%)	8 11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	B	118	ASN
1	B	125	TYR
1	B	106	SER
1	A	61	ASN
1	A	107	ARG
1	A	191	ARG
1	B	175	ASP
1	B	103	ASP
1	B	65	VAL

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	292/329 (89%)	284 (97%)	8 (3%)	40 60
1	B	294/329 (89%)	283 (96%)	11 (4%)	29 46
All	All	586/658 (89%)	567 (97%)	19 (3%)	33 52

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	32	GLU
1	A	65	VAL
1	A	70	LEU
1	A	108	THR
1	A	116	VAL

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Mol	Chain	Res	Type
1	A	130	ASP
1	A	330	ASP
1	B	21	ARG
1	B	38	ASP
1	B	59	ILE
1	B	65	VAL
1	B	73	VAL
1	B	119	THR
1	B	121	PHE
1	B	166	HIS
1	B	170	LYS
1	B	288	GLU
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	35	ASN
1	A	115	HIS
1	A	117	ASN
1	A	310	GLN
1	B	29	HIS
1	B	286	HIS

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

16 ligands are 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
2	SO4	A	401	-	4,4,4	0.20	0	6,6,6	0.28	0
2	SO4	A	409	-	4,4,4	0.36	0	6,6,6	0.44	0
2	SO4	A	402	-	4,4,4	0.35	0	6,6,6	0.38	0
2	SO4	A	404	-	4,4,4	0.22	0	6,6,6	0.44	0
2	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.66	0
2	SO4	A	407	-	4,4,4	0.28	0	6,6,6	0.40	0
4	A1IVS	B	407	-	11,12,12	1.68	3 (27%)	10,17,17	2.87	3 (30%)
4	A1IVS	A	406	-	11,12,12	1.45	2 (18%)	10,17,17	2.99	3 (30%)
2	SO4	B	405	-	4,4,4	0.30	0	6,6,6	0.25	0
3	PEG	B	401	-	6,6,6	0.42	0	5,5,5	0.25	0
2	SO4	B	402	-	4,4,4	0.41	0	6,6,6	0.38	0
4	A1IVS	B	404	-	11,12,12	1.73	3 (27%)	10,17,17	5.02	3 (30%)
2	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.29	0
2	SO4	A	408	-	4,4,4	0.26	0	6,6,6	0.47	0
3	PEG	A	405	-	6,6,6	0.19	0	5,5,5	0.21	0
2	SO4	B	406	-	4,4,4	0.20	0	6,6,6	0.18	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
4	A1IVS	B	407	-	-	-	0/2/2/2
4	A1IVS	A	406	-	-	-	0/2/2/2
3	PEG	B	401	-	-	3/4/4/4	-
4	A1IVS	B	404	-	-	-	0/2/2/2
3	PEG	A	405	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	A1IVS	C04-C05	-3.35	1.38	1.43
4	B	407	A1IVS	C04-C05	-3.20	1.38	1.43
4	B	404	A1IVS	C09-C05	3.19	1.44	1.41
4	B	404	A1IVS	C04-C05	-2.98	1.38	1.43
4	B	407	A1IVS	C03-C02	2.97	1.41	1.36
4	A	406	A1IVS	C03-C02	2.50	1.40	1.36
4	B	404	A1IVS	C03-C02	2.39	1.40	1.36
4	B	407	A1IVS	C11-C09	2.23	1.39	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	A1IVS	F10-C09-C05	14.54	123.27	117.40
4	B	407	A1IVS	F10-C09-C05	6.68	120.10	117.40
4	A	406	A1IVS	F10-C09-C05	6.52	120.03	117.40
4	A	406	A1IVS	C03-C02-C11	-4.94	120.19	124.09
4	B	407	A1IVS	C03-C02-C11	-4.65	120.42	124.09
4	B	404	A1IVS	C03-C02-C11	-4.41	120.61	124.09
4	B	404	A1IVS	C09-C11-C02	4.15	120.40	116.64
4	A	406	A1IVS	C09-C11-C02	4.01	120.27	116.64
4	B	407	A1IVS	C09-C11-C02	3.22	119.55	116.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	PEG	C4-C3-O2-C2
3	A	405	PEG	C4-C3-O2-C2
3	B	401	PEG	O1-C1-C2-O2
3	A	405	PEG	O1-C1-C2-O2
3	B	401	PEG	O2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 12 short contacts:

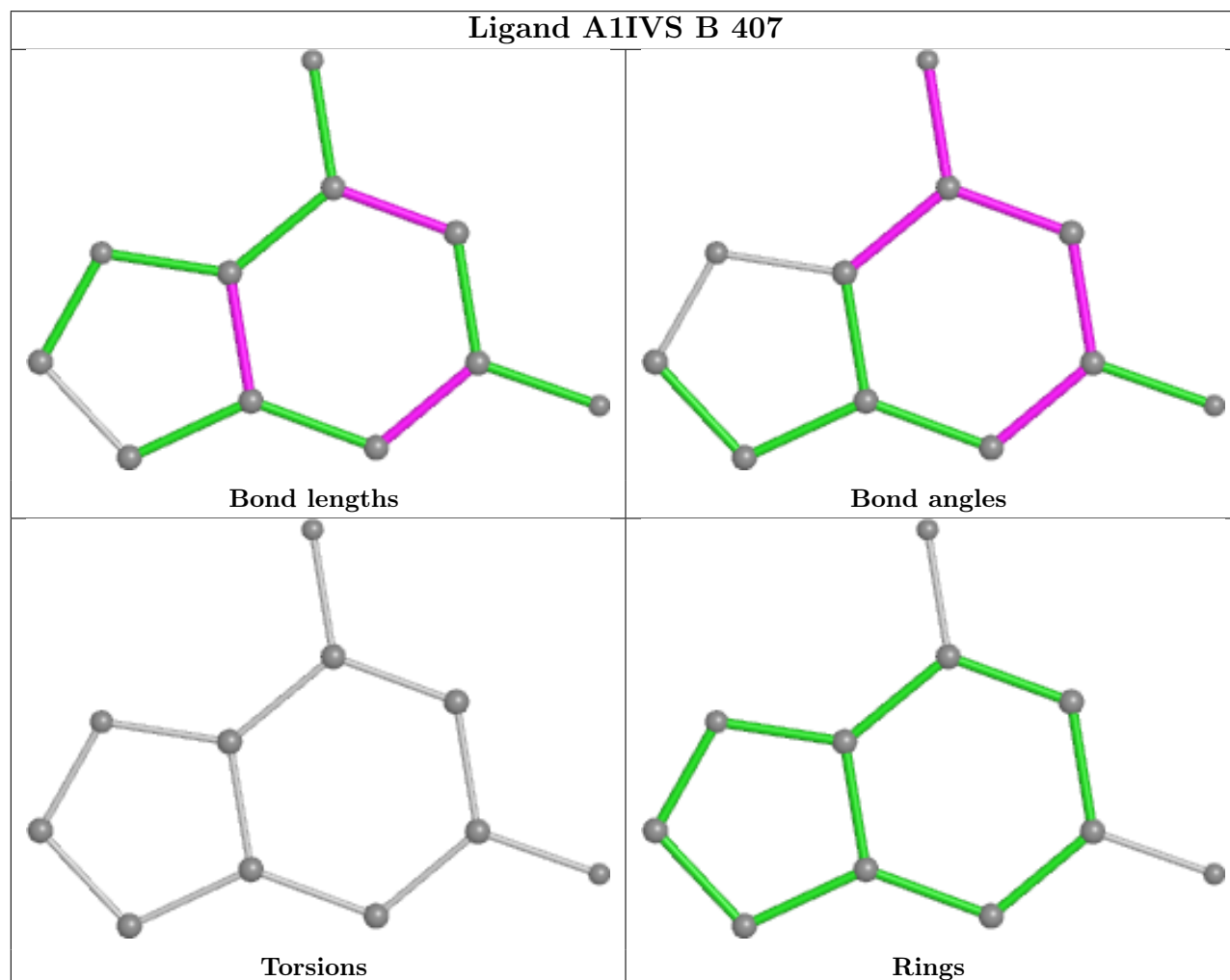
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	SO4	1	0
2	A	407	SO4	1	0
4	A	406	A1IVS	1	0
3	B	401	PEG	4	0
2	B	402	SO4	2	0
2	A	408	SO4	1	0

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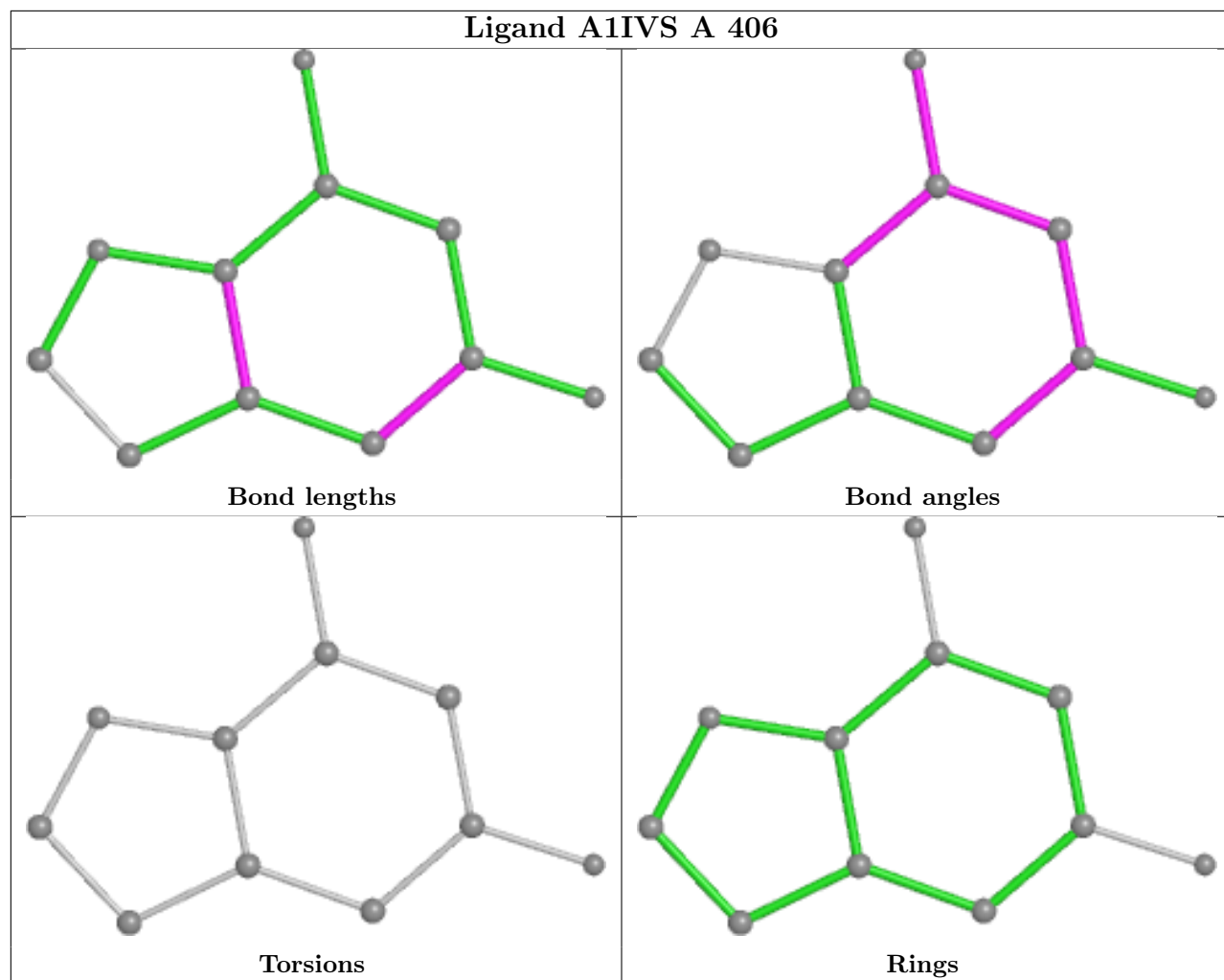
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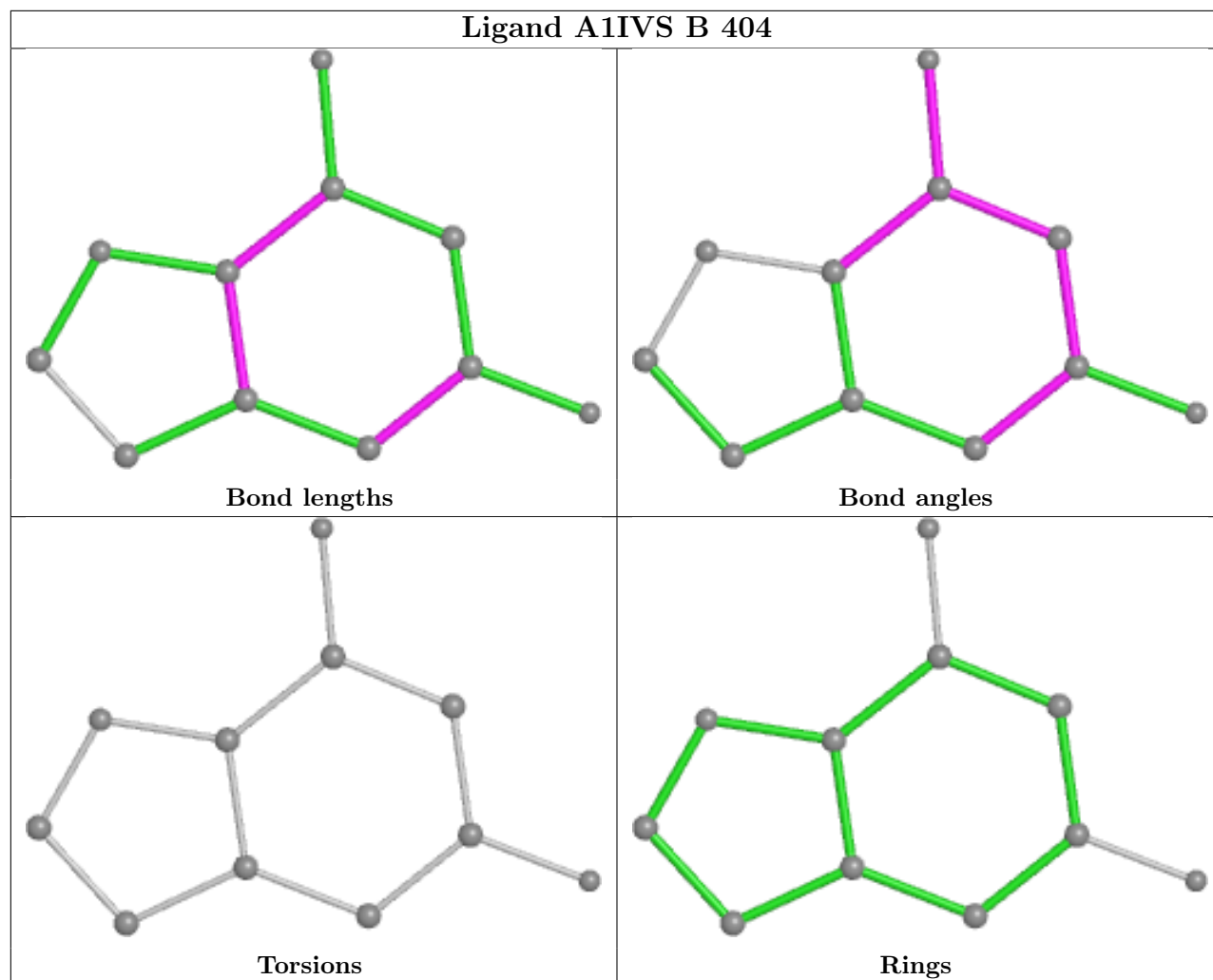
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	PEG	2	0

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



Ligand A1IVS A 406





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	331/359 (92%)	-0.04	13 (3%) 44 42	34, 49, 90, 119	1 (0%)
1	B	328/359 (91%)	0.09	21 (6%) 27 25	33, 50, 90, 146	1 (0%)
All	All	659/718 (91%)	0.02	34 (5%) 34 33	33, 49, 90, 146	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	PHE	5.0
1	B	123	GLN	4.8
1	B	105	VAL	4.6
1	A	50	TYR	4.4
1	B	51	SER	4.1
1	B	107	ARG	4.0
1	B	125	TYR	4.0
1	B	120	ASP	3.9
1	B	119	THR	3.7
1	A	125	TYR	3.5
1	A	47	ARG	3.4
1	B	332	ALA	3.4
1	B	127	THR	3.2
1	A	120	ASP	3.2
1	A	270	ASN	3.1
1	A	332	ALA	3.0
1	B	270	ASN	2.7
1	A	107	ARG	2.7
1	A	268	ARG	2.6
1	B	268	ARG	2.5
1	B	104	PRO	2.5
1	B	124	LEU	2.4
1	B	236	HIS	2.4
1	B	47	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	118	ASN	2.3
1	B	118	ASN	2.3
1	B	121	PHE	2.2
1	B	106	SER	2.2
1	B	74	LYS	2.2
1	A	63	GLU	2.1
1	B	325	TYR	2.1
1	A	2	SER	2.0
1	A	126	GLN	2.0
1	B	2	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	403	5/5	0.53	0.19	88,91,96,101	0
2	SO4	B	406	5/5	0.53	0.18	67,68,76,77	5
2	SO4	A	401	5/5	0.79	0.14	77,86,87,95	0
4	A1IVS	B	404	11/11	0.81	0.13	59,61,74,77	0
2	SO4	A	409	5/5	0.84	0.24	52,54,66,71	0
3	PEG	A	405	7/7	0.84	0.17	59,65,66,69	0
2	SO4	B	405	5/5	0.84	0.11	70,72,77,83	0
2	SO4	A	407	5/5	0.86	0.24	55,63,66,72	5
2	SO4	A	402	5/5	0.87	0.19	52,53,58,61	5
4	A1IVS	B	407	11/11	0.87	0.12	47,59,75,77	0
2	SO4	B	402	5/5	0.89	0.22	52,59,68,68	0
3	PEG	B	401	7/7	0.89	0.14	51,54,56,58	0
2	SO4	A	408	5/5	0.91	0.20	49,54,60,62	0

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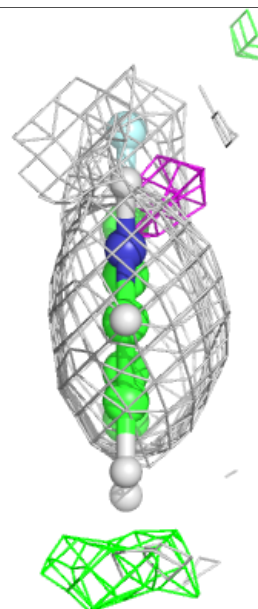
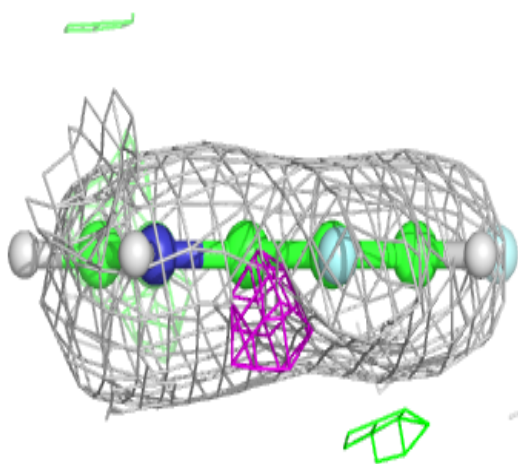
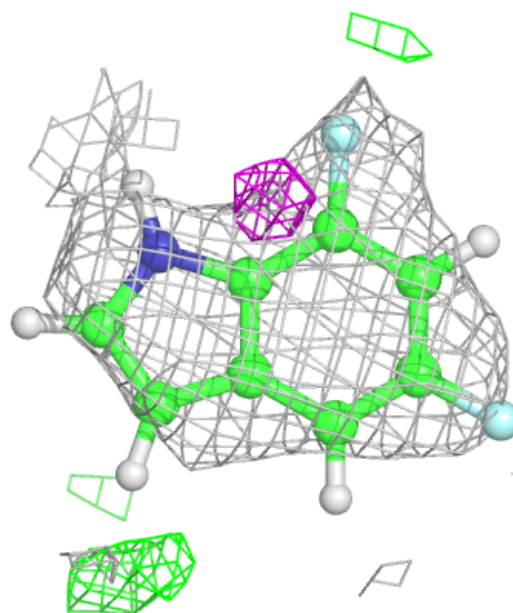
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	404	5/5	0.93	0.12	51,52,58,59	0
4	A1IVS	A	406	11/11	0.93	0.08	49,53,62,64	0
2	SO4	B	403	5/5	0.94	0.14	48,49,51,54	0

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.

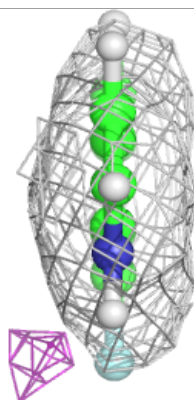
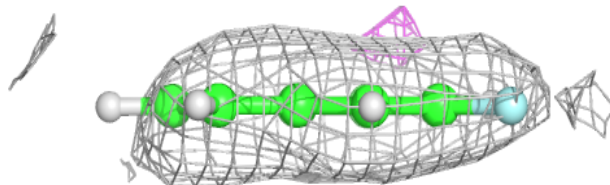
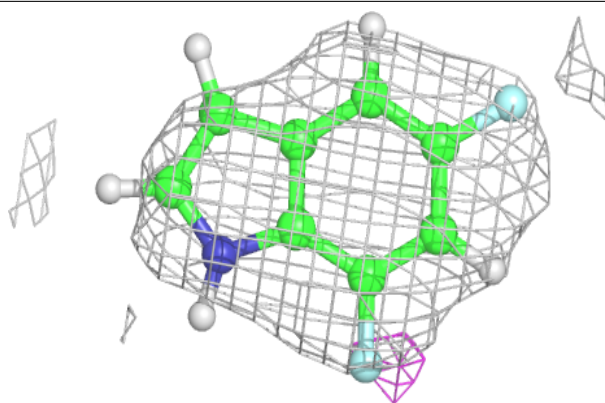
Electron density around A1IVS B 404:

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

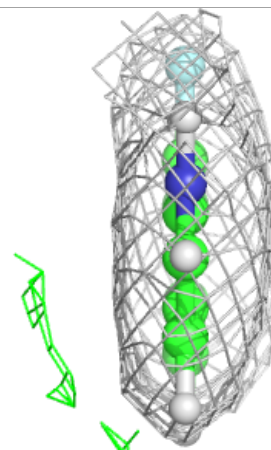
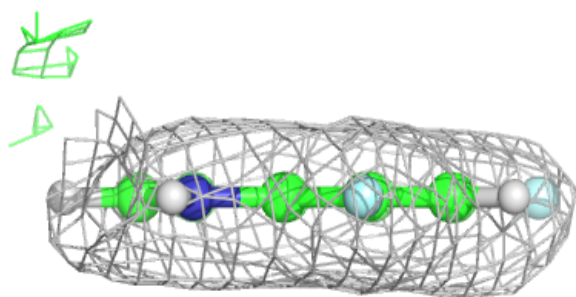
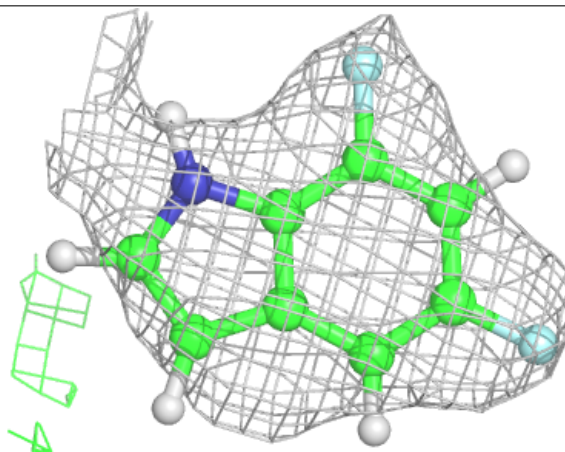


Electron density around A1IVS B 407:

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

**Electron density around A1IVS A 406:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.