Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:08 PM JST

PDB ID	:	7EFN / pdb_00007efn
Title	:	Crystal structure of the gastric proton pump K791S/E820D/Y340N/E936V in (BYK)E2BeF state
Authors	:	Abe, K.; Yamamoto, K.; Irie, K.
Deposited on	:	2021-03-22
Resolution	:	3.20 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:

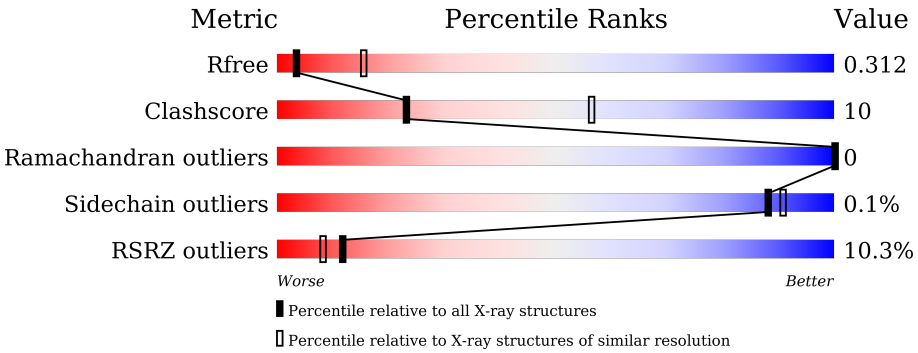
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 <=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	985	10% 77% 23%
2	B	261	13% 76% 24%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9845 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 Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	985	Total	C	N	O	S	0	0	0
			7637	4874	1290	1420	53			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	ASN	TYR	engineered mutation	UNP A0A5G2QYH2
A	791	SER	LYS	engineered mutation	UNP A0A5G2QYH2
A	820	ASP	GLU	engineered mutation	UNP A0A5G2QYH2
A	936	VAL	GLU	engineered mutation	UNP A0A5G2QYH2
A	1005	SER	GLY	conflict	UNP A0A5G2QYH2

- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			2092	1359	347	375	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

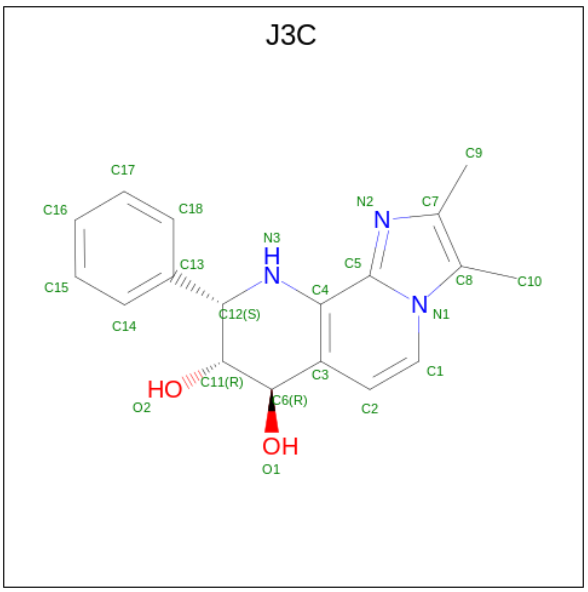
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Rb	0	0
			4	4		

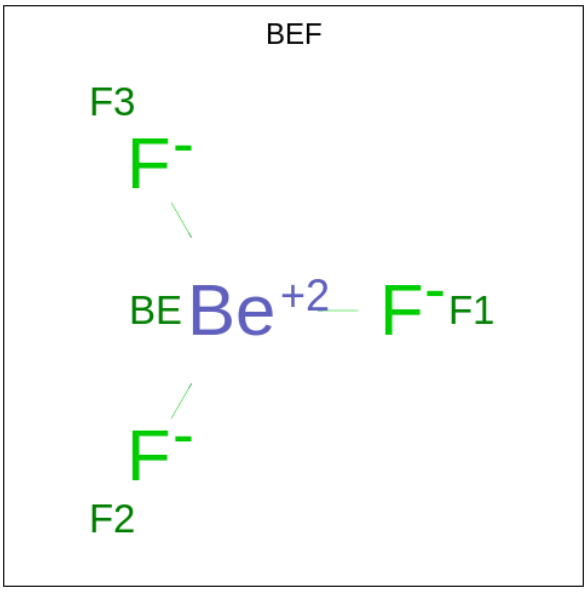
- Molecule 5 is (7R,8R,9S)-2,3-dimethyl-9-phenyl-7,8,9,10-tetrahydroimidazo[1,2-h][1,7]naphthyridine-7,8-diol (CCD ID: J3C) (formula: $C_{18}H_{19}N_3O_2$) (labeled as "Ligand of Interest"

by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 23 18 3 2	0	0

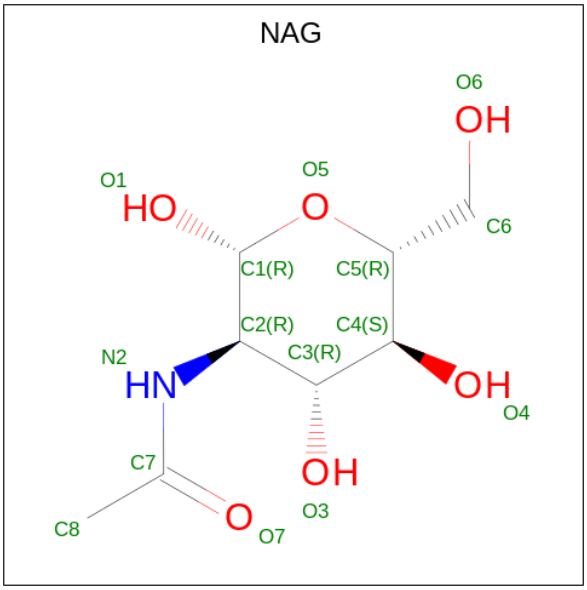
- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Be F 4 1 3	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	36	Total O 36 36	0	0
8	B	6	Total O 6 6	0	0

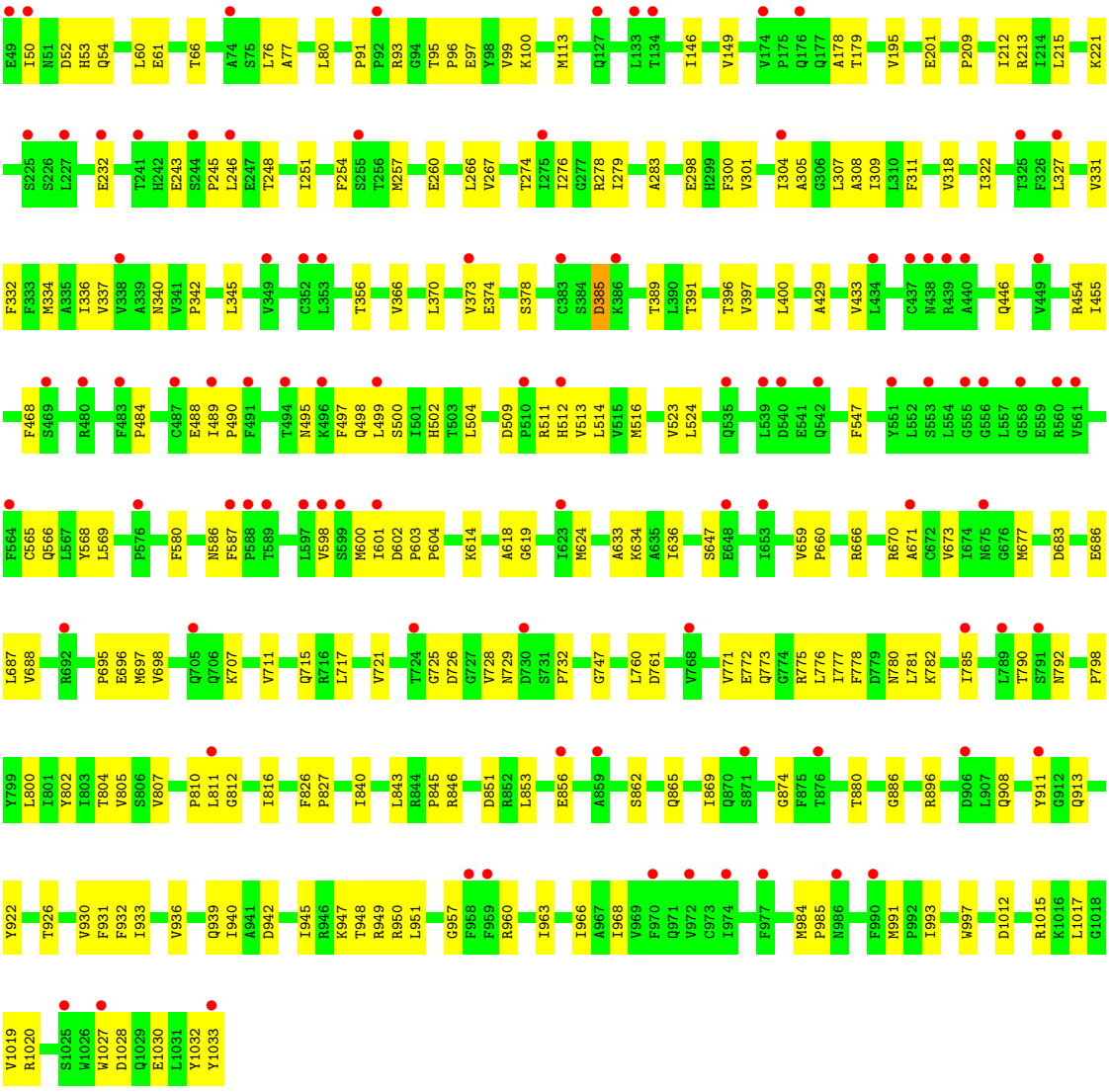
3 Residue-property plots (i)

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: Sodium/potassium-transporting ATPase subunit alpha

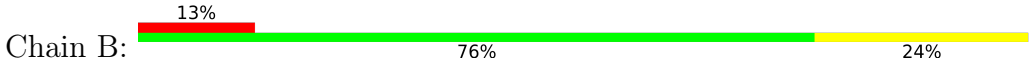
Chain A:

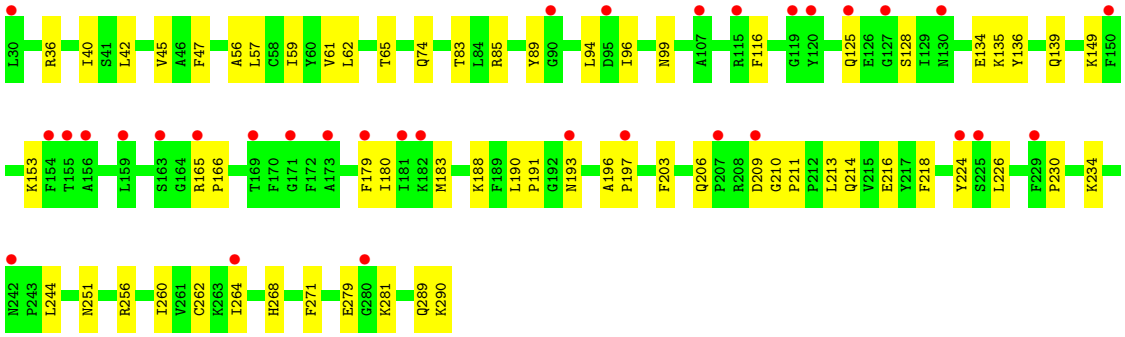




• Molecule 2: Potassium-transporting ATPase subunit beta

Chain B:


13%
76%
24%


L30 R36 I40 S41 L42 V45 A46 F47 A56 L57 C58 I59 Y60 V61 L62 T65 Q74 T83 L84 R85 Y89 G90 L94 D95 I96 N99 A107 R115 F116 G119 Y120 Q125 E126 G127 S128 I129 N130 E134 K135 Y136 Q139 K149 F150
K153 F154 T155 A156 L159 S163 G164 R165 P166 T169 F170 G171 F172 A173 F179 I180 I181 K182 M183 K188 F189 L190 P191 G192 N193 A196 P197 F203 Q206 P207 R208 D209 G210 P211 P212 L213 Q214 V215 E216 Y217 F218 Y224 S225 L226 F229 P230 K234
N242 P243 L244 N251 R256 I260 V261 C262 K263 I264 H268 F271 E279 G280 K281 Q289 K290

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.94Å 105.94Å 372.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.71 – 3.20 48.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	81.8 (48.71-3.20) 81.7 (48.71-3.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.268 , 0.308 0.269 , 0.312	Depositor DCC
R_{free} test set	1663 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	9845	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: RB, J3C, NAG, BEF, MG

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	0.23	1/7794 (0.0%)	0.46	0/10590
2	B	0.22	0/2159	0.49	0/2937
All	All	0.22	1/9953 (0.0%)	0.47	0/13527

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	ASP	CG-OD2	10.01	1.44	1.25

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	7637	0	7662	158	1
2	B	2092	0	2037	47	1
3	A	1	0	0	0	0
4	A	4	0	0	0	0
5	A	23	0	0	0	0
6	A	4	0	0	1	0
7	B	42	0	39	0	0
8	A	36	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	6	0	0	1	0
All	All	9845	0	9738	202	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 10.

All (202) 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:54:GLN:NE2	1:A:243:GLU:OE2	2.07	0.88
1:A:385:ASP:O	1:A:389:THR:OG1	1.97	0.81
1:A:53:HIS:HB3	1:A:251:ILE:HD11	1.64	0.80
1:A:516:MET:SD	8:A:1202:HOH:O	2.40	0.78
2:B:83:THR:HG22	2:B:85:ARG:HH12	1.48	0.77
1:A:811:LEU:HD13	1:A:931:PHE:HB3	1.67	0.76
1:A:800:LEU:O	1:A:804:THR:OG1	2.02	0.75
1:A:374:GLU:HB2	1:A:777:ILE:HD11	1.67	0.75
2:B:125:GLN:O	2:B:153:LYS:NZ	2.22	0.73
1:A:940:ILE:HD13	1:A:968:ILE:HG23	1.70	0.72
1:A:580:PHE:HA	1:A:586:ASN:HD21	1.55	0.71
1:A:624:MET:HE1	1:A:633:ALA:HB1	1.71	0.71
2:B:96:ILE:HD12	2:B:179:PHE:HE2	1.56	0.71
1:A:490:PRO:HA	1:A:498:GLN:HG3	1.71	0.70
1:A:792:ASN:OD1	8:A:1201:HOH:O	2.09	0.70
2:B:197:PRO:HG2	2:B:224:TYR:HB2	1.75	0.69
1:A:516:MET:O	8:A:1202:HOH:O	2.12	0.67
2:B:128:SER:HB2	2:B:153:LYS:HG2	1.77	0.67
2:B:149:LYS:NZ	8:B:401:HOH:O	2.29	0.65
1:A:502:HIS:HB2	1:A:513:VAL:HG23	1.79	0.65
2:B:83:THR:CG2	2:B:85:ARG:HH12	2.10	0.65
1:A:356:THR:HB	1:A:373:VAL:HG11	1.79	0.64
1:A:221:LYS:HB2	1:A:260:GLU:HG3	1.81	0.62
1:A:245:PRO:HA	1:A:248:THR:HG22	1.82	0.62
2:B:188:LYS:HA	2:B:230:PRO:HB3	1.81	0.62
2:B:165:ARG:NH2	2:B:166:PRO:HA	2.14	0.61
1:A:332:PHE:O	1:A:336:ILE:HG12	2.02	0.60
1:A:76:LEU:O	1:A:80:LEU:HG	2.02	0.59
1:A:96:PRO:HB2	1:A:99:VAL:HG12	1.83	0.59
2:B:139:GLN:HB3	2:B:149:LYS:HD3	1.84	0.59
1:A:777:ILE:O	1:A:781:LEU:N	2.34	0.59
1:A:274:THR:O	1:A:278:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:THR:HG22	2:B:85:ARG:NH1	2.18	0.58
1:A:619:GLY:HA3	1:A:845:PRO:HD3	1.86	0.58
1:A:775:ARG:HD3	1:A:840:ILE:HG23	1.84	0.58
1:A:846:ARG:HG2	1:A:851:ASP:HB2	1.85	0.58
1:A:498:GLN:O	1:A:516:MET:HA	2.04	0.58
1:A:782:LYS:HD3	1:A:853:LEU:O	2.04	0.57
1:A:97:GLU:HA	1:A:100:LYS:HD3	1.87	0.56
1:A:391:THR:HG22	1:A:636:ILE:HG21	1.85	0.56
2:B:96:ILE:HD12	2:B:179:PHE:CE2	2.38	0.56
1:A:215:LEU:HD11	1:A:266:LEU:HG	1.88	0.56
2:B:89:TYR:CE2	2:B:94:LEU:HG	2.40	0.56
1:A:345:LEU:HD21	1:A:785:ILE:HG22	1.87	0.56
1:A:798:PRO:HG3	1:A:931:PHE:CZ	2.41	0.56
1:A:389:THR:HG21	1:A:725:GLY:HA2	1.88	0.55
1:A:1015:ARG:HA	1:A:1027:TRP:CZ2	2.41	0.55
1:A:948:THR:OG1	1:A:951:LEU:O	2.20	0.55
1:A:53:HIS:HE1	1:A:243:GLU:HA	1.70	0.55
2:B:191:PRO:HA	2:B:268:HIS:HB2	1.88	0.55
1:A:683:ASP:N	1:A:686:GLU:OE2	2.28	0.55
1:A:1012:ASP:HA	1:A:1015:ARG:HG2	1.88	0.55
2:B:85:ARG:HB2	2:B:180:ILE:HG12	1.89	0.55
1:A:512:HIS:HB2	1:A:569:LEU:HB2	1.88	0.55
1:A:647:SER:HB2	1:A:670:ARG:HD3	1.88	0.54
2:B:165:ARG:NE	2:B:165:ARG:HA	2.23	0.54
1:A:880:THR:HA	2:B:62:LEU:HD21	1.90	0.54
1:A:1030:GLU:OE1	2:B:40:ILE:HD12	2.08	0.54
1:A:308:ALA:HB1	1:A:337:VAL:HA	1.90	0.53
1:A:499:LEU:HD11	1:A:514:LEU:HG	1.89	0.53
1:A:504:LEU:HD21	1:A:568:TYR:HE1	1.73	0.53
1:A:374:GLU:OE2	1:A:378:SER:OG	2.27	0.53
1:A:601:ILE:O	1:A:603:PRO:HD3	2.07	0.53
2:B:116:PHE:HE2	2:B:244:LEU:HD11	1.74	0.53
1:A:1017:LEU:HA	1:A:1020:ARG:HG2	1.91	0.53
1:A:91:PRO:O	1:A:93:ARG:HD2	2.08	0.52
2:B:203:PHE:HB3	2:B:206:GLN:HB2	1.91	0.52
1:A:805:VAL:HG12	1:A:807:VAL:HG13	1.92	0.52
1:A:1015:ARG:HH21	1:A:1032:TYR:HA	1.73	0.52
1:A:327:LEU:O	1:A:331:VAL:HG23	2.09	0.52
2:B:165:ARG:CZ	2:B:166:PRO:HA	2.40	0.52
1:A:942:ASP:HA	1:A:945:ILE:HG12	1.92	0.51
1:A:53:HIS:CE1	1:A:243:GLU:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:ILE:HA	1:A:936:VAL:HG22	1.93	0.51
1:A:113:MET:HE2	1:A:342:PRO:O	2.11	0.51
1:A:618:ALA:HB1	1:A:775:ARG:HH12	1.76	0.51
2:B:57:LEU:O	2:B:61:VAL:HG13	2.11	0.51
1:A:50:ILE:HD11	1:A:243:GLU:OE1	2.11	0.51
1:A:932:PHE:O	1:A:936:VAL:HG13	2.11	0.51
1:A:495:ASN:HB2	1:A:497:PHE:CZ	2.47	0.50
1:A:397:VAL:HG12	1:A:600:MET:HG2	1.93	0.50
1:A:495:ASN:HB2	1:A:497:PHE:CE2	2.46	0.50
2:B:206:GLN:HE22	2:B:256:ARG:HH22	1.60	0.50
1:A:276:ILE:HD13	1:A:728:VAL:HG21	1.94	0.50
1:A:1015:ARG:HA	1:A:1027:TRP:HZ2	1.76	0.50
1:A:318:VAL:O	1:A:322:ILE:HG12	2.11	0.49
1:A:254:PHE:HB3	1:A:276:ILE:HG13	1.94	0.49
1:A:308:ALA:HB2	1:A:340:ASN:HB2	1.93	0.49
1:A:601:ILE:HG12	1:A:602:ASP:H	1.77	0.49
1:A:886:GLY:HA2	1:A:911:TYR:CE2	2.48	0.49
1:A:524:LEU:HD22	1:A:547:PHE:CD1	2.47	0.49
2:B:271:PHE:HA	2:B:279:GLU:O	2.13	0.49
1:A:396:THR:OG1	1:A:603:PRO:HG3	2.13	0.49
1:A:397:VAL:HG21	1:A:468:PHE:CG	2.48	0.49
1:A:677:MET:SD	1:A:677:MET:N	2.86	0.48
1:A:670:ARG:HA	1:A:695:PRO:HD2	1.94	0.48
1:A:790:THR:HG22	1:A:862:SER:HB3	1.96	0.48
1:A:429:ALA:O	1:A:433:VAL:HG23	2.14	0.48
1:A:488:GLU:HA	1:A:499:LEU:O	2.14	0.48
1:A:52:ASP:O	1:A:213:ARG:HD2	2.14	0.48
1:A:580:PHE:HA	1:A:586:ASN:ND2	2.26	0.48
1:A:874:GLY:HA3	1:A:931:PHE:CE1	2.49	0.48
2:B:213:LEU:HD22	2:B:260:ILE:HG12	1.96	0.47
2:B:216:GLU:HG2	2:B:218:PHE:CZ	2.49	0.47
1:A:504:LEU:HD13	1:A:509:ASP:HB3	1.96	0.47
1:A:939:GLN:HA	1:A:942:ASP:HB2	1.96	0.47
1:A:963:ILE:HA	1:A:966:ILE:HD12	1.97	0.47
1:A:1015:ARG:NH2	1:A:1032:TYR:HA	2.30	0.47
2:B:190:LEU:CD2	2:B:230:PRO:HG3	2.45	0.47
1:A:826:PHE:HB3	1:A:827:PRO:HD3	1.96	0.47
1:A:957:GLY:HA3	1:A:960:ARG:HD3	1.96	0.47
2:B:214:GLN:HB2	2:B:251:ASN:HB2	1.97	0.47
1:A:772:GLU:HG3	1:A:773:GLN:H	1.81	0.46
2:B:183:MET:HE2	2:B:264:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:VAL:HA	1:A:698:VAL:O	2.15	0.46
2:B:85:ARG:HB2	2:B:180:ILE:CG1	2.46	0.46
1:A:949:ARG:HG2	1:A:1033:TYR:CZ	2.50	0.46
1:A:688:VAL:HG12	1:A:717:LEU:HD11	1.98	0.46
1:A:856:GLU:H	1:A:856:GLU:CD	2.23	0.46
1:A:1019:VAL:HG23	1:A:1028:ASP:OD1	2.16	0.46
1:A:489:ILE:HD11	1:A:587:PHE:CZ	2.50	0.46
2:B:209:ASP:OD2	2:B:210:GLY:N	2.49	0.46
1:A:624:MET:HE2	1:A:624:MET:HB3	1.76	0.46
1:A:179:THR:OG1	1:A:201:GLU:HB3	2.15	0.46
1:A:500:SER:HB3	1:A:502:HIS:NE2	2.31	0.46
1:A:659:VAL:HG12	1:A:660:PRO:O	2.16	0.46
1:A:775:ARG:NH2	1:A:843:LEU:O	2.49	0.45
1:A:776:LEU:O	1:A:780:ASN:N	2.41	0.45
1:A:95:THR:N	1:A:96:PRO:HD3	2.31	0.45
1:A:257:MET:HE3	1:A:257:MET:HB3	1.84	0.45
2:B:190:LEU:HD21	2:B:230:PRO:HG3	1.97	0.45
2:B:211:PRO:HG2	2:B:251:ASN:OD1	2.15	0.45
1:A:812:GLY:O	1:A:816:ILE:HG23	2.15	0.45
1:A:601:ILE:HG12	1:A:602:ASP:N	2.32	0.45
1:A:802:TYR:CE1	1:A:896:ARG:HG3	2.52	0.45
1:A:366:VAL:HG13	1:A:760:LEU:HD11	1.99	0.45
1:A:984:MET:N	1:A:985:PRO:HD2	2.32	0.45
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.79	0.44
1:A:726:ASP:HB2	1:A:747:GLY:HA2	1.99	0.44
1:A:77:ALA:HA	1:A:195:VAL:HG21	2.00	0.44
2:B:42:LEU:HA	2:B:45:VAL:HG12	1.98	0.44
2:B:74:GLN:O	2:B:74:GLN:HG3	2.18	0.44
1:A:300:PHE:O	1:A:304:ILE:HG12	2.17	0.44
1:A:604:PRO:HG3	1:A:636:ILE:HG23	1.98	0.44
1:A:947:LYS:HG3	1:A:948:THR:HG23	1.99	0.44
1:A:446:GLN:HE22	1:A:455:ILE:HB	1.82	0.44
1:A:761:ASP:OD1	1:A:761:ASP:N	2.44	0.44
1:A:373:VAL:HG12	1:A:777:ILE:HD13	1.98	0.44
1:A:305:ALA:O	1:A:309:ILE:HD12	2.18	0.44
1:A:991:MET:HB2	1:A:991:MET:HE3	1.39	0.44
1:A:950:ARG:O	1:A:1020:ARG:HD3	2.18	0.44
2:B:56:ALA:O	2:B:59:ILE:HG12	2.18	0.44
1:A:523:VAL:HG13	1:A:565:CYS:HB2	2.00	0.43
1:A:865:GLN:O	1:A:869:ILE:HG13	2.18	0.43
1:A:279:ILE:HD13	8:A:1232:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:ALA:HB1	2:B:224:TYR:O	2.19	0.43
2:B:262:CYS:O	2:B:281:LYS:HA	2.19	0.43
1:A:146:ILE:O	1:A:149:VAL:HG22	2.19	0.43
1:A:614:LYS:HB3	1:A:614:LYS:HE2	1.88	0.43
1:A:886:GLY:HA2	1:A:911:TYR:CD2	2.54	0.43
1:A:61:GLU:HB2	1:A:66:THR:O	2.19	0.42
1:A:777:ILE:HG13	1:A:778:PHE:N	2.33	0.42
2:B:135:LYS:O	2:B:226:LEU:HB3	2.19	0.42
2:B:136:TYR:HE2	2:B:193:ASN:OD1	2.02	0.42
1:A:670:ARG:HE	1:A:670:ARG:HB2	1.65	0.42
1:A:504:LEU:HD12	1:A:511:ARG:O	2.19	0.42
1:A:671:ALA:HA	1:A:696:GLU:O	2.19	0.42
2:B:234:LYS:HA	2:B:234:LYS:HD3	1.68	0.42
1:A:298:GLU:HA	1:A:301:VAL:HG22	2.00	0.42
1:A:634:LYS:HE3	1:A:673:VAL:HG21	2.01	0.42
1:A:908:GLN:HA	1:A:913:GLN:O	2.19	0.42
2:B:116:PHE:CE2	2:B:244:LEU:HD11	2.55	0.42
1:A:212:ILE:CD1	1:A:267:VAL:HG22	2.50	0.42
1:A:356:THR:HB	1:A:373:VAL:CG1	2.50	0.42
1:A:666:ARG:H	1:A:666:ARG:HG2	1.50	0.42
1:A:771:VAL:O	1:A:775:ARG:N	2.46	0.42
1:A:446:GLN:HB3	1:A:454:ARG:HG2	2.00	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.90	0.41
1:A:697:MET:HE2	1:A:697:MET:HB2	1.79	0.41
2:B:65:THR:HG22	2:B:65:THR:O	2.20	0.41
1:A:707:LYS:O	1:A:711:VAL:HG23	2.20	0.41
1:A:922:TYR:O	1:A:991:MET:HE1	2.21	0.41
1:A:729:ASN:ND2	6:A:1107:BEF:F1	2.44	0.41
2:B:36:ARG:HA	2:B:36:ARG:HD3	1.94	0.41
1:A:484:PRO:O	1:A:502:HIS:HA	2.20	0.41
1:A:178:ALA:HB2	1:A:209:PRO:HB3	2.02	0.41
1:A:400:LEU:HD23	1:A:598:VAL:HG22	2.03	0.41
1:A:865:GLN:HA	2:B:47:PHE:CE2	2.56	0.41
1:A:715:GLN:HG3	1:A:721:VAL:HG23	2.01	0.41
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.87	0.40
1:A:514:LEU:O	1:A:566:GLN:HA	2.21	0.40
1:A:624:MET:HE2	1:A:698:VAL:HG22	2.02	0.40
1:A:798:PRO:HB3	1:A:810:PRO:HB2	2.03	0.40
2:B:134:GLU:H	2:B:134:GLU:CD	2.28	0.40
1:A:283:ALA:HB2	1:A:732:PRO:HD3	2.03	0.40
1:A:311:PHE:HB3	1:A:336:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:TYR:HE1	1:A:896:ARG:HG3	1.86	0.40
1:A:926:THR:O	1:A:930:VAL:HG13	2.21	0.40
1:A:334:MET:O	1:A:337:VAL:HG22	2.21	0.40
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.76	0.40
1:A:993:ILE:HG23	1:A:997:TRP:HE3	1.86	0.40
2:B:99:ASN:HA	2:B:289:GLN:O	2.21	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:232:GLU:OE1	2:B:290:LYS:NZ[2_545]	2.19	0.01

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	983/985 (100%)	955 (97%)	28 (3%)	0	100	100
2	B	259/261 (99%)	256 (99%)	3 (1%)	0	100	100
All	All	1242/1246 (100%)	1211 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	833/833 (100%)	832 (100%)	1 (0%)	88 91
2	B	228/228 (100%)	228 (100%)	0	100 100
All	All	1061/1061 (100%)	1060 (100%)	1 (0%)	88 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU

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

Mol	Chain	Res	Type
1	A	512	HIS
1	A	678	GLN
1	A	870	GLN
1	A	923	GLN
1	A	939	GLN
2	B	255	ASN
2	B	268	HIS
2	B	275	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
7	NAG	B	301	2	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
6	BEF	A	1107	1	0,3,3	-	-	-		
5	J3C	A	1104	-	23,26,26	1.38	4 (17%)	26,39,39	1.68	4 (15%)
7	NAG	B	302	2	14,14,15	0.67	1 (7%)	17,19,21	0.57	0
7	NAG	B	303	2	14,14,15	0.22	0	17,19,21	0.57	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
5	J3C	A	1104	-	-	2/4/20/20	0/4/4/4
7	NAG	B	301	2	-	2/6/23/26	0/1/1/1
7	NAG	B	303	2	-	2/6/23/26	0/1/1/1
7	NAG	B	302	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	J3C	C5-N1	-3.78	1.34	1.39
5	A	1104	J3C	C2-C3	-2.32	1.39	1.44
7	B	302	NAG	C1-C2	2.17	1.55	1.52
5	A	1104	J3C	C1-C2	2.04	1.39	1.35
5	A	1104	J3C	C13-C12	-2.03	1.49	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1104	J3C	C7-C8-N1	5.03	108.00	105.31
5	A	1104	J3C	C9-C7-N2	3.40	126.27	119.38
7	B	301	NAG	C1-O5-C5	2.74	115.90	112.19
5	A	1104	J3C	C10-C8-C7	-2.60	125.71	131.23
5	A	1104	J3C	N1-C5-N2	-2.52	109.08	111.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	303	NAG	O5-C5-C6-O6
7	B	301	NAG	O5-C5-C6-O6
7	B	303	NAG	C4-C5-C6-O6
7	B	302	NAG	C1-C2-N2-C7
7	B	301	NAG	C4-C5-C6-O6
5	A	1104	J3C	C11-C12-C13-C14
5	A	1104	J3C	C11-C12-C13-C18
7	B	302	NAG	C3-C2-N2-C7

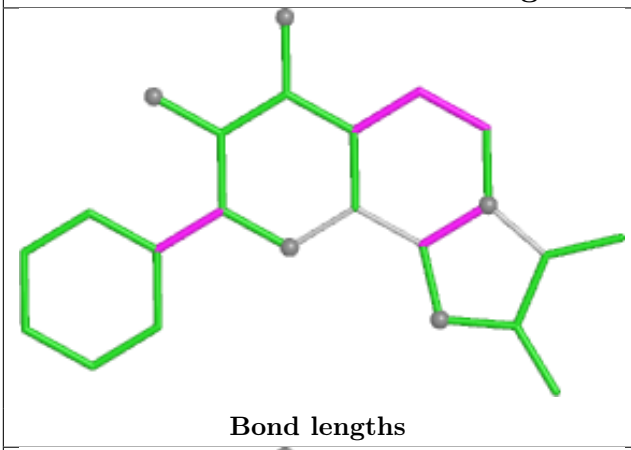
There are no ring outliers.

1 monomer is involved in 1 short contact:

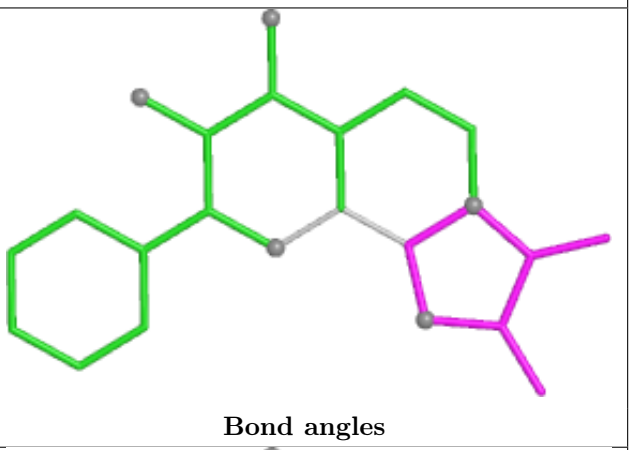
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1107	BEF	1	0

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 then 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.

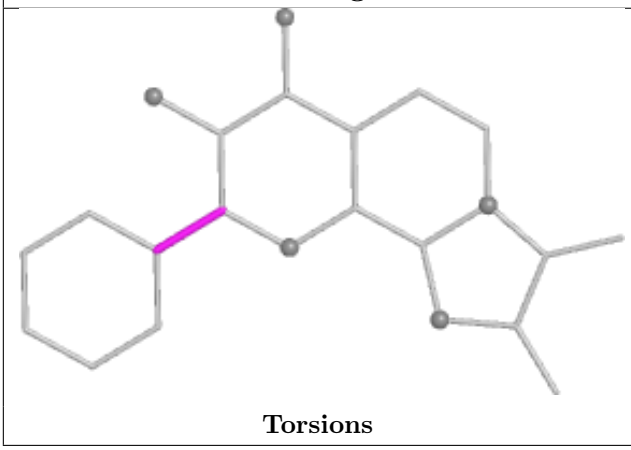
Ligand J3C A 1104



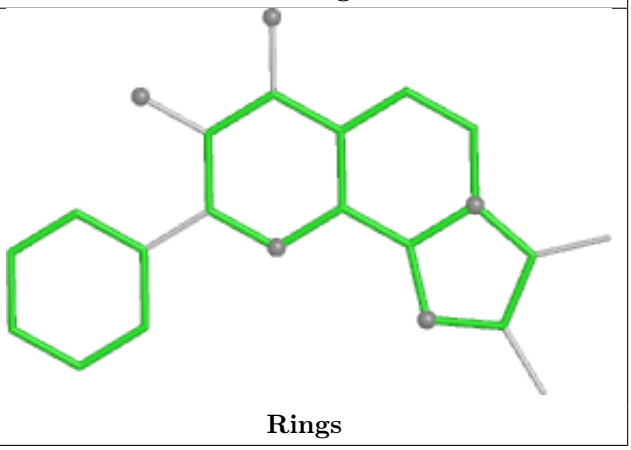
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	985/985 (100%)	0.81	95 (9%) 13 9	27, 52, 102, 158	0
2	B	261/261 (100%)	1.05	33 (12%) 8 6	37, 62, 104, 138	0
All	All	1246/1246 (100%)	0.86	128 (10%) 12 8	27, 54, 103, 158	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	GLU	8.0
1	A	440	ALA	6.2
1	A	487	CYS	6.0
1	A	227	LEU	5.5
2	B	30	LEU	4.4
1	A	598	VAL	4.3
1	A	50	ILE	4.3
2	B	150	PHE	4.3
1	A	246	LEU	4.2
2	B	130	ASN	4.1
1	A	491	PHE	4.0
1	A	560	ARG	4.0
1	A	558	GLY	3.9
2	B	95	ASP	3.9
1	A	373	VAL	3.7
2	B	125	GLN	3.7
1	A	275	ILE	3.7
2	B	127	GLY	3.7
1	A	494	THR	3.7
1	A	483	PHE	3.6
1	A	134	THR	3.6
1	A	434	LEU	3.5
1	A	675	ASN	3.5
1	A	785	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	977	PHE	3.3
1	A	255	SER	3.3
1	A	958	PHE	3.2
1	A	539	LEU	3.2
1	A	327	LEU	3.2
1	A	338	VAL	3.2
1	A	489	ILE	3.2
1	A	601	ILE	3.2
2	B	179	PHE	3.1
2	B	159	LEU	3.1
2	B	280	GLY	3.1
1	A	553	SER	3.1
2	B	225	SER	3.0
2	B	181	ILE	3.0
2	B	165	ARG	3.0
1	A	589	THR	3.0
2	B	242	ASN	3.0
1	A	555	GLY	2.9
1	A	92	PRO	2.9
1	A	789	LEU	2.9
1	A	438	ASN	2.9
2	B	182	LYS	2.9
2	B	264	ILE	2.9
2	B	90	GLY	2.9
2	B	163	SER	2.8
2	B	173	ALA	2.8
1	A	648	GLU	2.8
1	A	724	THR	2.7
1	A	349	VAL	2.7
1	A	127	GLN	2.7
2	B	171	GLY	2.7
1	A	353	LEU	2.7
1	A	768	VAL	2.7
2	B	107	ALA	2.7
1	A	437	CYS	2.6
1	A	692	ARG	2.6
2	B	229	PHE	2.6
1	A	671	ALA	2.6
1	A	542	GLN	2.6
1	A	561	VAL	2.6
1	A	564	PHE	2.5
1	A	241	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	535	GLN	2.5
1	A	439	ARG	2.5
1	A	244	SER	2.5
1	A	540	ASP	2.5
1	A	1027	TRP	2.5
1	A	597	LEU	2.5
1	A	232	GLU	2.5
1	A	990	PHE	2.5
2	B	209	ASP	2.5
1	A	588	PRO	2.5
1	A	959	PHE	2.4
2	B	197	PRO	2.4
2	B	169	THR	2.4
1	A	856	GLU	2.4
2	B	154	PHE	2.4
2	B	224	TYR	2.4
1	A	623	ILE	2.4
1	A	587	PHE	2.4
2	B	155	THR	2.4
1	A	1033	TYR	2.4
1	A	174	VAL	2.4
1	A	556	GLY	2.3
1	A	974	ILE	2.3
1	A	730	ASP	2.3
1	A	512	HIS	2.3
1	A	859	ALA	2.3
1	A	986	ASN	2.3
1	A	496	LYS	2.3
2	B	115	ARG	2.3
1	A	653	ILE	2.3
1	A	705	GLN	2.2
1	A	480	ARG	2.2
1	A	599	SER	2.2
1	A	871	SER	2.2
1	A	383	CYS	2.2
1	A	911	TYR	2.2
1	A	352	CYS	2.2
2	B	120	TYR	2.2
2	B	119	GLY	2.2
1	A	906	ASP	2.2
1	A	449	VAL	2.1
1	A	551	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	510	PRO	2.1
1	A	499	LEU	2.1
1	A	176	GLN	2.1
2	B	207	PRO	2.1
1	A	225	SER	2.1
2	B	193	ASN	2.1
1	A	576	PRO	2.1
1	A	1025	SER	2.1
1	A	325	THR	2.1
2	B	156	ALA	2.1
1	A	386	LYS	2.0
1	A	133	LEU	2.0
1	A	304	ILE	2.0
1	A	876	THR	2.0
1	A	811	LEU	2.0
1	A	469	SER	2.0
1	A	791	SER	2.0
1	A	74	ALA	2.0
1	A	970	PHE	2.0
1	A	972	VAL	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, 95^{th} 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	NAG	B	302	14/15	0.53	0.19	80,92,97,100	0
4	RB	A	1106	1/1	0.54	0.11	165,165,165,165	0
6	BEF	A	1107	4/4	0.79	0.20	46,50,57,64	0

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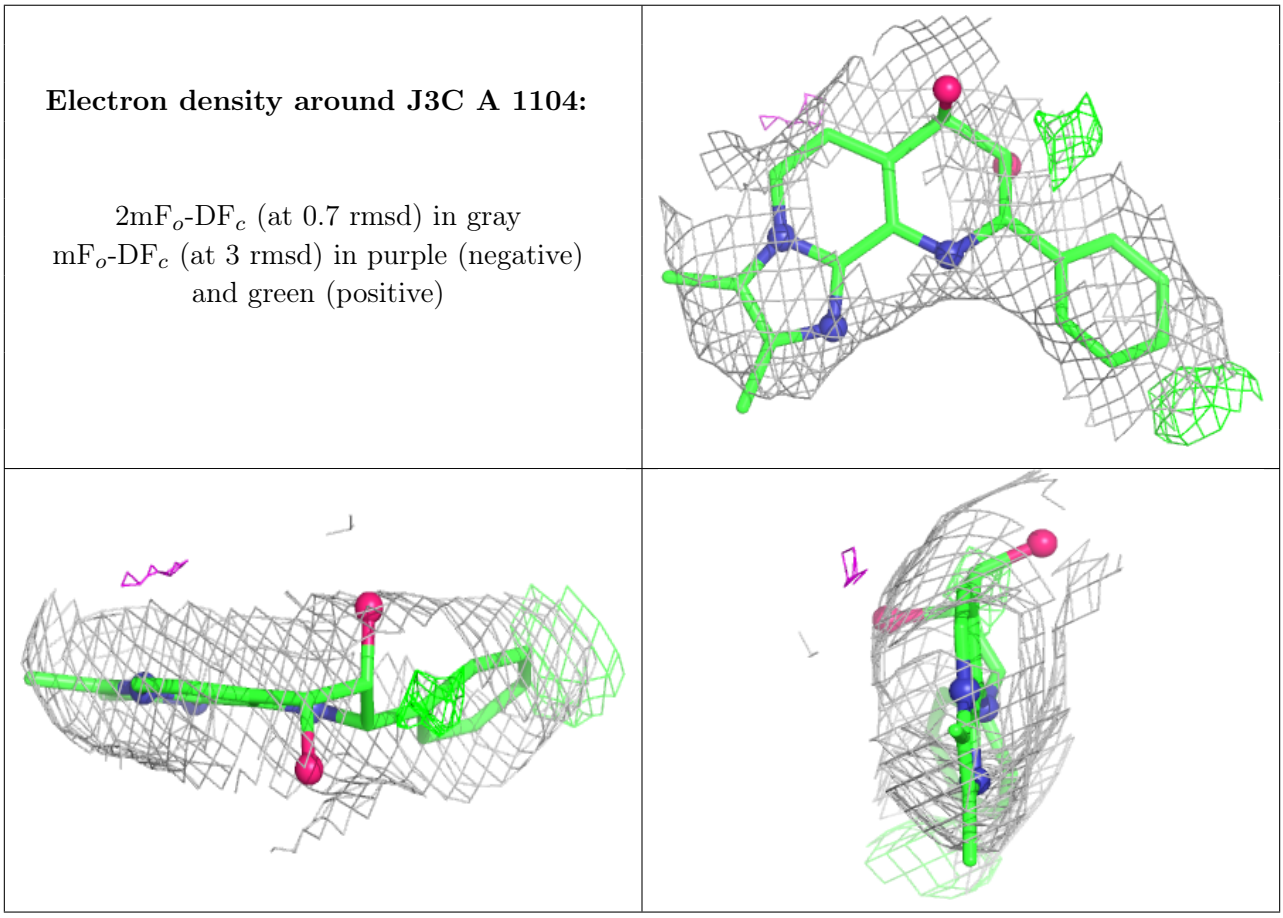
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1101	1/1	0.81	0.19	41,41,41,41	0
7	NAG	B	301	14/15	0.84	0.16	49,54,59,61	0
7	NAG	B	303	14/15	0.85	0.12	53,64,74,81	0
5	J3C	A	1104	23/23	0.88	0.15	33,48,50,56	0
4	RB	A	1103	1/1	0.94	0.06	78,78,78,78	0
4	RB	A	1105	1/1	0.96	0.18	66,66,66,66	0
4	RB	A	1102	1/1	0.97	0.08	70,70,70,70	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 J3C A 1104:

$2mF_o$-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.