wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 05:35 PM EDT

PDB ID	:	2AJL
Title	:	X-ray Structure of Novel Biaryl-Based Dipeptidyl peptidase IV inhibitor
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Deposited on	:	2005-08-02
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

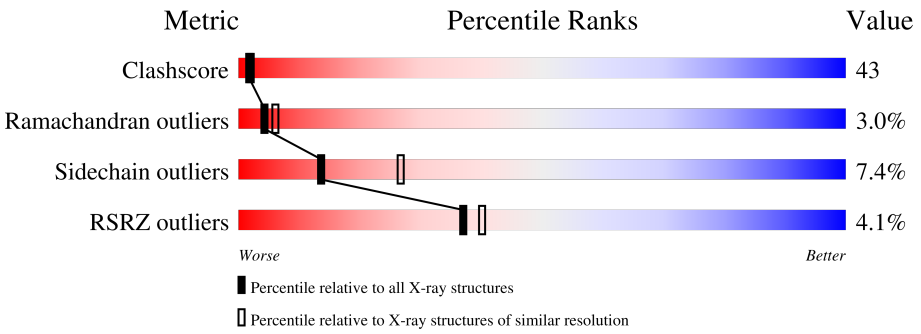
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	I	728	4%, 41%, 50%, 8%
1	J	728	4%, 42%, 51%, 6%

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	NAG	I	768	X	-	-	-
2	NAG	I	771	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	J	767	-	-	X	-
2	NAG	J	769	X	-	-	-
2	NAG	J	771	X	-	-	-
3	JNH	J	1	X	-	-	-

2 Entry composition (i)

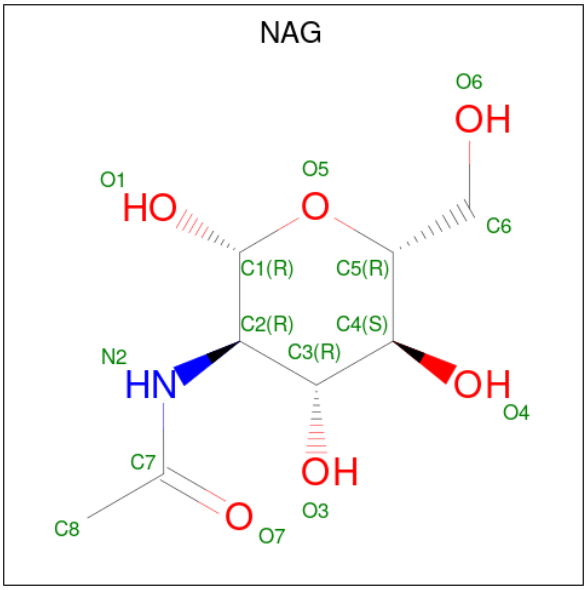
There are 4 unique types of molecules in this entry. The entry contains 12558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	726	5947	3818	977	1126	26	0	0	0
1	J	728	5964	3827	982	1129	26	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	I	1	14	8	1	5	0	0
2	I	1	14	8	1	5	0	0
2	I	1	14	8	1	5	0	0
2	I	1	14	8	1	5	0	0

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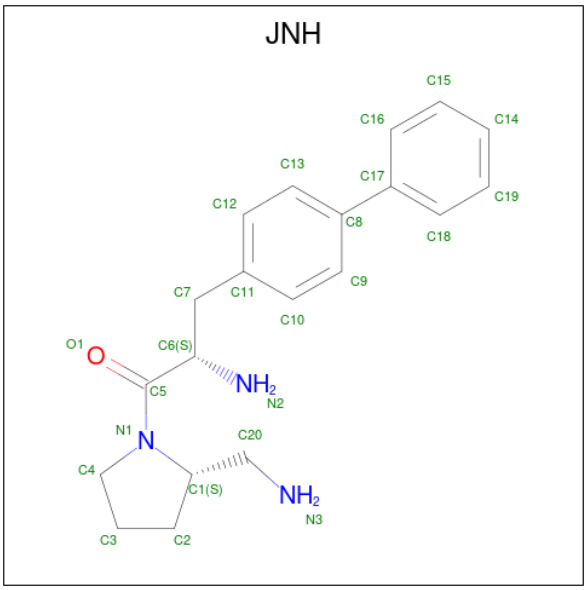
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	I	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0
2	J	1	14	8	1	5	0	0

- Molecule 3 is 1-[2-(S)-AMINO-3-BIPHENYL-4-YL-PROPIONYL]-PYRROLIDINE-2-(S)-CARBONITRILE (three-letter code: JNH) (formula: $C_{20}H_{25}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	I	1	24	20	3	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	J	1	24	20	3	1	0	0

- Molecule 4 is water.

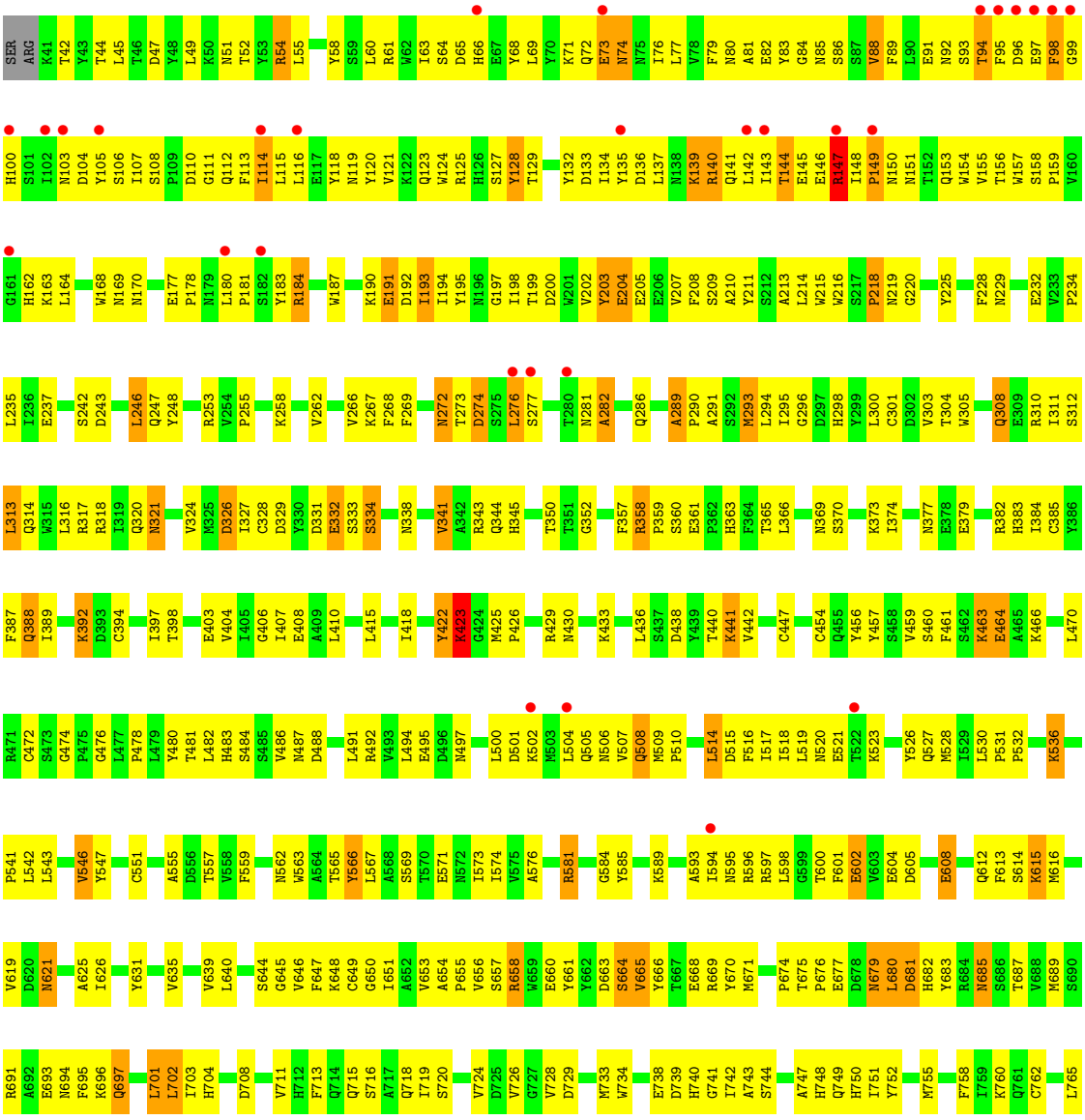
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	I	190	190	190	0	0
			Total	O		
4	J	213	213	213	0	0

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: Dipeptidyl peptidase 4

Chain I: 4% 41% 50% 8%



P766

- Molecule 1: Dipeptidyl peptidase 4

Chain J: 4% 42% 51% 6%

S39 R40 Y43 T44 L45 T46 D47 Y48 L49 K50 N51 T52 Y53 R54 L55 K56 L57 Y58 S59 L60 R61 W62 D65 L69 Y70 K71 Q72 E73 N74 N75 I76 L77 V78 F79 N80 A81 E82 Y83 G84 N85 S86 S87 V88 F89 L90 E91 N92 S93 T94 F95 D96 E97 F98 G99 H100 S101 I102

N103 D104 Y105 S106 I107 S108 P109 D110 G111 Q112 F113 I114 L115 L116 E117 Y118 N119 Y120 Q123 W124 R125 H126 S127 Y128 T129 A130 S131 Y132 D133 I134 Y135 D136 L137 N138 K139 R140 Q141 L142 I143 T144 E145 E146 R147 I148 P149 N150 Q153 W154 V155 T156 W157 S158 P159 V160 G161 H162 K163

V167 W168 N169 N170 D171 I172 Y173 V174 K175 I176 E177 P178 L180 P181 S182 Y183 R184 W187 G197 Y203 E204 E205 E206 V207 F208 S209 A210 Y211 S212 A213 L214 W215 W216 S217 P218 N219 G220 T221 F222 L223 Q227 F228 N229 E232 W233 P234 L235 I236 E237 F240 Y241 S242

L246 Q247 Y248 P249 K250 V254 P255 Y256 P257 K258 V262 T265 V266 K267 F268 V271 N272 T273 D274 S275 L276 S277 S278 V279 T280 N281 Q286 I287 T288 A289 P290 M293 D297 H298 Y299 L300 C301 D302 V303 T304 Q308 E309 R310 L313 Q314 W315 R318 I319 Q320 N321

M325 D326 I327 G328 D329 Y330 D331 E332 S333 S334 G335 R336 W337 Q344 H345 I346 E347 M348 R358 P359 S360 E361 Y372 K373 I374 I375 S376 N377 E378 E379 G380 Y381 R382 H383 I384 C385 Y386 F387 Q388 I389 D390 K391 K392 I397 T398 K399 G400 T401 I407 E408 A409 L410 T411 S412

D413 Y414 L415 I418 Y422 K423 G427 G428 R429 N430 L431 Y432 K433 I434 Q435 L436 S437 D438 Y439 T440 K441 V442 T443 C444 L445 S446 C447 E448 L449 N450 P451 E452 R453 C454 Q455 Y456 Y457 S458 V459 S460 F461 S462 K463 E464 A465 K466 Y467 Y468 Q469 L470 R471 C472 S473 G474 P475 G476 L477

P478 L479 Y480 S484 S485 V486 N487 D488 K489 G490 L491 L494 E495 D496 N497 L500 D501 K502 M503 L504 Q505 N506 V507 Q508 M509 P510 S511 K512 K513 L514 D515 F516 I517 I518 T522 K523 F524 W525 Y526 Q527 M528 I529 L530 P531 P532 H533 F534 D535 Y540 P541 L542 L543 L544 D545 V546

Y547 Q553 K554 A555 D556 T557 V558 F559 N562 T565 Y566 L567 A568 S569 T570 E571 N572 I573 A576 S577 F578 D579 G580 R581 H592 R596 R597 L598 G599 T600 F601 E602 V603 E604 D605 Q606 I607 E608 A609 A610 R611 Q612 F613 S614 K615 M616 G617 F618 V619 D620 N621 K622 R623

I626 W627 Y631 G632 G633 V639 L640 C649 G650 I651 P655 V656 S657 R658 W659 E660 Y661 Y662 D663 S664 V665 Y666 T667 E668 R669 Y670 M671 G672 L673 P674 T675 P676 E677 D678 N679 L680 Y683 T687 V688 M689 S690 E699 Y700 L701 L702 I703 H704 V711 H712 F713 Q714 Q715

Q718 I719 S720 K721 V724 D725 V726 G727 V728 Q731 A732 M733 W734 Y735 T736 D737 E738 D739 H740 G741 I742 H750 I751 H754 M755 I759 K760 F763 S764 L765 P766

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.28Å 126.88Å 110.83Å 90.00° 99.41° 90.00°	Depositor
Resolution (Å)	64.10 – 2.50 64.40 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.8 (64.10-2.50) 91.6 (64.40-2.51)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.303 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12558	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, JNH

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	I	0.36	0/6119	0.68	4/8322 (0.0%)
1	J	0.37	0/6136	0.67	4/8344 (0.0%)
All	All	0.36	0/12255	0.68	8/16666 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	766	PRO	CA-C-O	9.57	143.17	120.20
1	J	766	PRO	CA-C-O	9.20	142.28	120.20
1	I	388	GLN	N-CA-C	-6.01	94.77	111.00
1	I	300	LEU	N-CA-C	-5.72	95.55	111.00
1	J	240	PHE	N-CA-C	-5.27	96.78	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	700	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	I	5947	0	5666	532	0
1	J	5964	0	5684	500	0
2	I	70	0	65	8	0
2	J	126	0	117	22	0
3	I	24	0	24	7	0
3	J	24	0	23	7	0
4	I	190	0	0	18	0
4	J	213	0	0	13	0
All	All	12558	0	11579	1029	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 43.

The worst 5 of 1029 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:J:489:LYS:HE3	1:J:491:LEU:HD21	1.27	1.14
1:I:289:ALA:HB1	1:I:290:PRO:HA	1.28	1.13
1:I:107:ILE:HG13	1:I:114:ILE:HG12	1.23	1.11
1:I:310:ARG:HD3	1:I:329:ASP:OD1	1.51	1.10
1:I:626:ILE:HD13	1:I:639:VAL:HG21	1.34	1.10

There are no symmetry-related clashes.

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	I	724/728 (100%)	607 (84%)	86 (12%)	31 (4%)	2 3
1	J	726/728 (100%)	632 (87%)	82 (11%)	12 (2%)	9 16
All	All	1450/1456 (100%)	1239 (85%)	168 (12%)	43 (3%)	4 6

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	94	THR
1	I	98	PHE
1	I	99	GLY
1	I	140	ARG
1	I	147	ARG

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	I	651/653 (100%)	603 (93%)	48 (7%)	13 27
1	J	653/653 (100%)	605 (93%)	48 (7%)	13 27
All	All	1304/1306 (100%)	1208 (93%)	96 (7%)	13 27

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	221	THR
1	J	387	PHE
1	J	246	LEU
1	J	325	MET
1	J	445	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	682	HIS

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Mol	Chain	Res	Type
1	J	679	ASN
1	J	112	GLN
1	J	606	GLN
1	J	345	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	NAG	J	773	-	14,14,15	2.92	3 (21%)	17,19,21	2.39	5 (29%)
2	NAG	I	769	-	14,14,15	2.52	2 (14%)	17,19,21	2.01	4 (23%)
2	NAG	J	775	-	14,14,15	2.74	3 (21%)	17,19,21	2.75	8 (47%)
2	NAG	I	768	-	14,14,15	2.67	3 (21%)	17,19,21	3.40	4 (23%)
2	NAG	J	767	-	14,14,15	2.69	3 (21%)	17,19,21	3.05	9 (52%)
2	NAG	J	769	-	14,14,15	2.71	2 (14%)	17,19,21	2.59	7 (41%)
2	NAG	I	767	-	14,14,15	2.88	3 (21%)	17,19,21	2.24	5 (29%)
3	JNH	I	1	1	24,26,26	1.59	5 (20%)	30,35,35	1.62	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	I	771	-	14,14,15	2.68	2 (14%)	17,19,21	1.74	5 (29%)
2	NAG	I	770	-	14,14,15	2.67	2 (14%)	17,19,21	2.63	7 (41%)
2	NAG	J	772	-	14,14,15	2.70	2 (14%)	17,19,21	3.34	6 (35%)
2	NAG	J	768	-	14,14,15	2.75	3 (21%)	17,19,21	2.96	6 (35%)
3	JNH	J	1	1	24,26,26	1.46	4 (16%)	30,35,35	2.03	8 (26%)
2	NAG	J	774	-	14,14,15	2.74	3 (21%)	17,19,21	3.07	7 (41%)
2	NAG	J	771	-	14,14,15	3.07	5 (35%)	17,19,21	5.66	8 (47%)
2	NAG	J	770	-	14,14,15	2.96	4 (28%)	17,19,21	2.46	7 (41%)

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
2	NAG	J	773	-	-	3/6/23/26	0/1/1/1
2	NAG	I	769	-	-	3/6/23/26	0/1/1/1
2	NAG	J	775	-	-	3/6/23/26	0/1/1/1
2	NAG	I	768	-	2/2/5/7	1/6/23/26	0/1/1/1
2	NAG	J	769	-	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	J	767	-	-	4/6/23/26	0/1/1/1
2	NAG	I	767	-	-	2/6/23/26	0/1/1/1
3	JNH	I	1	1	-	4/14/28/28	0/3/3/3
2	NAG	I	771	-	1/1/5/7	4/6/23/26	0/1/1/1
3	JNH	J	1	1	1/1/4/4	6/14/28/28	0/3/3/3
2	NAG	I	770	-	-	2/6/23/26	0/1/1/1
2	NAG	J	768	-	-	1/6/23/26	0/1/1/1
2	NAG	J	772	-	-	3/6/23/26	0/1/1/1
2	NAG	J	774	-	-	2/6/23/26	0/1/1/1
2	NAG	J	771	-	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	J	770	-	-	2/6/23/26	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	771	NAG	O7-C7	9.24	1.44	1.23
2	J	773	NAG	O7-C7	9.22	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	770	NAG	O7-C7	9.17	1.44	1.23
2	I	767	NAG	O7-C7	8.92	1.43	1.23
2	J	768	NAG	O7-C7	8.90	1.43	1.23

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	771	NAG	C2-N2-C7	-18.31	96.83	122.90
2	I	768	NAG	C2-N2-C7	-11.99	105.83	122.90
2	J	771	NAG	C1-O5-C5	-9.69	99.06	112.19
2	J	768	NAG	C2-N2-C7	-9.06	110.00	122.90
2	J	772	NAG	C2-N2-C7	-8.92	110.20	122.90

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	768	NAG	C3
2	I	768	NAG	C5
2	I	771	NAG	C5
2	J	769	NAG	C4
2	J	771	NAG	C3

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	767	NAG	C8-C7-N2-C2
2	I	767	NAG	O7-C7-N2-C2
2	I	768	NAG	C8-C7-N2-C2
2	I	769	NAG	C8-C7-N2-C2
2	I	769	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	773	NAG	1	0
2	I	768	NAG	5	0
2	J	767	NAG	7	0
2	J	769	NAG	3	0
2	I	767	NAG	2	0
3	I	1	JNH	7	0

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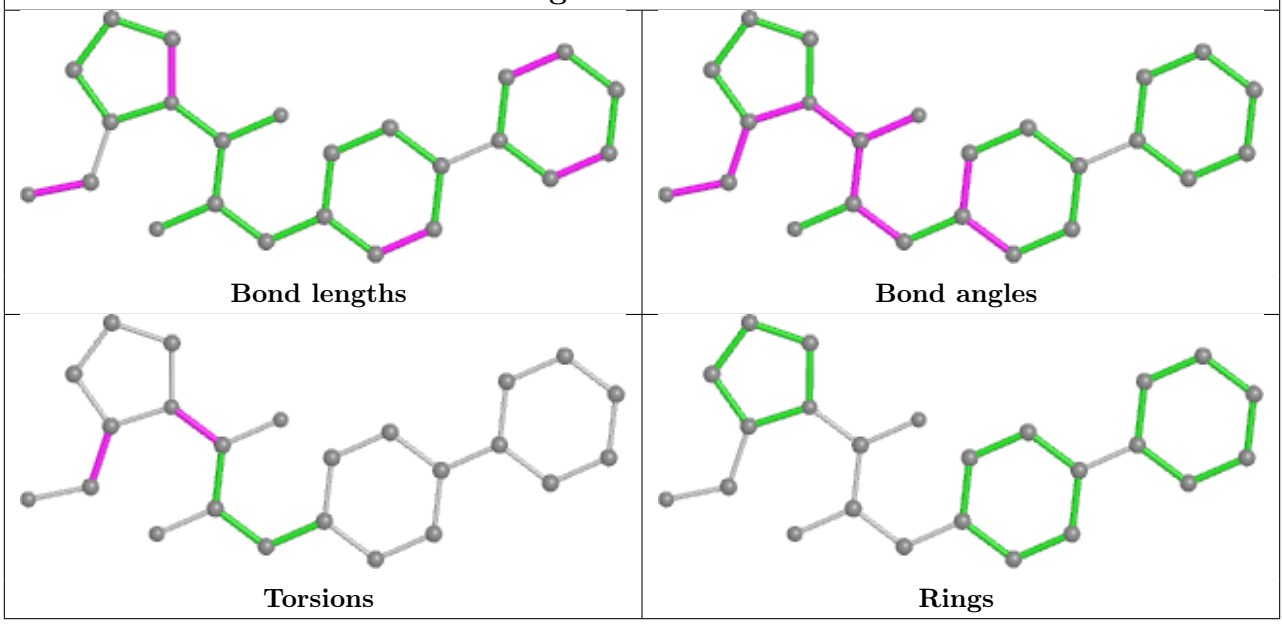
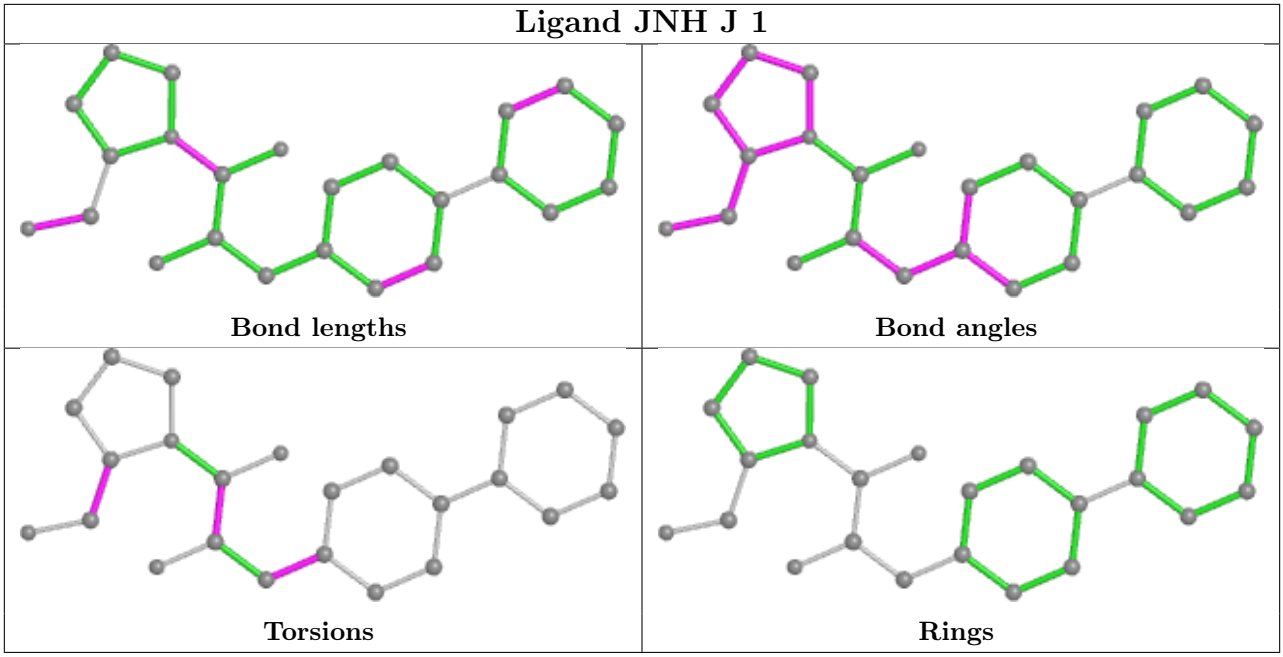
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	770	NAG	1	0
2	J	768	NAG	1	0
3	J	1	JNH	7	0
2	J	774	NAG	5	0
2	J	771	NAG	6	0
2	J	770	NAG	1	0

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 JNH I 1





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	I	726/728 (99%)	0.33	29 (3%)	38	41	3, 19, 50, 80	0
1	J	728/728 (100%)	0.31	30 (4%)	37	40	3, 16, 49, 86	0
All	All	1454/1456 (99%)	0.32	59 (4%)	37	40	3, 18, 49, 86	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	99	GLY	7.5
1	J	98	PHE	5.0
1	I	98	PHE	4.7
1	J	277	SER	4.7
1	J	389	ILE	4.5

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 monosaccharides in this entry.

6.4 Ligands (i)

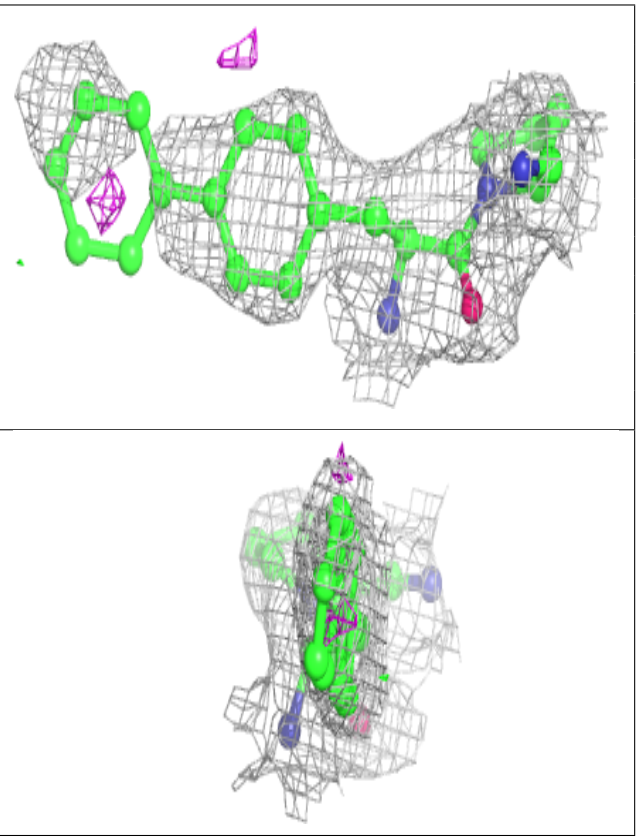
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	J	768	14/15	0.57	0.28	67,70,72,72	0
2	NAG	I	771	14/15	0.61	0.29	78,82,86,86	0
2	NAG	J	770	14/15	0.65	0.35	56,62,69,70	0
2	NAG	I	769	14/15	0.70	0.27	59,61,65,66	0
2	NAG	I	770	14/15	0.74	0.28	77,80,81,82	0
2	NAG	I	767	14/15	0.74	0.21	38,40,42,43	0
2	NAG	J	769	14/15	0.75	0.24	45,50,53,55	0
2	NAG	J	775	14/15	0.76	0.23	48,57,60,64	0
2	NAG	J	772	14/15	0.77	0.25	56,60,65,65	0
2	NAG	J	773	14/15	0.78	0.18	31,38,41,45	0
2	NAG	J	767	14/15	0.78	0.24	39,46,49,50	0
2	NAG	J	771	14/15	0.81	0.22	18,21,30,31	0
2	NAG	J	774	14/15	0.83	0.20	35,38,41,42	0
2	NAG	I	768	14/15	0.83	0.28	35,40,42,43	0
3	JNH	I	1	24/24	0.86	0.27	27,32,38,41	0
3	JNH	J	1	24/24	0.86	0.22	19,24,30,30	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.

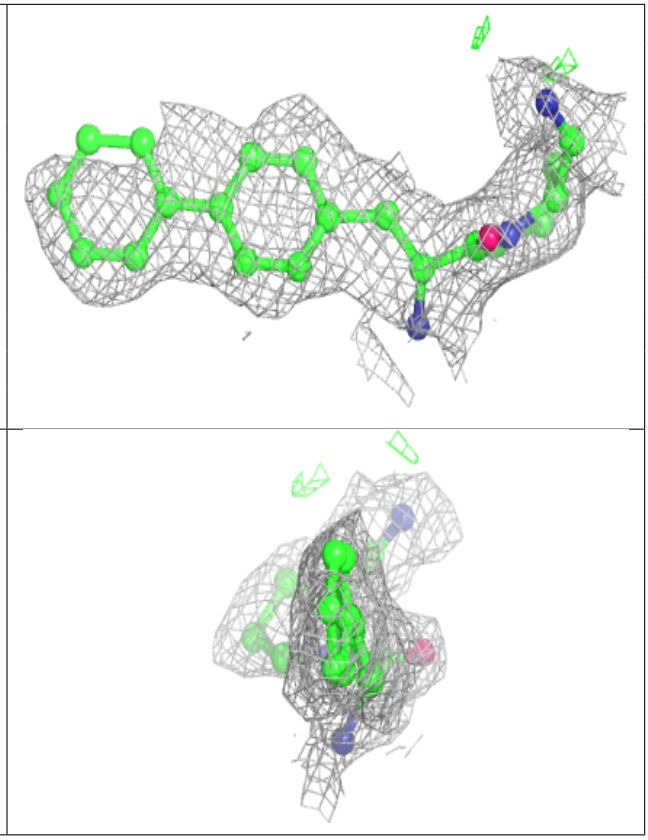
Electron density around JNH I 1:

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 JNH J 1:

$2mF_o$-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.