



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 07:38 AM EDT

PDB ID : 3JSW
Title : Human PDE9 in complex with selective inhibitor
Authors : Liu, S.
Deposited on : 2009-09-11
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

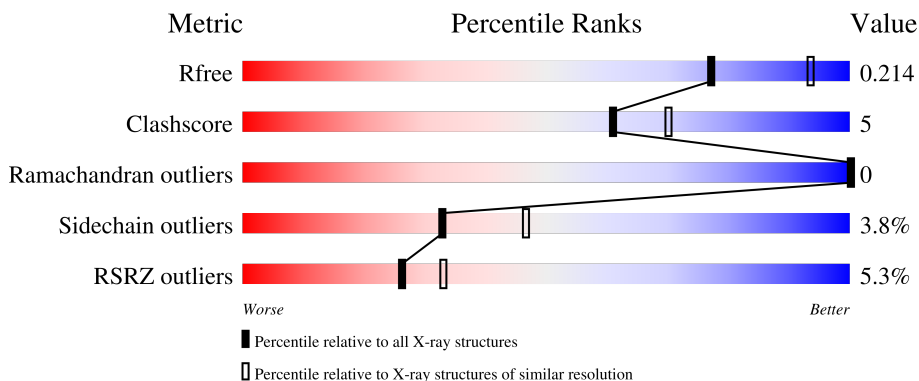
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


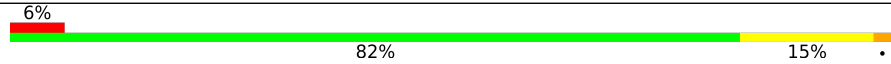
The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	329	
1	B	329	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5770 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 High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2706	1732	449	494	31	0	0	0
1	B	328	2706	1732	449	494	31	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	GLY	-	expression tag	UNP O76083
A	179	SER	-	expression tag	UNP O76083
A	180	HIS	-	expression tag	UNP O76083
A	181	MET	-	expression tag	UNP O76083
B	178	GLY	-	expression tag	UNP O76083
B	179	SER	-	expression tag	UNP O76083
B	180	HIS	-	expression tag	UNP O76083
B	181	MET	-	expression tag	UNP O76083

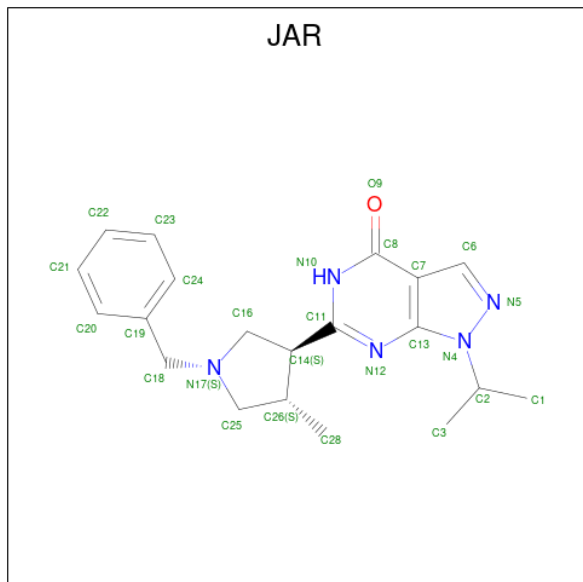
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 6-[(3S,4S)-1-benzyl-4-methylpyrrolidin-3-yl]-1-(1-methylethyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (three-letter code: JAR) (formula: C₂₀H₂₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	26	20	5	1	0	0
4	B	1	26	20	5	1	0	0

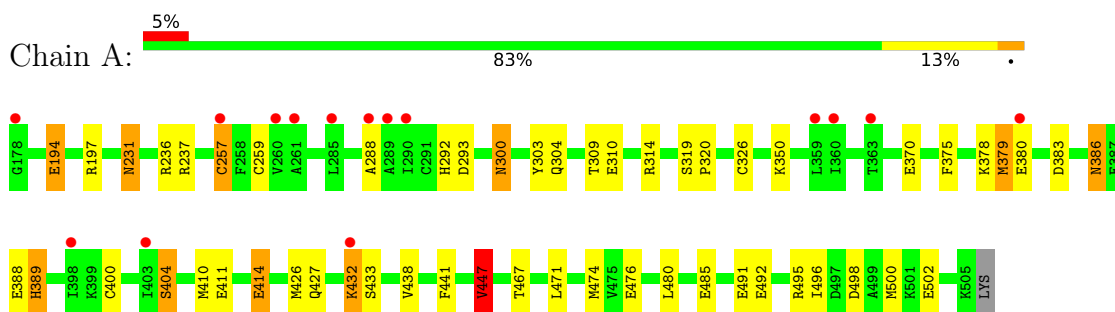
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	164	164	164	0	0
5	B	138	138	138	0	0

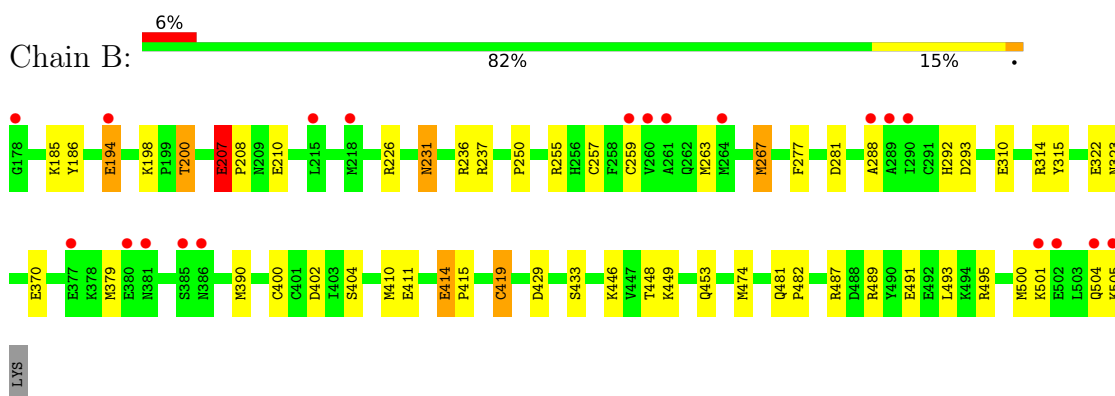
3 Residue-property plots [i](#)

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: High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A



- Molecule 1: High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.28Å 103.28Å 270.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 36.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.30) 99.7 (36.51-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.179 , 0.212 0.186 , 0.214	Depositor DCC
R_{free} test set	6633 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.371	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5770	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: JAR, ZN, 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	1.34	22/2776 (0.8%)	1.09	15/3759 (0.4%)
1	B	1.27	15/2776 (0.5%)	1.08	14/3759 (0.4%)
All	All	1.30	37/5552 (0.7%)	1.08	29/7518 (0.4%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	CYS	CB-SG	-11.42	1.62	1.82
1	B	370	GLU	CG-CD	10.84	1.68	1.51
1	A	411	GLU	CG-CD	10.73	1.68	1.51
1	A	370	GLU	CG-CD	10.24	1.67	1.51
1	B	411	GLU	CG-CD	9.24	1.65	1.51
1	A	411	GLU	CD-OE1	9.22	1.35	1.25
1	B	370	GLU	CB-CG	7.79	1.67	1.52
1	B	310	GLU	CD-OE2	7.57	1.33	1.25
1	A	370	GLU	CD-OE2	7.55	1.33	1.25
1	B	194	GLU	CD-OE1	7.42	1.33	1.25
1	B	194	GLU	CG-CD	7.38	1.63	1.51
1	B	446	LYS	CE-NZ	7.26	1.67	1.49
1	A	411	GLU	CD-OE2	7.04	1.33	1.25
1	A	259	CYS	CB-SG	-6.52	1.71	1.82
1	B	231	ASN	CB-CG	6.48	1.66	1.51
1	B	310	GLU	CD-OE1	6.48	1.32	1.25
1	A	194	GLU	CD-OE1	6.40	1.32	1.25
1	A	350	LYS	CE-NZ	6.38	1.65	1.49
1	A	310	GLU	CB-CG	6.18	1.63	1.52
1	A	414	GLU	CG-CD	6.18	1.61	1.51
1	B	210	GLU	CD-OE1	6.10	1.32	1.25
1	A	404	SER	CB-OG	6.09	1.50	1.42
1	A	476	GLU	CD-OE1	-5.87	1.19	1.25
1	A	370	GLU	CB-CG	5.80	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	ARG	CG-CD	5.73	1.66	1.51
1	B	207	GLU	CB-CG	-5.67	1.41	1.52
1	A	231	ASN	CB-CG	5.64	1.64	1.51
1	A	404	SER	CA-CB	5.59	1.61	1.52
1	A	414	GLU	CD-OE1	5.54	1.31	1.25
1	B	186	TYR	CG-CD2	5.53	1.46	1.39
1	A	492	GLU	CD-OE2	-5.49	1.19	1.25
1	A	380	GLU	CG-CD	5.33	1.59	1.51
1	A	350	LYS	CD-CE	5.22	1.64	1.51
1	B	322	GLU	CB-CG	5.21	1.62	1.52
1	A	485	GLU	CD-OE1	5.13	1.31	1.25
1	B	259	CYS	CB-SG	-5.04	1.73	1.81
1	B	419	CYS	CB-SG	-5.02	1.73	1.81

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ARG	NE-CZ-NH2	-17.20	111.70	120.30
1	A	237	ARG	NE-CZ-NH2	-16.07	112.27	120.30
1	A	197	ARG	NE-CZ-NH2	-14.21	113.19	120.30
1	A	237	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	B	237	ARG	NE-CZ-NH1	12.47	126.54	120.30
1	B	293	ASP	CB-CG-OD1	9.66	127.00	118.30
1	A	236	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	B	236	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	B	267	MET	CG-SD-CE	-7.52	88.17	100.20
1	A	197	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	B	495	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	489	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	447	VAL	CB-CA-C	-6.99	98.12	111.40
1	A	197	ARG	CG-CD-NE	-6.60	97.95	111.80
1	B	429	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	A	498	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	379	MET	CG-SD-CE	-6.19	90.30	100.20
1	A	236	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	293	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	B	237	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	500	MET	CG-SD-CE	-5.62	91.20	100.20
1	B	402	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	255	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	495	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	426	MET	CG-SD-CE	5.22	108.55	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	237	ARG	CD-NE-CZ	5.16	130.83	123.60
1	B	310	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	A	257	CYS	CA-CB-SG	5.02	123.04	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2706	0	2643	27	0
1	B	2706	0	2643	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	25	0	0
4	B	26	0	25	2	0
5	A	164	0	0	8	0
5	B	138	0	0	4	1
All	All	5770	0	5336	49	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 5.

All (49) 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:231:ASN:HB2	5:B:550:HOH:O	1.26	1.33
1:A:231:ASN:HB2	5:A:559:HOH:O	1.43	1.15
1:B:226:ARG:HD2	5:B:557:HOH:O	1.57	1.00
1:B:453:GLN:HE22	4:B:900:JAR:HN10	1.09	0.97
1:A:414:GLU:HG3	5:A:553:HOH:O	1.70	0.91
1:A:314:ARG:HD3	1:B:314:ARG:HD3	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:THR:HG21	5:B:176:HOH:O	1.84	0.77
1:A:231:ASN:ND2	5:A:527:HOH:O	2.23	0.72
1:A:386:ASN:HD21	1:A:388:GLU:HB2	1.57	0.70
1:A:441:PHE:HA	1:A:447:VAL:HG13	1.81	0.62
1:A:467:THR:HG22	5:A:514:HOH:O	1.98	0.62
1:B:207:GLU:HG3	1:B:208:PRO:HD2	1.80	0.62
1:A:383:ASP:H	1:A:389:HIS:HD2	1.50	0.59
1:A:386:ASN:ND2	1:A:388:GLU:HB2	2.17	0.58
1:A:400:CYS:O	1:A:404:SER:HB3	2.05	0.56
1:B:414:GLU:OE2	1:B:449:LYS:NZ	2.28	0.56
1:A:300:ASN:ND2	1:A:303:TYR:H	2.05	0.54
1:A:375:PHE:CZ	1:A:379:MET:HE1	2.42	0.54
1:A:432:LYS:HE3	1:A:438:VAL:HG21	1.89	0.53
1:A:375:PHE:CZ	1:A:379:MET:CE	2.92	0.53
1:A:375:PHE:CE1	1:A:379:MET:HE1	2.43	0.52
1:A:491:GLU:HG2	5:A:569:HOH:O	2.07	0.52
1:B:207:GLU:HG3	1:B:208:PRO:CD	2.39	0.52
1:B:500:MET:O	1:B:504:GLN:HG3	2.09	0.52
1:B:263:MET:O	1:B:267:MET:HG3	2.10	0.51
1:B:453:GLN:NE2	4:B:900:JAR:HN10	1.92	0.50
1:A:378:LYS:HE2	5:A:566:HOH:O	2.12	0.50
1:B:379:MET:HA	1:B:379:MET:HE2	1.94	0.50
1:A:300:ASN:ND2	1:A:427:GLN:HE22	2.10	0.49
1:A:300:ASN:HD22	1:A:303:TYR:H	1.59	0.49
1:A:410:MET:HB2	5:A:64:HOH:O	2.13	0.49
1:B:250:PRO:O	1:B:419:CYS:HB3	2.12	0.48
1:A:300:ASN:HD22	1:A:300:ASN:C	2.17	0.47
1:A:319:SER:N	1:A:320:PRO:HD3	2.29	0.47
1:B:400:CYS:O	1:B:404:SER:HB3	2.15	0.46
1:B:198:LYS:HB2	1:B:200:THR:HG22	1.98	0.45
1:A:386:ASN:HD22	1:A:386:ASN:C	2.21	0.43
1:B:474:MET:HE2	5:B:521:HOH:O	2.18	0.43
1:B:481:GLN:N	1:B:482:PRO:HD2	2.34	0.43
1:B:185:LYS:NZ	1:B:207:GLU:OE1	2.51	0.43
1:B:414:GLU:HG3	1:B:415:PRO:N	2.34	0.42
1:B:315:TYR:CE1	1:B:323:ASN:HB3	2.54	0.42
1:B:277:PHE:CE1	1:B:390:MET:CE	3.03	0.42
1:B:288:ALA:O	1:B:292:HIS:HB3	2.20	0.42
1:B:487:ARG:O	1:B:491:GLU:HG3	2.20	0.42
1:A:304:GLN:NE2	1:A:309:THR:OG1	2.51	0.41
1:A:432:LYS:HG2	5:A:120:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:N	1:A:389:HIS:HD2	2.17	0.41
1:A:288:ALA:O	1:A:292:HIS:HB3	2.20	0.41

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)
5:B:554:HOH:O	5:B:559:HOH:O[7_645]	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	326/329 (99%)	324 (99%)	2 (1%)	0	100	100
1	B	326/329 (99%)	322 (99%)	4 (1%)	0	100	100
All	All	652/658 (99%)	646 (99%)	6 (1%)	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	304/305 (100%)	291 (96%)	13 (4%)	29	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	304/305 (100%)	294 (97%)	10 (3%)	38	53
All	All	608/610 (100%)	585 (96%)	23 (4%)	33	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	257	CYS
1	A	300	ASN
1	A	386	ASN
1	A	389	HIS
1	A	432	LYS
1	A	433	SER
1	A	447	VAL
1	A	471	LEU
1	A	474	MET
1	A	480	LEU
1	A	496	ILE
1	A	502	GLU
1	B	194	GLU
1	B	200	THR
1	B	207	GLU
1	B	257	CYS
1	B	410	MET
1	B	414	GLU
1	B	433	SER
1	B	493	LEU
1	B	501	LYS
1	B	505	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	300	ASN
1	A	304	GLN
1	A	351	GLN
1	A	386	ASN
1	A	389	HIS
1	B	304	GLN
1	B	389	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	453	GLN

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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JAR	B	900	-	26,29,29	1.31	1 (3%)	23,42,42	2.10	5 (21%)
4	JAR	A	900	-	26,29,29	1.37	5 (19%)	23,42,42	2.42	9 (39%)

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	JAR	B	900	-	-	1/8/24/24	0/4/4/4
4	JAR	A	900	-	-	0/8/24/24	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	JAR	C14-C26	-4.45	1.51	1.55
4	A	900	JAR	C25-N17	-3.15	1.42	1.47
4	A	900	JAR	N5-N4	2.42	1.40	1.36
4	A	900	JAR	C14-C26	-2.14	1.53	1.55
4	A	900	JAR	C20-C19	2.07	1.43	1.38
4	A	900	JAR	C21-C20	2.00	1.43	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	JAR	C8-N10-C11	6.12	126.85	123.78
4	B	900	JAR	C25-N17-C16	5.84	112.88	104.19
4	A	900	JAR	C6-C7-C13	5.16	108.90	103.80
4	B	900	JAR	C6-C7-C13	4.70	108.44	103.80
4	A	900	JAR	C16-C14-C26	4.13	106.26	102.70
4	B	900	JAR	C18-N17-C16	3.75	119.64	113.27
4	A	900	JAR	C18-N17-C25	-3.01	108.17	113.27
4	A	900	JAR	C19-C18-N17	-2.79	107.72	113.12
4	A	900	JAR	C28-C26-C25	2.79	117.08	113.67
4	A	900	JAR	C18-N17-C16	-2.71	108.67	113.27
4	A	900	JAR	N10-C11-N12	-2.37	119.93	123.39
4	B	900	JAR	C16-C14-C26	2.36	104.73	102.70
4	B	900	JAR	C3-C2-C1	2.25	120.22	113.28
4	A	900	JAR	C25-N17-C16	2.11	107.32	104.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	900	JAR	C19-C18-N17-C16

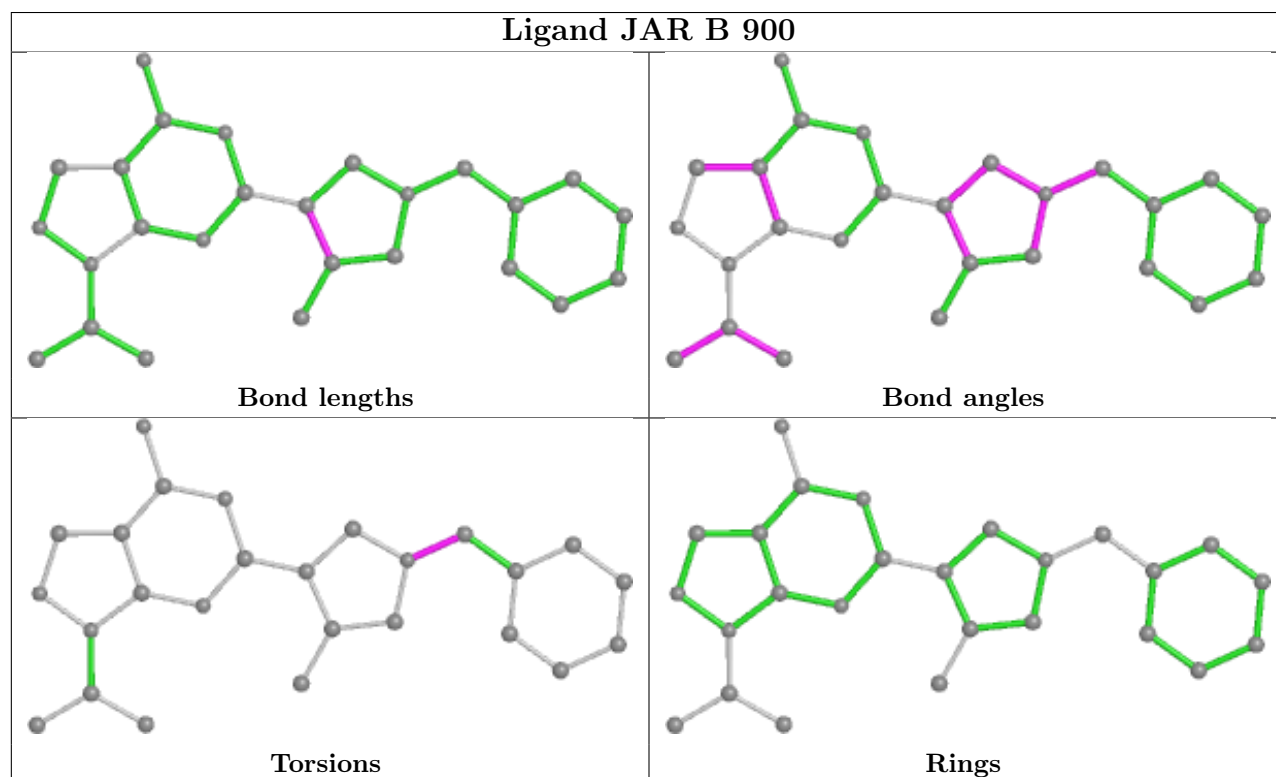
There are no ring outliers.

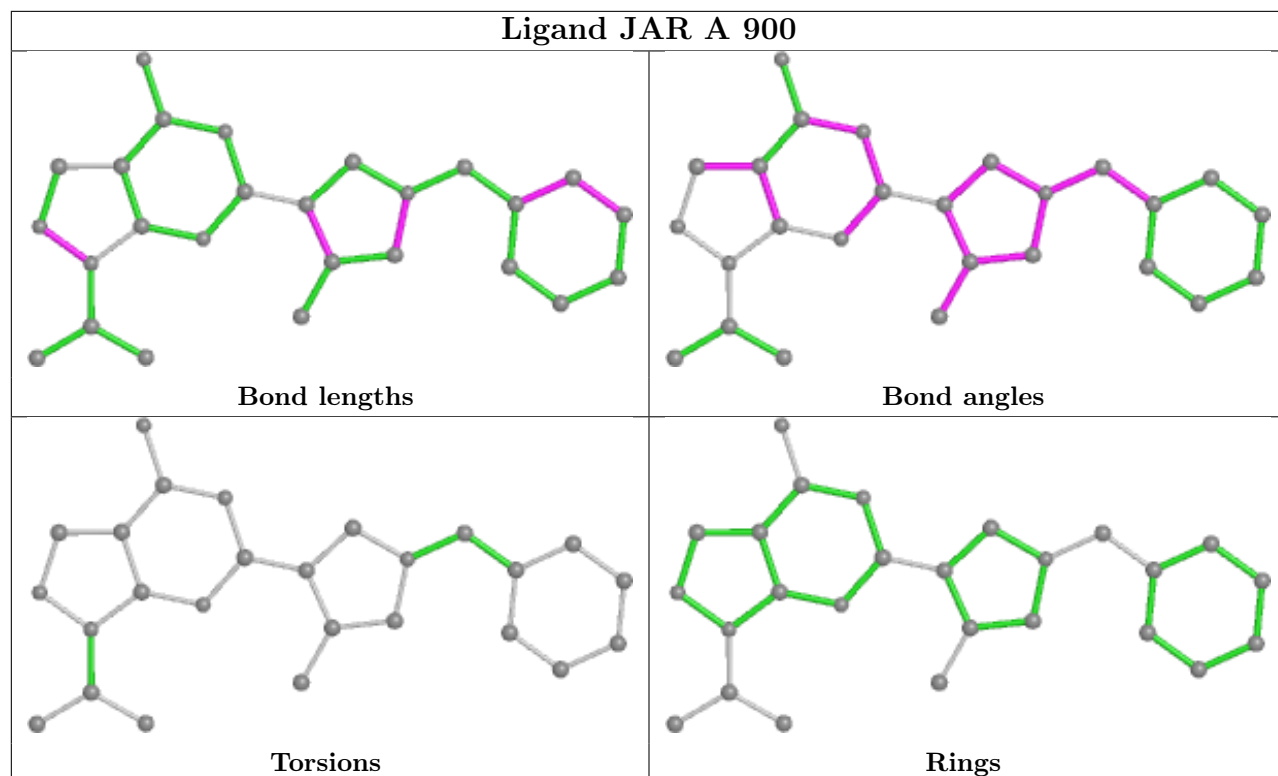
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	900	JAR	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.





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	328/329 (99%)	0.03	15 (4%) 32 39	32, 40, 51, 62	0
1	B	328/329 (99%)	0.10	20 (6%) 21 27	32, 40, 53, 71	0
All	All	656/658 (99%)	0.06	35 (5%) 26 33	32, 40, 52, 71	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	LYS	6.4
1	A	260	VAL	3.5
1	A	290	ILE	3.4
1	A	178	GLY	3.4
1	B	380	GLU	3.3
1	B	290	ILE	3.1
1	B	381	ASN	3.0
1	A	261	ALA	3.0
1	B	502	GLU	2.9
1	B	289	ALA	2.7
1	B	259	CYS	2.7
1	B	260	VAL	2.7
1	B	385	SER	2.6
1	A	289	ALA	2.6
1	A	360	ILE	2.6
1	A	398	ILE	2.6
1	B	261	ALA	2.4
1	B	178	GLY	2.4
1	A	257	CYS	2.4
1	A	432	LYS	2.3
1	B	501	LYS	2.3
1	A	288	ALA	2.3
1	B	288	ALA	2.3
1	B	386	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	363	THR	2.2
1	B	504	GLN	2.1
1	B	377	GLU	2.1
1	B	218	MET	2.1
1	B	264	MET	2.1
1	A	403	ILE	2.0
1	A	359	LEU	2.0
1	B	215	LEU	2.0
1	A	380	GLU	2.0
1	B	194	GLU	2.0
1	A	285	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

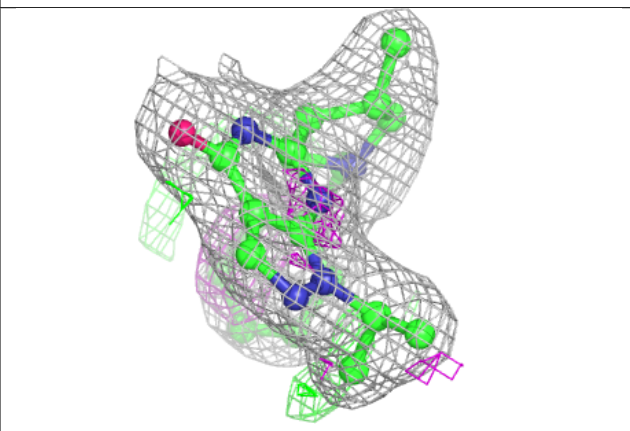
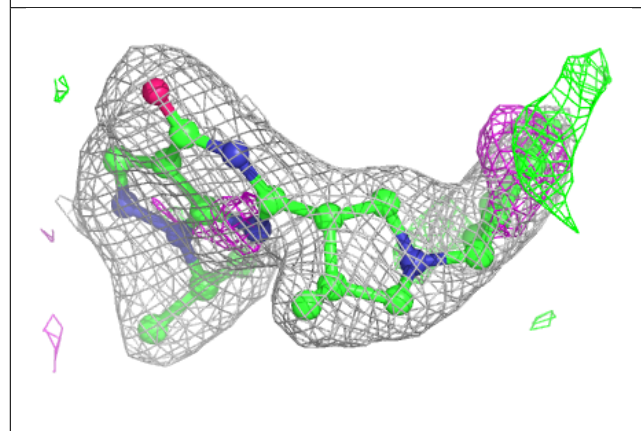
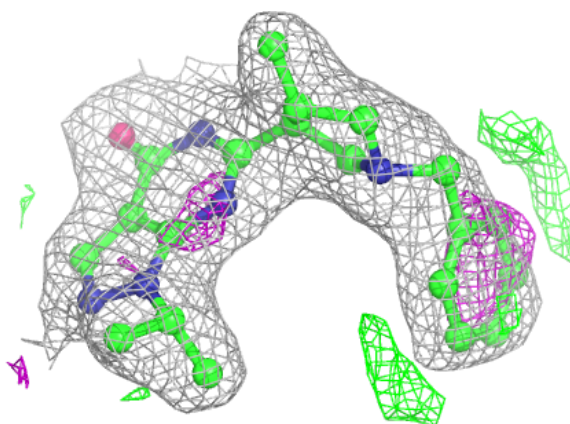
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	902	1/1	0.81	0.28	45,45,45,45	0
2	ZN	B	901	1/1	0.94	0.04	74,74,74,74	0
2	ZN	A	901	1/1	0.94	0.04	68,68,68,68	0
3	MG	B	902	1/1	0.94	0.17	40,40,40,40	0
4	JAR	A	900	26/26	0.95	0.12	33,35,54,55	0
4	JAR	B	900	26/26	0.96	0.09	41,44,54,55	0

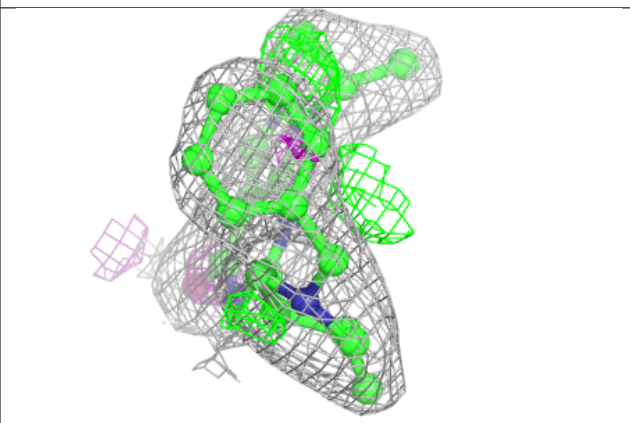
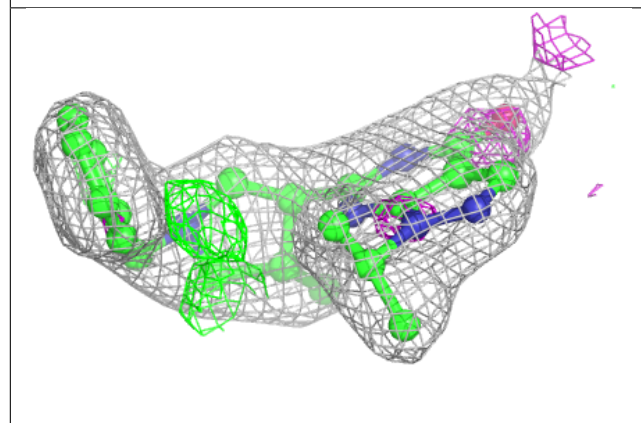
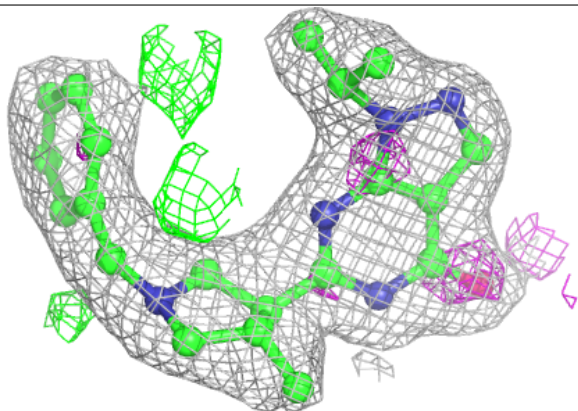
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JAR A 900:

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

**Electron density around JAR B 900:**

$2mF_o-DF_c$ (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.