Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2024 – 12:09 PM JST

PDB ID	:	8GOG
Title	:	Structure of streptavidin mutant (S112Y-K121E) complexed with biotin-cycl opentadienyl-rhodium (III)(Cp*-Rh(III))
Authors	:	Sairaman, A.; Mukherjee, P.; Maiti, D.; Bhaumik, P.
Deposited on	:	2022-08-24
Resolution	:	2.00 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:

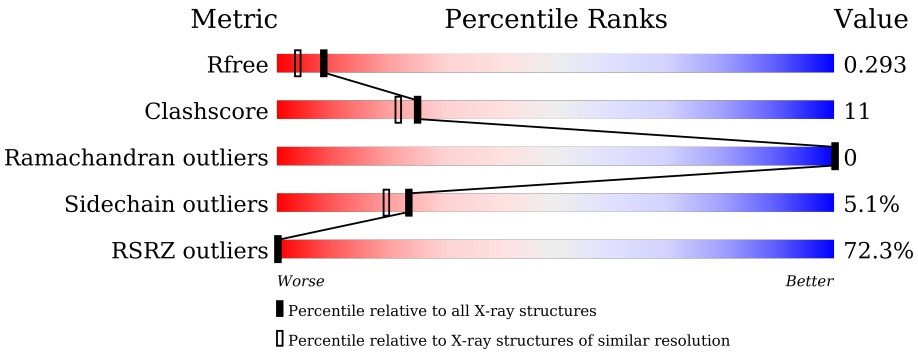
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	121	74% 84% 12% ·
1	B	121	70% 74% 24% ·

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
3	JSU	A	302[A]	-	-	-	X
3	JSU	A	302[B]	-	-	-	X
4	GOL	B	308	-	-	-	X
4	GOL	B	310	-	-	X	X
6	SO4	A	311	-	-	X	-
6	SO4	B	311	-	-	-	X
6	SO4	B	312	-	-	-	X
6	SO4	B	313	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 2064 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 Streptavidin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	121	Total 910	C 568	N 156	O 186	3	0	0
1	B	121	Total 917	C 572	N 157	O 188	0	1	0

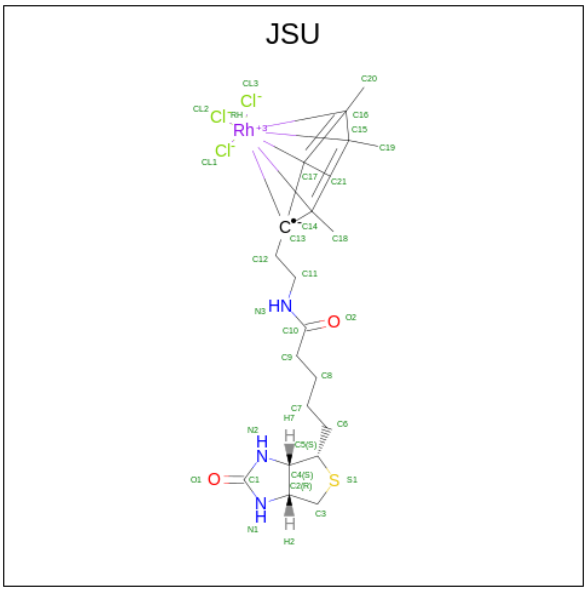
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	-	expression tag	UNP P22629
A	14	GLN	-	expression tag	UNP P22629
A	112	TYR	SER	engineered mutation	UNP P22629
A	121	GLU	LYS	engineered mutation	UNP P22629
B	13	ASP	-	expression tag	UNP P22629
B	14	GLN	-	expression tag	UNP P22629
B	112	TYR	SER	engineered mutation	UNP P22629
B	121	GLU	LYS	engineered mutation	UNP P22629

- Molecule 2 is RHODIUM(III) ION (three-letter code: RH3) (formula: Rh).

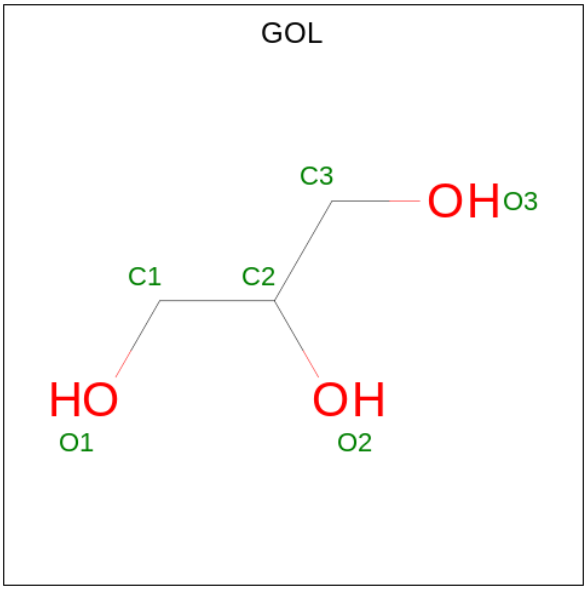
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Rh 2	0	0
2	B	2	Total 2	Rh 2	0	0

- Molecule 3 is trichloro((3 {a} {S},4 {S},6 {a} {R})-4-[(5 {R})-5-oxidanyl-5-[2-(2,3,4,5-tetramethylcyclopenta-2,4-dien-1-ylidene)ethylamino]pentyl]-1,3,3 {a},4,6,6 {a}-hexahydrothieno[3,4-d]imidazol-2-one)rhodium(3+) (three-letter code: JSU) (formula: $C_{21}H_{32}Cl_3N_3O_2RhS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	Rh	S	0	1
			42	32	2	3	2	2	1		
3	B	1	Total	C	Cl	N	O	Rh	S	0	1
			42	32	2	3	2	2	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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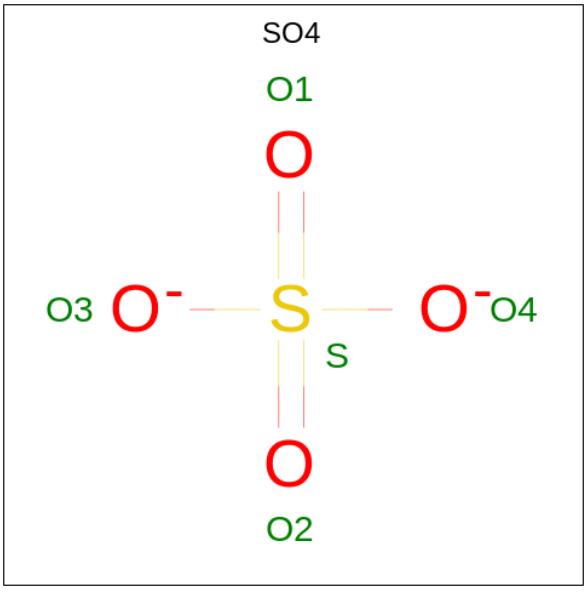
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

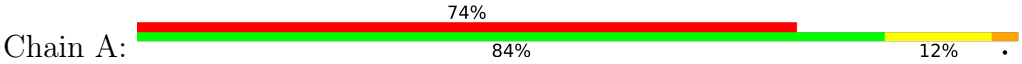
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	32	Total O 32 32	0	0
7	B	34	Total O 34 34	0	0

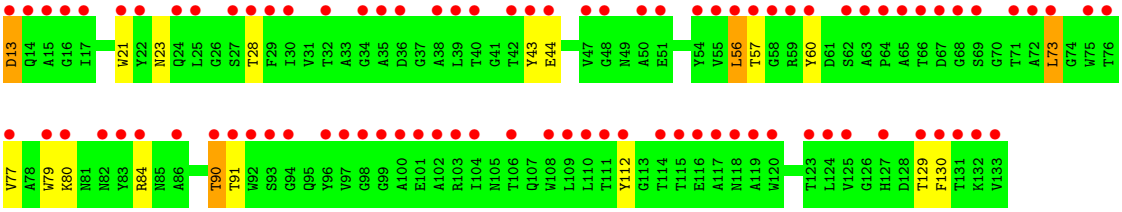
3 Residue-property plots (i)

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: Streptavidin

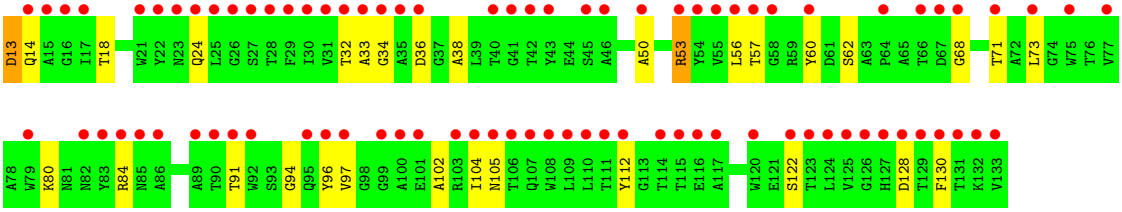
Chain A:





• Molecule 1: Streptavidin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	79.45Å 81.39Å 90.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 2.00 39.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.73-2.00) 98.7 (39.73-2.00)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	32.12 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.251 , 0.294 0.250 , 0.293	Depositor DCC
R_{free} test set	994 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2064	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 52.03 % 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 5.1534e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CL, SO4, RH3, JSU, GOL

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	0.49	0/933	0.77	1/1279 (0.1%)
1	B	0.54	0/940	0.75	0/1289
All	All	0.52	0/1873	0.76	1/2568 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	LEU	CA-CB-CG	5.37	127.66	115.30

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	910	0	837	18	0
1	B	917	0	843	23	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	42	0	0	2	0
3	B	42	0	0	2	0
4	A	18	0	24	2	0
4	B	36	0	48	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	10	0	0	2	0
6	B	15	0	0	4	0
7	A	32	0	0	0	0
7	B	34	0	0	0	0
All	All	2064	0	1752	40	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 11.

All (40) 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:80:LYS:NZ	6:B:313:SO4:S	2.53	0.82
1:B:80:LYS:NZ	6:B:313:SO4:O3	2.22	0.73
1:A:80:LYS:NZ	6:A:311:SO4:S	2.62	0.72
1:A:79:TRP:HE1	1:A:90:THR:HG23	1.55	0.70
1:A:44:GLU:HG2	4:A:304:GOL:H12	1.74	0.69
1:A:79:TRP:HE1	1:A:90:THR:CG2	2.09	0.66
1:A:112:TYR:CZ	3:A:302[B]:JSU:CL1	2.85	0.66
1:B:71[B]:THR:HG22	1:B:96:TYR:HB3	1.79	0.64
1:B:24:GLN:HE22	1:B:128:ASP:HA	1.65	0.61
1:B:104:ILE:HB	1:B:130:PHE:HB2	1.82	0.60
1:B:112:TYR:CE1	1:B:122:SER:HA	2.39	0.58
1:A:57:THR:HG21	4:B:310:GOL:H31	1.87	0.54
1:A:91:THR:HB	1:B:91:THR:HB	1.88	0.54
1:B:94:GLY:HA3	1:B:105:ASN:O	2.07	0.54
1:B:112:TYR:CZ	3:B:303[A]:JSU:CL1	3.00	0.52
1:B:38:ALA:HB1	4:B:310:GOL:H32	1.91	0.52
1:B:97:VAL:O	1:B:102:ALA:HA	2.12	0.49
1:B:57:THR:OG1	4:B:310:GOL:O3	2.23	0.49
1:A:23:ASN:HA	1:A:129:THR:O	2.13	0.49
1:A:28:THR:OG1	4:A:304:GOL:O1	2.26	0.47
1:A:21:TRP:HB3	1:A:130:PHE:HB3	1.97	0.46
1:B:14:GLN:HG3	1:B:33:ALA:O	2.15	0.46
1:B:112:TYR:CE1	3:B:303[A]:JSU:CL1	3.05	0.46
1:A:43:TYR:HB2	1:A:56:LEU:HD23	1.98	0.46
1:A:80:LYS:NZ	6:A:311:SO4:O3	2.49	0.45
1:A:112:TYR:OH	3:A:302[B]:JSU:CL1	2.72	0.45
1:B:68:GLY:HA2	6:B:312:SO4:O2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TYR:CB	1:A:73:LEU:HB3	2.48	0.44
1:B:50:ALA:N	1:B:84:ARG:HH11	2.16	0.44
1:B:57:THR:HG1	4:B:310:GOL:HO3	1.56	0.44
1:B:80:LYS:NZ	6:B:313:SO4:O2	2.51	0.43
1:A:79:TRP:NE1	1:A:90:THR:HG23	2.28	0.43
1:B:53:ARG:HE	1:B:53:ARG:HB3	1.56	0.43
1:B:34:GLY:O	1:B:60:TYR:OH	2.30	0.43
1:A:56:LEU:HB3	1:A:77:VAL:HG22	2.01	0.42
1:A:13:ASP:OD1	1:A:13:ASP:N	2.53	0.42
1:B:18:THR:HG23	1:B:32:THR:HA	2.00	0.42
1:B:56:LEU:HD12	1:B:56:LEU:C	2.41	0.41
1:B:13:ASP:OD1	1:B:13:ASP:N	2.54	0.40

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	A	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
1	B	120/121 (99%)	115 (96%)	5 (4%)	0	100	100
All	All	239/242 (99%)	229 (96%)	10 (4%)	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	89/89 (100%)	85 (96%)	4 (4%)	27 24
1	B	90/89 (101%)	85 (94%)	5 (6%)	21 17
All	All	179/178 (101%)	170 (95%)	9 (5%)	24 20

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	73	LEU
1	A	84	ARG
1	A	90	THR
1	B	13	ASP
1	B	36	ASP
1	B	53	ARG
1	B	62	SER
1	B	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	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)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	B	309	-	5,5,5	0.83	0	5,5,5	0.99	0
4	GOL	A	304	-	5,5,5	0.80	0	5,5,5	1.02	0
3	JSU	A	302[B]	-	20,35,37	3.98	9 (45%)	27,71,84	3.06	8 (29%)
4	GOL	B	308	-	5,5,5	1.17	0	5,5,5	0.82	0
4	GOL	B	310	-	5,5,5	1.25	0	5,5,5	0.75	0
6	SO4	A	311	-	4,4,4	0.50	0	6,6,6	0.07	0
4	GOL	B	305	-	5,5,5	0.83	0	5,5,5	0.97	0
3	JSU	B	303[A]	-	20,35,37	3.96	9 (45%)	27,71,84	2.28	13 (48%)
3	JSU	B	303[B]	-	20,35,37	4.01	10 (50%)	27,71,84	2.33	14 (51%)
6	SO4	B	312	-	4,4,4	0.14	0	6,6,6	0.11	0
4	GOL	B	306	-	5,5,5	0.87	0	5,5,5	0.87	0
4	GOL	B	307	-	5,5,5	0.91	0	5,5,5	0.94	0
6	SO4	B	313	-	4,4,4	0.19	0	6,6,6	0.20	0
4	GOL	A	309	-	5,5,5	0.82	0	5,5,5	1.06	0
6	SO4	A	310	-	4,4,4	0.15	0	6,6,6	0.15	0
6	SO4	B	311	-	4,4,4	0.14	0	6,6,6	0.09	0
4	GOL	A	308	-	5,5,5	0.89	0	5,5,5	1.03	0
3	JSU	A	302[A]	-	20,35,37	4.02	9 (45%)	27,71,84	3.20	9 (33%)

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	GOL	B	309	-	-	3/4/4/4	-
4	GOL	A	304	-	-	3/4/4/4	-
3	JSU	A	302[B]	-	-	2/11/140/170	0/8/7/7
4	GOL	B	308	-	-	2/4/4/4	-
4	GOL	B	310	-	-	3/4/4/4	-
4	GOL	B	305	-	-	2/4/4/4	-
3	JSU	B	303[A]	-	-	2/11/140/170	0/8/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JSU	B	303[B]	-	-	3/11/140/170	0/8/7/7
4	GOL	B	306	-	-	1/4/4/4	-
4	GOL	B	307	-	-	2/4/4/4	-
4	GOL	A	309	-	-	0/4/4/4	-
4	GOL	A	308	-	-	0/4/4/4	-
3	JSU	A	302[A]	-	-	3/11/140/170	0/8/7/7

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[A]	JSU	C2-N1	12.98	1.65	1.46
3	A	302[B]	JSU	C2-N1	12.98	1.65	1.46
3	B	303[A]	JSU	C2-N1	12.52	1.65	1.46
3	B	303[B]	JSU	C2-N1	12.52	1.65	1.46
3	B	303[A]	JSU	C1-N1	-7.10	1.23	1.35
3	B	303[B]	JSU	C1-N1	-7.10	1.23	1.35
3	A	302[A]	JSU	C1-N1	-6.96	1.23	1.35
3	A	302[B]	JSU	C1-N1	-6.96	1.23	1.35
3	B	303[A]	JSU	C4-N2	6.53	1.57	1.45
3	B	303[B]	JSU	C4-N2	6.53	1.57	1.45
3	A	302[A]	JSU	C4-N2	5.71	1.55	1.45
3	A	302[B]	JSU	C4-N2	5.71	1.55	1.45
3	A	302[A]	JSU	C3-C2	4.74	1.61	1.53
3	A	302[B]	JSU	C3-C2	4.74	1.61	1.53
3	B	303[A]	JSU	C3-C2	4.67	1.61	1.53
3	B	303[B]	JSU	C3-C2	4.67	1.61	1.53
3	B	303[B]	JSU	C11-N3	3.40	1.53	1.46
3	A	302[A]	JSU	O2-C10	3.32	1.30	1.23
3	A	302[B]	JSU	O2-C10	3.32	1.30	1.23
3	A	302[A]	JSU	C11-N3	3.22	1.53	1.46
3	A	302[A]	JSU	C9-C10	3.19	1.57	1.51
3	A	302[B]	JSU	C9-C10	3.19	1.57	1.51
3	B	303[A]	JSU	O2-C10	3.05	1.29	1.23
3	B	303[B]	JSU	O2-C10	3.05	1.29	1.23
3	A	302[A]	JSU	C8-C9	2.76	1.62	1.52
3	A	302[B]	JSU	C8-C9	2.76	1.62	1.52
3	B	303[A]	JSU	C8-C9	2.75	1.62	1.52
3	B	303[B]	JSU	C8-C9	2.75	1.62	1.52
3	B	303[A]	JSU	C5-C4	-2.67	1.47	1.53
3	B	303[B]	JSU	C5-C4	-2.67	1.47	1.53
3	B	303[A]	JSU	C9-C10	2.53	1.56	1.51
3	B	303[B]	JSU	C9-C10	2.53	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[A]	JSU	C10-N3	2.43	1.38	1.33
3	A	302[B]	JSU	C10-N3	2.43	1.38	1.33
3	A	302[B]	JSU	C11-N3	2.05	1.50	1.46
3	B	303[A]	JSU	C10-N3	2.05	1.38	1.33
3	B	303[B]	JSU	C10-N3	2.05	1.38	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302[A]	JSU	C5-C4-N2	-7.78	106.16	113.13
3	A	302[B]	JSU	C5-C4-N2	-7.78	106.16	113.13
3	A	302[A]	JSU	C3-C2-C4	-7.73	101.95	108.66
3	A	302[B]	JSU	C3-C2-C4	-7.73	101.95	108.66
3	A	302[A]	JSU	C11-N3-C10	-5.66	112.33	122.84
3	A	302[B]	JSU	C11-N3-C10	-5.59	112.46	122.84
3	B	303[A]	JSU	C11-N3-C10	-5.54	112.55	122.84
3	B	303[B]	JSU	C12-C11-N3	5.33	122.73	111.28
3	B	303[A]	JSU	C3-C2-C4	-4.81	104.48	108.66
3	B	303[B]	JSU	C3-C2-C4	-4.81	104.48	108.66
3	A	302[A]	JSU	C12-C11-N3	4.70	121.36	111.28
3	A	302[A]	JSU	C2-C4-N2	-4.27	98.08	102.67
3	A	302[B]	JSU	C2-C4-N2	-4.27	98.08	102.67
3	A	302[A]	JSU	C7-C6-C5	-3.94	105.86	113.86
3	A	302[B]	JSU	C7-C6-C5	-3.94	105.86	113.86
3	A	302[A]	JSU	N2-C1-N1	3.92	112.44	108.76
3	A	302[B]	JSU	N2-C1-N1	3.92	112.44	108.76
3	B	303[A]	JSU	C2-C4-N2	-3.90	98.48	102.67
3	B	303[B]	JSU	C2-C4-N2	-3.90	98.48	102.67
3	A	302[A]	JSU	C5-C4-C2	3.83	113.38	108.94
3	A	302[B]	JSU	C5-C4-C2	3.83	113.38	108.94
3	A	302[A]	JSU	C4-N2-C1	3.20	115.60	112.62
3	A	302[B]	JSU	C4-N2-C1	3.20	115.60	112.62
3	B	303[B]	JSU	C11-N3-C10	-2.91	117.43	122.84
3	B	303[A]	JSU	O1-C1-N1	-2.72	122.04	125.94
3	B	303[B]	JSU	O1-C1-N1	-2.72	122.04	125.94
3	B	303[A]	JSU	C7-C6-C5	-2.65	108.48	113.86
3	B	303[B]	JSU	C7-C6-C5	-2.65	108.48	113.86
3	B	303[A]	JSU	N2-C1-N1	2.57	111.17	108.76
3	B	303[B]	JSU	N2-C1-N1	2.57	111.17	108.76
3	B	303[A]	JSU	C5-C4-N2	-2.56	110.84	113.13
3	B	303[B]	JSU	C5-C4-N2	-2.56	110.84	113.13
3	B	303[A]	JSU	C6-C5-C4	-2.40	107.75	114.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	303[B]	JSU	C6-C5-C4	-2.40	107.75	114.73
3	B	303[A]	JSU	O2-C10-C9	-2.33	117.75	122.02
3	B	303[B]	JSU	O2-C10-C9	-2.33	117.75	122.02
3	B	303[A]	JSU	C8-C9-C10	-2.32	106.74	113.26
3	B	303[B]	JSU	C8-C9-C10	-2.32	106.74	113.26
3	B	303[A]	JSU	C5-C4-C2	2.17	111.46	108.94
3	B	303[B]	JSU	C5-C4-C2	2.17	111.46	108.94
3	B	303[A]	JSU	C4-N2-C1	2.16	114.64	112.62
3	B	303[B]	JSU	C4-N2-C1	2.16	114.64	112.62
3	B	303[A]	JSU	C7-C8-C9	-2.06	105.80	113.19
3	B	303[B]	JSU	C7-C8-C9	-2.06	105.80	113.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302[A]	JSU	S1-C5-C6-C7
3	A	302[A]	JSU	C4-C5-C6-C7
3	A	302[B]	JSU	S1-C5-C6-C7
3	A	302[B]	JSU	C4-C5-C6-C7
3	B	303[A]	JSU	S1-C5-C6-C7
3	B	303[B]	JSU	S1-C5-C6-C7
4	A	304	GOL	O1-C1-C2-C3
4	B	307	GOL	C1-C2-C3-O3
4	B	308	GOL	C1-C2-C3-O3
4	B	308	GOL	O2-C2-C3-O3
4	B	309	GOL	O1-C1-C2-C3
4	B	310	GOL	C1-C2-C3-O3
4	B	310	GOL	O2-C2-C3-O3
3	B	303[B]	JSU	C12-C11-N3-C10
4	B	307	GOL	O2-C2-C3-O3
4	B	309	GOL	O1-C1-C2-O2
4	B	305	GOL	O1-C1-C2-C3
3	A	302[A]	JSU	C12-C11-N3-C10
4	B	305	GOL	O1-C1-C2-O2
3	B	303[A]	JSU	C4-C5-C6-C7
3	B	303[B]	JSU	C4-C5-C6-C7
4	A	304	GOL	O1-C1-C2-O2
4	B	310	GOL	O1-C1-C2-O2
4	A	304	GOL	O2-C2-C3-O3
4	B	306	GOL	O1-C1-C2-C3
4	B	309	GOL	O2-C2-C3-O3

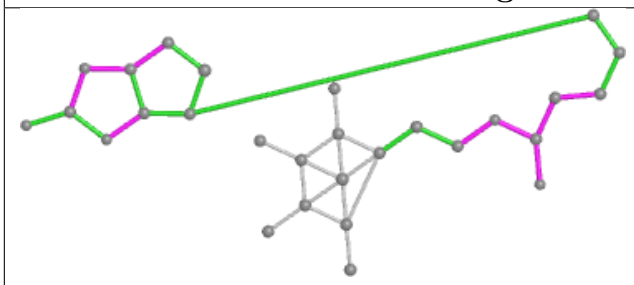
There are no ring outliers.

7 monomers are involved in 16 short contacts:

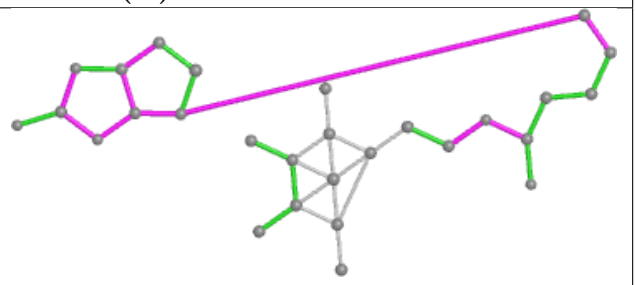
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	GOL	2	0
3	A	302[B]	JSU	2	0
4	B	310	GOL	4	0
6	A	311	SO4	2	0
3	B	303[A]	JSU	2	0
6	B	312	SO4	1	0
6	B	313	SO4	3	0

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.

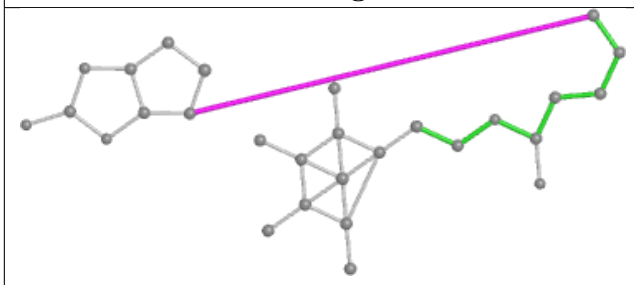
Ligand JSU A 302 (B)



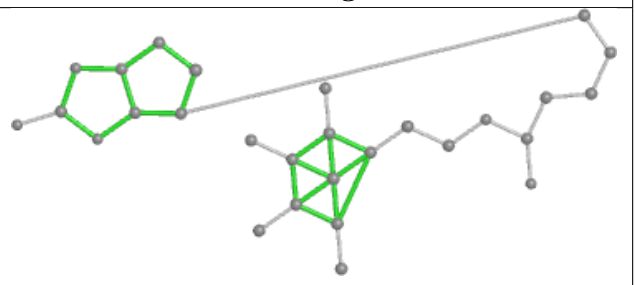
Bond lengths



Bond angles

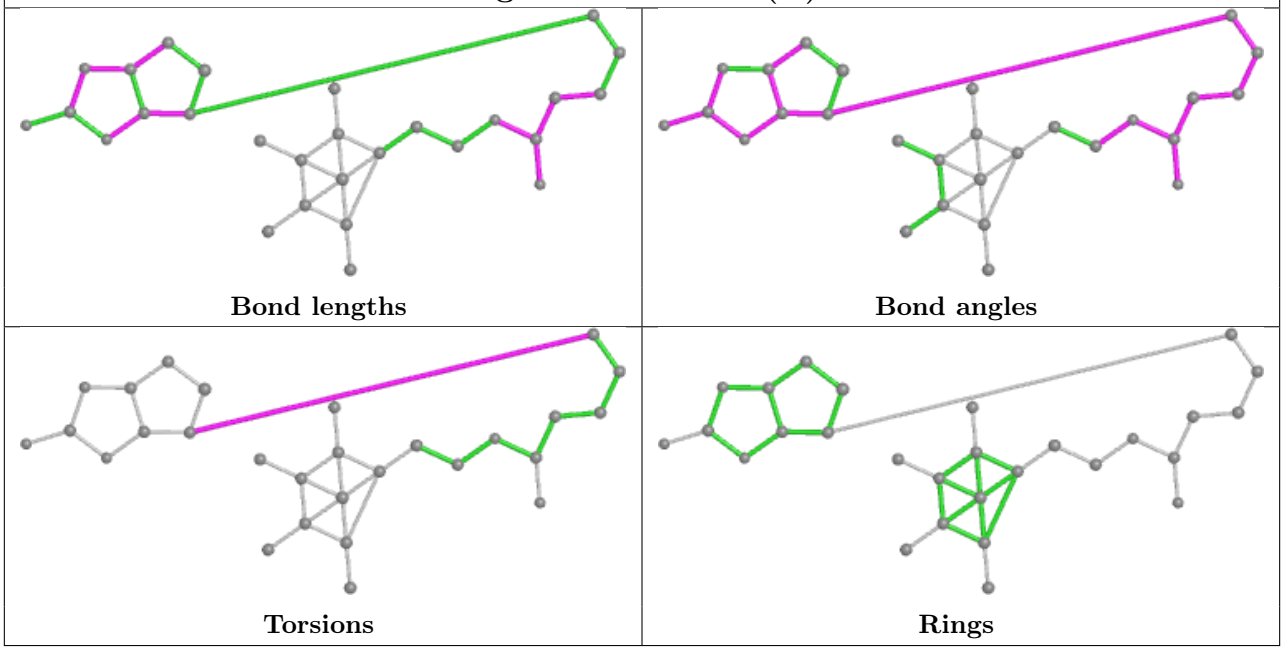


Torsions

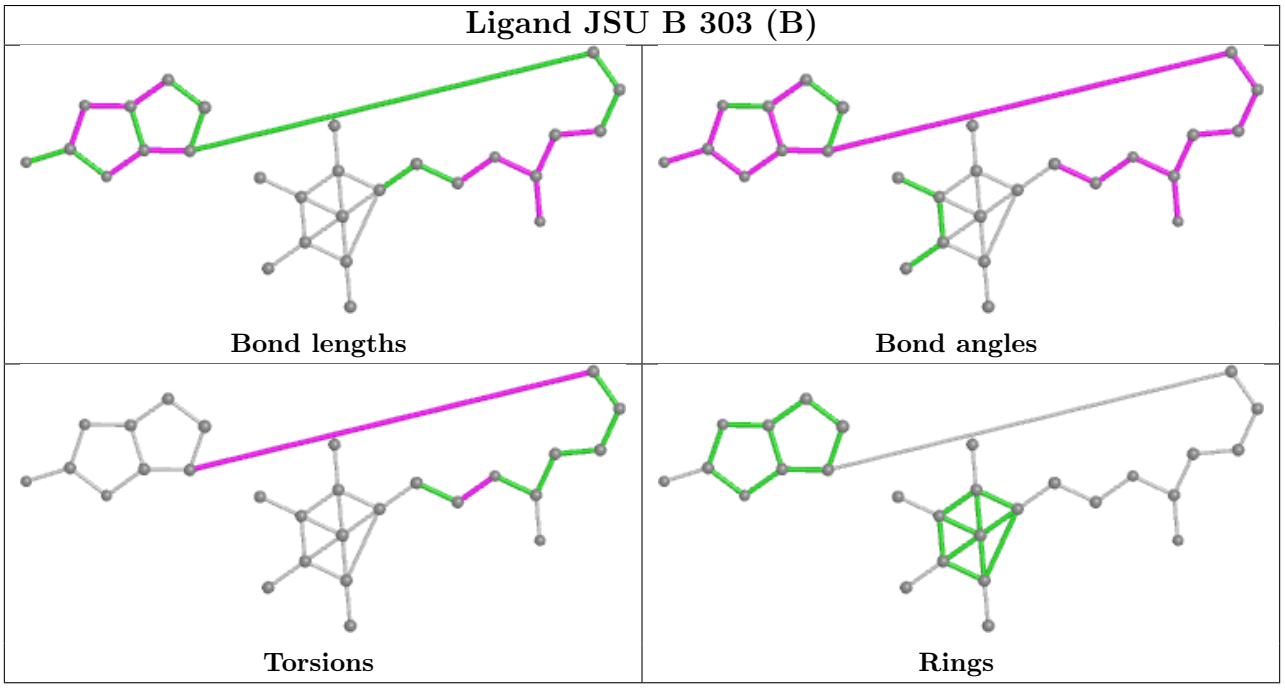


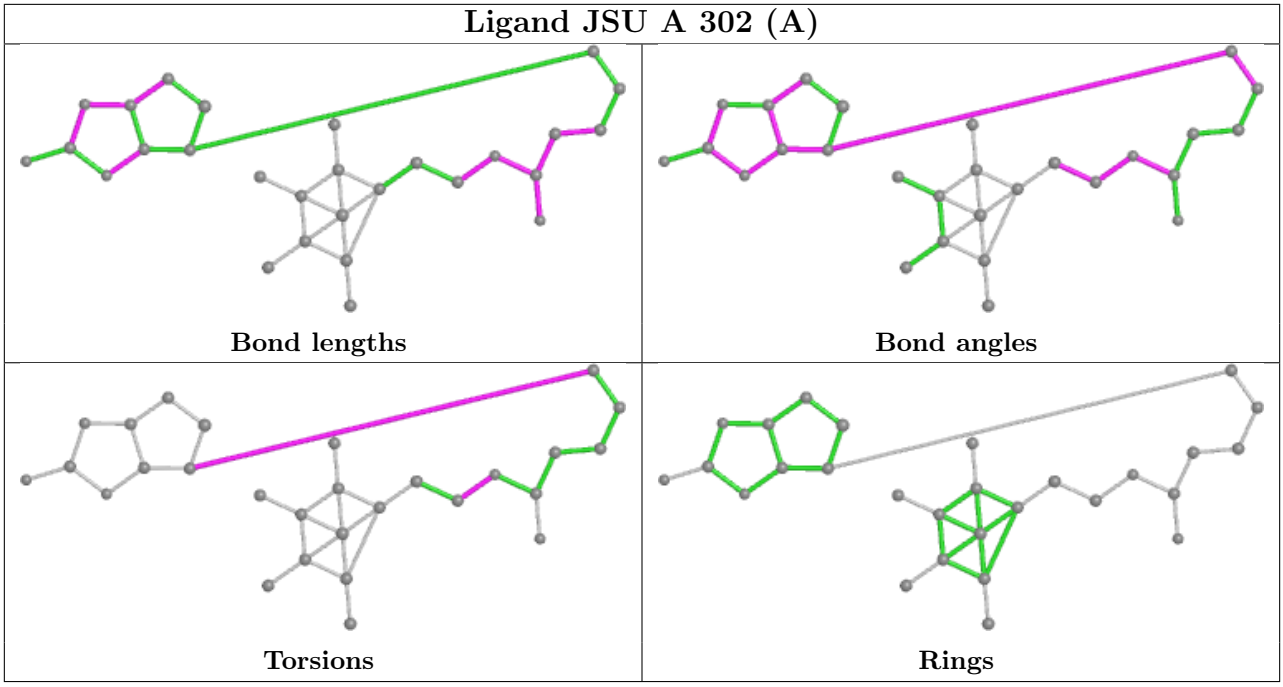
Rings

Ligand JSU B 303 (A)



Ligand JSU B 303 (B)





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	121/121 (100%)	2.98	90 (74%)	0	0	18, 28, 46, 57	1 (0%)
1	B	121/121 (100%)	2.90	85 (70%)	0	0	15, 29, 42, 51	0
All	All	242/242 (100%)	2.94	175 (72%)	0	0	15, 29, 45, 57	1 (0%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	ALA	11.7
1	A	15	ALA	10.1
1	A	66	THR	9.6
1	B	68	GLY	8.8
1	A	116	GLU	8.6
1	A	65	ALA	7.9
1	B	29	PHE	7.7
1	A	133	VAL	7.6
1	A	83	TYR	7.4
1	B	112	TYR	7.2
1	A	50	ALA	6.7
1	B	116	GLU	6.7
1	A	99	GLY	6.6
1	B	83	TYR	6.5
1	B	96	TYR	6.3
1	A	112	TYR	5.8
1	B	104	ILE	5.8
1	A	84	ARG	5.6
1	A	127	HIS	5.5
1	B	66	THR	5.4
1	A	67	ASP	5.3
1	A	120	TRP	5.3
1	A	117	ALA	5.2
1	B	16	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	47	VAL	4.7
1	A	60	TYR	4.6
1	B	14	GLN	4.5
1	A	36	ASP	4.4
1	A	38	ALA	4.3
1	B	117	ALA	4.3
1	B	133	VAL	4.3
1	A	68	GLY	4.3
1	A	130	PHE	4.3
1	B	100	ALA	4.3
1	B	106	THR	4.2
1	B	67	ASP	4.2
1	B	21	TRP	4.2
1	B	31	VAL	4.2
1	B	71[A]	THR	4.2
1	A	82	ASN	4.2
1	B	53	ARG	4.2
1	B	92	TRP	4.1
1	B	130	PHE	4.1
1	B	99	GLY	4.1
1	B	111	THR	4.1
1	B	25	LEU	4.0
1	B	115	THR	4.0
1	A	103	ARG	4.0
1	B	75	TRP	4.0
1	A	104	ILE	3.9
1	A	101	GLU	3.8
1	A	77	VAL	3.8
1	B	43	TYR	3.8
1	B	124	LEU	3.7
1	A	71	THR	3.7
1	B	97	VAL	3.6
1	B	103	ARG	3.6
1	B	129	THR	3.6
1	B	35	ALA	3.5
1	B	73	LEU	3.5
1	A	108	TRP	3.5
1	A	98	GLY	3.5
1	A	79	TRP	3.5
1	A	131	THR	3.4
1	B	54	TYR	3.4
1	B	55	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	77	VAL	3.4
1	B	90	THR	3.4
1	A	39	LEU	3.4
1	A	125	VAL	3.3
1	A	124	LEU	3.3
1	A	75	TRP	3.3
1	A	56	LEU	3.3
1	A	73	LEU	3.3
1	A	55	VAL	3.3
1	B	123	THR	3.2
1	B	33	ALA	3.2
1	A	21	TRP	3.2
1	A	34	GLY	3.2
1	A	63	ALA	3.1
1	B	28	THR	3.1
1	B	50	ALA	3.1
1	A	14	GLN	3.1
1	B	30	ILE	3.1
1	A	62	SER	3.1
1	A	91	THR	3.1
1	A	86	ALA	3.0
1	A	111	THR	3.0
1	B	110	LEU	3.0
1	A	43	TYR	3.0
1	B	84	ARG	3.0
1	B	26	GLY	3.0
1	B	36	ASP	3.0
1	A	17	ILE	2.9
1	A	28	THR	2.9
1	A	90	THR	2.9
1	A	115	THR	2.9
1	A	48	GLY	2.9
1	A	58	GLY	2.9
1	A	110	LEU	2.9
1	B	58	GLY	2.8
1	A	64	PRO	2.8
1	B	86	ALA	2.8
1	A	114	THR	2.8
1	B	91	THR	2.8
1	B	122	SER	2.8
1	A	96	TYR	2.8
1	A	32	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	102	ALA	2.7
1	A	40	THR	2.7
1	B	79	TRP	2.7
1	B	64	PRO	2.7
1	A	25	LEU	2.7
1	B	22	TYR	2.6
1	A	129	THR	2.6
1	A	97	VAL	2.6
1	A	100	ALA	2.6
1	B	57	THR	2.6
1	B	85	ASN	2.6
1	B	120	TRP	2.5
1	A	92	TRP	2.5
1	B	56	LEU	2.5
1	B	131	THR	2.5
1	A	118	ASN	2.5
1	B	108	TRP	2.5
1	A	123	THR	2.5
1	B	82	ASN	2.5
1	A	13	ASP	2.5
1	A	72	ALA	2.5
1	A	59	ARG	2.5
1	A	51	GLU	2.5
1	B	114	THR	2.4
1	B	24	GLN	2.4
1	B	125	VAL	2.4
1	A	27	SER	2.4
1	B	17	ILE	2.4
1	B	107	GLN	2.4
1	A	42	THR	2.4
1	A	76	THR	2.4
1	A	80	LYS	2.4
1	A	69	SER	2.4
1	B	126	GLY	2.4
1	A	24	GLN	2.4
1	A	22	TYR	2.3
1	A	119	ALA	2.3
1	B	46	ALA	2.3
1	B	128	ASP	2.3
1	B	27	SER	2.3
1	A	57	THR	2.3
1	A	29	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	40	THR	2.2
1	B	45	SER	2.2
1	B	132	LYS	2.2
1	B	23	ASN	2.2
1	A	106	THR	2.2
1	B	32	THR	2.2
1	B	101	GLU	2.2
1	B	105	ASN	2.1
1	B	95	GLN	2.1
1	A	30	ILE	2.1
1	B	109	LEU	2.1
1	A	16	GLY	2.1
1	A	35	ALA	2.1
1	B	34	GLY	2.1
1	B	89	ALA	2.1
1	A	93	SER	2.1
1	B	42	THR	2.1
1	A	132	LYS	2.1
1	B	41	GLY	2.0
1	B	60	TYR	2.0
1	B	127	HIS	2.0
1	A	44	GLU	2.0
1	A	94	GLY	2.0
1	A	54	TYR	2.0
1	A	109	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)

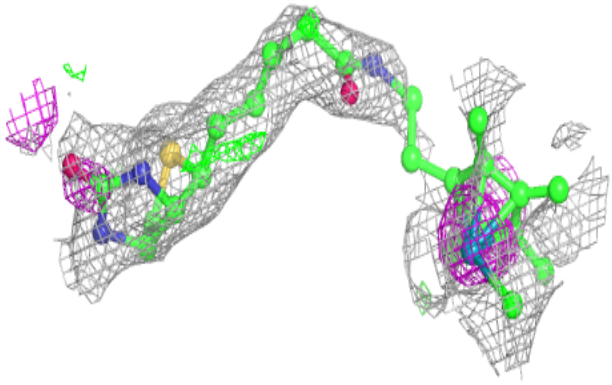
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

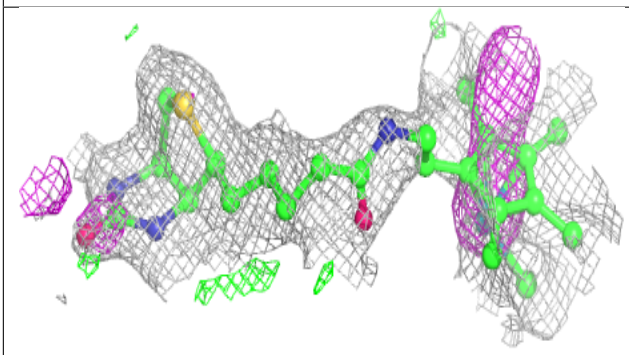
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	308	6/6	0.22	0.41	50,56,60,64	0
6	SO4	A	310	5/5	0.31	0.29	82,85,93,93	0
6	SO4	B	311	5/5	0.31	0.84	64,65,72,77	2
4	GOL	B	310	6/6	0.45	1.01	31,39,41,42	0
4	GOL	A	308	6/6	0.53	0.21	53,54,58,62	0
4	GOL	A	309	6/6	0.56	0.21	67,71,73,76	0
4	GOL	B	305	6/6	0.59	0.39	52,56,59,64	0
3	JSU	B	303[B]	29/31	0.61	0.39	27,36,58,74	13
3	JSU	A	302[A]	29/31	0.61	0.42	28,39,57,77	13
5	CL	A	307	1/1	0.61	0.18	76,76,76,76	0
3	JSU	A	302[B]	29/31	0.61	0.42	28,39,57,59	13
3	JSU	B	303[A]	29/31	0.61	0.39	27,36,57,62	13
4	GOL	B	309	6/6	0.62	0.25	48,51,52,52	0
6	SO4	B	312	5/5	0.64	0.71	68,72,81,82	0
6	SO4	A	311	5/5	0.65	0.24	50,54,65,69	0
6	SO4	B	313	5/5	0.66	0.27	47,50,57,58	0
4	GOL	B	307	6/6	0.70	0.33	61,64,66,67	0
4	GOL	B	306	6/6	0.73	0.32	42,50,52,64	0
5	CL	A	305	1/1	0.81	0.26	67,67,67,67	0
2	RH3	A	303	1/1	0.83	0.12	71,71,71,71	0
2	RH3	A	301	1/1	0.83	0.12	92,92,92,92	0
4	GOL	A	304	6/6	0.86	0.24	35,40,46,54	0
5	CL	B	304	1/1	0.90	0.31	77,77,77,77	0
5	CL	A	306	1/1	0.94	0.14	63,63,63,63	0
2	RH3	B	301	1/1	0.95	0.15	77,77,77,77	0
2	RH3	B	302	1/1	0.96	0.14	66,66,66,66	0

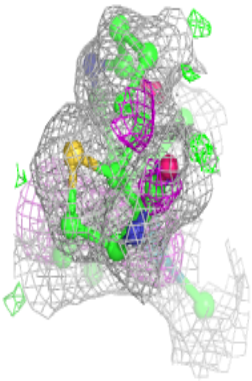
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JSU B 303 (B):

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

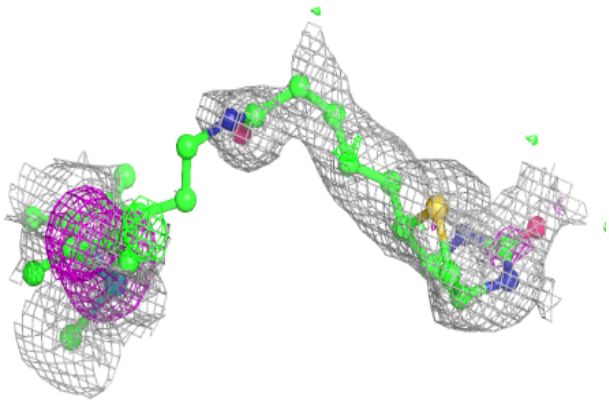


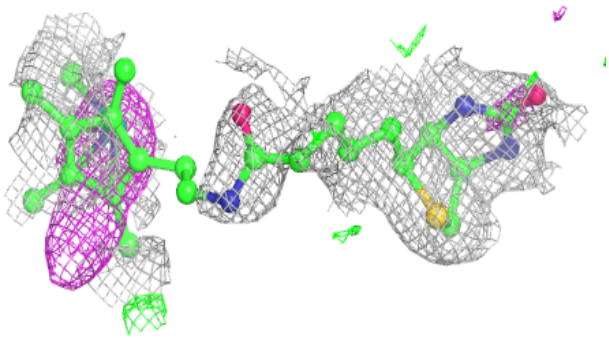


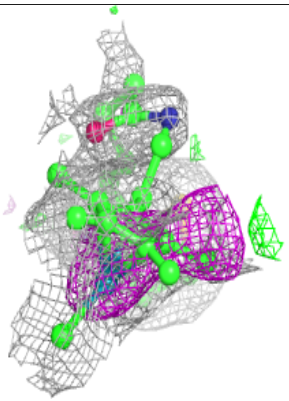


Electron density around JSU A 302 (A):

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

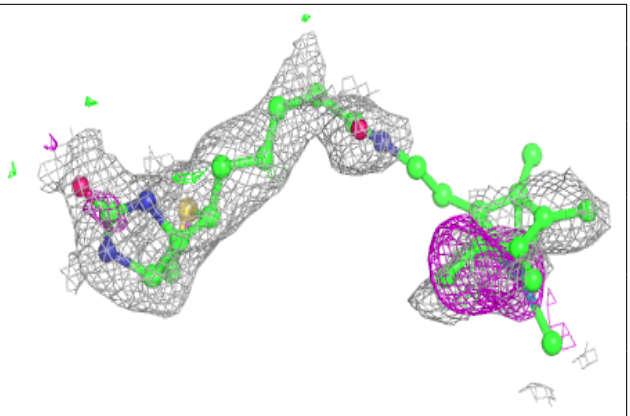


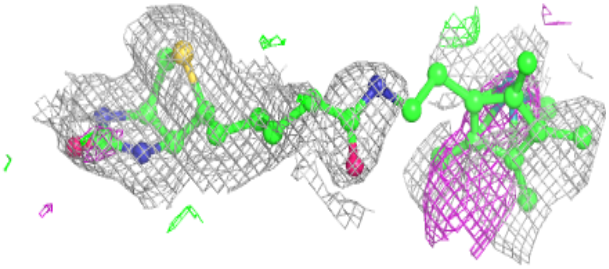


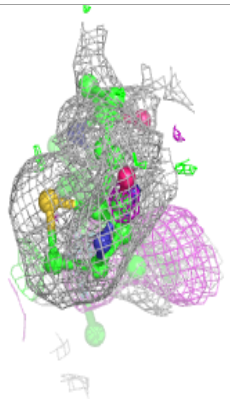


Electron density around JSU A 302 (B):

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

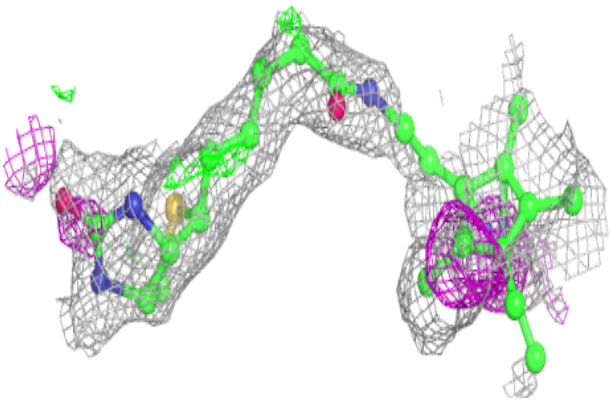


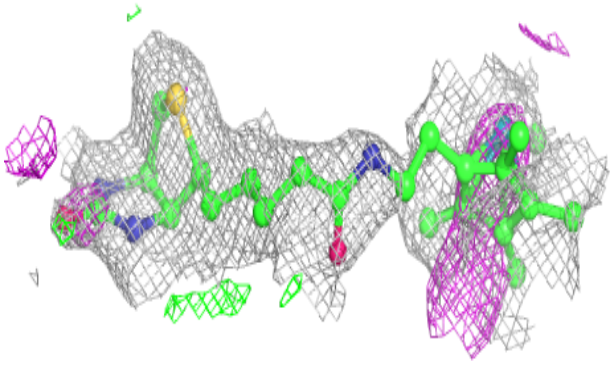


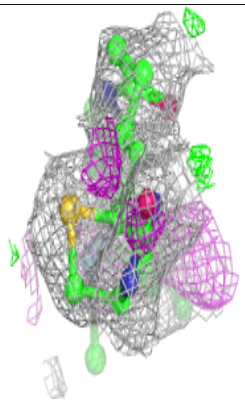


Electron density around JSU B 303 (A):

$2mF_o$-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.