



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:52 AM UTC

PDB ID : 6QS9 / pdb_00006qs9
Title : Bovine Serum Albumin in complex with Ketoprofen
Authors : Donini, S.; Parisini, E.
Deposited on : 2019-02-20
Resolution : 2.80 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 ⓘ 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

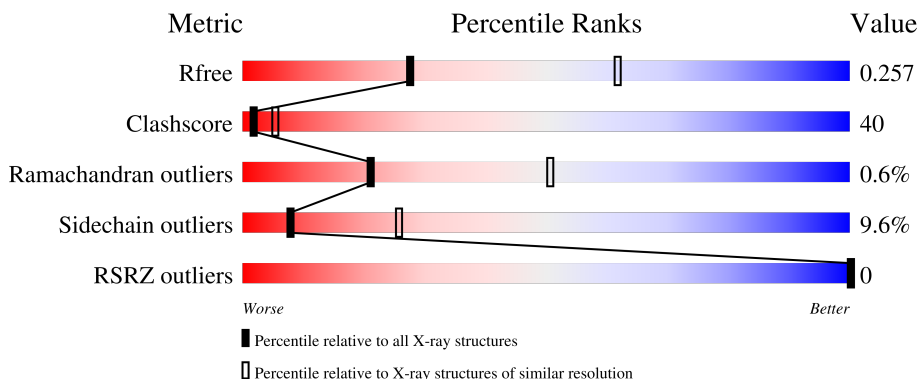
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

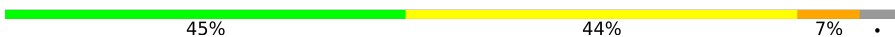
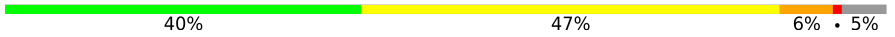
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	607	
1	B	607	

2 Entry composition [i](#)

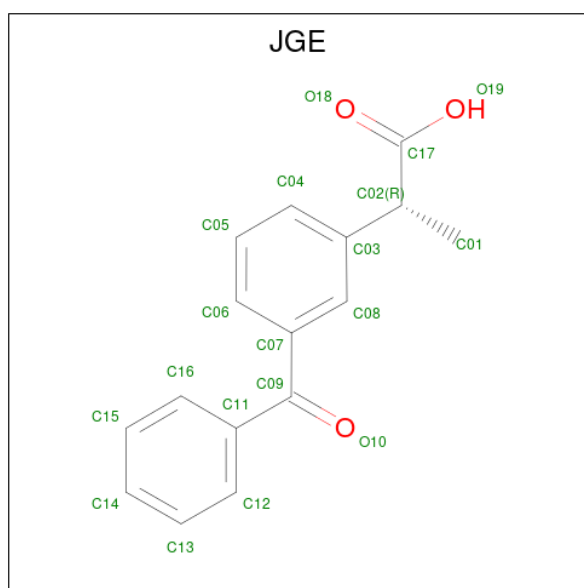
There are 4 unique types of molecules in this entry. The entry contains 9371 atoms, of which 26 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4626	2920	776	891	39			
1	B	576	Total	C	N	O	S	0	0	0
			4600	2905	773	883	39			

- Molecule 2 is (R)-Ketoprofen (CCD ID: JGE) (formula: $C_{16}H_{14}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			32	16	13	3		
2	B	1	Total	C	H	O	0	0
			32	16	13	3		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	B	2	Total 2	Ca 2	0	0

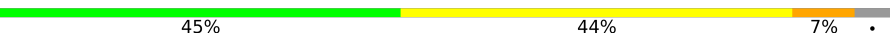
- Molecule 4 is water.

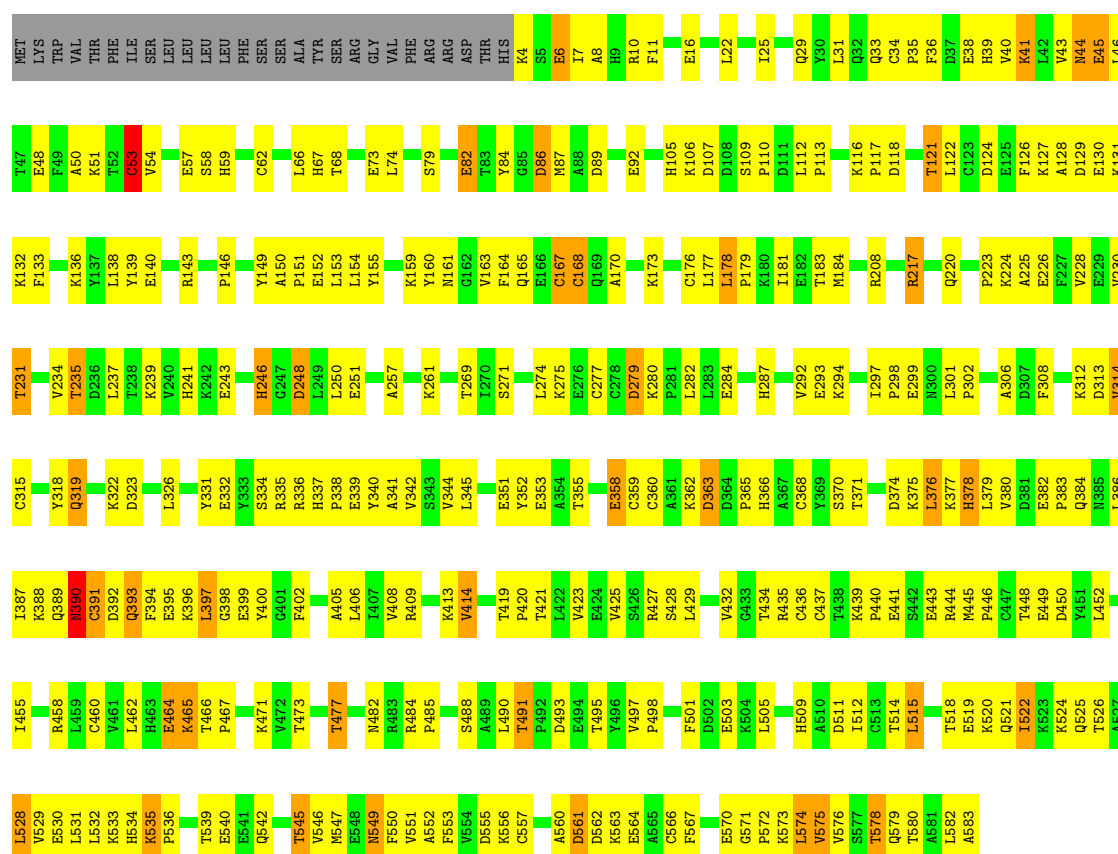
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total 46	O 46	0	0
4	B	31	Total 31	O 31	0	0

3 Residue-property plots

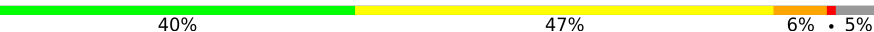
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

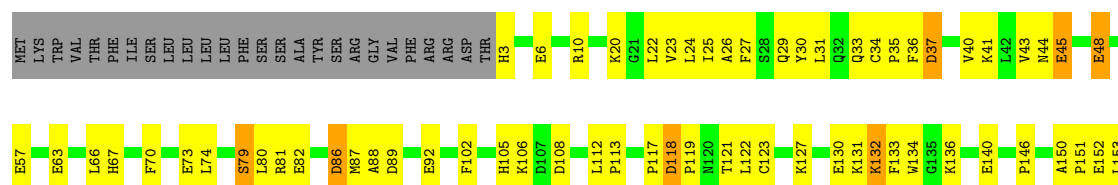
• Molecule 1: Serum albumin

Chain A: 



• Molecule 1: Serum albumin

Chain B: 



Q521	L452	K388	Y318	T231	L154
K524	L456	Q389	Q319	K232	Y156
Q525	L457	N390	K322	L233	A157
L528	R458	Q393	D323	V234	N158
V529	L459	F394	G327	T235	K159
E530	G460	E395	S328	D236	Y160
L531	V461	K396	F329	K239	V163
L532	L462	L397	L330	E243	F164
K533	H463	G398	Y331	C244	Q165
H534	H464	E399	E332	C245	E166
K535	K465	Y400	Y333	H246	C167
P536	T466	G401	S334	G247	C168
T539	P467	F402	R335	L248	Q169
E540	K471	Q403	R336	L249	A170
E541	V472	N404	A405	Y262	E171
Q542	T473	L406	E339	L269	D172
L543	K474	I407	Y340	T270	L177
K544	T477	V408	A341	L271	L178
T545	E478	R409	V342	S271	P179
V546	S479	Y410	S343	L274	K180
M547	L480	T411	V344	K275	T183
E548	L481	R412	L345	E276	A190
K549	M482	K413	L348	C277	S191
F550	R483	P415	A349	C278	S192
V551	R484	Q416	Y352	D279	Q195
A552	P485	V417	L356	K280	R196
F553	P485	S418	E357	P281	L197
V554	A489	T419	Q1U	L282	I202
D555	L490	P420	C359	L283	F205
K556	P491	T421	C360	E284	R208
C557	P492	L422	A361	H287	A209
C558	D493	V423	LYS	V292	L210
ALA	V497	E424	D363	E293	K211
ASP	P498	S426	D364	A296	A212
D562	F501	S428	H366	I297	A213
K563	D602	V432	Y369	P298	S214
E564	E503	Q433	S370	E299	V215
A565	K504	T434	F373	K300	A216
G566	L505	R435	D374	L301	R217
F567	F506	C436	K375	L304	L218
A568	T507	T438	L376	T305	S219
V569	F508	K439	K377	F308	Q220
E570	H509	P440	H378	A309	K221
G571	A510	E441	L379	E310	F222
P572	D511	S442	V380	D311	P223
K573	I512	E443	R444	K312	K224
L574	C513	R444	M445	E382	
V575	T514	M445	P446	P383	
V576	T515	P446	G447	Q384	
V577	L515	T448	E449	N385	
S577	T518	L582		K316	
T578	P516			V314	
T579	D517			C315	
T580	T518			N317	
A581	E519				
L582	K520				
A583					

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.49Å 44.37Å 142.72Å 90.00° 113.24° 90.00°	Depositor
Resolution (Å)	46.59 – 2.80 46.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.59-2.80) 99.2 (46.59-2.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.215 , 0.272 (Not available) , 0.257	Depositor DCC
R_{free} test set	1526 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9371	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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

5.1 Standard geometry

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

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	0.69	2/4720 (0.0%)	1.03	13/6371 (0.2%)
1	B	0.65	0/4692	1.02	20/6329 (0.3%)
All	All	0.67	2/9412 (0.0%)	1.03	33/12700 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	CYS	CB-SG	5.17	1.98	1.81
1	A	62	CYS	CB-SG	5.15	1.98	1.81

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	CYS	N-CA-C	-8.58	102.80	113.18
1	A	390	ASN	N-CA-C	7.54	122.90	112.04
1	B	118	ASP	CA-C-N	7.39	128.04	119.47
1	B	118	ASP	C-N-CA	7.39	128.04	119.47
1	B	489	ALA	CA-C-N	-6.95	110.18	122.07

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	4626	0	4542	323	0
1	B	4600	0	4513	405	0
2	A	19	13	0	2	0
2	B	19	13	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	46	0	0	21	0
4	B	31	0	0	14	0
All	All	9345	26	9055	728	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 40.

The worst 5 of 728 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:314:VAL:HG21	1:B:369:TYR:CZ	1.32	1.58
1:B:314:VAL:CG2	1:B:369:TYR:CZ	1.92	1.48
1:B:314:VAL:CG2	1:B:369:TYR:CE2	2.00	1.45
1:A:400:TYR:CE1	4:A:701:HOH:O	1.84	1.27
1:A:400:TYR:HE1	4:A:701:HOH:O	1.10	1.26

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	578/607 (95%)	550 (95%)	24 (4%)	4 (1%)	18 47
1	B	568/607 (94%)	541 (95%)	24 (4%)	3 (0%)	24 55
All	All	1146/1214 (94%)	1091 (95%)	48 (4%)	7 (1%)	21 51

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	SER
1	B	299	GLU
1	A	377	LYS
1	A	562	ASP
1	B	167	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/542 (95%)	469 (91%)	48 (9%)	8	27
1	B	515/542 (95%)	464 (90%)	51 (10%)	7	24
All	All	1032/1084 (95%)	933 (90%)	99 (10%)	8	26

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	132	LYS
1	B	343	SER
1	B	177	LEU
1	B	275	LYS
1	B	384	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	GLN
1	B	67	HIS
1	B	169	GLN
1	B	161	ASN
1	A	385	ASN

5.3.3 RNA ⓘ

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 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	$\# Z > 2$
2	JGE	A	601	-	20,20,20	1.25	3 (15%)	27,27,27	1.22	3 (11%)
2	JGE	B	601	-	20,20,20	1.11	3 (15%)	27,27,27	0.96	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
2	JGE	A	601	-	-	2/16/16/16	0/2/2/2
2	JGE	B	601	-	-	2/16/16/16	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JGE	C07-C09	3.09	1.54	1.49
2	A	601	JGE	C11-C09	2.67	1.53	1.49
2	B	601	JGE	O10-C09	-2.65	1.18	1.22
2	B	601	JGE	C07-C09	2.36	1.53	1.49
2	B	601	JGE	C11-C09	2.19	1.53	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	JGE	O19-C17-O18	-3.17	116.89	124.08
2	A	601	JGE	C06-C07-C09	2.14	125.25	120.55
2	A	601	JGE	O10-C09-C11	-2.06	116.85	120.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

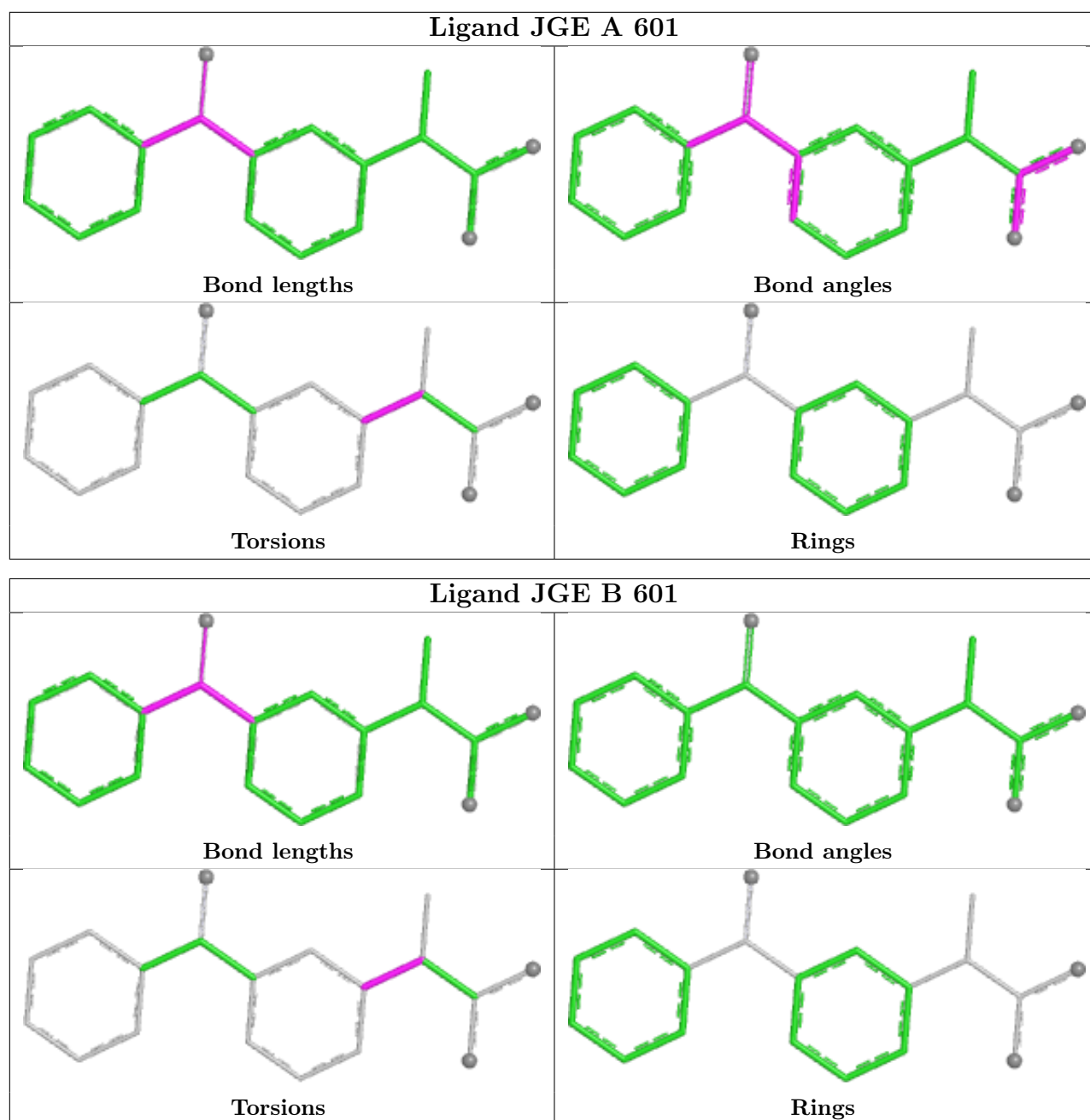
Mol	Chain	Res	Type	Atoms
2	A	601	JGE	C17-C02-C03-C04
2	B	601	JGE	C17-C02-C03-C04
2	B	601	JGE	C17-C02-C03-C08
2	A	601	JGE	C17-C02-C03-C08

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	JGE	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 [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	A	580/607 (95%)	-0.63	0 100 100	30, 60, 111, 125	0
1	B	576/607 (94%)	-0.53	0 100 100	27, 69, 116, 142	0
All	All	1156/1214 (95%)	-0.58	0 100 100	27, 64, 112, 142	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

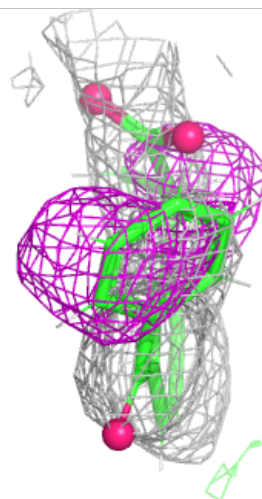
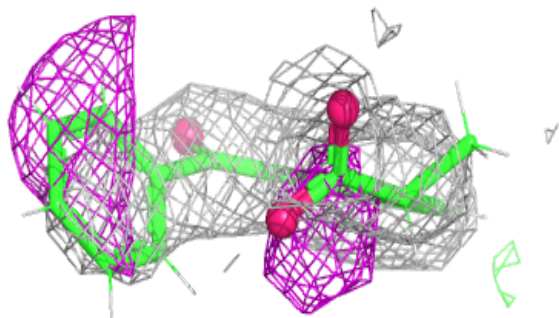
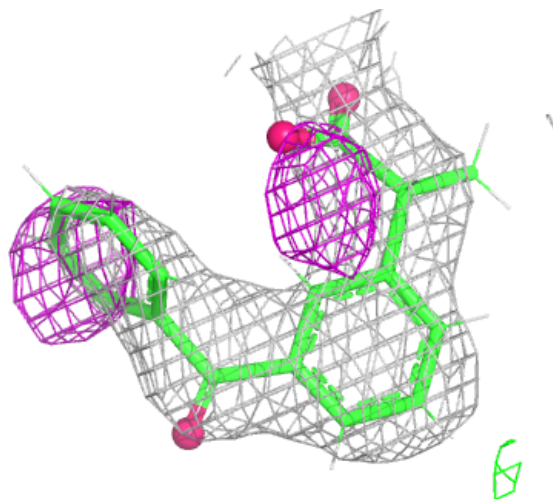
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	A	603	1/1	0.75	0.11	91,91,91,91	0
2	JGE	A	601	19/19	0.82	0.09	44,54,65,66	0
2	JGE	B	601	19/19	0.86	0.09	46,55,67,75	0
3	CA	B	603	1/1	0.89	0.07	76,76,76,76	0
3	CA	B	602	1/1	0.96	0.05	65,65,65,65	0
3	CA	A	602	1/1	0.96	0.03	67,67,67,67	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.

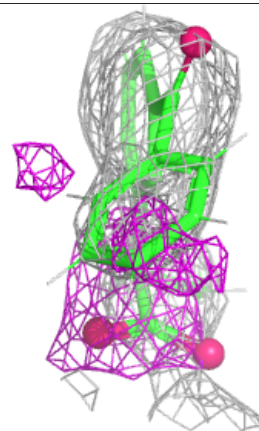
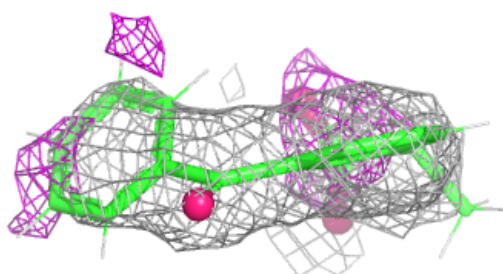
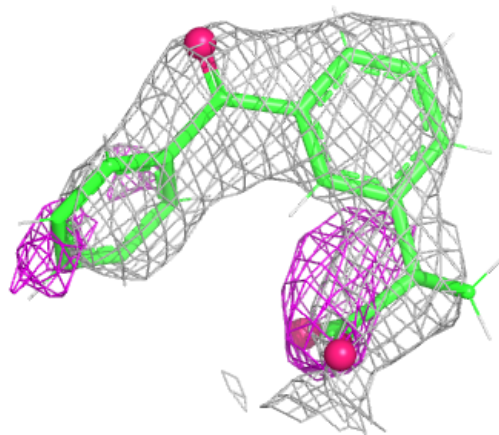
Electron density around JGE A 601:

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



Electron density around JGE B 601:

$2mF_o-DF_c$ (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.