



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:12 AM UTC

PDB ID : 6R27 / pdb_00006r27
Title : Crystallographic superstructure of the photosensory core module (PAS-GAF-PHY) of the bacterial phytochrome Agp1 (AtBphP1) locked in a Pr-like state
Authors : Scheerer, P.; Michael, N.; Lamparter, T.; Krauss, N.
Deposited on : 2019-03-15
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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

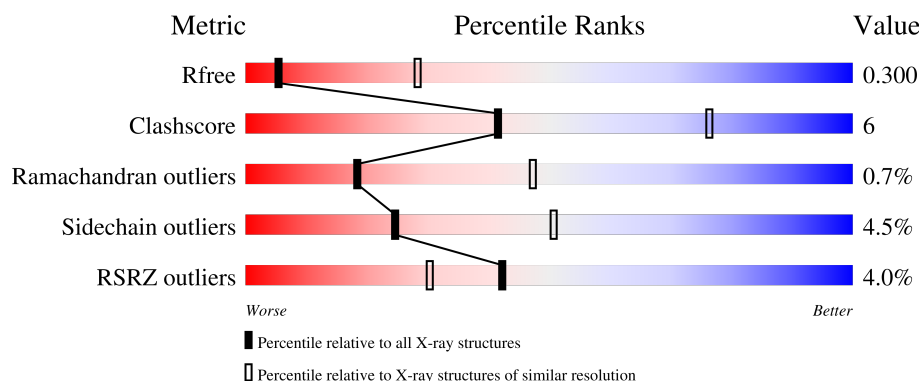
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

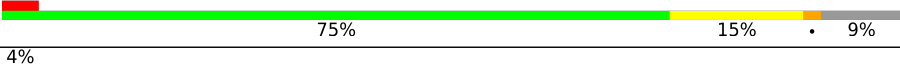
The reported resolution of this entry is 3.40 Å.

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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	510	
1	B	510	
1	C	510	
1	D	510	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14122 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 Bacteriophytochrome protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	Se	0	0	0
			3559	2252	623	671	3	10			
1	B	466	Total	C	N	O	S	Se	0	0	0
			3462	2195	605	649	3	10			
1	C	475	Total	C	N	O	S	Se	0	0	0
			3547	2242	620	672	3	10			
1	D	463	Total	C	N	O	S	Se	0	0	0
			3378	2138	581	647	3	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q7CY45
A	2	GLN	-	expression tag	UNP Q7CY45
A	3	ARG	-	expression tag	UNP Q7CY45
A	4	GLU	-	expression tag	UNP Q7CY45
A	5	ARG	-	expression tag	UNP Q7CY45
A	6	LEU	-	expression tag	UNP Q7CY45
A	7	GLU	-	expression tag	UNP Q7CY45
A	8	LYS	-	expression tag	UNP Q7CY45
A	9	VAL	-	expression tag	UNP Q7CY45
A	10	MSE	-	expression tag	UNP Q7CY45
A	505	HIS	-	expression tag	UNP Q7CY45
A	506	HIS	-	expression tag	UNP Q7CY45
A	507	HIS	-	expression tag	UNP Q7CY45
A	508	HIS	-	expression tag	UNP Q7CY45
A	509	HIS	-	expression tag	UNP Q7CY45
A	510	HIS	-	expression tag	UNP Q7CY45
B	1	MSE	-	initiating methionine	UNP Q7CY45
B	2	GLN	-	expression tag	UNP Q7CY45
B	3	ARG	-	expression tag	UNP Q7CY45
B	4	GLU	-	expression tag	UNP Q7CY45
B	5	ARG	-	expression tag	UNP Q7CY45

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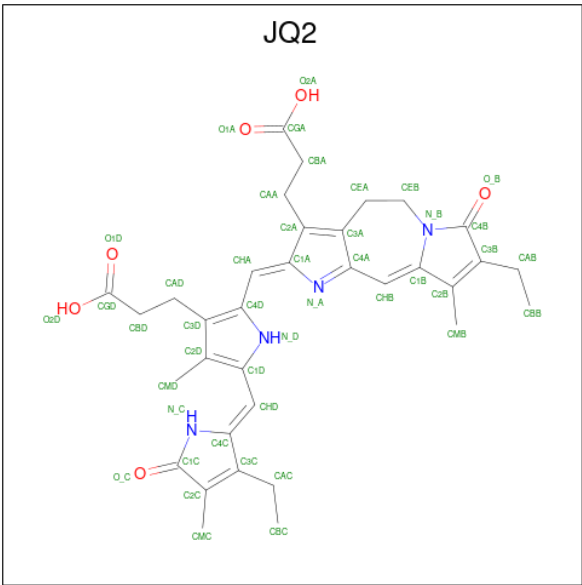
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	LEU	-	expression tag	UNP Q7CY45
B	7	GLU	-	expression tag	UNP Q7CY45
B	8	LYS	-	expression tag	UNP Q7CY45
B	9	VAL	-	expression tag	UNP Q7CY45
B	10	MSE	-	expression tag	UNP Q7CY45
B	505	HIS	-	expression tag	UNP Q7CY45
B	506	HIS	-	expression tag	UNP Q7CY45
B	507	HIS	-	expression tag	UNP Q7CY45
B	508	HIS	-	expression tag	UNP Q7CY45
B	509	HIS	-	expression tag	UNP Q7CY45
B	510	HIS	-	expression tag	UNP Q7CY45
C	1	MSE	-	initiating methionine	UNP Q7CY45
C	2	GLN	-	expression tag	UNP Q7CY45
C	3	ARG	-	expression tag	UNP Q7CY45
C	4	GLU	-	expression tag	UNP Q7CY45
C	5	ARG	-	expression tag	UNP Q7CY45
C	6	LEU	-	expression tag	UNP Q7CY45
C	7	GLU	-	expression tag	UNP Q7CY45
C	8	LYS	-	expression tag	UNP Q7CY45
C	9	VAL	-	expression tag	UNP Q7CY45
C	10	MSE	-	expression tag	UNP Q7CY45
C	505	HIS	-	expression tag	UNP Q7CY45
C	506	HIS	-	expression tag	UNP Q7CY45
C	507	HIS	-	expression tag	UNP Q7CY45
C	508	HIS	-	expression tag	UNP Q7CY45
C	509	HIS	-	expression tag	UNP Q7CY45
C	510	HIS	-	expression tag	UNP Q7CY45
D	1	MSE	-	initiating methionine	UNP Q7CY45
D	2	GLN	-	expression tag	UNP Q7CY45
D	3	ARG	-	expression tag	UNP Q7CY45
D	4	GLU	-	expression tag	UNP Q7CY45
D	5	ARG	-	expression tag	UNP Q7CY45
D	6	LEU	-	expression tag	UNP Q7CY45
D	7	GLU	-	expression tag	UNP Q7CY45
D	8	LYS	-	expression tag	UNP Q7CY45
D	9	VAL	-	expression tag	UNP Q7CY45
D	10	MSE	-	expression tag	UNP Q7CY45
D	505	HIS	-	expression tag	UNP Q7CY45
D	506	HIS	-	expression tag	UNP Q7CY45
D	507	HIS	-	expression tag	UNP Q7CY45
D	508	HIS	-	expression tag	UNP Q7CY45
D	509	HIS	-	expression tag	UNP Q7CY45

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Chain	Residue	Modelled	Actual	Comment	Reference
D	510	HIS	-	expression tag	UNP Q7CY45

- Molecule 2 is 3-[2-[({Z})-[12-ethyl-6-(3-hydroxy-3-oxopropyl)-13-methyl-11-oxidanylidene-4,10-diazatricyclo[8.3.0.0[^]{3,7}]trideca-1,3,6,12-tetraen-5-ylidene)methyl]-5-[({Z})-(3-ethyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-4-methyl-1 {H}-pyrrol-3-yl]propanoic acid (CCD ID: JQ2) (formula: C₃₄H₃₈N₄O₆) (labeled as "Ligand of Interest" by depositor).

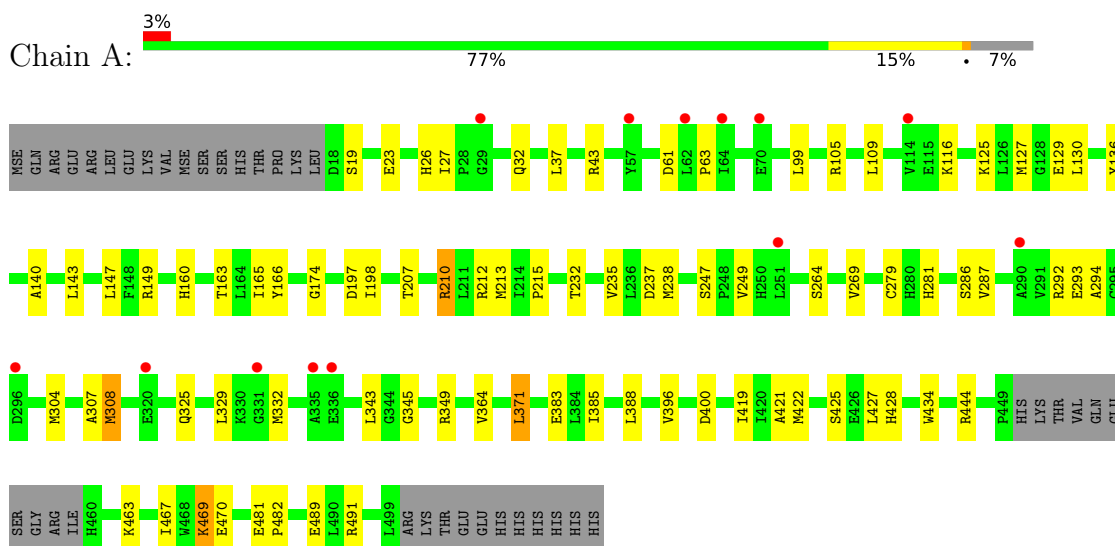


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	34	4	6		
2	B	1	Total	C	N	O	0	0
			44	34	4	6		
2	C	1	Total	C	N	O	0	0
			44	34	4	6		
2	D	1	Total	C	N	O	0	0
			44	34	4	6		

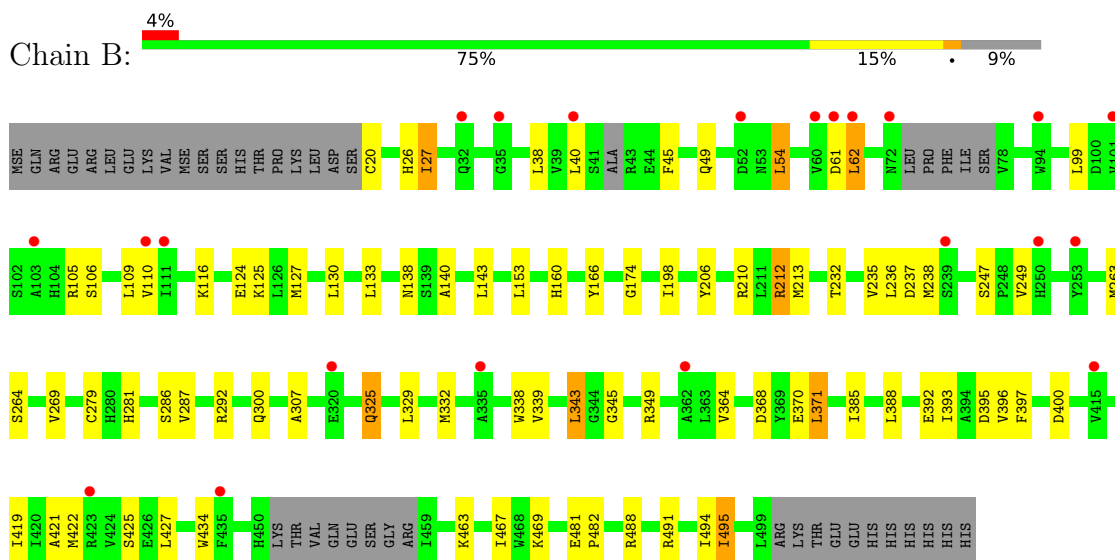
3 Residue-property plots [i](#)

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.

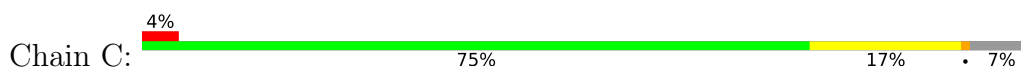
• Molecule 1: Bacteriophytochrome protein



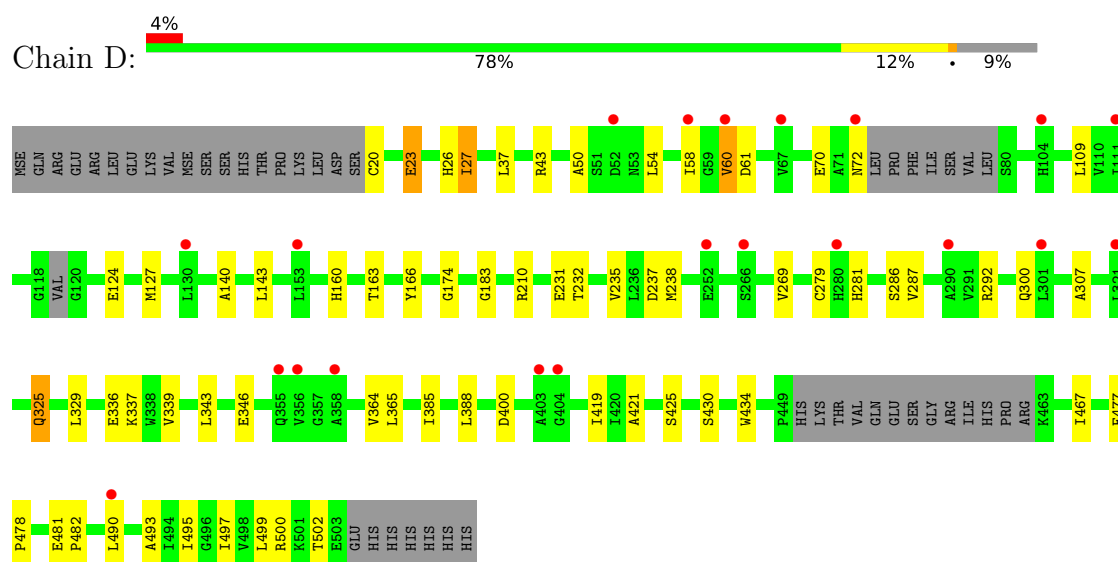
• Molecule 1: Bacteriophytochrome protein



• Molecule 1: Bacteriophytochrome protein



- Molecule 1: Bacteriophytochrome protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	240.22Å 240.22Å 160.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.89 – 3.40 47.89 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.89-3.40) 96.4 (47.89-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.255 , 0.297 0.257 , 0.300	Depositor DCC
R_{free} test set	1578 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14122	wwPDB-VP
Average B, all atoms (Å ²)	87.0	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 46.40 % 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 1.1516e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: JQ2

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	1.00	0/3626	1.49	4/4918 (0.1%)
1	B	1.01	0/3526	1.48	2/4786 (0.0%)
1	C	1.02	0/3613	1.49	8/4901 (0.2%)
1	D	1.03	0/3438	1.49	3/4676 (0.1%)
All	All	1.01	0/14203	1.49	17/19281 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	GLU	CB-CA-C	6.21	116.95	109.31
1	B	263	MSE	CG-SE-CE	5.65	111.35	98.92
1	C	213	MSE	CG-SE-CE	5.64	111.32	98.92
1	A	19	SER	CA-C-N	5.49	127.90	120.65
1	A	19	SER	C-N-CA	5.49	127.90	120.65
1	C	495	ILE	CA-C-N	5.35	125.89	120.00
1	C	495	ILE	C-N-CA	5.35	125.89	120.00
1	B	213	MSE	CG-SE-CE	5.35	110.69	98.92
1	A	308	MSE	CG-SE-CE	5.24	110.45	98.92
1	C	19	SER	CA-C-N	5.16	127.14	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	SER	C-N-CA	5.16	127.14	120.44
1	C	346	GLU	CA-C-N	5.13	125.64	120.00
1	C	346	GLU	C-N-CA	5.13	125.64	120.00
1	A	213	MSE	CG-SE-CE	5.10	110.14	98.92
1	D	346	GLU	CA-C-N	5.05	125.56	120.00
1	D	346	GLU	C-N-CA	5.05	125.56	120.00
1	C	308	MSE	CG-SE-CE	5.03	109.98	98.92

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	427	LEU	Peptide
1	D	60	VAL	Peptide

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	3559	0	3480	42	0
1	B	3462	0	3333	49	0
1	C	3547	0	3414	60	0
1	D	3378	0	3177	37	0
2	A	44	0	0	1	0
2	B	44	0	0	1	0
2	C	44	0	0	1	0
2	D	44	0	0	0	0
All	All	14122	0	13404	175	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 6.

All (175) 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:C:343:LEU:HD11	1:C:363:LEU:HD23	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:HG22	1:B:343:LEU:HD11	1.61	0.82
1:C:332:MSE:SE	1:C:494:ILE:CD1	2.78	0.81
1:B:287:VAL:O	1:B:292:ARG:NH1	2.18	0.77
1:A:287:VAL:O	1:A:292:ARG:NH1	2.17	0.77
1:C:287:VAL:O	1:C:292:ARG:NH1	2.18	0.76
1:D:287:VAL:O	1:D:292:ARG:NH1	2.19	0.76
1:A:329:LEU:HD23	1:A:332:MSE:HE3	1.68	0.75
1:B:329:LEU:HD23	1:B:332:MSE:HE3	1.69	0.73
1:B:395:ASP:OD2	1:B:488:ARG:NH1	2.23	0.72
1:C:495:ILE:HG22	1:D:495:ILE:HG22	1.71	0.71
1:C:332:MSE:SE	1:C:494:ILE:HD13	2.42	0.68
1:B:106:SER:O	1:B:109:LEU:HD13	1.94	0.68
1:C:48:VAL:HG11	1:C:229:ASN:ND2	2.10	0.67
1:B:40:LEU:HB2	1:B:110:VAL:CG1	2.25	0.67
1:C:141:PRO:HD2	1:C:305:ARG:HE	1.59	0.66
1:C:329:LEU:HD21	1:C:493:ALA:HB1	1.78	0.65
1:C:371:LEU:CD2	1:C:371:LEU:N	2.59	0.65
1:B:345:GLY:O	1:B:349:ARG:HG3	1.98	0.64
1:C:343:LEU:CD1	1:C:363:LEU:HD23	2.25	0.63
1:B:210:ARG:HH21	1:B:300:GLN:HE21	1.47	0.62
1:A:396:VAL:HG12	1:A:422:MSE:HG3	1.81	0.62
1:A:247:SER:OG	1:A:249:VAL:HG12	2.00	0.62
1:B:40:LEU:HB2	1:B:110:VAL:HG12	1.82	0.62
1:B:247:SER:OG	1:B:249:VAL:HG12	2.00	0.61
1:C:64:ILE:HD13	1:C:226:PRO:HD3	1.81	0.61
1:C:422:MSE:HE3	1:C:491:ARG:HA	1.83	0.61
1:C:130:LEU:HD11	1:C:294:ALA:HB1	1.83	0.60
1:C:332:MSE:SE	1:C:494:ILE:HD12	2.51	0.60
1:B:396:VAL:HG12	1:B:422:MSE:HG3	1.83	0.59
1:C:365:LEU:HD23	1:C:430:SER:OG	2.02	0.59
1:C:64:ILE:CD1	1:C:226:PRO:HD3	2.33	0.59
1:A:130:LEU:HD11	1:A:294:ALA:HB1	1.83	0.59
1:A:304:MSE:HG3	1:B:138:ASN:HD21	1.69	0.58
1:C:342:LEU:HB2	1:C:343:LEU:HD12	1.84	0.58
1:A:269:VAL:HG13	1:A:307:ALA:HB2	1.87	0.57
1:A:166:TYR:CZ	1:A:174:GLY:HA3	2.40	0.56
1:B:160:HIS:CG	1:B:279:CYS:HB3	2.40	0.56
1:C:160:HIS:CG	1:C:279:CYS:HB3	2.41	0.56
1:D:210:ARG:HH21	1:D:300:GLN:HE21	1.51	0.56
1:B:166:TYR:CZ	1:B:174:GLY:HA3	2.39	0.56
1:B:419:ILE:HA	1:B:434:TRP:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:TYR:CZ	1:C:174:GLY:HA3	2.40	0.56
1:D:419:ILE:HA	1:D:434:TRP:O	2.05	0.56
1:A:419:ILE:HA	1:A:434:TRP:O	2.05	0.56
1:D:166:TYR:CZ	1:D:174:GLY:HA3	2.39	0.56
1:D:329:LEU:HD21	1:D:493:ALA:HB1	1.88	0.56
1:D:160:HIS:CG	1:D:279:CYS:HB3	2.41	0.56
1:A:160:HIS:CG	1:A:279:CYS:HB3	2.41	0.56
1:A:371:LEU:HD23	1:A:371:LEU:N	2.21	0.55
1:C:419:ILE:HA	1:C:434:TRP:O	2.06	0.55
1:A:444:ARG:NH1	1:D:183:GLY:O	2.36	0.55
1:B:425:SER:OG	1:B:427:LEU:O	2.15	0.55
1:C:339:VAL:HG21	1:C:365:LEU:HD11	1.89	0.55
1:A:427:LEU:HD13	1:A:428:HIS:O	2.06	0.55
1:B:106:SER:O	1:B:109:LEU:CD1	2.56	0.54
1:C:371:LEU:N	1:C:371:LEU:HD23	2.21	0.54
1:A:130:LEU:HD12	1:B:127:MSE:HE1	1.90	0.54
1:B:371:LEU:N	1:B:371:LEU:HD23	2.22	0.54
1:A:127:MSE:HE1	1:B:130:LEU:CD1	2.37	0.54
1:B:206:TYR:OH	2:B:601:JQ2:O1D	2.17	0.54
1:B:49:GLN:OE1	1:B:236:LEU:HB2	2.08	0.54
1:B:232:THR:O	1:C:200:PRO:HG2	2.08	0.54
1:A:425:SER:OG	1:A:427:LEU:O	2.17	0.53
1:B:109:LEU:HD11	1:B:232:THR:HG21	1.89	0.53
1:A:304:MSE:HG3	1:B:138:ASN:ND2	2.24	0.53
1:B:364:VAL:HG21	1:B:385:ILE:CD1	2.38	0.52
1:C:364:VAL:HG21	1:C:385:ILE:CD1	2.40	0.52
1:D:339:VAL:HG11	1:D:365:LEU:HD11	1.92	0.52
1:D:425:SER:HB3	1:D:430:SER:OG	2.09	0.52
1:B:269:VAL:HG13	1:B:307:ALA:HB2	1.93	0.51
1:A:212:ARG:HD2	1:A:264:SER:HB2	1.92	0.51
1:D:60:VAL:HG13	1:D:60:VAL:O	2.10	0.51
1:B:212:ARG:HD2	1:B:264:SER:HB2	1.92	0.51
1:B:38:LEU:HB2	1:B:54:LEU:CD1	2.41	0.50
1:C:48:VAL:O	1:C:64:ILE:HD12	2.11	0.50
1:B:393:ILE:HG12	1:B:397:PHE:HB2	1.92	0.50
1:A:364:VAL:HG21	1:A:385:ILE:CD1	2.42	0.50
1:C:58:ILE:HD12	1:C:94:TRP:HZ3	1.77	0.50
1:D:364:VAL:HG21	1:D:385:ILE:CD1	2.42	0.50
1:D:109:LEU:HD11	1:D:232:THR:HG21	1.92	0.50
1:C:263:MSE:HE1	1:C:295:CYS:SG	2.52	0.49
1:C:269:VAL:HG22	1:C:274:TRP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ARG:HD2	1:C:264:SER:HB2	1.94	0.49
1:B:422:MSE:HG2	1:B:491:ARG:HD2	1.96	0.48
1:D:497:ILE:HG12	1:D:500:ARG:NH2	2.29	0.48
1:B:343:LEU:HD22	1:B:370:GLU:HB3	1.96	0.48
1:C:332:MSE:HE1	1:C:494:ILE:HD13	1.96	0.48
1:C:127:MSE:HA	1:D:127:MSE:HE1	1.95	0.47
1:B:388:LEU:HD13	1:B:421:ALA:HB1	1.97	0.47
1:C:499:LEU:HD13	1:D:499:LEU:CD1	2.45	0.47
1:D:481:GLU:N	1:D:482:PRO:CD	2.78	0.47
1:B:364:VAL:HG21	1:B:385:ILE:HD11	1.97	0.47
1:C:58:ILE:HD12	1:C:94:TRP:CZ3	2.49	0.47
1:A:345:GLY:O	1:A:349:ARG:HG2	2.15	0.46
1:B:343:LEU:HA	1:B:349:ARG:HG2	1.97	0.46
1:A:481:GLU:N	1:A:482:PRO:CD	2.79	0.46
1:B:110:VAL:O	1:B:110:VAL:HG13	2.15	0.46
1:C:343:LEU:CD2	1:C:370:GLU:HB3	2.45	0.46
1:C:495:ILE:HG23	1:D:499:LEU:HD22	1.98	0.46
1:A:325:GLN:OE1	1:A:489:GLU:HB3	2.16	0.46
1:D:497:ILE:HG12	1:D:500:ARG:HH22	1.81	0.46
1:C:137:LEU:O	1:C:305:ARG:HD3	2.16	0.45
1:C:481:GLU:N	1:C:482:PRO:CD	2.79	0.45
1:A:388:LEU:HD13	1:A:421:ALA:HB1	1.99	0.45
1:B:61:ASP:O	1:B:62:LEU:C	2.59	0.45
1:B:481:GLU:N	1:B:482:PRO:CD	2.79	0.45
1:A:207:THR:O	1:A:210:ARG:NH1	2.48	0.45
1:A:325:GLN:O	1:A:329:LEU:HG	2.17	0.44
1:B:329:LEU:HD23	1:B:332:MSE:CE	2.44	0.44
1:A:109:LEU:HD11	1:A:232:THR:HG21	2.00	0.44
1:A:364:VAL:HG21	1:A:385:ILE:HD11	2.00	0.44
1:A:160:HIS:HA	1:A:281:HIS:HD2	1.82	0.44
1:D:388:LEU:HD13	1:D:421:ALA:HB1	2.00	0.44
1:B:133:LEU:HD22	1:B:153:LEU:HD13	2.00	0.44
1:D:61:ASP:CB	1:D:72:ASN:HA	2.48	0.43
1:A:197:ASP:HA	2:A:601:JQ2:O_C	2.16	0.43
1:C:371:LEU:HD12	1:C:375:THR:OG1	2.18	0.43
1:C:499:LEU:HD13	1:D:499:LEU:HD12	2.00	0.43
1:C:364:VAL:HG21	1:C:385:ILE:HD11	2.00	0.43
1:C:388:LEU:HD13	1:C:421:ALA:HB1	2.00	0.43
1:D:269:VAL:HG13	1:D:307:ALA:HB2	2.00	0.43
1:B:325:GLN:O	1:B:329:LEU:HG	2.18	0.43
1:C:391:ARG:NE	1:C:397:PHE:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:HIS:HA	1:B:281:HIS:HD2	1.83	0.43
1:C:136:TYR:CD2	1:C:149:ARG:HG2	2.53	0.43
1:C:424:VAL:CG2	1:C:430:SER:OG	2.67	0.43
1:D:26:HIS:CD2	1:D:27:ILE:HG23	2.53	0.43
1:D:477:PHE:CD1	1:D:478:PRO:HD2	2.54	0.43
1:D:237:ASP:C	1:D:237:ASP:OD1	2.62	0.43
1:D:364:VAL:HG21	1:D:385:ILE:HD11	2.01	0.43
1:B:425:SER:HA	1:B:495:ILE:HG13	2.01	0.43
1:C:237:ASP:OD1	1:C:237:ASP:C	2.62	0.42
1:B:26:HIS:CD2	1:B:27:ILE:HG23	2.54	0.42
1:D:58:ILE:HG13	1:D:60:VAL:H	1.84	0.42
1:A:422:MSE:CG	1:A:491:ARG:HD2	2.49	0.42
1:A:37:LEU:HD13	1:A:238:MSE:HE3	2.00	0.42
1:B:237:ASP:OD1	1:B:237:ASP:C	2.61	0.42
1:C:339:VAL:HG21	1:C:365:LEU:CD1	2.50	0.42
1:D:160:HIS:HA	1:D:281:HIS:HD2	1.84	0.42
1:C:26:HIS:CD2	1:C:27:ILE:HG23	2.55	0.42
1:A:237:ASP:OD1	1:A:237:ASP:C	2.62	0.42
1:A:136:TYR:CD2	1:A:149:ARG:HG2	2.54	0.42
1:C:250:HIS:CE1	2:C:601:JQ2:C1A	3.03	0.42
1:A:23:GLU:OE1	1:A:247:SER:OG	2.37	0.42
1:B:109:LEU:H	1:B:109:LEU:HD12	1.84	0.42
1:C:325:GLN:OE1	1:C:490:LEU:HA	2.20	0.42
1:D:329:LEU:CD2	1:D:493:ALA:HB1	2.48	0.42
1:A:304:MSE:HB3	1:A:308:MSE:HE2	2.02	0.41
1:C:37:LEU:HD13	1:C:238:MSE:HE3	2.02	0.41
1:A:163:THR:HG23	1:A:279:CYS:SG	2.60	0.41
1:C:191:LEU:HA	1:C:444:ARG:O	2.20	0.41
1:C:329:LEU:CD2	1:C:493:ALA:HB1	2.47	0.41
1:D:50:ALA:HB1	1:D:54:LEU:HD22	2.02	0.41
1:A:469:LYS:HG2	1:A:470:GLU:N	2.35	0.41
1:B:338:TRP:CH2	1:B:494:ILE:HG23	2.55	0.41
1:D:163:THR:HG23	1:D:279:CYS:SG	2.60	0.41
1:C:99:LEU:HD23	1:C:116:LYS:HA	2.02	0.41
1:A:147:LEU:O	1:A:165:ILE:HD12	2.21	0.41
1:B:109:LEU:HD11	1:B:232:THR:CG2	2.51	0.41
1:C:163:THR:HG23	1:C:279:CYS:SG	2.60	0.41
1:C:91:ARG:NH2	1:D:124:GLU:OE2	2.54	0.41
1:A:26:HIS:CD2	1:A:27:ILE:HG23	2.55	0.41
1:C:332:MSE:CE	1:C:494:ILE:HD13	2.50	0.41
1:D:37:LEU:HD13	1:D:238:MSE:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:OE1	1:A:215:PRO:HD2	2.21	0.41
1:D:336:GLU:HG2	1:D:337:LYS:N	2.35	0.41
1:A:99:LEU:HD23	1:A:116:LYS:HA	2.02	0.40
1:C:61:ASP:C	1:C:63:PRO:HD3	2.46	0.40
1:C:391:ARG:HG2	1:C:392:GLU:N	2.36	0.40
1:A:61:ASP:C	1:A:63:PRO:HD3	2.46	0.40
1:C:39:VAL:HG21	1:C:236:LEU:HD13	2.03	0.40
1:D:325:GLN:OE1	1:D:490:LEU:HA	2.21	0.40
1:B:99:LEU:HD23	1:B:116:LYS:HA	2.02	0.40
1:C:127:MSE:HA	1:D:127:MSE:CE	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	468/510 (92%)	429 (92%)	36 (8%)	3 (1%)	21	50
1	B	458/510 (90%)	424 (93%)	30 (7%)	4 (1%)	14	42
1	C	469/510 (92%)	431 (92%)	35 (8%)	3 (1%)	21	50
1	D	455/510 (89%)	419 (92%)	33 (7%)	3 (1%)	18	47
All	All	1850/2040 (91%)	1703 (92%)	134 (7%)	13 (1%)	18	47

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	B	467	ILE
1	C	43	ARG
1	D	43	ARG
1	D	467	ILE

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Mol	Chain	Res	Type
1	A	467	ILE
1	B	392	GLU
1	A	140	ALA
1	B	62	LEU
1	B	140	ALA
1	C	140	ALA
1	D	140	ALA
1	C	467	ILE

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	363/401 (90%)	348 (96%)	15 (4%)	27	52
1	B	342/401 (85%)	321 (94%)	21 (6%)	17	43
1	C	353/401 (88%)	339 (96%)	14 (4%)	28	53
1	D	324/401 (81%)	312 (96%)	12 (4%)	30	55
All	All	1382/1604 (86%)	1320 (96%)	62 (4%)	24	51

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	125	LYS
1	A	129	GLU
1	A	143	LEU
1	A	198	ILE
1	A	210	ARG
1	A	235	VAL
1	A	286	SER
1	A	293	GLU
1	A	343	LEU
1	A	371	LEU
1	A	383	GLU
1	A	400	ASP

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Mol	Chain	Res	Type
1	A	463	LYS
1	A	469	LYS
1	B	20	CYS
1	B	27	ILE
1	B	45	PHE
1	B	54	LEU
1	B	105	ARG
1	B	124	GLU
1	B	125	LYS
1	B	143	LEU
1	B	198	ILE
1	B	212	ARG
1	B	235	VAL
1	B	238	MSE
1	B	286	SER
1	B	325	GLN
1	B	343	LEU
1	B	368	ASP
1	B	371	LEU
1	B	400	ASP
1	B	463	LYS
1	B	469	LYS
1	B	495	ILE
1	C	20	CYS
1	C	64	ILE
1	C	105	ARG
1	C	143	LEU
1	C	235	VAL
1	C	238	MSE
1	C	286	SER
1	C	293	GLU
1	C	325	GLN
1	C	346	GLU
1	C	348	GLU
1	C	371	LEU
1	C	400	ASP
1	C	502	THR
1	D	20	CYS
1	D	23	GLU
1	D	27	ILE
1	D	70	GLU
1	D	143	LEU

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Mol	Chain	Res	Type
1	D	231	GLU
1	D	235	VAL
1	D	286	SER
1	D	325	GLN
1	D	343	LEU
1	D	400	ASP
1	D	502	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	138	ASN
1	A	152	GLN
1	A	250	HIS
1	A	281	HIS
1	A	405	ASN
1	B	34	HIS
1	B	138	ASN
1	B	152	GLN
1	B	250	HIS
1	B	300	GLN
1	B	405	ASN
1	C	152	GLN
1	C	250	HIS
1	C	405	ASN
1	D	34	HIS
1	D	56	ASN
1	D	138	ASN
1	D	152	GLN
1	D	270	ASN
1	D	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

4 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	JQ2	C	601	-	46,48,48	2.86	14 (30%)	61,71,71	1.62	15 (24%)
2	JQ2	B	601	-	46,48,48	2.88	14 (30%)	61,71,71	1.63	15 (24%)
2	JQ2	D	601	-	46,48,48	2.85	15 (32%)	61,71,71	1.84	17 (27%)
2	JQ2	A	601	-	46,48,48	2.85	13 (28%)	61,71,71	1.63	14 (22%)

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	JQ2	C	601	-	-	6/22/83/83	0/5/5/5
2	JQ2	B	601	-	-	7/22/83/83	0/5/5/5
2	JQ2	D	601	-	-	8/22/83/83	0/5/5/5
2	JQ2	A	601	-	-	8/22/83/83	0/5/5/5

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	JQ2	C4A-C3A	-7.69	1.33	1.45
2	A	601	JQ2	C4A-C3A	-7.57	1.33	1.45
2	D	601	JQ2	C4A-C3A	-7.50	1.34	1.45
2	B	601	JQ2	C4A-C3A	-7.32	1.34	1.45
2	B	601	JQ2	CAB-C3B	-6.92	1.33	1.51
2	D	601	JQ2	CAB-C3B	-6.84	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	JQ2	CAB-C3B	-6.78	1.33	1.51
2	A	601	JQ2	CAB-C3B	-6.74	1.33	1.51
2	D	601	JQ2	C1A-C2A	-6.72	1.35	1.45
2	B	601	JQ2	C1A-C2A	-6.69	1.35	1.45
2	A	601	JQ2	C1A-C2A	-6.43	1.35	1.45
2	C	601	JQ2	C1A-C2A	-6.21	1.36	1.45
2	B	601	JQ2	C1B-C2B	-5.52	1.34	1.45
2	C	601	JQ2	CEA-C3A	-5.40	1.40	1.50
2	D	601	JQ2	C1B-C2B	-5.26	1.34	1.45
2	A	601	JQ2	C1B-C2B	-5.23	1.35	1.45
2	B	601	JQ2	CEA-C3A	-5.22	1.41	1.50
2	B	601	JQ2	C4B-C3B	-5.17	1.32	1.47
2	A	601	JQ2	CEA-C3A	-5.14	1.41	1.50
2	C	601	JQ2	C4C-C3C	-5.13	1.35	1.44
2	A	601	JQ2	C4C-C3C	-5.12	1.35	1.44
2	A	601	JQ2	C4B-C3B	-5.10	1.33	1.47
2	C	601	JQ2	C4B-C3B	-5.09	1.33	1.47
2	B	601	JQ2	C4C-C3C	-5.01	1.35	1.44
2	D	601	JQ2	C4B-C3B	-5.00	1.33	1.47
2	C	601	JQ2	C1B-C2B	-5.00	1.35	1.45
2	A	601	JQ2	C1C-C2C	-4.97	1.36	1.48
2	D	601	JQ2	CEA-C3A	-4.91	1.41	1.50
2	B	601	JQ2	C1C-C2C	-4.49	1.37	1.48
2	C	601	JQ2	C1C-C2C	-4.45	1.37	1.48
2	D	601	JQ2	C4C-C3C	-4.42	1.36	1.44
2	D	601	JQ2	C4D-C3D	-4.15	1.33	1.42
2	D	601	JQ2	C1C-C2C	-3.83	1.39	1.48
2	C	601	JQ2	C4D-C3D	-3.77	1.34	1.42
2	B	601	JQ2	C4D-C3D	-3.67	1.34	1.42
2	D	601	JQ2	C1B-N_B	-3.65	1.34	1.39
2	A	601	JQ2	C4D-C3D	-3.63	1.34	1.42
2	B	601	JQ2	C1D-C2D	-3.61	1.32	1.41
2	C	601	JQ2	C1D-C2D	-3.53	1.33	1.41
2	B	601	JQ2	C1B-N_B	-3.45	1.34	1.39
2	D	601	JQ2	C1D-C2D	-3.36	1.33	1.41
2	C	601	JQ2	C1B-N_B	-3.32	1.34	1.39
2	A	601	JQ2	C1D-C2D	-3.26	1.33	1.41
2	A	601	JQ2	C1B-N_B	-3.13	1.35	1.39
2	B	601	JQ2	C4B-N_B	-3.12	1.32	1.40
2	D	601	JQ2	C4B-N_B	-2.81	1.33	1.40
2	A	601	JQ2	C4B-N_B	-2.76	1.33	1.40
2	C	601	JQ2	C4B-N_B	-2.72	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	JQ2	C3D-C2D	-2.65	1.32	1.38
2	A	601	JQ2	C3D-C2D	-2.49	1.32	1.38
2	C	601	JQ2	C3D-C2D	-2.43	1.32	1.38
2	B	601	JQ2	C3D-C2D	-2.41	1.32	1.38
2	D	601	JQ2	C1A-N_A	-2.13	1.34	1.38
2	D	601	JQ2	CAC-C3C	2.11	1.56	1.51
2	C	601	JQ2	CAA-C2A	2.09	1.56	1.51
2	B	601	JQ2	C4C-N_C	-2.08	1.34	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	JQ2	CMC-C2C-C1C	4.56	130.74	121.21
2	C	601	JQ2	CMC-C2C-C1C	4.33	130.27	121.21
2	B	601	JQ2	CMC-C2C-C1C	4.25	130.09	121.21
2	A	601	JQ2	CMC-C2C-C1C	4.02	129.62	121.21
2	B	601	JQ2	C4C-N_C-C1C	-3.91	105.86	110.66
2	D	601	JQ2	CHA-C4D-N_D	3.66	133.56	125.29
2	D	601	JQ2	CEA-CEB-N_B	-3.62	106.80	112.53
2	D	601	JQ2	CHA-C4D-C3D	-3.61	119.45	127.22
2	D	601	JQ2	C4C-N_C-C1C	-3.39	106.50	110.66
2	A	601	JQ2	C1A-C2A-C3A	3.30	109.67	106.72
2	C	601	JQ2	C4C-N_C-C1C	-3.30	106.61	110.66
2	A	601	JQ2	C4C-N_C-C1C	-3.22	106.71	110.66
2	B	601	JQ2	CHA-C4D-N_D	3.14	132.38	125.29
2	A	601	JQ2	CAC-C3C-C4C	2.95	128.23	124.39
2	C	601	JQ2	CBB-CAB-C3B	2.93	120.38	112.42
2	C	601	JQ2	CAB-C3B-C4B	2.93	126.38	122.13
2	B	601	JQ2	CHA-C4D-C3D	-2.90	120.99	127.22
2	D	601	JQ2	CBB-CAB-C3B	2.86	120.17	112.42
2	A	601	JQ2	CBB-CAB-C3B	2.85	120.15	112.42
2	D	601	JQ2	CHA-C1A-N_A	2.85	130.58	124.60
2	B	601	JQ2	CBB-CAB-C3B	2.84	120.11	112.42
2	D	601	JQ2	CHD-C1D-C2D	-2.81	120.64	127.53
2	C	601	JQ2	CHA-C4D-N_D	2.81	131.63	125.29
2	D	601	JQ2	C1A-C2A-C3A	2.81	109.23	106.72
2	B	601	JQ2	CEA-CEB-N_B	-2.80	108.10	112.53
2	A	601	JQ2	CHA-C1A-N_A	2.80	130.48	124.60
2	D	601	JQ2	CAB-C3B-C4B	2.74	126.11	122.13
2	C	601	JQ2	CEA-CEB-N_B	-2.74	108.20	112.53
2	D	601	JQ2	CBC-CAC-C3C	2.72	119.78	112.42
2	D	601	JQ2	CHD-C1D-N_D	2.71	131.42	125.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	JQ2	CAA-C2A-C3A	-2.66	123.01	129.24
2	C	601	JQ2	CHA-C4D-C3D	-2.65	121.52	127.22
2	B	601	JQ2	C1A-C2A-C3A	2.65	109.09	106.72
2	A	601	JQ2	CHA-C4D-N_D	2.55	131.06	125.29
2	A	601	JQ2	CHA-C4D-C3D	-2.53	121.78	127.22
2	B	601	JQ2	CHA-C1A-N_A	2.50	129.84	124.60
2	A	601	JQ2	C2A-C1A-N_A	-2.47	106.55	110.04
2	D	601	JQ2	CAA-CBA-CGA	-2.47	107.13	113.67
2	C	601	JQ2	CAA-C2A-C3A	-2.44	123.52	129.24
2	B	601	JQ2	C1D-CHD-C4C	-2.42	123.86	130.82
2	C	601	JQ2	CAC-C3C-C4C	2.37	127.47	124.39
2	D	601	JQ2	CAC-C3C-C4C	2.36	127.46	124.39
2	D	601	JQ2	C3C-C4C-N_C	2.32	110.69	107.32
2	C	601	JQ2	CHD-C1D-C2D	-2.28	121.93	127.53
2	B	601	JQ2	CAB-C3B-C4B	2.28	125.44	122.13
2	A	601	JQ2	CAB-C3B-C4B	2.27	125.43	122.13
2	B	601	JQ2	CAA-C2A-C3A	-2.27	123.90	129.24
2	B	601	JQ2	CHD-C1D-C2D	-2.23	122.06	127.53
2	B	601	JQ2	C3C-C4C-N_C	2.15	110.44	107.32
2	C	601	JQ2	CMB-C2B-C1B	2.14	128.50	124.73
2	D	601	JQ2	O1A-CGA-CBA	-2.12	116.38	123.09
2	D	601	JQ2	CAD-CBD-CGD	-2.11	108.06	113.67
2	C	601	JQ2	C1D-CHD-C4C	-2.11	124.74	130.82
2	C	601	JQ2	CHA-C1A-N_A	2.10	129.01	124.60
2	B	601	JQ2	C2A-C1A-N_A	-2.07	107.11	110.04
2	A	601	JQ2	O1A-CGA-CBA	-2.05	116.60	123.09
2	C	601	JQ2	CHD-C1D-N_D	2.05	129.91	125.29
2	A	601	JQ2	CHD-C1D-N_D	2.03	129.88	125.29
2	B	601	JQ2	CAC-C3C-C4C	2.03	127.03	124.39
2	A	601	JQ2	C1D-CHD-C4C	-2.03	124.99	130.82
2	C	601	JQ2	C1A-C2A-C3A	2.01	108.52	106.72

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	JQ2	C2C-C3C-CAC-CBC
2	D	601	JQ2	C2C-C3C-CAC-CBC
2	D	601	JQ2	C4C-C3C-CAC-CBC
2	A	601	JQ2	C2A-CAA-CBA-CGA
2	B	601	JQ2	C4C-C3C-CAC-CBC
2	C	601	JQ2	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	D	601	JQ2	C2B-C3B-CAB-CBB
2	B	601	JQ2	C2A-CAA-CBA-CGA
2	A	601	JQ2	C2C-C3C-CAC-CBC
2	A	601	JQ2	C4C-C3C-CAC-CBC
2	D	601	JQ2	C2A-CAA-CBA-CGA
2	A	601	JQ2	CAA-CBA-CGA-O1A
2	D	601	JQ2	CAD-CBD-CGD-O1D
2	A	601	JQ2	CAD-CBD-CGD-O2D
2	A	601	JQ2	CAA-CBA-CGA-O2A
2	D	601	JQ2	CAA-CBA-CGA-O2A
2	D	601	JQ2	CAD-CBD-CGD-O2D
2	D	601	JQ2	CAA-CBA-CGA-O1A
2	B	601	JQ2	CAA-CBA-CGA-O2A
2	C	601	JQ2	CAA-CBA-CGA-O1A
2	C	601	JQ2	CAD-CBD-CGD-O2D
2	C	601	JQ2	CAD-CBD-CGD-O1D
2	A	601	JQ2	CAD-CBD-CGD-O1D
2	B	601	JQ2	CAA-CBA-CGA-O1A
2	B	601	JQ2	CAD-CBD-CGD-O2D
2	C	601	JQ2	CAA-CBA-CGA-O2A
2	B	601	JQ2	CAD-CBD-CGD-O1D
2	A	601	JQ2	N_A-C1A-CHA-C4D
2	C	601	JQ2	C4C-C3C-CAC-CBC

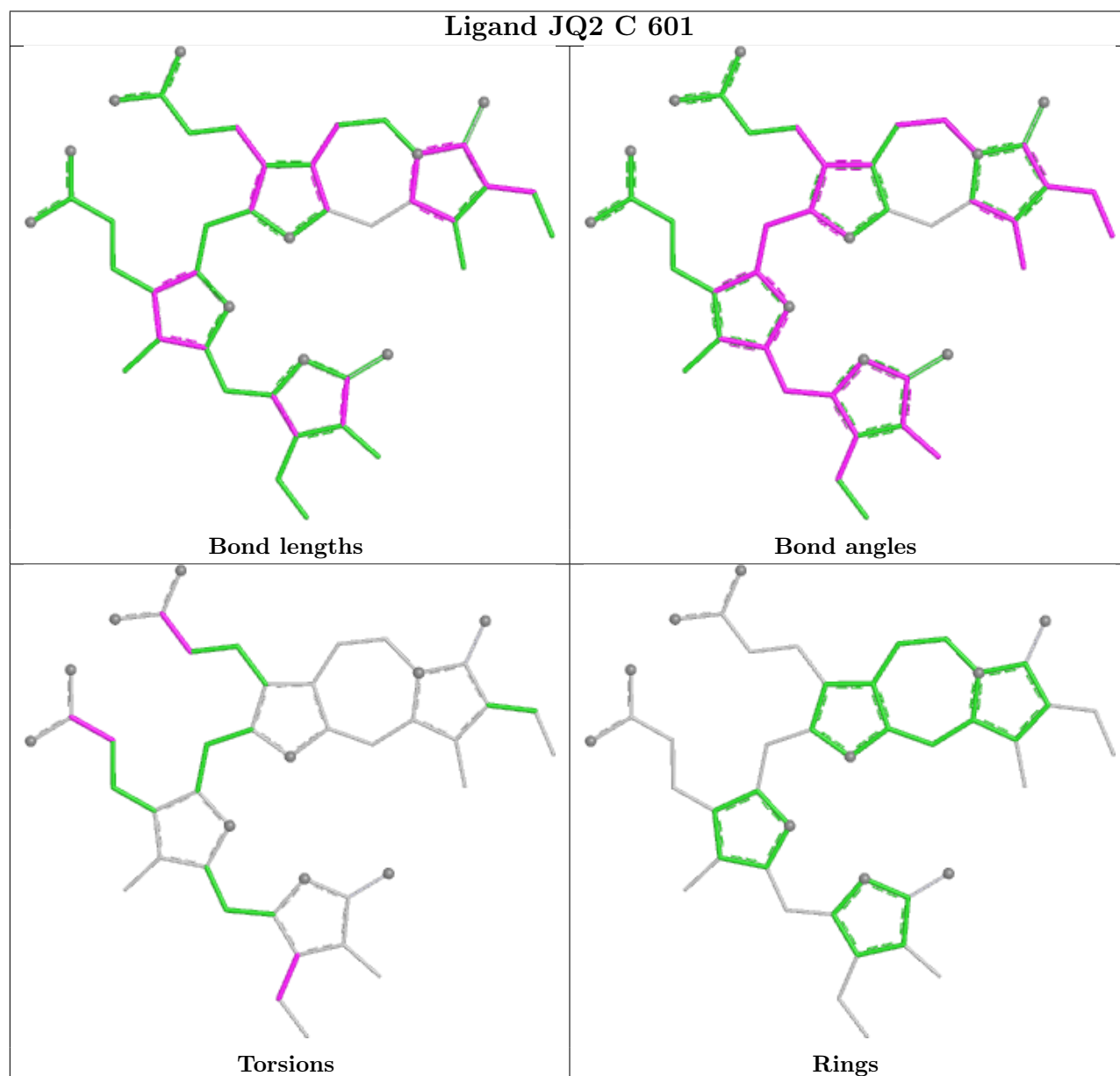
There are no ring outliers.

3 monomers are involved in 3 short contacts:

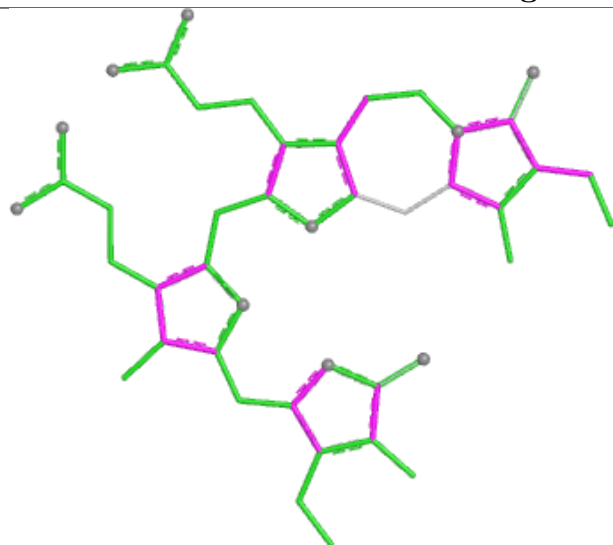
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	JQ2	1	0
2	B	601	JQ2	1	0
2	A	601	JQ2	1	0

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 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.

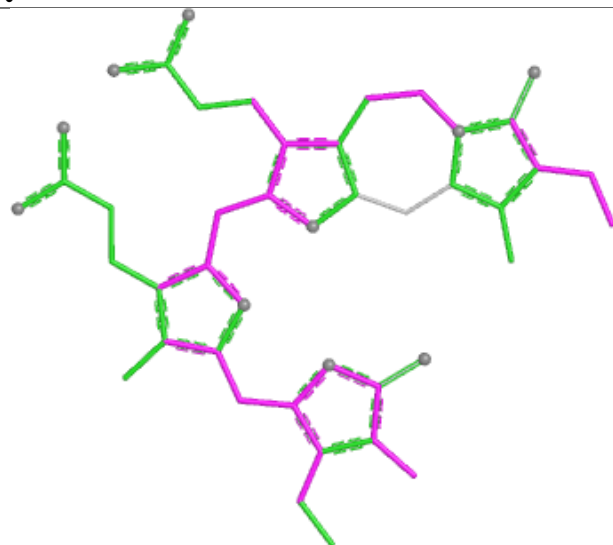
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



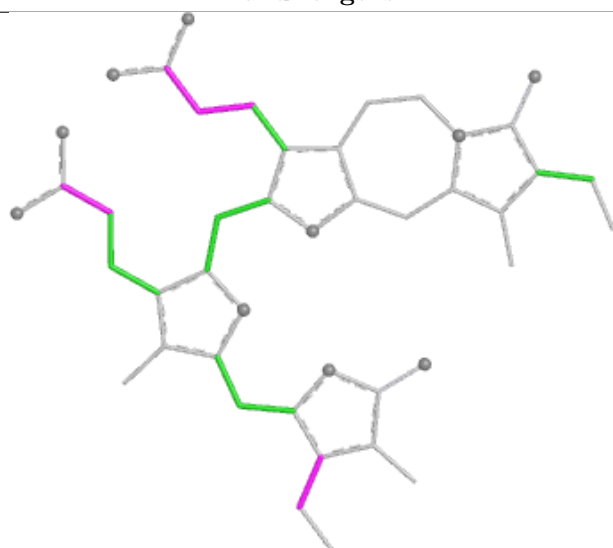
Ligand JQ2 B 601



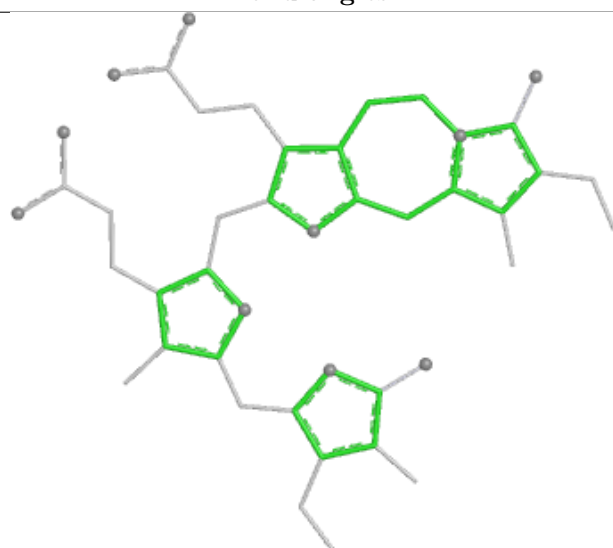
Bond lengths



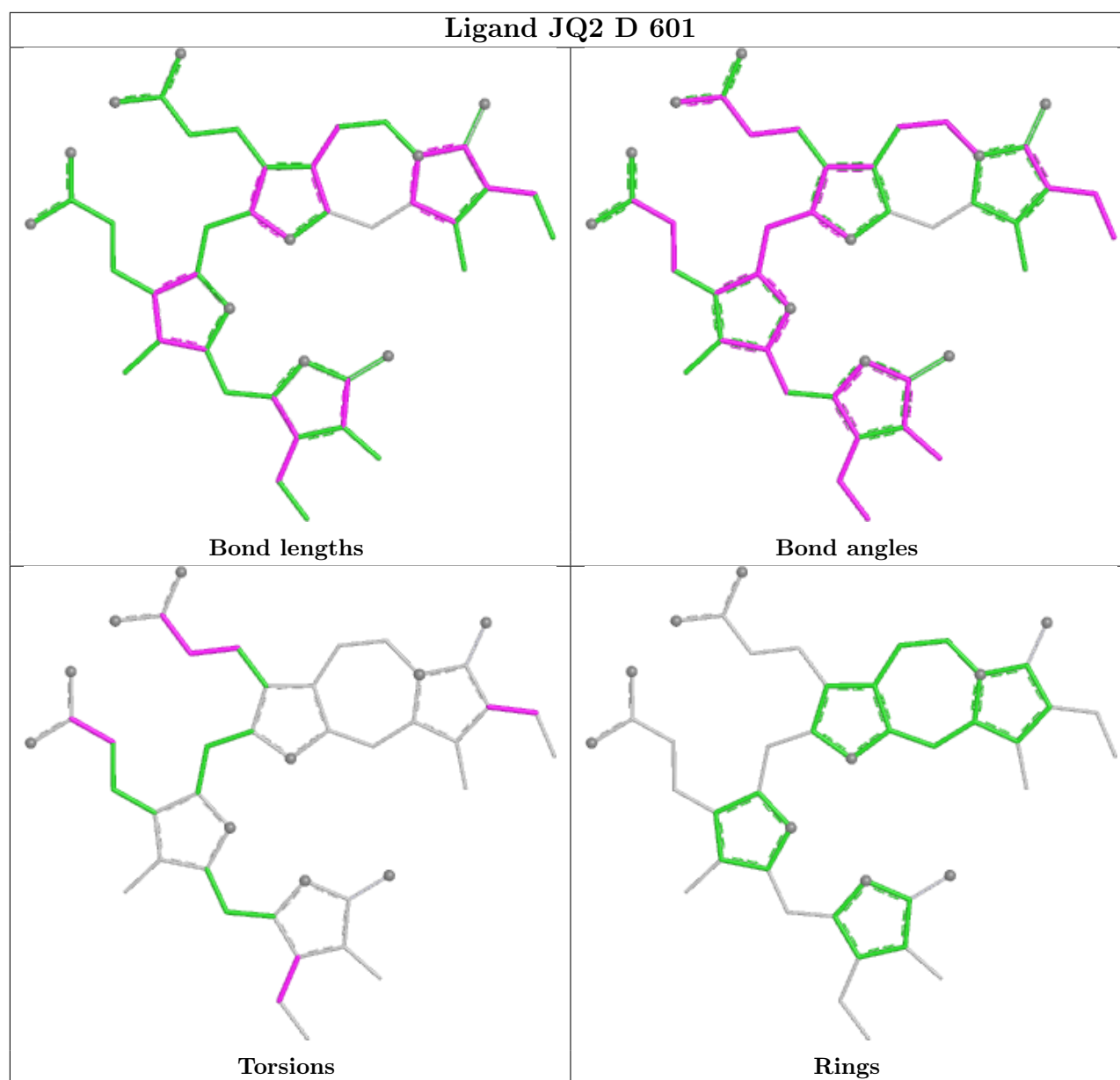
Bond angles

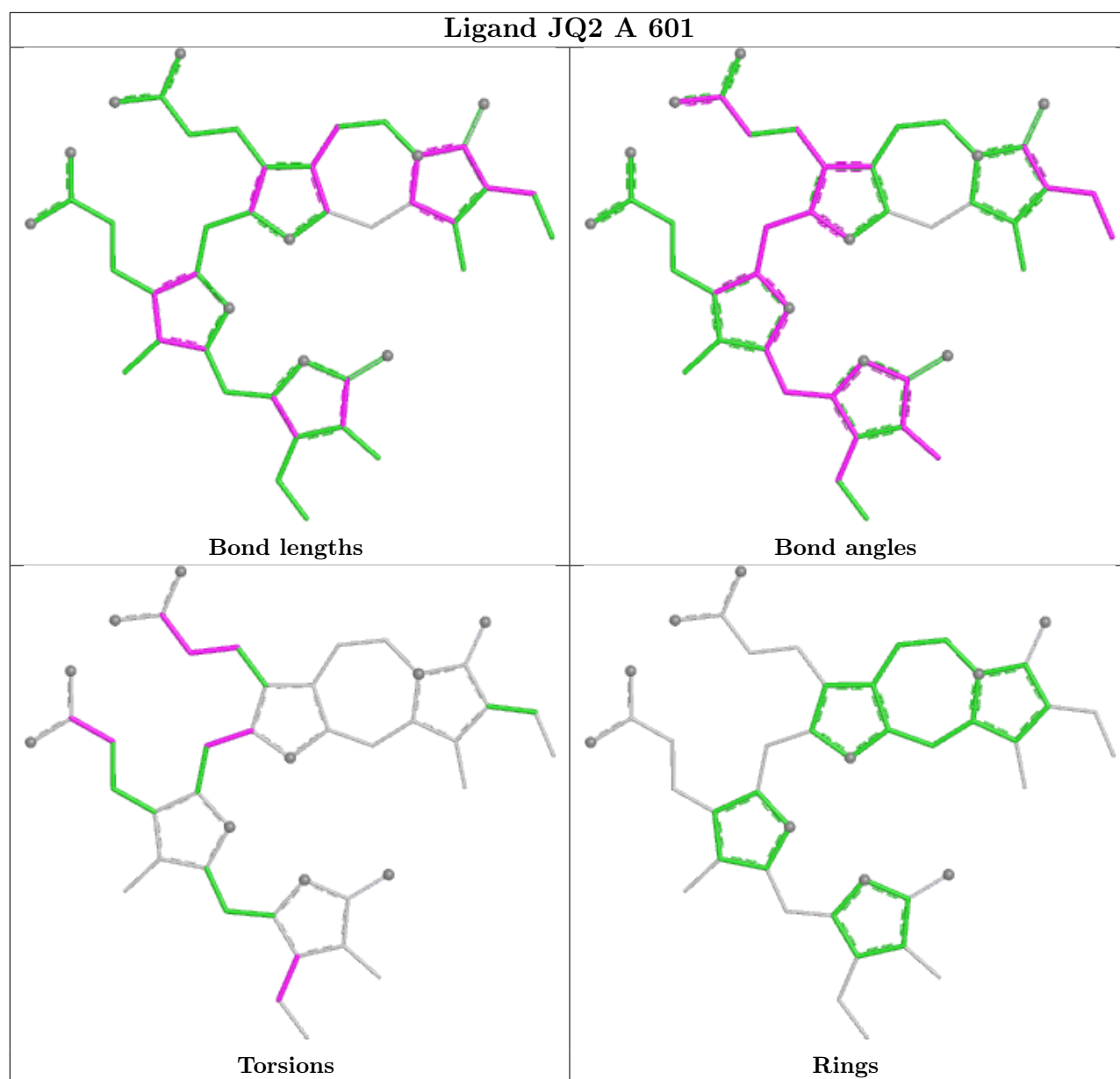


Torsions



Rings





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	462/510 (90%)	0.24	13 (2%)	55 41	50, 73, 107, 138	0
1	B	456/510 (89%)	0.50	22 (4%)	35 26	55, 87, 138, 180	0
1	C	465/510 (91%)	0.42	18 (3%)	43 31	60, 84, 120, 149	0
1	D	453/510 (88%)	0.49	21 (4%)	37 27	62, 95, 128, 157	0
All	All	1836/2040 (90%)	0.41	74 (4%)	42 30	50, 85, 127, 180	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	GLN	4.4
1	B	435	PHE	4.1
1	B	415	VAL	3.9
1	D	321	LEU	3.8
1	B	72	ASN	3.7
1	B	239	SER	3.5
1	A	320	GLU	3.4
1	D	290	ALA	3.4
1	D	111	ILE	3.4
1	A	335	ALA	3.3
1	C	316	SER	3.2
1	B	250	HIS	3.2
1	C	250	HIS	3.2
1	B	423	ARG	3.2
1	A	336	GLU	3.2
1	B	61	ASP	3.2
1	B	253	TYR	3.1
1	D	60	VAL	3.1
1	B	62	LEU	3.1
1	B	52	ASP	3.1
1	A	114	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	290	ALA	3.0
1	B	335	ALA	3.0
1	C	358	ALA	3.0
1	D	67	VAL	2.9
1	A	62	LEU	2.8
1	C	319	VAL	2.8
1	C	290	ALA	2.8
1	A	57	TYR	2.8
1	D	358	ALA	2.8
1	A	251	LEU	2.8
1	B	111	ILE	2.8
1	D	72	ASN	2.7
1	C	45	PHE	2.6
1	A	29	GLY	2.6
1	D	404	GLY	2.5
1	C	62	LEU	2.5
1	C	137	LEU	2.5
1	D	252	GLU	2.5
1	C	180	ALA	2.4
1	A	70	GLU	2.4
1	B	362	ALA	2.4
1	D	301	LEU	2.4
1	B	35	GLY	2.4
1	B	94	TRP	2.4
1	B	320	GLU	2.4
1	C	159	GLY	2.3
1	A	296	ASP	2.3
1	D	356	VAL	2.3
1	D	104	HIS	2.3
1	D	130	LEU	2.3
1	D	490	LEU	2.3
1	D	280	HIS	2.3
1	C	53	ASN	2.3
1	C	320	GLU	2.2
1	C	259	THR	2.2
1	A	64	ILE	2.2
1	B	103	ALA	2.2
1	C	126	LEU	2.2
1	C	357	GLY	2.2
1	B	101	VAL	2.2
1	C	249	VAL	2.2
1	D	58	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	355	GLN	2.2
1	D	403	ALA	2.2
1	C	20	CYS	2.2
1	B	110	VAL	2.1
1	D	52	ASP	2.1
1	A	331	GLY	2.1
1	B	60	VAL	2.1
1	C	61	ASP	2.1
1	B	40	LEU	2.0
1	D	266	SER	2.0
1	D	153	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

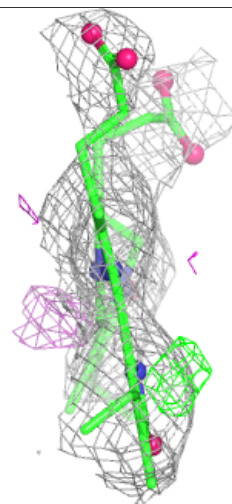
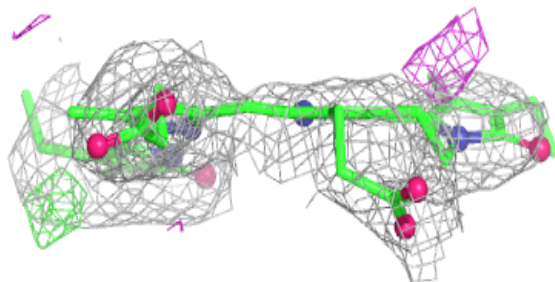
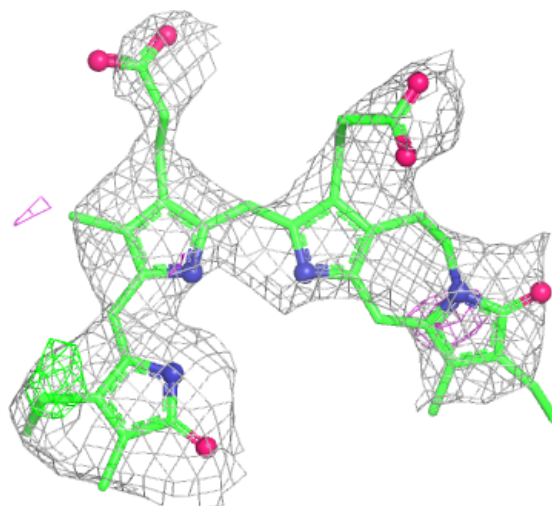
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	JQ2	C	601	44/44	0.86	0.14	67,88,95,98	0
2	JQ2	B	601	44/44	0.89	0.12	61,82,109,119	0
2	JQ2	A	601	44/44	0.89	0.10	54,67,72,73	0
2	JQ2	D	601	44/44	0.89	0.13	65,81,96,98	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.

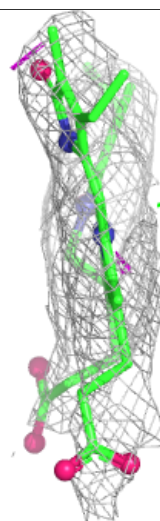
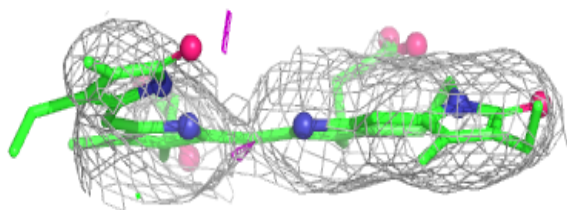
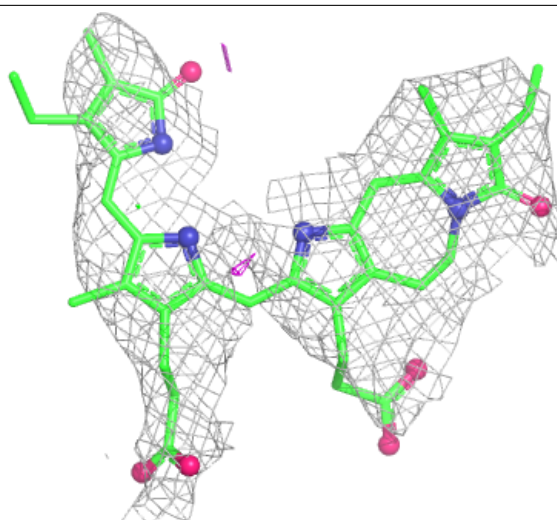
Electron density around JQ2 C 601:

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



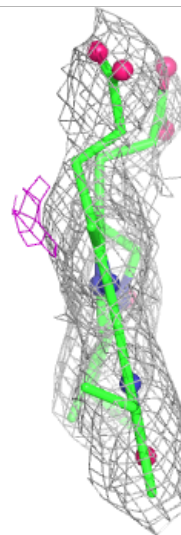
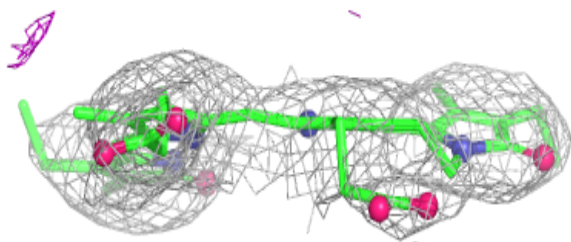
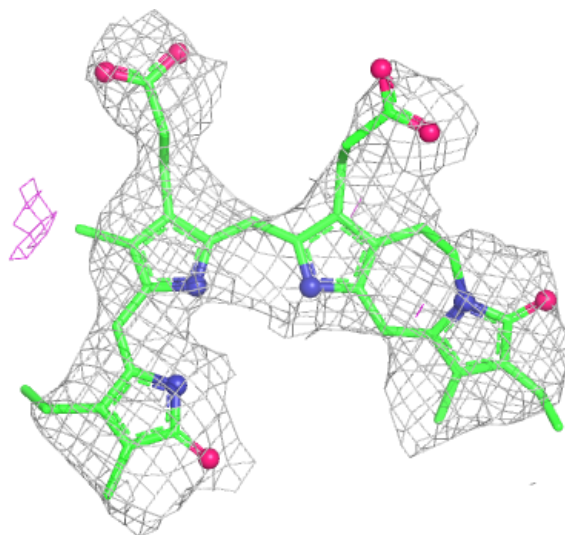
Electron density around JQ2 B 601:

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



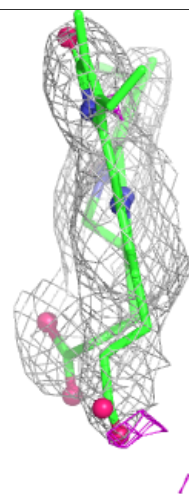
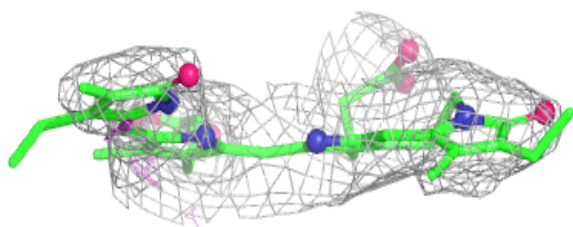
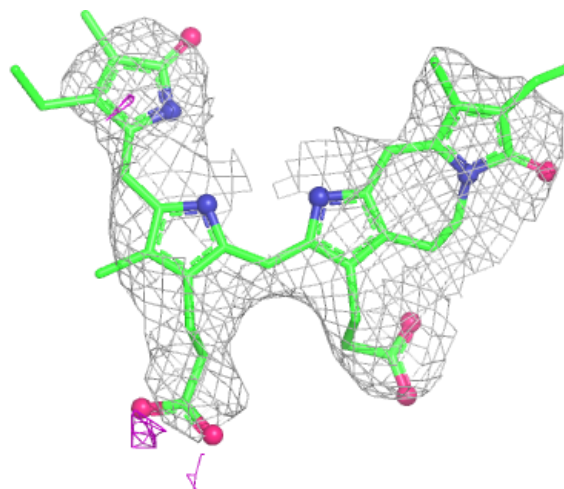
Electron density around JQ2 A 601:

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



Electron density around JQ2 D 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.