WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:07 pm BST

PDB ID	:	6R27
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)

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	:	2.11
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)	:	2.11

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.
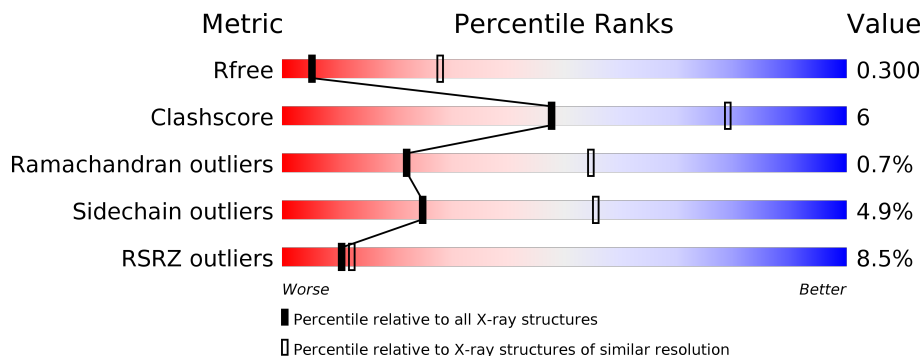
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	510	3% / 77% / 15% / · / 7%
1	B	510	9% / 75% / 15% / · / 9%
1	C	510	7% / 76% / 17% / · / 7%
1	D	510	12% / 78% / 13% / 9%

2 Entry composition (i)

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 3559	C 2252	N 623	O 671	S 3	Se 10	0	0	0
1	B	466	Total 3462	C 2195	N 605	O 649	S 3	Se 10	0	0	0
1	C	475	Total 3547	C 2242	N 620	O 672	S 3	Se 10	0	0	0
1	D	463	Total 3378	C 2138	N 581	O 647	S 3	Se 9	0	0	0

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 (three-letter code: JQ2) (formula: $C_{34}H_{38}N_4O_6$) (labeled as "Ligand of Interest" by author).
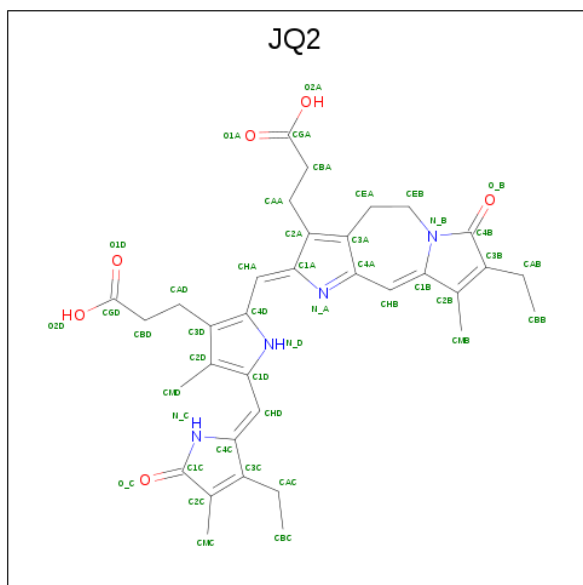

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	34	4	6		
2	B	1	Total	C	N	O	0	0
			44	34	4	6		
2	C	1	Total	C	N	O	0	0
			44	34	4	6		
2	D	1	Total	C	N	O	0	0
			44	34	4	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.
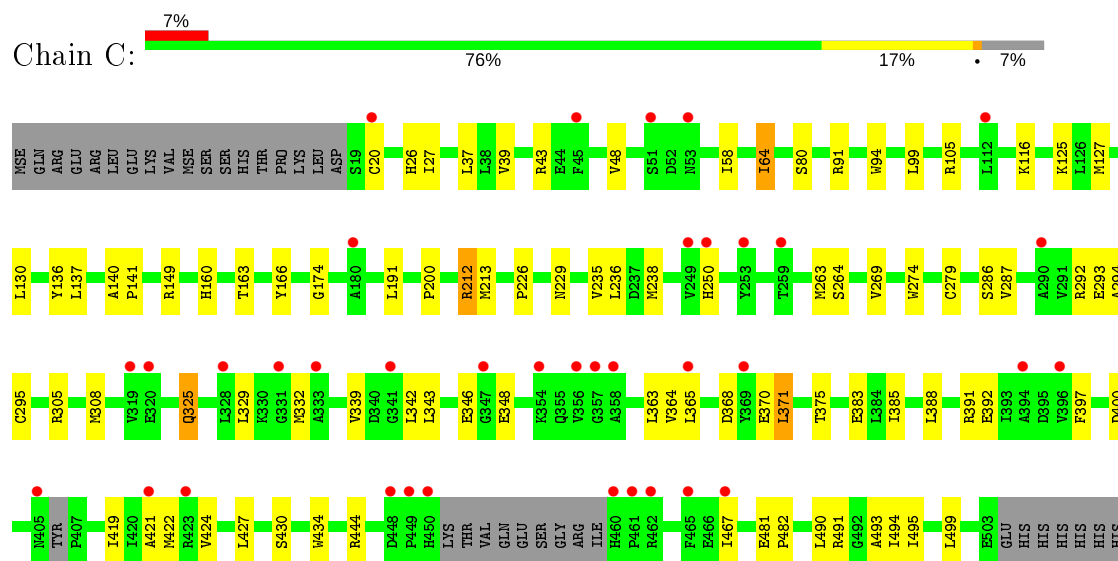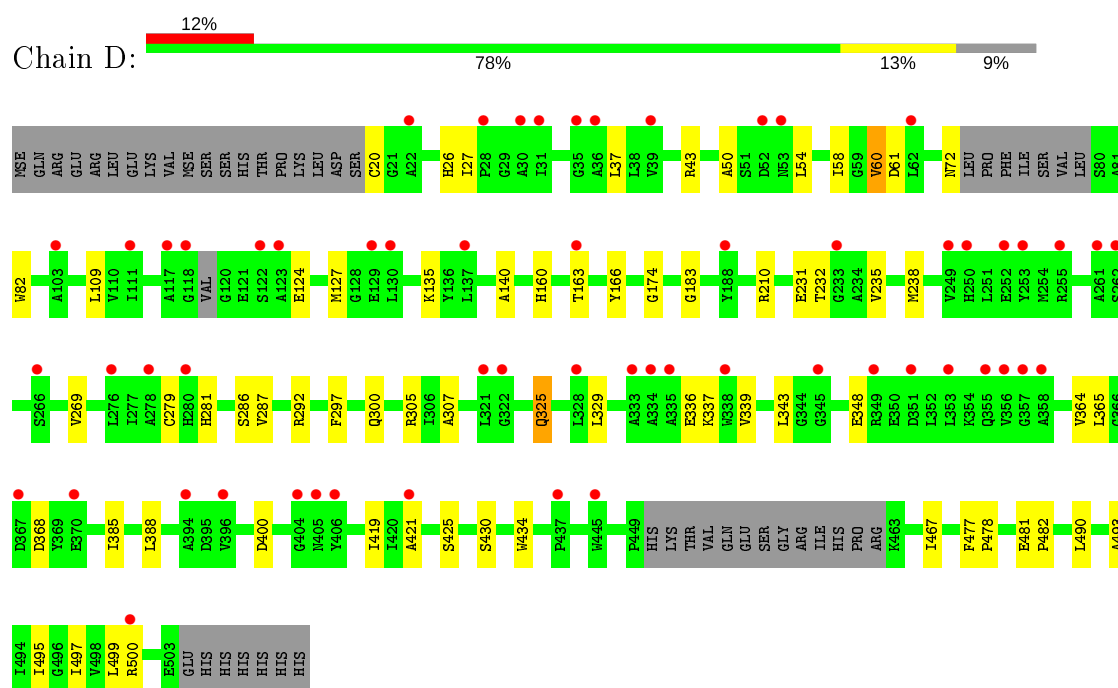
• Molecule 1: Bacteriophytochrome protein
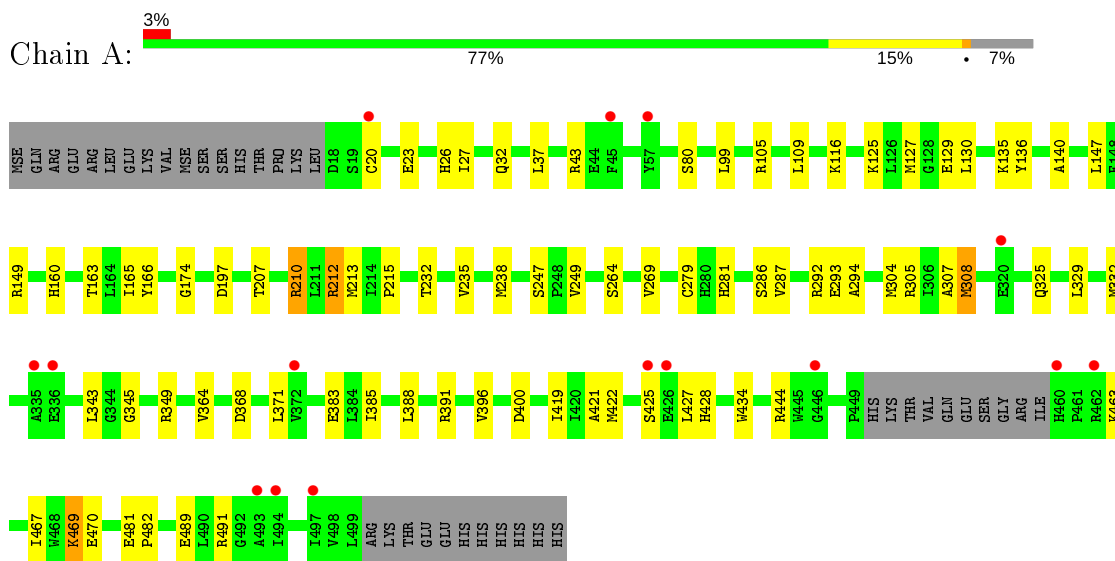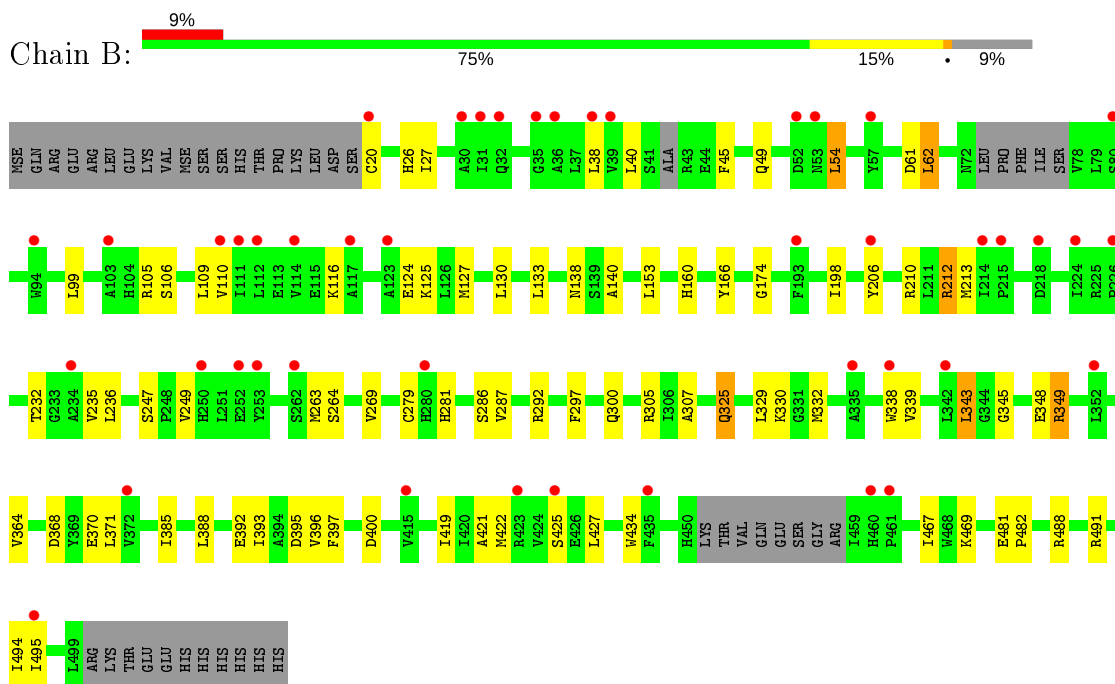
Chain A:

• Molecule 1: Bacteriophytochrome protein

Chain B:

• Molecule 1: Bacteriophytochrome protein

Chain C:

• Molecule 1: Bacteriophytochrome protein

Chain D:

4 Data and refinement statistics (i)

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) 96.5 (47.89-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.04%)	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)	0.29 , 34.8	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	0/3626	0.81	2/4918 (0.0%)
1	B	0.66	0/3526	0.81	2/4786 (0.0%)
1	C	0.67	0/3613	0.81	2/4901 (0.0%)
1	D	0.68	0/3438	0.80	0/4676
All	All	0.66	0/14203	0.80	6/19281 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($°$)	Ideal($°$)
1	B	263	MSE	CG-SE-CE	5.66	111.35	98.90
1	C	213	MSE	CG-SE-CE	5.65	111.32	98.90
1	B	213	MSE	CG-SE-CE	5.36	110.69	98.90
1	A	308	MSE	CG-SE-CE	5.25	110.45	98.90
1	A	213	MSE	CG-SE-CE	5.11	110.14	98.90
1	C	308	MSE	CG-SE-CE	5.04	109.98	98.90

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3559	0	3480	40	0
1	B	3462	0	3333	48	0
1	C	3547	0	3414	58	0
1	D	3378	0	3177	36	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	169	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 (169) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:371:LEU:CD2	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
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:N	1:A:371:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:B:371:LEU:N	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
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:B:110:VAL:O	1:B:110:VAL:HG13	2.15	0.47
1:A:345:GLY:O	1:A:349:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:391:ARG:HG2	1:C:392:GLU:N	2.36	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:B:61:ASP:O	1:B:62:LEU:C	2.59	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 (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	468/510 (92%)	429 (92%)	36 (8%)	3 (1%)	25	57
1	B	458/510 (90%)	424 (93%)	30 (7%)	4 (1%)	17	49
1	C	469/510 (92%)	431 (92%)	35 (8%)	3 (1%)	25	57
1	D	455/510 (89%)	419 (92%)	33 (7%)	3 (1%)	22	55
All	All	1850/2040 (91%)	1703 (92%)	134 (7%)	13 (1%)	22	55

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
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 (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	363/401 (90%)	344 (95%)	19 (5%)	23	53
1	B	342/401 (85%)	322 (94%)	20 (6%)	20	50
1	C	353/401 (88%)	337 (96%)	16 (4%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	324/401 (81%)	311 (96%)	13 (4%)	31	60
All	All	1382/1604 (86%)	1314 (95%)	68 (5%)	25	55

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	CYS
1	A	80	SER
1	A	105	ARG
1	A	125	LYS
1	A	129	GLU
1	A	135	LYS
1	A	210	ARG
1	A	212	ARG
1	A	235	VAL
1	A	286	SER
1	A	293	GLU
1	A	305	ARG
1	A	343	LEU
1	A	368	ASP
1	A	383	GLU
1	A	391	ARG
1	A	400	ASP
1	A	463	LYS
1	A	469	LYS
1	B	20	CYS
1	B	45	PHE
1	B	54	LEU
1	B	105	ARG
1	B	124	GLU
1	B	125	LYS
1	B	198	ILE
1	B	212	ARG
1	B	235	VAL
1	B	286	SER
1	B	297	PHE
1	B	305	ARG
1	B	325	GLN
1	B	330	LYS
1	B	343	LEU
1	B	348	GLU
1	B	349	ARG

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Mol	Chain	Res	Type
1	B	368	ASP
1	B	400	ASP
1	B	469	LYS
1	C	20	CYS
1	C	64	ILE
1	C	80	SER
1	C	105	ARG
1	C	125	LYS
1	C	212	ARG
1	C	235	VAL
1	C	286	SER
1	C	293	GLU
1	C	325	GLN
1	C	346	GLU
1	C	348	GLU
1	C	368	ASP
1	C	371	LEU
1	C	383	GLU
1	C	400	ASP
1	D	20	CYS
1	D	82	TRP
1	D	135	LYS
1	D	231	GLU
1	D	235	VAL
1	D	286	SER
1	D	297	PHE
1	D	305	ARG
1	D	325	GLN
1	D	343	LEU
1	D	348	GLU
1	D	368	ASP
1	D	400	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	152	GLN
1	B	138	ASN
1	B	300	GLN
1	D	34	HIS
1	D	152	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates 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	1	36,48,48	2.96	12 (33%)	39,71,71	1.61	9 (23%)
2	JQ2	B	601	1	36,48,48	3.01	13 (36%)	39,71,71	1.58	9 (23%)
2	JQ2	D	601	1	36,48,48	2.95	13 (36%)	39,71,71	1.78	11 (28%)
2	JQ2	A	601	1	36,48,48	2.97	11 (30%)	39,71,71	1.62	10 (25%)

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	1	-	3/18/83/83	0/5/5/5
2	JQ2	B	601	1	-	3/18/83/83	0/5/5/5
2	JQ2	D	601	1	-	4/18/83/83	0/5/5/5
2	JQ2	A	601	1	-	4/18/83/83	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	JQ2	C4A-C3A	-7.54	1.33	1.45
2	A	601	JQ2	C4A-C3A	-7.43	1.33	1.45
2	D	601	JQ2	C4A-C3A	-7.36	1.34	1.45
2	B	601	JQ2	C4A-C3A	-7.18	1.34	1.45
2	B	601	JQ2	CAB-C3B	-6.91	1.33	1.51
2	D	601	JQ2	CAB-C3B	-6.82	1.33	1.51
2	C	601	JQ2	CAB-C3B	-6.77	1.33	1.51
2	A	601	JQ2	CAB-C3B	-6.73	1.33	1.51
2	D	601	JQ2	C1A-C2A	-6.59	1.35	1.45
2	B	601	JQ2	C1A-C2A	-6.56	1.35	1.45
2	A	601	JQ2	C1A-C2A	-6.31	1.35	1.45
2	C	601	JQ2	C1A-C2A	-6.08	1.36	1.45
2	B	601	JQ2	C1B-C2B	-5.53	1.34	1.45
2	D	601	JQ2	C1B-C2B	-5.27	1.34	1.45
2	B	601	JQ2	C4B-C3B	-5.25	1.32	1.47
2	A	601	JQ2	C1B-C2B	-5.24	1.35	1.45
2	C	601	JQ2	CEA-C3A	-5.23	1.40	1.50
2	A	601	JQ2	C4B-C3B	-5.18	1.33	1.47
2	C	601	JQ2	C4B-C3B	-5.17	1.33	1.47
2	D	601	JQ2	C4B-C3B	-5.08	1.33	1.47
2	B	601	JQ2	CEA-C3A	-5.05	1.41	1.50
2	C	601	JQ2	C4C-C3C	-5.02	1.35	1.45
2	A	601	JQ2	C4C-C3C	-5.02	1.35	1.45
2	C	601	JQ2	C1B-C2B	-5.01	1.35	1.45
2	A	601	JQ2	CEA-C3A	-4.98	1.41	1.50
2	B	601	JQ2	C4C-C3C	-4.90	1.35	1.45
2	D	601	JQ2	CEA-C3A	-4.76	1.41	1.50
2	D	601	JQ2	C4C-C3C	-4.33	1.36	1.45
2	A	601	JQ2	C1C-C2C	-4.23	1.36	1.47
2	B	601	JQ2	C1C-C2C	-3.81	1.37	1.47
2	C	601	JQ2	C1C-C2C	-3.77	1.37	1.47
2	D	601	JQ2	C1B-N_B	-3.73	1.34	1.39
2	B	601	JQ2	C1B-N_B	-3.53	1.34	1.39
2	C	601	JQ2	C1B-N_B	-3.39	1.34	1.39
2	D	601	JQ2	C1C-C2C	-3.22	1.39	1.47
2	A	601	JQ2	C1B-N_B	-3.20	1.35	1.39
2	B	601	JQ2	C4B-N_B	-2.99	1.32	1.39
2	D	601	JQ2	C4B-N_B	-2.68	1.33	1.39
2	A	601	JQ2	C4B-N_B	-2.64	1.33	1.39
2	C	601	JQ2	C4B-N_B	-2.60	1.33	1.39
2	A	601	JQ2	CHA-C1A	2.17	1.36	1.35
2	B	601	JQ2	CHA-C1A	2.14	1.36	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	JQ2	C1C-N_C	-2.14	1.33	1.38
2	B	601	JQ2	C4C-N_C	-2.12	1.34	1.37
2	C	601	JQ2	C1C-N_C	-2.11	1.33	1.38
2	D	601	JQ2	C1A-N_A	-2.10	1.34	1.38
2	D	601	JQ2	CAC-C3C	2.09	1.56	1.51
2	C	601	JQ2	CAA-C2A	2.09	1.56	1.51
2	B	601	JQ2	C1C-N_C	-2.03	1.33	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	JQ2	CMC-C2C-C1C	3.98	130.74	121.39
2	B	601	JQ2	C4C-N_C-C1C	-3.78	105.86	110.67
2	C	601	JQ2	CMC-C2C-C1C	3.77	130.27	121.39
2	B	601	JQ2	CMC-C2C-C1C	3.70	130.09	121.39
2	A	601	JQ2	CMC-C2C-C1C	3.50	129.62	121.39
2	A	601	JQ2	C1A-C2A-C3A	3.33	109.67	106.69
2	D	601	JQ2	CAA-CBA-CGA	-3.30	107.13	112.67
2	D	601	JQ2	C4C-N_C-C1C	-3.28	106.50	110.67
2	C	601	JQ2	C4C-N_C-C1C	-3.18	106.61	110.67
2	A	601	JQ2	C4C-N_C-C1C	-3.11	106.71	110.67
2	A	601	JQ2	CAA-C2A-C3A	-3.09	123.01	129.51
2	C	601	JQ2	CAB-C3B-C4B	2.89	126.38	122.15
2	C	601	JQ2	CBB-CAB-C3B	2.88	120.38	112.43
2	A	601	JQ2	CAC-C3C-C4C	2.85	128.23	124.38
2	C	601	JQ2	CAA-C2A-C3A	-2.84	123.52	129.51
2	D	601	JQ2	C1A-C2A-C3A	2.83	109.23	106.69
2	D	601	JQ2	CBB-CAB-C3B	2.81	120.17	112.43
2	A	601	JQ2	CBB-CAB-C3B	2.80	120.15	112.43
2	B	601	JQ2	CBB-CAB-C3B	2.79	120.11	112.43
2	D	601	JQ2	CAD-CBD-CGD	-2.75	108.06	112.67
2	D	601	JQ2	CAB-C3B-C4B	2.70	126.11	122.15
2	B	601	JQ2	C1A-C2A-C3A	2.67	109.09	106.69
2	D	601	JQ2	CBC-CAC-C3C	2.67	119.78	112.43
2	B	601	JQ2	CAA-C2A-C3A	-2.66	123.90	129.51
2	A	601	JQ2	C2A-C1A-N_A	-2.41	106.55	110.05
2	D	601	JQ2	C3C-C4C-N_C	2.32	110.69	107.30
2	D	601	JQ2	CAA-C2A-C3A	-2.31	124.64	129.51
2	C	601	JQ2	CAD-CBD-CGD	-2.31	108.79	112.67
2	C	601	JQ2	CAC-C3C-C4C	2.29	127.47	124.38
2	D	601	JQ2	CAC-C3C-C4C	2.28	127.46	124.38
2	B	601	JQ2	CAB-C3B-C4B	2.24	125.44	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	JQ2	CAB-C3B-C4B	2.24	125.43	122.15
2	B	601	JQ2	C3C-C4C-N_C	2.15	110.44	107.30
2	C	601	JQ2	CMB-C2B-C1B	2.15	128.50	124.71
2	B	601	JQ2	CAD-CBD-CGD	-2.14	109.08	112.67
2	A	601	JQ2	CAC-C3C-C2C	-2.08	123.98	127.53
2	C	601	JQ2	C1A-C2A-C3A	2.04	108.52	106.69
2	A	601	JQ2	CBD-CAD-C3D	-2.02	108.75	112.49
2	B	601	JQ2	C2A-C1A-N_A	-2.02	107.11	110.05

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

There are no ring outliers.
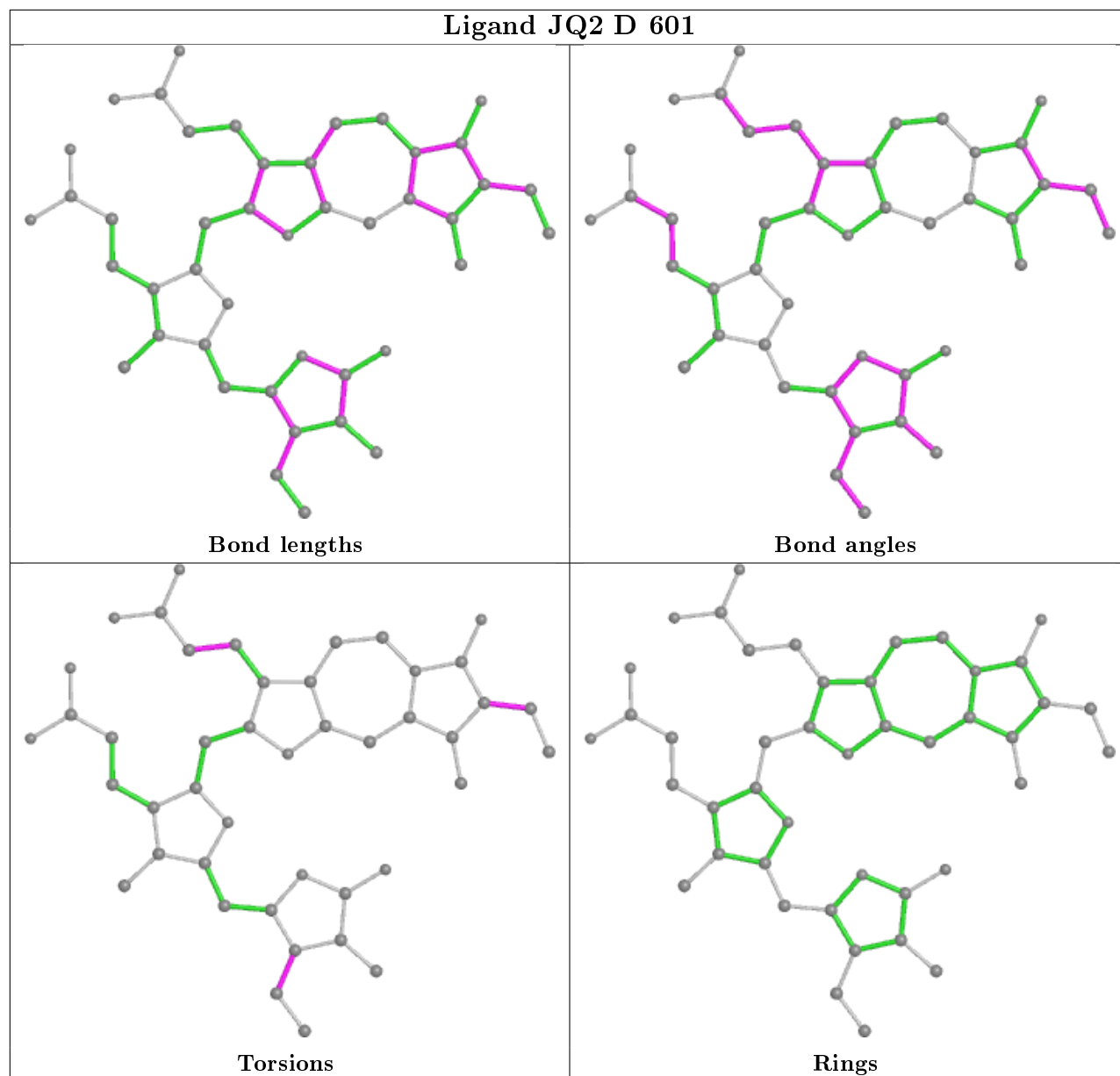
3 monomers are involved in 3 short contacts:

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 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
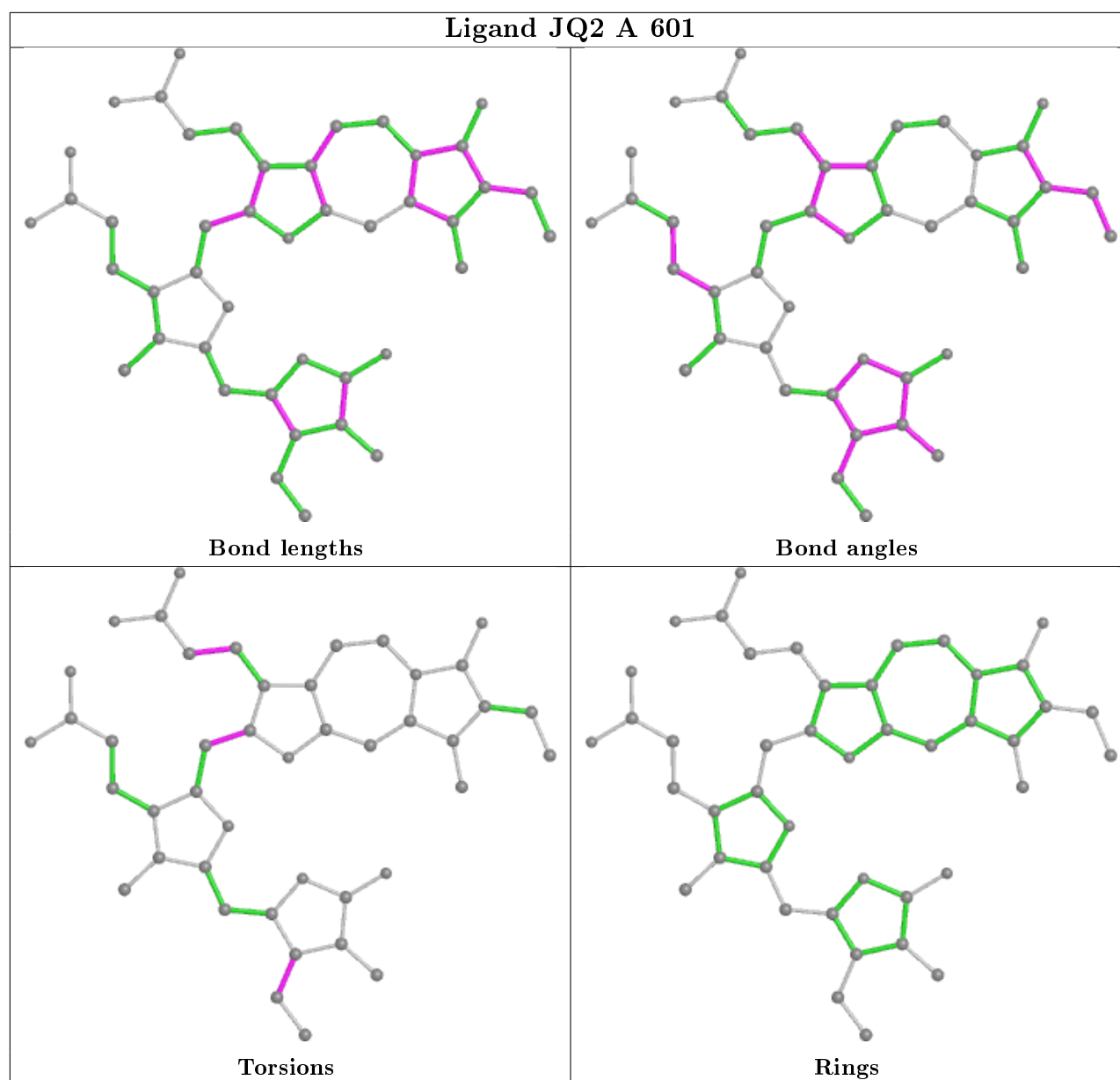
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 JQ2 C 601

Bond lengths

Bond angles

Torsions

Rings

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Ligand JQ2 B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand JQ2 D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand JQ2 A 601

Bond lengths

Bond angles

Torsions

Rings
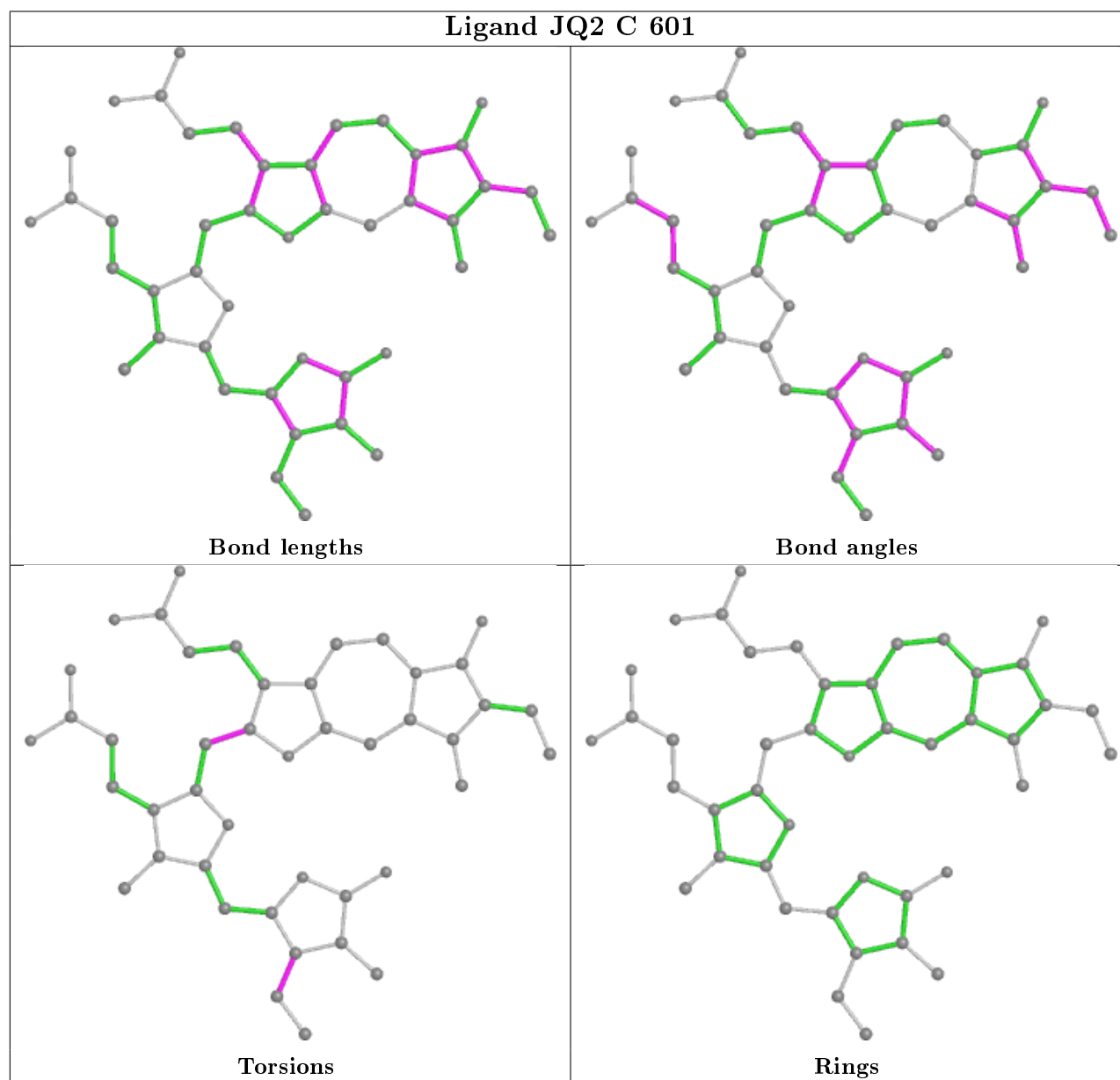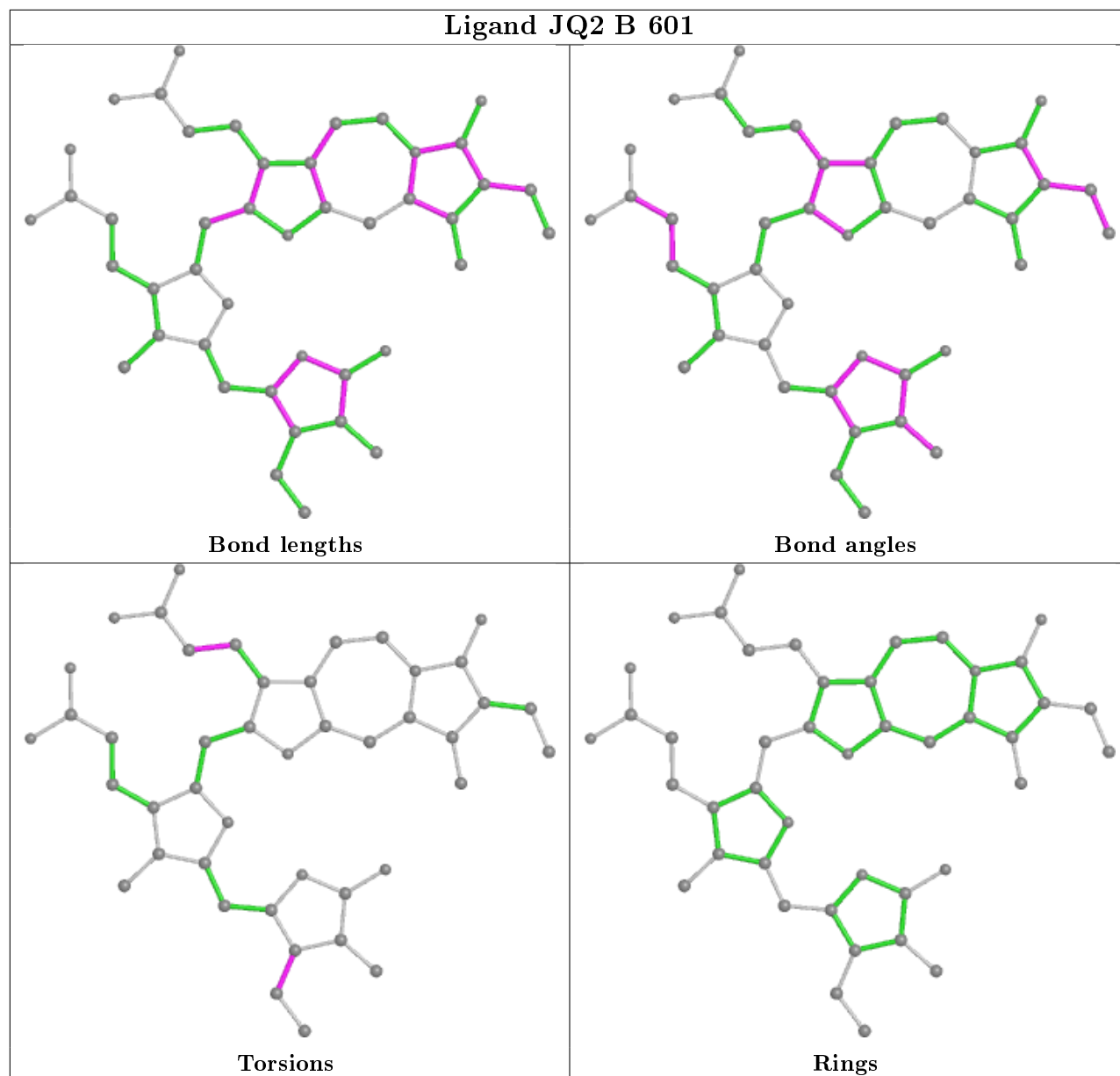
5.7 Other polymers (i)

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 (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(Å²)	Q<0.9
1	A	462/510 (90%)	0.24	15 (3%)	47	46	50, 73, 107, 138	0
1	B	456/510 (89%)	0.59	45 (9%)	7	8	55, 87, 138, 180	0
1	C	465/510 (91%)	0.49	37 (7%)	12	13	60, 84, 120, 149	0
1	D	453/510 (88%)	0.77	59 (13%)	3	4	62, 95, 128, 157	0
All	All	1836/2040 (90%)	0.52	156 (8%)	10	12	50, 85, 127, 180	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	GLY	4.8
1	D	357	GLY	4.7
1	B	38	LEU	4.6
1	D	333	ALA	4.4
1	D	356	VAL	4.4
1	D	280	HIS	4.3
1	D	421	ALA	4.3
1	B	36	ALA	4.2
1	B	110	VAL	4.1
1	D	321	LEU	4.1
1	D	123	ALA	4.1
1	D	111	ILE	4.0
1	B	32	GLN	4.0
1	D	396	VAL	3.9
1	C	357	GLY	3.9
1	C	53	ASN	3.9
1	D	117	ALA	3.9
1	C	396	VAL	3.9
1	D	394	ALA	3.9
1	C	421	ALA	3.8
1	C	250	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	52	ASP	3.6
1	C	462	ARG	3.6
1	C	20	CYS	3.6
1	D	253	TYR	3.6
1	C	461	PRO	3.5
1	D	36	ALA	3.5
1	B	52	ASP	3.5
1	B	111	ILE	3.5
1	C	423	ARG	3.4
1	A	497	ILE	3.4
1	B	57	TYR	3.4
1	B	280	HIS	3.4
1	A	425	SER	3.4
1	D	334	ALA	3.4
1	B	206	TYR	3.4
1	B	253	TYR	3.4
1	A	336	GLU	3.4
1	B	20	CYS	3.3
1	B	250	HIS	3.3
1	A	493	ALA	3.3
1	D	30	ALA	3.3
1	A	57	TYR	3.3
1	D	328	LEU	3.2
1	D	358	ALA	3.2
1	B	39	VAL	3.2
1	B	112	LEU	3.2
1	C	465	PHE	3.1
1	C	259	THR	3.1
1	C	347	GLY	3.1
1	C	341	GLY	3.1
1	D	445	TRP	3.1
1	B	460	HIS	3.1
1	B	435	PHE	3.1
1	A	462	ARG	3.1
1	B	35	GLY	3.0
1	D	252	GLU	3.0
1	C	333	ALA	3.0
1	B	103	ALA	3.0
1	D	355	GLN	3.0
1	D	129	GLU	3.0
1	B	94	TRP	2.9
1	B	415	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	331	GLY	2.9
1	D	103	ALA	2.9
1	B	226	PRO	2.9
1	D	404	GLY	2.9
1	A	494	ILE	2.8
1	D	35	GLY	2.8
1	D	353	LEU	2.8
1	C	319	VAL	2.8
1	B	31	ILE	2.8
1	B	262	SER	2.8
1	B	123	ALA	2.8
1	B	425	SER	2.7
1	A	426	GLU	2.7
1	C	358	ALA	2.7
1	C	51	SER	2.7
1	B	338	TRP	2.7
1	D	261	ALA	2.7
1	B	372	VAL	2.6
1	A	335	ALA	2.6
1	D	53	ASN	2.6
1	D	163	THR	2.6
1	B	423	ARG	2.6
1	A	20	CYS	2.6
1	D	338	TRP	2.6
1	D	122	SER	2.6
1	B	80	SER	2.6
1	B	252	GLU	2.5
1	A	446	GLY	2.5
1	D	349	ARG	2.5
1	D	262	SER	2.5
1	B	53	ASN	2.5
1	B	335	ALA	2.5
1	D	118	GLY	2.5
1	C	448	ASP	2.5
1	C	450	HIS	2.5
1	D	22	ALA	2.4
1	B	218	ASP	2.4
1	B	214	ILE	2.4
1	C	320	GLU	2.4
1	C	45	PHE	2.4
1	C	405	ASN	2.4
1	D	335	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	460	HIS	2.3
1	C	180	ALA	2.3
1	D	250	HIS	2.3
1	D	500	ARG	2.3
1	D	233	GLY	2.3
1	C	356	VAL	2.3
1	B	224	ILE	2.3
1	D	278	ALA	2.3
1	D	130	LEU	2.3
1	B	461	PRO	2.3
1	C	253	TYR	2.3
1	D	351	ASP	2.3
1	B	117	ALA	2.3
1	D	370	GLU	2.2
1	B	114	VAL	2.2
1	D	345	GLY	2.2
1	D	188	TYR	2.2
1	C	249	VAL	2.2
1	D	31	ILE	2.2
1	B	30	ALA	2.2
1	A	45	PHE	2.2
1	A	320	GLU	2.2
1	C	467	ILE	2.2
1	D	28	PRO	2.2
1	C	460	HIS	2.1
1	D	367	ASP	2.1
1	B	215	PRO	2.1
1	D	266	SER	2.1
1	C	449	PRO	2.1
1	D	62	LEU	2.1
1	D	255	ARG	2.1
1	D	406	TYR	2.1
1	B	342	LEU	2.1
1	C	290	ALA	2.1
1	D	437	PRO	2.1
1	D	39	VAL	2.1
1	A	372	VAL	2.1
1	C	354	LYS	2.1
1	D	276	LEU	2.1
1	B	495	ILE	2.1
1	B	234	ALA	2.0
1	D	137	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	394	ALA	2.0
1	B	352	LEU	2.0
1	C	112	LEU	2.0
1	C	328	LEU	2.0
1	B	193	PHE	2.0
1	D	405	ASN	2.0
1	C	365	LEU	2.0
1	C	369	TYR	2.0
1	D	249	VAL	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 carbohydrates 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	0.88	0.56	67,88,95,98	0
2	JQ2	D	601	44/44	0.88	0.47	65,81,96,98	0
2	JQ2	B	601	44/44	0.90	0.48	61,82,109,119	0
2	JQ2	A	601	44/44	0.92	0.44	54,67,72,73	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.
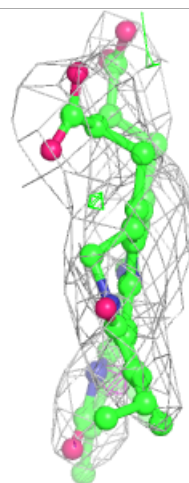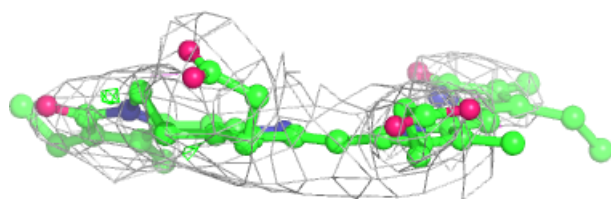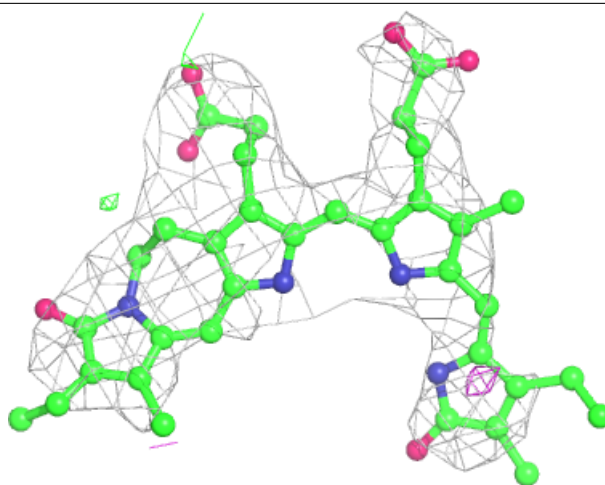
Electron density around JQ2 C 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
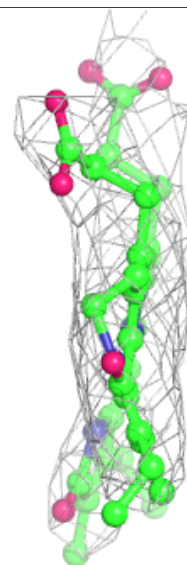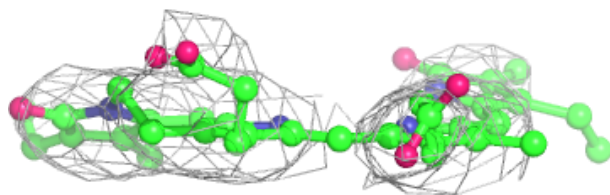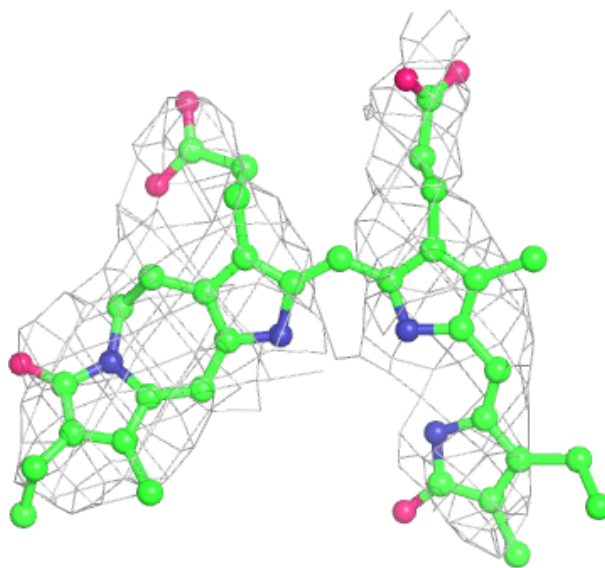and green (positive)
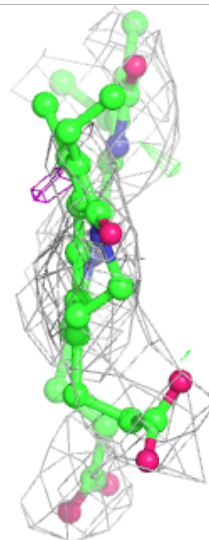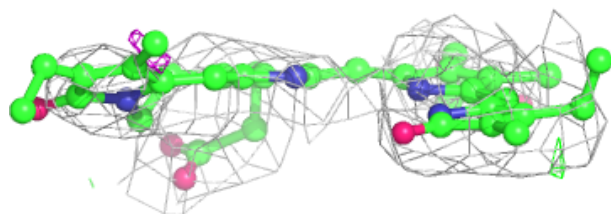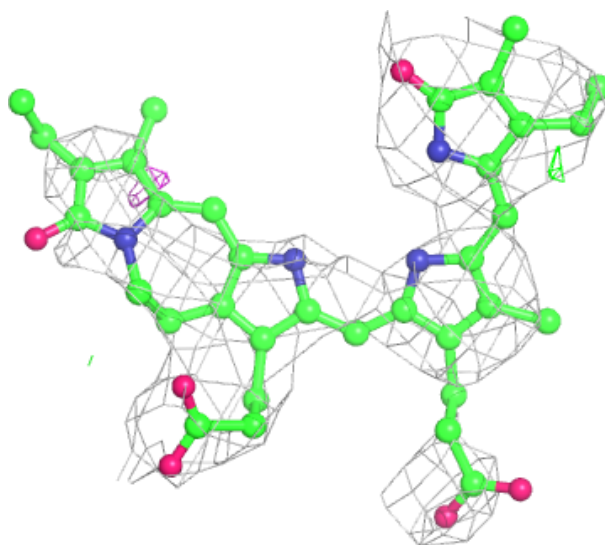
Electron density around JQ2 D 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
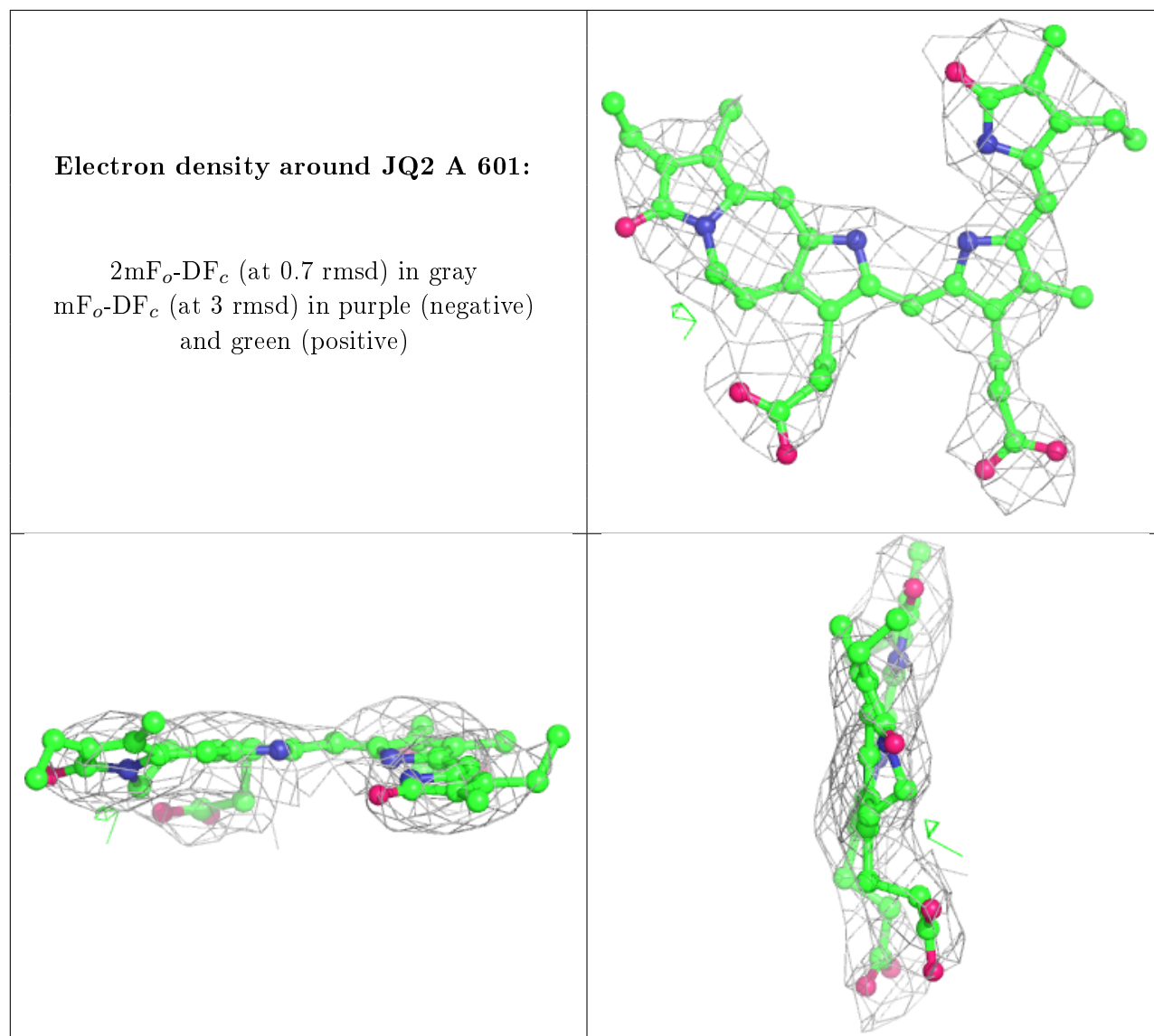
Electron density around JQ2 B 601:

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:

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

6.5 Other polymers (i)

There are no such residues in this entry.