wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 07:07 AM EDT

PDB ID	:	4UQI
Title	:	AP2 controls clathrin polymerization with a membrane-activated switch
Authors	:	Kelly, B.T.; Graham, S.C.; Liska, N.; Dannhauser, P.N.; Hoening, S.; Ungewickell, E.J.; Owen, D.J.
Deposited on	:	2014-06-23
Resolution	:	2.79 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 (i) 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 (i)) were used in the production of this report:

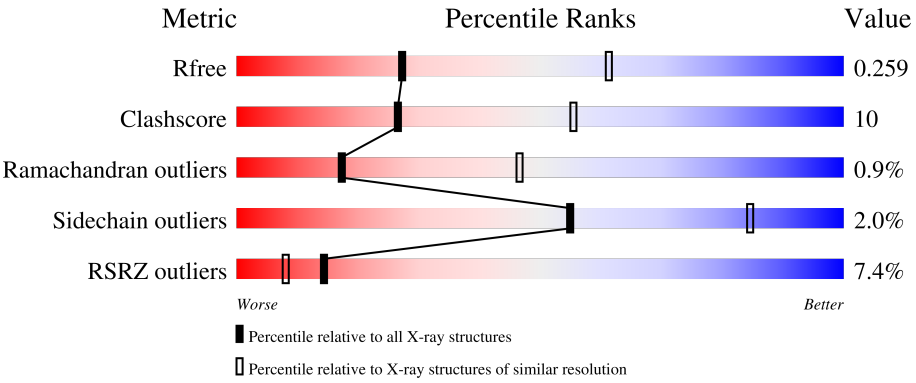
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	628	82% 14% ·
2	B	657	17% 60% 28% · 9%
3	M	446	3% 71% 17% · 11%
4	S	142	93% 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13889 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 AP-2 COMPLEX SUBUNIT ALPHA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	600	4737	3017	815	884	21	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	GLU	conflict	UNP P18484
A	272	GLU	-	insertion	UNP P18484
A	622	GLY	-	expression tag	UNP P18484
A	623	SER	-	expression tag	UNP P18484
A	624	GLY	-	expression tag	UNP P18484
A	625	LEU	-	expression tag	UNP P18484
A	626	VAL	-	expression tag	UNP P18484
A	627	PRO	-	expression tag	UNP P18484
A	628	ARG	-	expression tag	UNP P18484

- Molecule 2 is a protein called AP-2 COMPLEX SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	597	4720	3007	783	905	25	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	652	HIS	-	expression tag	UNP P63010
B	653	HIS	-	expression tag	UNP P63010
B	654	HIS	-	expression tag	UNP P63010
B	655	HIS	-	expression tag	UNP P63010
B	656	HIS	-	expression tag	UNP P63010
B	657	HIS	-	expression tag	UNP P63010

- Molecule 3 is a protein called AP-2 COMPLEX SUBUNIT MU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	396	Total	C	N	O	S	0	0	0
			3192	2053	559	561	19			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	236A	MET	-	insertion	UNP P84092
M	236B	GLU	-	insertion	UNP P84092
M	236C	GLN	-	insertion	UNP P84092
M	236D	LYS	-	insertion	UNP P84092
M	236E	LEU	-	insertion	UNP P84092
M	236F	ILE	-	insertion	UNP P84092
M	236G	SER	-	insertion	UNP P84092
M	236H	GLU	-	insertion	UNP P84092
M	236I	GLU	-	insertion	UNP P84092
M	236J	ASP	-	insertion	UNP P84092
M	236K	LEU	-	insertion	UNP P84092

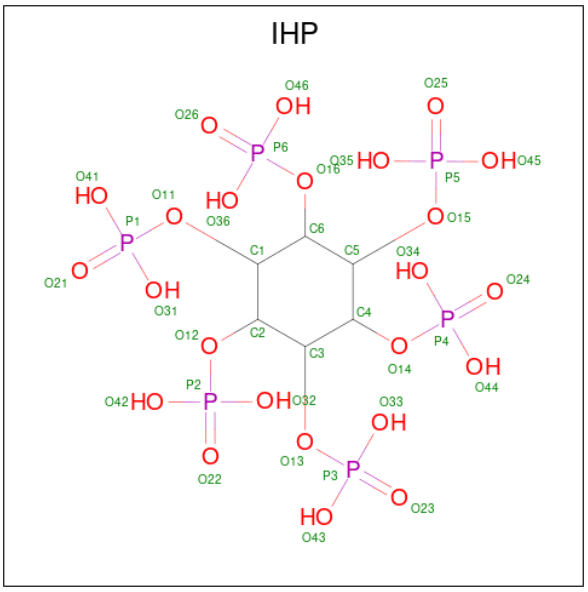
- Molecule 4 is a protein called AP-2 COMPLEX SUBUNIT SIGMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			

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

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

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O P 36 6 24 6	0	0

- Molecule 7 is water.

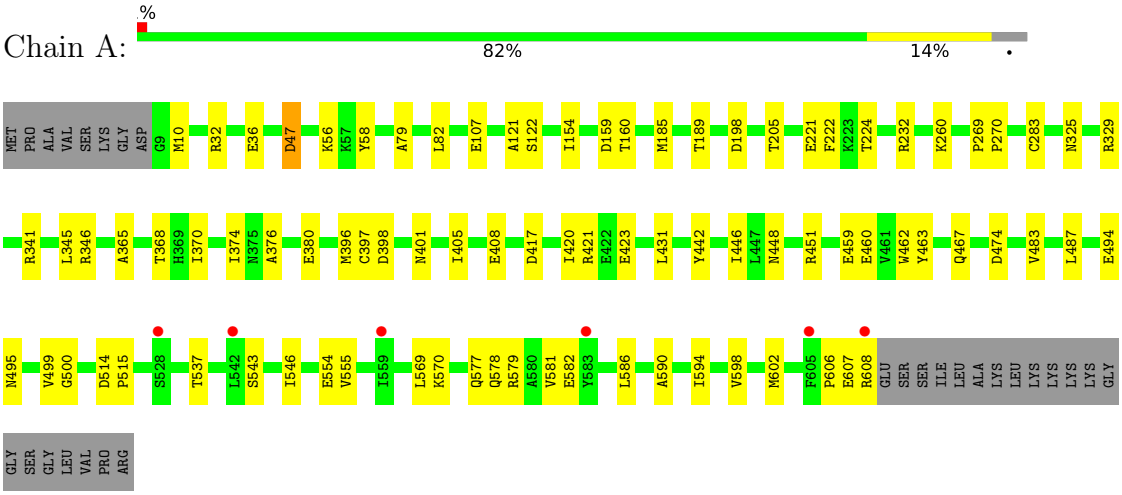
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	B	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

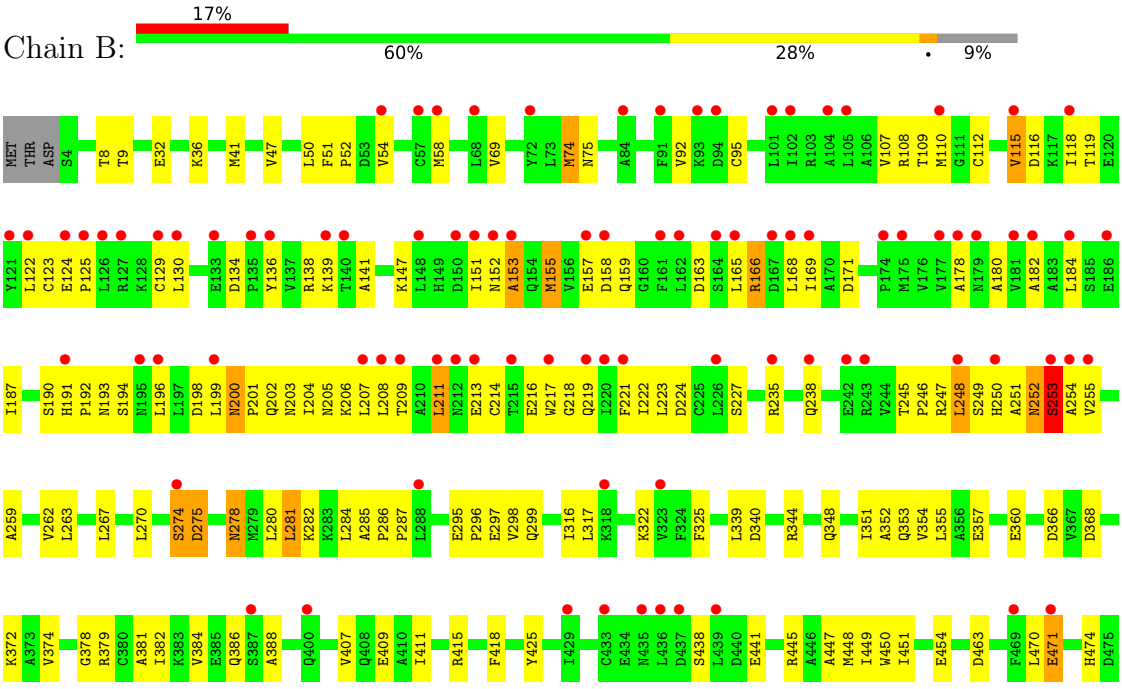
• Molecule 1: AP-2 COMPLEX SUBUNIT ALPHA-2

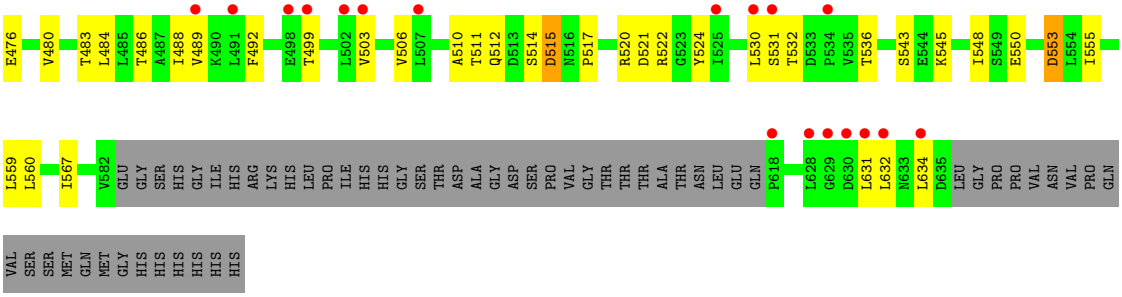
Chain A:



• Molecule 2: AP-2 COMPLEX SUBUNIT BETA

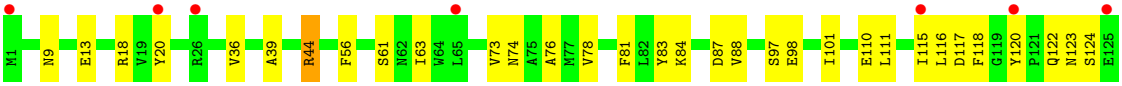
Chain B:

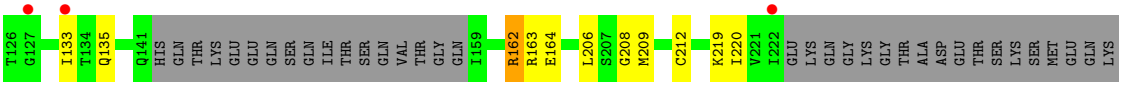




• Molecule 3: AP-2 COMPLEX SUBUNIT MU

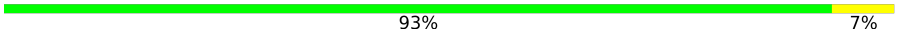
Chain M:





• Molecule 4: AP-2 COMPLEX SUBUNIT SIGMA

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.30Å 121.30Å 259.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.37 – 2.79 97.37 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.9 (97.37-2.79) 99.9 (97.37-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.203 , 0.259 0.204 , 0.259	Depositor DCC
R_{free} test set	2824 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13889	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0/4822	0.76	0/6541
2	B	0.53	0/4793	0.72	1/6503 (0.0%)
3	M	0.64	0/3255	0.82	2/4382 (0.0%)
4	S	0.78	0/1224	0.80	0/1650
All	All	0.62	0/14094	0.76	3/19076 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	162	ARG	NE-CZ-NH1	6.73	123.67	120.30
3	M	323	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	B	366	ASP	CB-CG-OD1	5.36	123.12	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4737	0	4830	64	0
2	B	4720	0	4831	180	1
3	M	3192	0	3295	55	0
4	S	1200	0	1195	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	36	0	6	1	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
All	All	13889	0	14157	290	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 290 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:A:198:ASP:O	1:A:232:ARG:NH2	2.01	0.92
1:A:495:ASN:O	1:A:499:VAL:HG23	1.71	0.88
2:B:204:ILE:HG22	2:B:208:LEU:HD12	1.59	0.85
1:A:365:ALA:O	1:A:368:THR:HB	1.75	0.84
2:B:211:LEU:O	2:B:211:LEU:HG	1.76	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLU:O	2:B:213:GLU:O[4_555]	2.10	0.10

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	598/628 (95%)	581 (97%)	17 (3%)	0	100 100
2	B	593/657 (90%)	522 (88%)	57 (10%)	14 (2%)	6 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	M	388/446 (87%)	364 (94%)	22 (6%)	2 (0%)	29 61
4	S	140/142 (99%)	135 (96%)	5 (4%)	0	100 100
All	All	1719/1873 (92%)	1602 (93%)	101 (6%)	16 (1%)	17 46

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	ASN
2	B	211	LEU
2	B	247	ARG
2	B	252	ASN
2	B	253	SER

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	526/548 (96%)	521 (99%)	5 (1%)	76 93
2	B	535/589 (91%)	516 (96%)	19 (4%)	35 69
3	M	353/398 (89%)	347 (98%)	6 (2%)	60 87
4	S	131/131 (100%)	130 (99%)	1 (1%)	81 94
All	All	1545/1666 (93%)	1514 (98%)	31 (2%)	55 84

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	253	SER
3	M	331	SER
2	B	282	LYS
3	M	348	GLU
3	M	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	305	ASN
4	S	46	HIS
2	B	435	ASN
4	S	48	ASN
3	M	72	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
6	IHP	A	1609	-	36,36,36	2.55	14 (38%)	54,60,60	2.35	13 (24%)

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
6	IHP	A	1609	-	-	10/30/54/54	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1609	IHP	P1-O41	4.69	1.72	1.54
6	A	1609	IHP	P1-O31	4.60	1.72	1.54
6	A	1609	IHP	P5-O35	4.44	1.72	1.54
6	A	1609	IHP	P5-O45	4.42	1.71	1.54
6	A	1609	IHP	P4-O44	4.37	1.71	1.54

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1609	IHP	O11-C1-C6	-8.32	89.08	108.69
6	A	1609	IHP	O16-C6-C5	6.85	124.83	108.69
6	A	1609	IHP	C6-C1-C2	5.73	122.96	110.41
6	A	1609	IHP	O15-C5-C4	5.01	120.51	108.69
6	A	1609	IHP	C4-C3-C2	-4.66	100.20	110.41

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1609	IHP	C1-C2-O12-P2
6	A	1609	IHP	C2-C3-O13-P3
6	A	1609	IHP	C4-C3-O13-P3
6	A	1609	IHP	C3-C4-O14-P4
6	A	1609	IHP	C5-C6-O16-P6

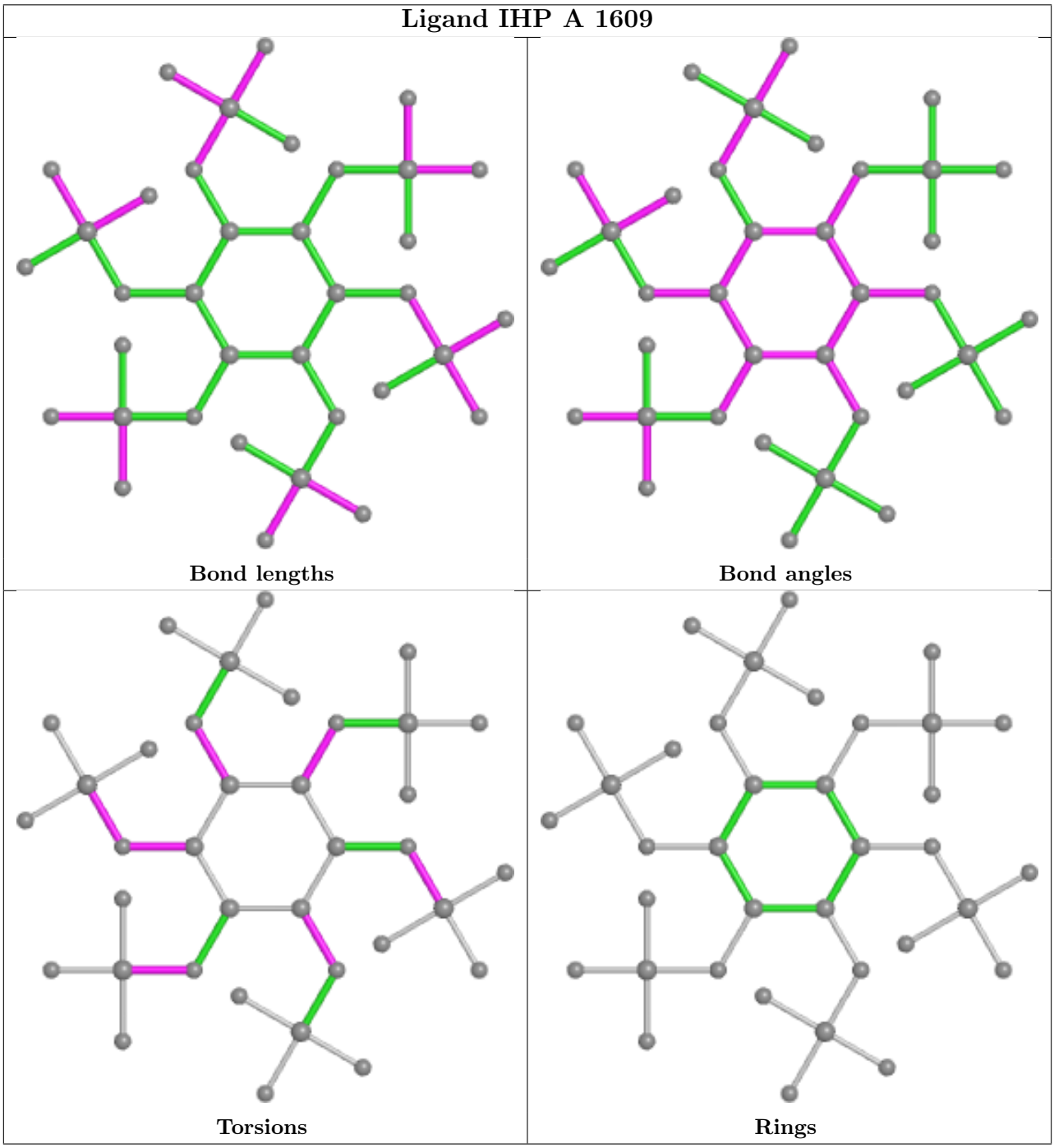
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1609	IHP	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.



5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	600/628 (95%)	0.27	6 (1%) 82 77	42, 72, 97, 130	0
2	B	597/657 (90%)	0.91	109 (18%) 1 1	69, 103, 136, 149	18 (3%)
3	M	396/446 (88%)	0.34	13 (3%) 46 36	48, 78, 111, 152	0
4	S	142/142 (100%)	0.23	0 100 100	45, 55, 74, 96	0
All	All	1735/1873 (92%)	0.50	128 (7%) 14 8	42, 81, 128, 152	18 (1%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	530	LEU	8.9
2	B	168	LEU	6.8
2	B	436	LEU	6.5
2	B	122	LEU	6.2
2	B	169	ILE	5.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

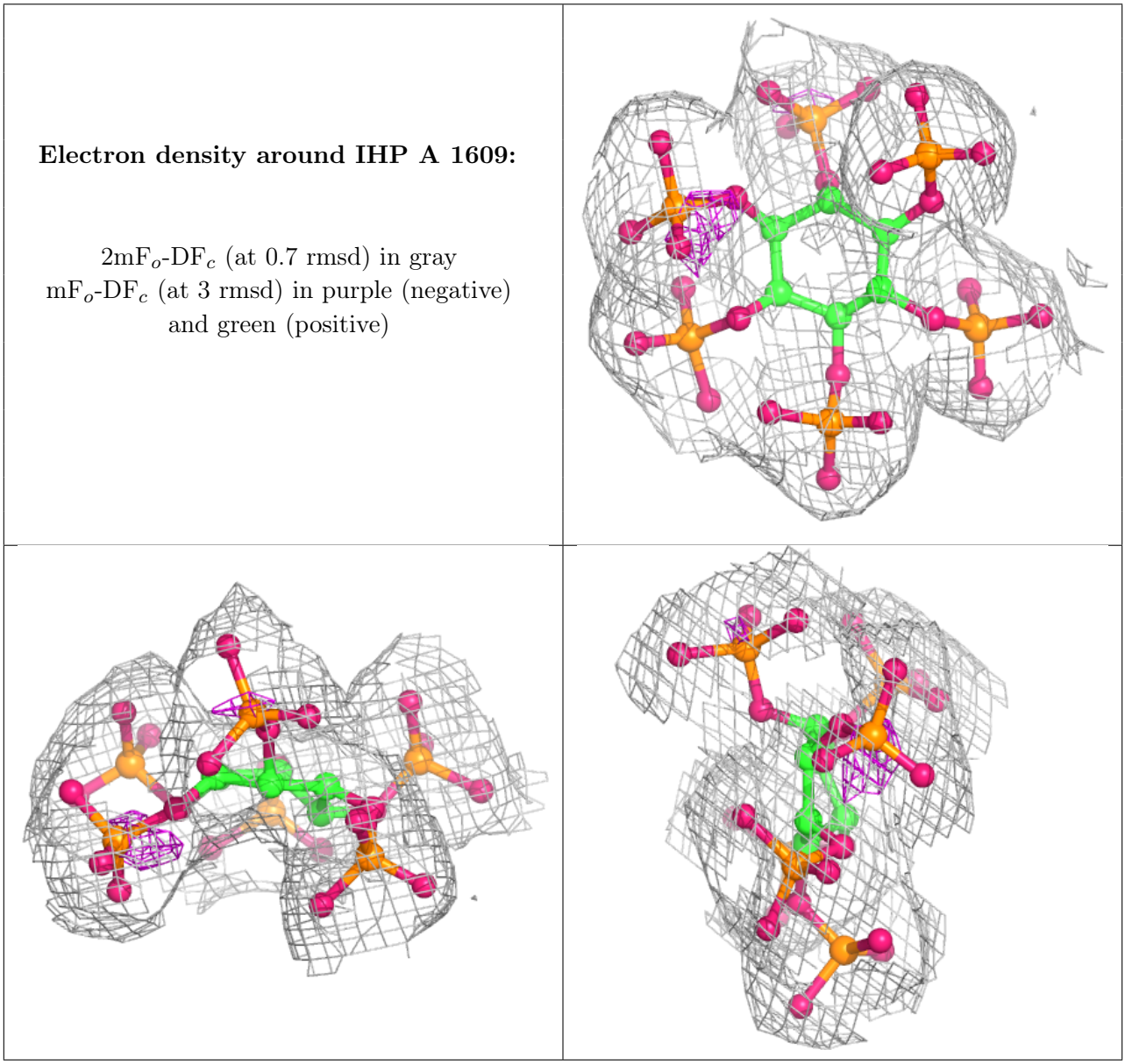
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IHP	A	1609	36/36	0.94	0.12	60,74,80,82	0
5	CL	A	1608	1/1	0.99	0.11	60,60,60,60	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 IHP A 1609:

$2mF_o$-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.