Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 12:39 AM EDT

PDB ID	:	2R0D
Title	:	Crystal Structure of Autoinhibited Form of Grp1 Arf GTPase Exchange Factor
Authors	:	DiNitto, J.P.; Delprato, A.; Gabe Lee, M.T.; Cronin, T.C.; Huang, S.; Guilherme, A.; Czech, M.P.; Lambright, D.G.
Deposited on	:	2007-08-18
Resolution	:	2.04 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	:	2.23.2
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)	:	2.23.2

1   Overall quality at a glance   ⓘ

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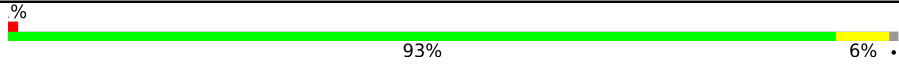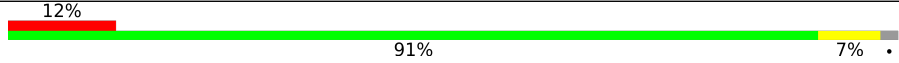*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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.
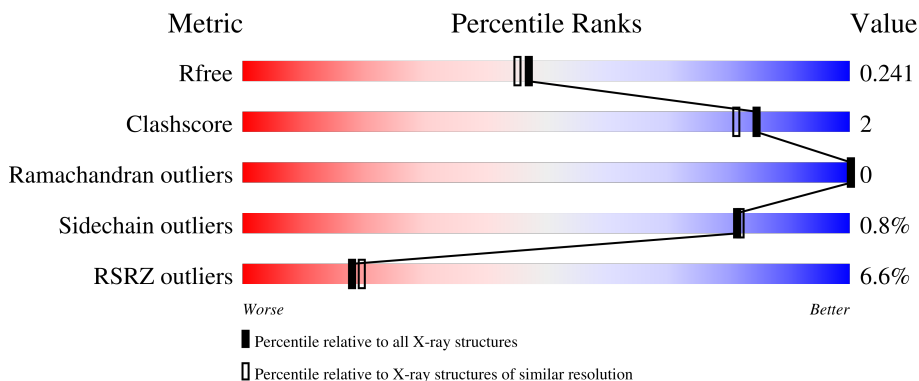
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	347	% 93% 6% ·
1	B	347	12% 91% 7% ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6231 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 Cytohesin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total 2806	C 1777	N 499	O 516	S 14	0	0	0
1	B	341	Total 2793	C 1768	N 497	O 514	S 14	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	MET	-	expression tag	UNP O08967
A	54	GLY	-	expression tag	UNP O08967
A	55	HIS	-	expression tag	UNP O08967
A	56	HIS	-	expression tag	UNP O08967
A	57	HIS	-	expression tag	UNP O08967
A	58	HIS	-	expression tag	UNP O08967
A	59	HIS	-	expression tag	UNP O08967
A	60	HIS	-	expression tag	UNP O08967
A	61	GLY	-	expression tag	UNP O08967
A	62	SER	-	expression tag	UNP O08967
A	68	ALA	LYS	engineered mutation	UNP O08967
B	53	MET	-	expression tag	UNP O08967
B	54	GLY	-	expression tag	UNP O08967
B	55	HIS	-	expression tag	UNP O08967
B	56	HIS	-	expression tag	UNP O08967
B	57	HIS	-	expression tag	UNP O08967
B	58	HIS	-	expression tag	UNP O08967
B	59	HIS	-	expression tag	UNP O08967
B	60	HIS	-	expression tag	UNP O08967
B	61	GLY	-	expression tag	UNP O08967
B	62	SER	-	expression tag	UNP O08967
B	68	ALA	LYS	engineered mutation	UNP O08967

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is INOSITOL-(1,3,4,5)-TETRAKISPHOSPHATE (three-letter code: 4IP) (formula: $C_6H_{16}O_{18}P_4$).
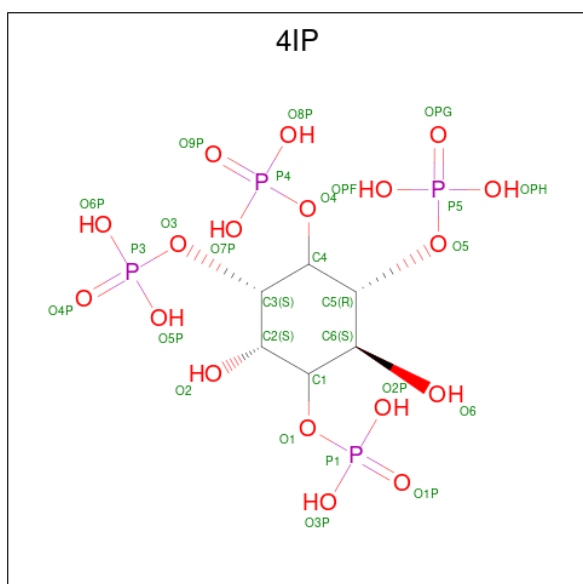
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 28	C 6	O 18	P 4	0	0
3	B	1	Total 28	C 6	O 18	P 4	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	B	1	Total 7	C 4	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	367	Total 367	O 367	0	0
5	B	168	Total 168	O 168	0	0

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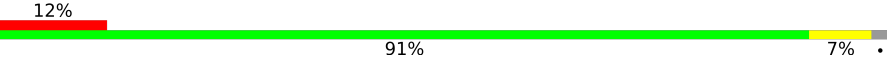
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cytohesin-3

Chain A:
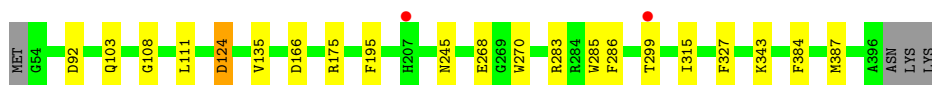
• Molecule 1: Cytohesin-3

Chain B:

4 Data and refinement statistics ⓘ

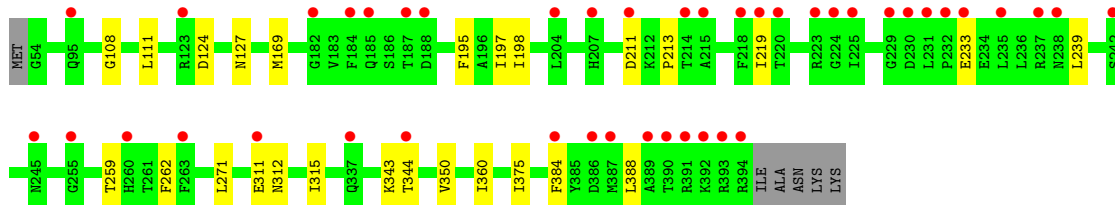| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.91Å 94.70Å 115.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.04 49.29 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.04) 99.0 (49.29-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.242 0.213 , 0.241	Depositor DCC
R_{free} test set	3253 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6231	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: PEG, 4IP, SO4

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	0.46	0/2874	0.52	0/3879
1	B	0.40	0/2861	0.50	0/3861
All	All	0.43	0/5735	0.51	0/7740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2806	0	2748	12	0
1	B	2793	0	2732	13	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	A	28	0	8	0	0
3	B	28	0	8	1	0
4	A	14	0	20	2	0
4	B	7	0	10	0	0
5	A	367	0	0	3	0
5	B	168	0	0	0	0
All	All	6231	0	5526	26	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 2.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:CE1	1:B:384:PHE:HE2	2.15	0.65
1:B:344:THR:HG22	1:B:350:VAL:HG22	1.80	0.62
1:A:270:TRP:HB2	4:A:404:PEG:H31	1.82	0.61
1:B:343:LYS:NZ	3:B:400:4IP:OPF	2.40	0.53
1:B:211:ASP:O	1:B:213:PRO:HD3	2.10	0.51
1:B:169:MET:HG3	1:B:195:PHE:CZ	2.46	0.51
1:A:268:GLU:HA	1:A:286:PHE:O	2.12	0.49
1:A:285:TRP:CD2	1:A:299:THR:HG22	2.48	0.48
1:A:315:ILE:HD11	1:A:327:PHE:CD1	2.48	0.48
1:B:315:ILE:HD11	1:B:375:ILE:HB	1.95	0.48
1:B:197:ILE:HD11	1:B:239:LEU:HD13	1.96	0.47
1:A:103:GLN:NE2	5:A:630:HOH:O	2.48	0.47
1:B:198:ILE:HG23	1:B:259:THR:HA	1.98	0.46
1:B:127:ASN:HD22	1:B:127:ASN:H	1.64	0.44
1:A:108:GLY:HA2	1:A:111:LEU:HD12	2.00	0.43
1:A:124:ASP:OD1	1:A:124:ASP:N	2.52	0.42
1:B:219:ILE:HD13	1:B:233:GLU:HG3	2.02	0.42
1:B:311:GLU:O	1:B:312:ASN:HB2	2.19	0.42
1:A:270:TRP:CE3	1:A:283:ARG:HG2	2.55	0.41
1:B:108:GLY:HA2	1:B:111:LEU:HD12	2.01	0.41
1:A:166:ASP:HB2	1:A:387:MET:CE	2.50	0.41
1:B:271:LEU:HD13	1:B:360:ILE:HG21	2.01	0.41
1:A:195:PHE:CZ	1:A:384:PHE:HZ	2.39	0.41
1:A:135:VAL:HG12	1:A:175:ARG:HG2	2.03	0.41
1:A:245:ASN:HB3	5:A:490:HOH:O	2.21	0.40
4:A:404:PEG:H12	5:A:722:HOH:O	2.21	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	341/347 (98%)	338 (99%)	3 (1%)	0	100	100
1	B	339/347 (98%)	332 (98%)	7 (2%)	0	100	100
All	All	680/694 (98%)	670 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	305/309 (99%)	302 (99%)	3 (1%)	76	75
1	B	304/309 (98%)	302 (99%)	2 (1%)	84	84
All	All	609/618 (98%)	604 (99%)	5 (1%)	81	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	124	ASP
1	A	343	LYS
1	B	124	ASP
1	B	388	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	B	65	GLN
1	B	86	GLN
1	B	127	ASN
1	B	208	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 ⓘ

9 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	$\#|Z| > 2$
4	PEG	A	404	-	6,6,6	0.43	0	5,5,5	0.25	0
2	SO4	A	401	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	1	-	4,4,4	0.23	0	6,6,6	0.40	0
2	SO4	A	400	-	4,4,4	0.15	0	6,6,6	0.14	0
3	4IP	A	402	-	28,28,28	0.79	0	42,46,46	1.00	3 (7%)
4	PEG	B	401	-	6,6,6	0.43	0	5,5,5	0.33	0
3	4IP	B	400	-	28,28,28	0.76	0	42,46,46	0.96	2 (4%)
4	PEG	A	403	-	6,6,6	0.48	0	5,5,5	0.24	0
2	SO4	B	1	-	4,4,4	0.16	0	6,6,6	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	404	-	-	3/4/4/4	-

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4IP	A	402	-	-	3/20/44/44	0/1/1/1
4	PEG	B	401	-	-	1/4/4/4	-
3	4IP	B	400	-	-	4/20/44/44	0/1/1/1
4	PEG	A	403	-	-	3/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	4IP	C5-C6-C1	2.38	113.90	108.96
3	B	400	4IP	O1-P1-O1P	-2.28	100.58	109.39
3	A	402	4IP	O6P-P3-O5P	2.16	115.91	107.64
3	A	402	4IP	O1-P1-O1P	-2.11	101.26	109.39
3	B	400	4IP	C5-C6-C1	2.06	113.25	108.96

There are no chirality outliers.

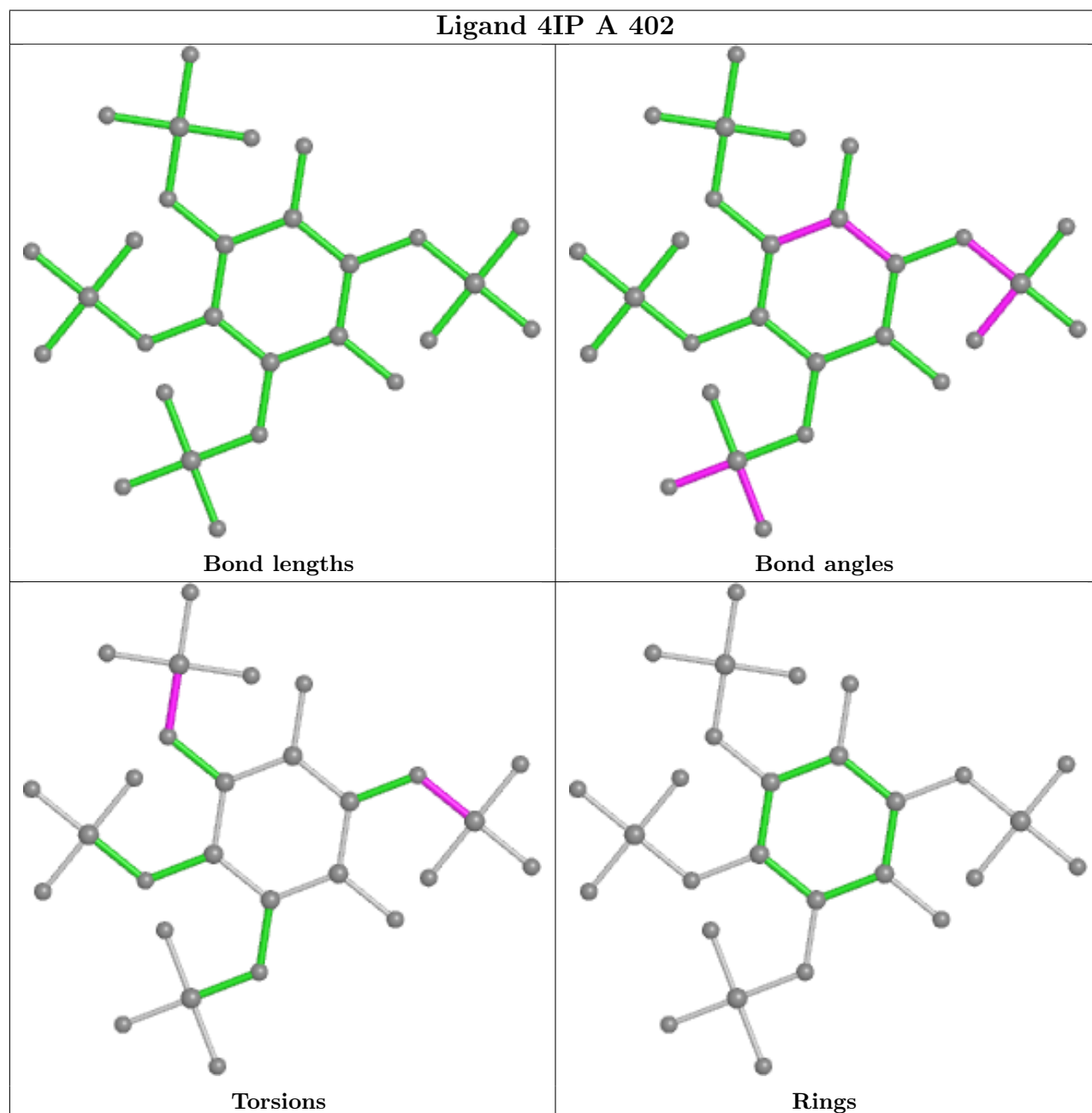All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	4IP	C1-O1-P1-O1P
3	A	402	4IP	C5-O5-P5-OPH
3	B	400	4IP	C1-O1-P1-O2P
3	B	400	4IP	C5-O5-P5-OPG
3	A	402	4IP	C5-O5-P5-OPG
3	B	400	4IP	C1-O1-P1-O1P
4	A	403	PEG	C1-C2-O2-C3
4	B	401	PEG	C1-C2-O2-C3
4	A	404	PEG	C4-C3-O2-C2
3	B	400	4IP	C5-O5-P5-OPH
4	A	404	PEG	O2-C3-C4-O4
4	A	403	PEG	C4-C3-O2-C2
4	A	404	PEG	C1-C2-O2-C3
4	A	403	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	PEG	2	0
3	B	400	4IP	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 4IP A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 4IP B 400

Bond lengths

Bond angles

Torsions

Rings
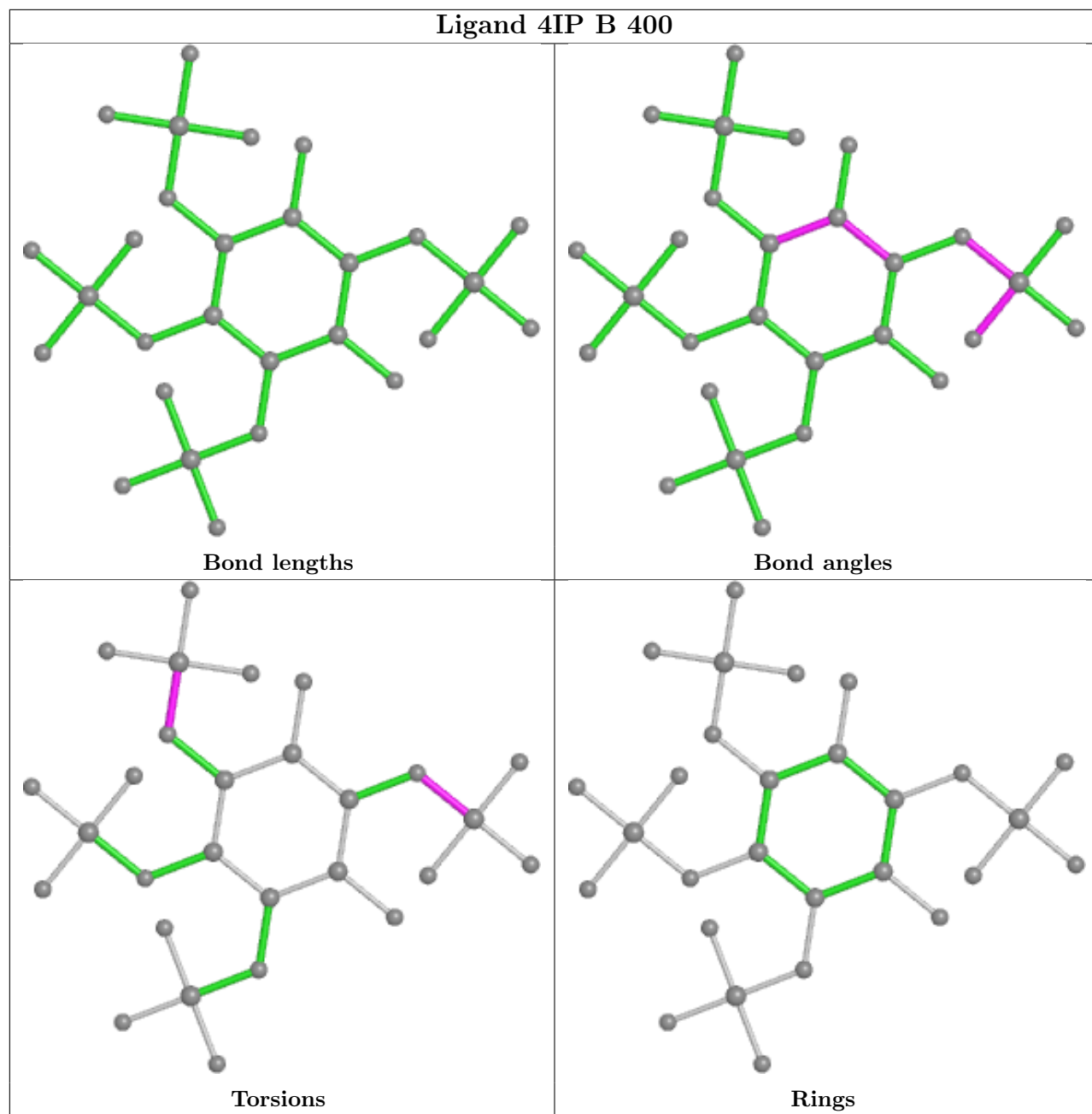
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	343/347 (98%)	0.16	2 (0%)	89	91	23, 33, 45, 52	0
1	B	341/347 (98%)	0.66	43 (12%)	3	3	28, 46, 75, 80	0
All	All	684/694 (98%)	0.41	45 (6%)	18	19	23, 38, 70, 80	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	ARG	6.5
1	B	235	LEU	5.1
1	B	184	PHE	4.8
1	B	392	LYS	4.7
1	B	233	GLU	4.2
1	B	391	ARG	4.0
1	B	219	ILE	3.9
1	B	393	ARG	3.8
1	B	123	ARG	3.8
1	B	245	ASN	3.7
1	B	389	ALA	3.7
1	B	225	ILE	3.6
1	B	231	LEU	3.5
1	B	220	THR	3.4
1	B	188	ASP	3.4
1	B	185	GLN	3.4
1	B	218	PHE	3.3
1	B	384	PHE	3.3
1	B	237	ARG	3.1
1	B	387	MET	3.0
1	B	214	THR	2.9
1	B	204	LEU	2.9
1	B	211	ASP	2.8
1	B	394	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	311	GLU	2.7
1	B	390	THR	2.6
1	B	187	THR	2.6
1	B	224	GLY	2.6
1	B	207	HIS	2.5
1	B	255	GLY	2.4
1	B	95	GLN	2.4
1	B	263	PHE	2.4
1	B	230	ASP	2.4
1	B	215	ALA	2.3
1	B	238	ASN	2.3
1	B	242	SER	2.3
1	B	337	GLN	2.3
1	B	229	GLY	2.1
1	B	232	PRO	2.1
1	B	386	ASP	2.1
1	A	299	THR	2.1
1	B	260	HIS	2.1
1	B	344	THR	2.1
1	B	182	GLY	2.1
1	A	207	HIS	2.0

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, 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
4	PEG	B	401	7/7	0.73	0.21	70,70,71,71	0
4	PEG	A	403	7/7	0.76	0.29	60,60,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	A	404	7/7	0.87	0.18	55,57,59,59	0
2	SO4	A	401	5/5	0.92	0.11	63,63,64,64	0
2	SO4	A	400	5/5	0.97	0.16	50,51,52,53	0
2	SO4	A	1	5/5	0.97	0.17	35,35,38,40	0
2	SO4	B	1	5/5	0.97	0.16	50,52,52,53	0
3	4IP	B	400	28/28	0.99	0.11	29,32,36,39	0
3	4IP	A	402	28/28	0.99	0.13	24,27,29,30	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 4IP B 400:

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

Electron density around 4IP A 402:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.