Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 10:14 PM EDT

PDB ID	:	9DP5
Title	:	Crystal Structure of Hydra Adenosine Deaminase Acting on RNA (ADAR) Deaminase Domain
Authors	:	Fisher, A.J.; Wilcox, X.E.
Deposited on	:	2024-09-20
Resolution	:	2.00 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:

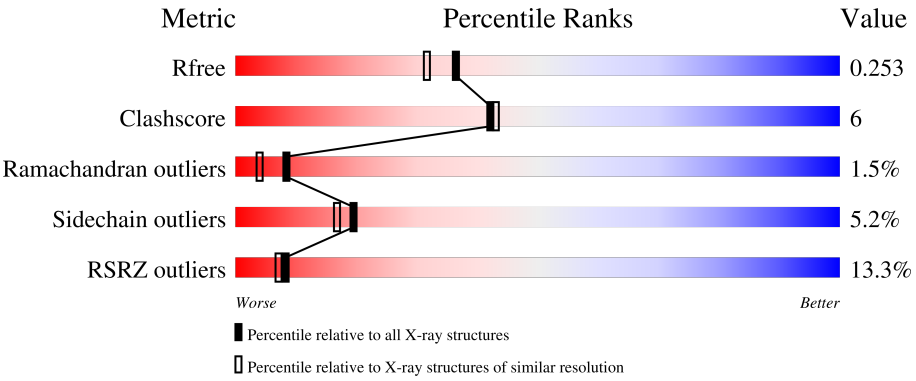
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	372	12% 80% 11% • 6%
1	B	372	13% 74% 16% • • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5683 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.

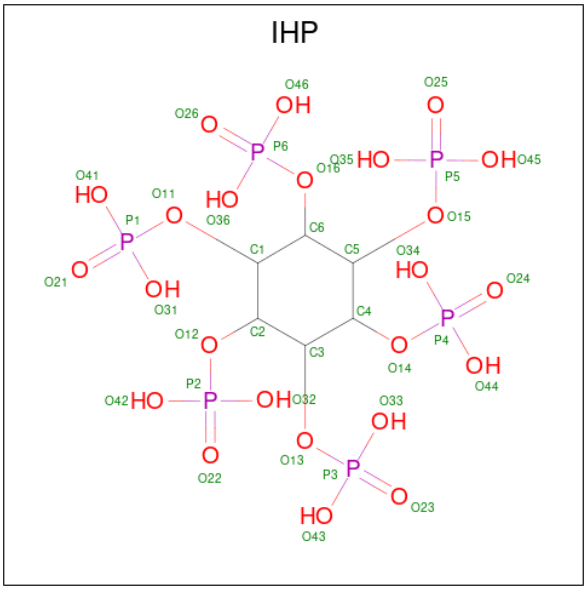
- Molecule 1 is a protein called Double-stranded RNA-specific editase Adar-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	2	0
			2768	1773	475	507	13			
1	B	349	Total	C	N	O	S	0	0	0
			2728	1746	462	507	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

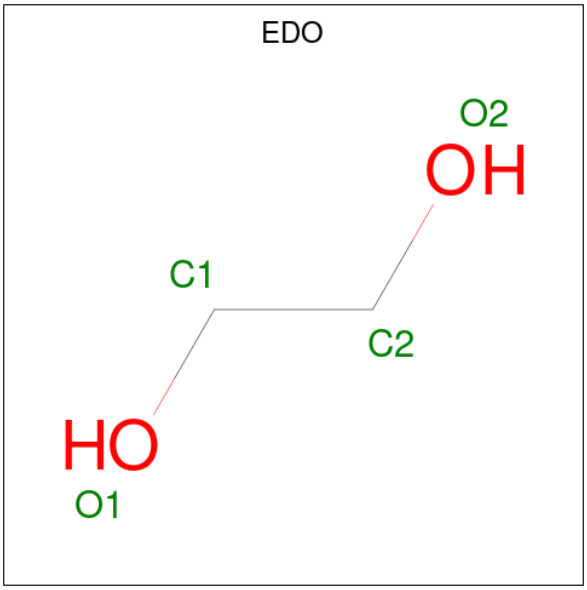
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

- Molecule 6 is water.

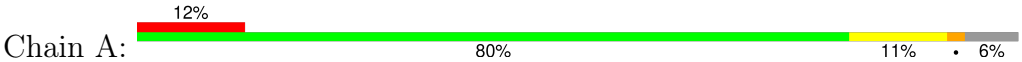
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	0
6	B	49	Total O 49 49	0	0

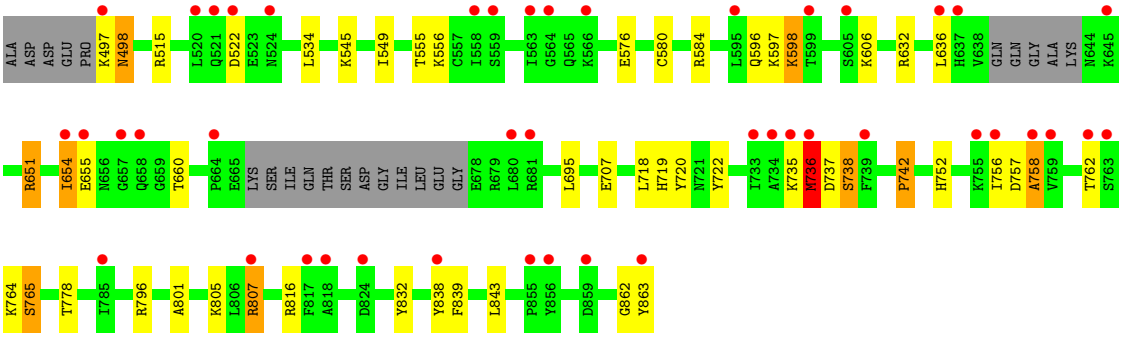
3 Residue-property plots (i)

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: Double-stranded RNA-specific editase Adar-like

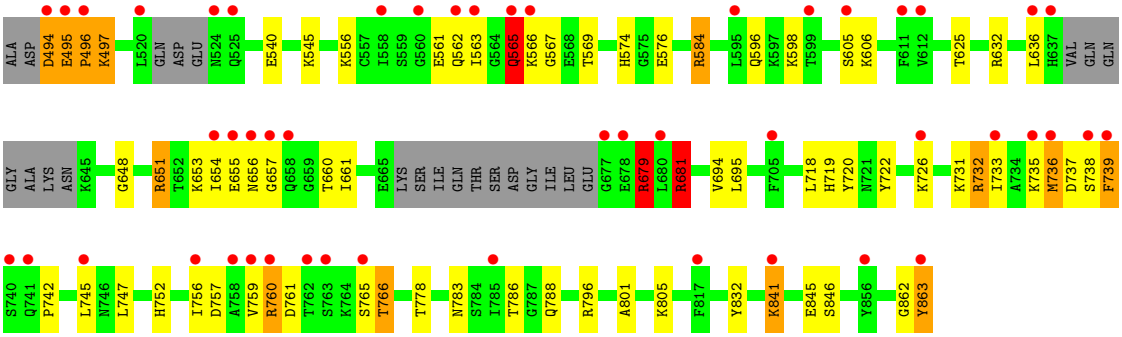
Chain A:





• Molecule 1: Double-stranded RNA-specific editase Adar-like

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.40Å 49.44Å 83.04Å 83.11° 80.17° 71.06°	Depositor
Resolution (Å)	39.38 – 2.00 39.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (39.38-2.00) 95.0 (39.38-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.211 , 0.243 0.222 , 0.253	Depositor DCC
R_{free} test set	2660 reflections (5.40%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.088 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5683	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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 (i)

5.1 Standard geometry (i)

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

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	0.42	0/2828	0.81	4/3809 (0.1%)
1	B	0.40	0/2781	0.85	10/3750 (0.3%)
All	All	0.41	0/5609	0.83	14/7559 (0.2%)

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	A	0	3
1	B	0	4
All	All	0	7

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	651	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	B	651	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	B	863	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	B	863	TYR	CB-CG-CD1	7.80	125.68	121.00
1	A	807	ARG	CB-CG-CD	-6.86	93.76	111.60
1	B	540	GLU	CB-CA-C	6.85	124.11	110.40
1	A	651	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	540	GLU	N-CA-CB	-6.40	99.09	110.60
1	B	841	LYS	N-CA-CB	6.10	121.58	110.60
1	B	863	TYR	CA-CB-CG	5.95	124.70	113.40
1	B	576	GLU	CB-CA-C	-5.43	99.54	110.40
1	B	863	TYR	N-CA-CB	-5.29	101.09	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	584	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	576	GLU	CB-CA-C	-5.17	100.06	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	ARG	Sidechain
1	A	807	ARG	Sidechain
1	A	816	ARG	Sidechain
1	B	584	ARG	Sidechain
1	B	679	ARG	Sidechain
1	B	732	ARG	Sidechain
1	B	760	ARG	Sidechain

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	2768	0	2798	25	0
1	B	2728	0	2726	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	6	0	0
3	B	36	0	6	0	0
4	A	8	0	12	0	0
4	B	16	0	24	2	0
5	A	1	0	0	0	0
6	A	39	0	0	0	0
6	B	49	0	0	0	0
All	All	5683	0	5572	69	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 (69) 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:497:LYS:O	1:A:722:TYR:OH	1.91	0.88
1:B:574:HIS:HE2	1:B:657:GLY:HA3	1.44	0.79
1:B:733:ILE:HD12	1:B:736:MET:HG3	1.73	0.69
1:B:654:ILE:HD11	1:B:661:ILE:HG23	1.75	0.69
1:B:783:ASN:HB3	1:B:786:THR:HG22	1.77	0.67
1:B:653:LYS:HB3	1:B:657:GLY:HA2	1.77	0.66
1:A:707:GLU:OE1	1:A:742:PRO:HG3	1.97	0.64
1:B:494:ASP:C	1:B:496:PRO:HD3	2.21	0.61
1:A:862:GLY:O	1:A:863:TYR:HB2	2.00	0.60
1:B:862:GLY:O	1:B:863:TYR:HB2	2.01	0.60
1:B:718:LEU:HD21	1:B:756:ILE:HG21	1.85	0.57
1:A:778:THR:HG23	1:A:796:ARG:HH12	1.71	0.56
1:B:737:ASP:O	1:B:738:SER:C	2.45	0.54
1:B:625:THR:HG23	1:B:718:LEU:HB2	1.90	0.54
1:B:745:LEU:HD21	1:B:747:LEU:HD21	1.91	0.52
1:B:574:HIS:NE2	1:B:657:GLY:HA3	2.21	0.52
1:B:745:LEU:CD2	1:B:747:LEU:HD21	2.39	0.52
1:B:569:THR:HB	4:B:905:EDO:O2	2.10	0.51
1:B:625:THR:HG22	1:B:632:ARG:HH12	1.76	0.51
1:A:720:TYR:CD2	1:A:752:HIS:HB2	2.46	0.50
1:A:555:THR:HG21	1:A:765:SER:HB2	1.93	0.50
1:A:718:LEU:HG	1:A:756:ILE:HG12	1.93	0.49
1:A:757:ASP:O	1:A:758:ALA:CB	2.59	0.49
1:A:580:CYS:SG	1:A:584[A]:ARG:NH1	2.85	0.49
1:B:718:LEU:CD2	1:B:756:ILE:HG21	2.43	0.49
1:B:733:ILE:CD1	1:B:736:MET:HG3	2.43	0.48
1:B:778:THR:HG23	1:B:796:ARG:HH12	1.78	0.48
1:A:737:ASP:O	1:A:738:SER:C	2.51	0.48
1:B:632:ARG:HH22	1:B:719:HIS:CE1	2.32	0.48
1:A:555:THR:HG23	1:A:556:LYS:HG2	1.96	0.48
1:B:556:LYS:HA	1:B:656:ASN:O	2.14	0.47
1:B:720:TYR:CD2	1:B:752:HIS:HB2	2.48	0.47
1:A:736:MET:O	1:A:838:TYR:OH	2.28	0.47
1:B:679:ARG:HH22	1:B:681:ARG:HE	1.61	0.47
1:A:632[B]:ARG:HH22	1:A:719:HIS:CE1	2.33	0.47
1:A:596:GLN:HB3	1:A:598:LYS:HE3	1.95	0.47
1:A:735:LYS:O	1:A:736:MET:C	2.54	0.46
1:B:694:VAL:HG13	1:B:739:PHE:CZ	2.51	0.46
1:B:731:LYS:HA	1:B:731:LYS:HD2	1.55	0.45
1:B:565:GLN:C	1:B:567:GLY:H	2.19	0.45
1:A:606:LYS:O	1:A:606:LYS:HG2	2.16	0.45
1:B:786:THR:HG23	1:B:788:GLN:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ARG:HD3	1:A:660:THR:OG1	2.17	0.44
1:B:651:ARG:HD3	1:B:660:THR:OG1	2.18	0.44
1:B:718:LEU:CD2	1:B:756:ILE:HG12	2.47	0.44
1:A:718:LEU:CD2	1:A:756:ILE:HG21	2.48	0.44
1:B:494:ASP:HB3	1:B:495:GLU:H	1.72	0.43
1:A:497:LYS:O	1:A:498:ASN:HB3	2.18	0.43
1:A:534:LEU:HG	1:A:549:ILE:HG13	2.00	0.43
1:B:695:LEU:HB3	1:B:832:TYR:CE2	2.54	0.43
1:B:565:GLN:HE21	1:B:565:GLN:HB2	1.70	0.43
1:A:801:ALA:O	1:A:805:LYS:HG2	2.19	0.42
1:B:765:SER:O	1:B:766:THR:HG22	2.19	0.42
1:B:801:ALA:O	1:B:805:LYS:HG2	2.20	0.42
1:B:722:TYR:OH	1:B:726:LYS:NZ	2.43	0.42
1:B:694:VAL:HG13	1:B:739:PHE:HZ	1.84	0.41
1:B:596:GLN:NE2	1:B:598:LYS:HE3	2.35	0.41
1:A:757:ASP:O	1:A:758:ALA:HB3	2.19	0.41
1:B:497:LYS:HD2	1:B:497:LYS:HA	1.44	0.41
1:B:632:ARG:HH12	1:B:719:HIS:CD2	2.38	0.41
1:B:733:ILE:HG22	1:B:846:SER:CB	2.51	0.41
1:A:654:ILE:HG23	1:A:655:GLU:HB2	2.03	0.41
1:A:839:PHE:CZ	1:A:843:LEU:HD11	2.56	0.41
1:B:783:ASN:HB3	1:B:786:THR:CG2	2.48	0.41
1:B:545:LYS:HA	4:B:903:EDO:H12	2.03	0.40
1:A:695:LEU:HB3	1:A:832:TYR:CE2	2.57	0.40
1:B:648:GLY:O	1:B:732:ARG:HD3	2.21	0.40
1:B:841:LYS:O	1:B:845:GLU:HG2	2.22	0.40
1:B:494:ASP:O	1:B:496:PRO:HD3	2.21	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	346/372 (93%)	321 (93%)	21 (6%)	4 (1%)	11 6
1	B	341/372 (92%)	310 (91%)	25 (7%)	6 (2%)	7 3
All	All	687/744 (92%)	631 (92%)	46 (7%)	10 (2%)	8 4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	ALA
1	B	759	VAL
1	A	498	ASN
1	A	522	ASP
1	B	496	PRO
1	B	681	ARG
1	B	735	LYS
1	A	736	MET
1	B	655	GLU
1	B	565	GLN

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	302/321 (94%)	291 (96%)	11 (4%)	30 30
1	B	296/321 (92%)	276 (93%)	20 (7%)	13 10
All	All	598/642 (93%)	567 (95%)	31 (5%)	19 17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	545	LYS
1	A	597	LYS
1	A	598	LYS
1	A	636	LEU
1	A	654	ILE
1	A	736	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	738	SER
1	A	742	PRO
1	A	762	THR
1	A	764	LYS
1	A	765	SER
1	B	494	ASP
1	B	495	GLU
1	B	497	LYS
1	B	561	GLU
1	B	562	GLN
1	B	563	ILE
1	B	565	GLN
1	B	566	LYS
1	B	605	SER
1	B	606	LYS
1	B	636	LEU
1	B	679	ARG
1	B	681	ARG
1	B	736	MET
1	B	739	PHE
1	B	742	PRO
1	B	757	ASP
1	B	760	ARG
1	B	761	ASP
1	B	766	THR

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

Mol	Chain	Res	Type
1	A	525	GLN
1	B	498	ASN
1	B	562	GLN
1	B	565	GLN
1	B	596	GLN
1	B	858	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	EDO	B	906	-	3,3,3	0.16	0	2,2,2	0.31	0
4	EDO	A	903	-	3,3,3	0.10	0	2,2,2	0.24	0
4	EDO	B	905	-	3,3,3	0.21	0	2,2,2	0.26	0
4	EDO	B	904	-	3,3,3	0.22	0	2,2,2	0.28	0
4	EDO	A	904	-	3,3,3	0.26	0	2,2,2	0.26	0
3	IHP	A	902	-	36,36,36	1.13	4 (11%)	60,60,60	2.16	13 (21%)
3	IHP	B	902	-	36,36,36	1.08	2 (5%)	60,60,60	2.08	15 (25%)
4	EDO	B	903	-	3,3,3	0.09	0	2,2,2	0.27	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	EDO	B	906	-	-	1/1/1/1	-
4	EDO	A	903	-	-	1/1/1/1	-
4	EDO	B	905	-	-	1/1/1/1	-
4	EDO	B	904	-	-	0/1/1/1	-
4	EDO	A	904	-	-	1/1/1/1	-
3	IHP	A	902	-	-	2/30/54/54	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IHP	B	902	-	-	3/30/54/54	0/1/1/1
4	EDO	B	903	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	IHP	P1-O11	3.39	1.65	1.59
3	B	902	IHP	P1-O11	2.87	1.64	1.59
3	B	902	IHP	P5-O15	2.81	1.64	1.59
3	A	902	IHP	P3-O13	2.43	1.63	1.59
3	A	902	IHP	P2-O32	-2.26	1.46	1.54
3	A	902	IHP	P5-O15	2.03	1.63	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	IHP	P4-O14-C4	11.20	153.35	123.43
3	B	902	IHP	P4-O14-C4	9.99	150.12	123.43
3	A	902	IHP	C5-C4-C3	4.90	121.17	110.43
3	B	902	IHP	C5-C4-C3	4.53	120.37	110.43
3	B	902	IHP	P3-O13-C3	-4.22	112.17	123.43
3	A	902	IHP	P3-O13-C3	-4.18	112.27	123.43
3	A	902	IHP	O14-C4-C5	3.47	116.14	108.76
3	B	902	IHP	P5-O15-C5	-3.35	114.50	123.43
3	A	902	IHP	O15-C5-C4	3.31	115.80	108.76
3	B	902	IHP	O14-C4-C5	3.20	115.56	108.76
3	B	902	IHP	O13-C3-C4	2.86	114.85	108.76
3	B	902	IHP	C6-C5-C4	2.77	116.50	110.43
3	B	902	IHP	O15-C5-C4	2.73	114.58	108.76
3	A	902	IHP	P5-O15-C5	-2.67	116.31	123.43
3	A	902	IHP	O13-C3-C4	2.66	114.41	108.76
3	B	902	IHP	C4-C3-C2	2.64	116.23	110.43
3	B	902	IHP	O14-C4-C3	2.63	114.36	108.76
3	A	902	IHP	O16-C6-C5	-2.58	103.27	108.76
3	A	902	IHP	C4-C3-C2	2.57	116.07	110.43
3	B	902	IHP	O11-P1-O21	-2.46	100.55	109.33
3	B	902	IHP	O44-P4-O14	-2.38	96.57	105.85
3	A	902	IHP	C6-C5-C4	2.36	115.60	110.43
3	B	902	IHP	O16-C6-C5	-2.32	103.83	108.76
3	B	902	IHP	O12-C2-C3	2.30	113.65	108.76
3	A	902	IHP	O12-C2-C3	2.24	113.52	108.76
3	B	902	IHP	O32-P2-O12	2.15	114.21	105.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	IHP	O12-P2-O22	2.05	116.63	109.33
3	A	902	IHP	O14-C4-C3	2.04	113.11	108.76

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	IHP	C5-C4-O14-P4
3	B	902	IHP	C5-C4-O14-P4
4	B	905	EDO	O1-C1-C2-O2
4	A	903	EDO	O1-C1-C2-O2
4	B	906	EDO	O1-C1-C2-O2
3	A	902	IHP	C4-O14-P4-O34
4	A	904	EDO	O1-C1-C2-O2
4	B	903	EDO	O1-C1-C2-O2
3	B	902	IHP	C5-O15-P5-O35
3	B	902	IHP	C3-C4-O14-P4

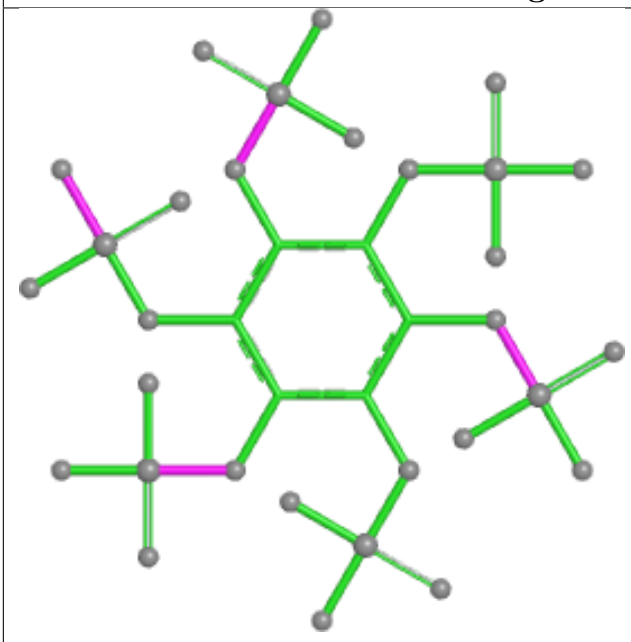
There are no ring outliers.

2 monomers are involved in 2 short contacts:

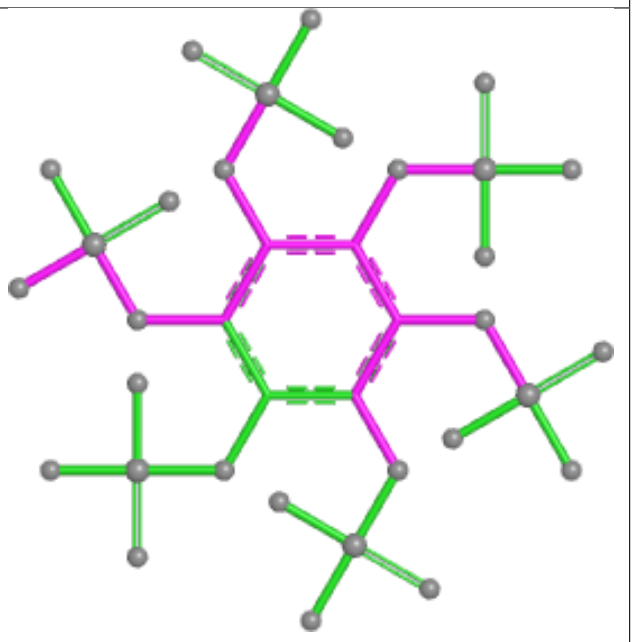
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	905	EDO	1	0
4	B	903	EDO	1	0

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.

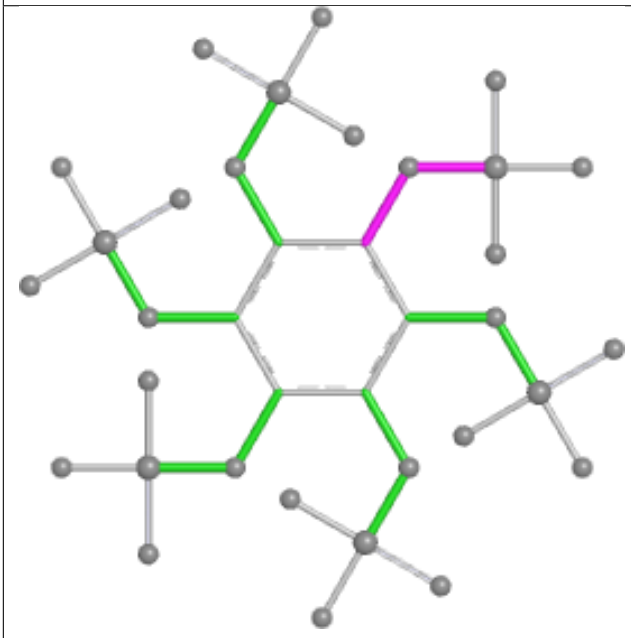
Ligand IHP A 902



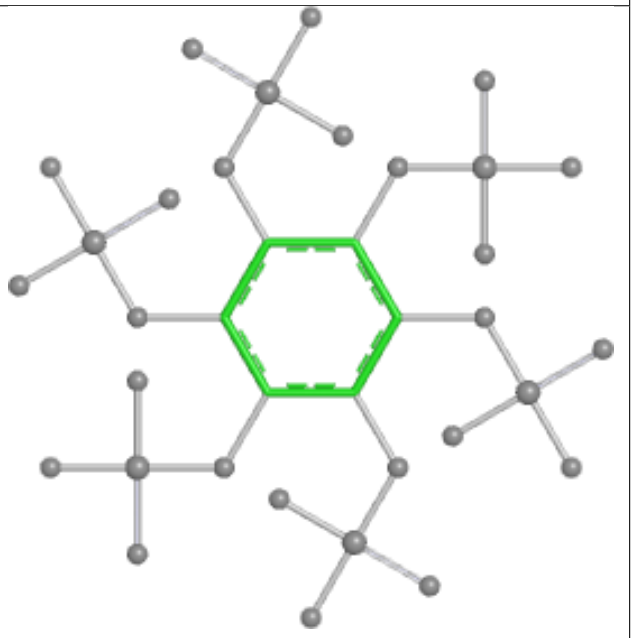
Bond lengths



Bond angles

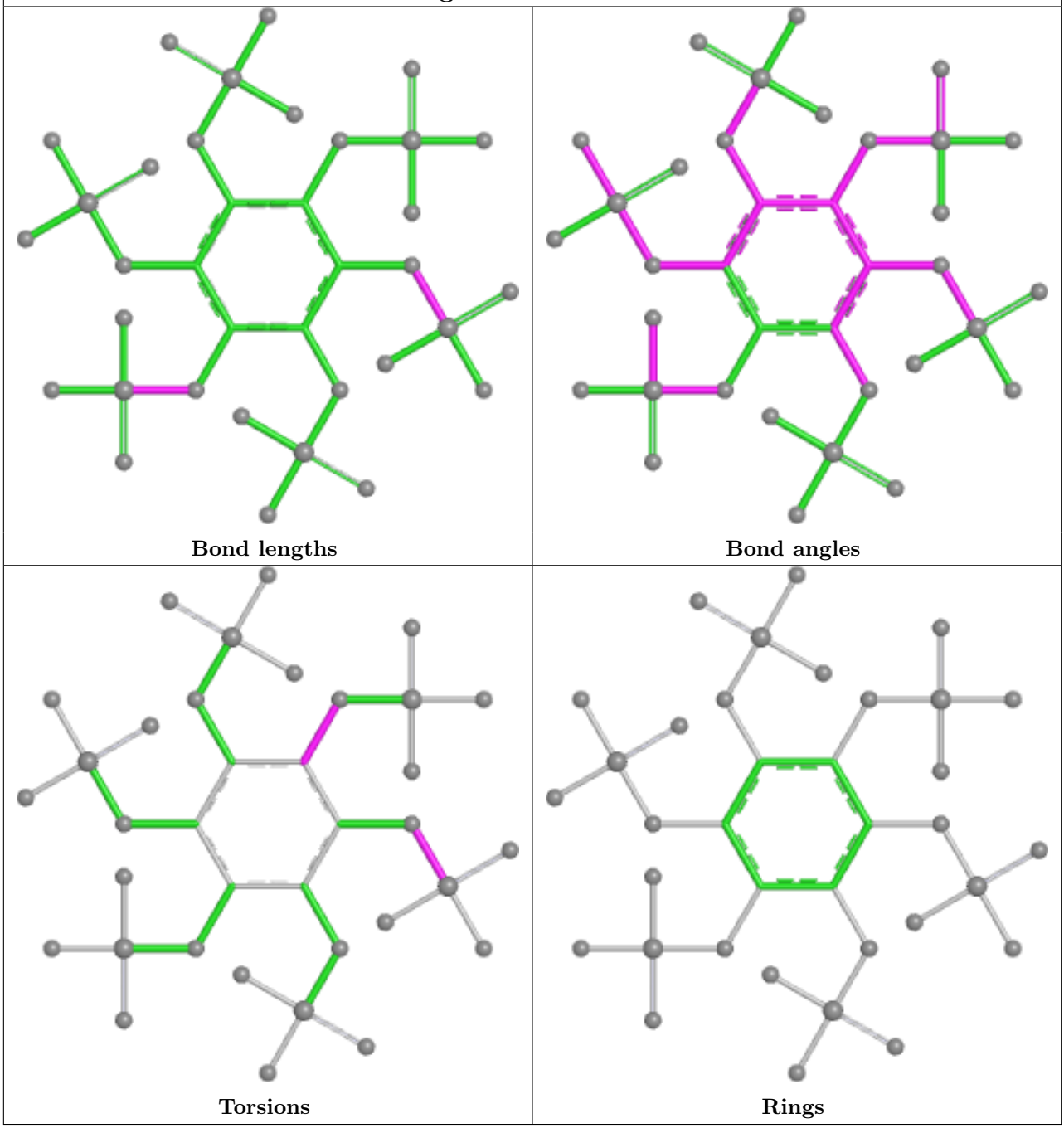


Torsions



Rings

Ligand IHP B 902



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, 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	350/372 (94%)	0.83	44 (12%)	9	8	18, 48, 106, 139	2 (0%)
1	B	349/372 (93%)	0.92	49 (14%)	7	6	24, 47, 109, 150	0
All	All	699/744 (93%)	0.88	93 (13%)	8	7	18, 47, 109, 150	2 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	654	ILE	6.8
1	A	680	LEU	5.3
1	B	736	MET	5.3
1	B	680	LEU	5.1
1	B	657	GLY	5.1
1	B	656	ASN	5.0
1	B	756	ILE	4.8
1	B	494	ASP	4.7
1	A	734	ALA	4.6
1	B	759	VAL	4.4
1	B	758	ALA	4.3
1	A	856	TYR	4.3
1	A	521	GLN	4.3
1	B	496	PRO	4.0
1	B	677	GLY	3.9
1	B	520	LEU	3.9
1	A	756	ILE	3.9
1	A	863	TYR	3.7
1	B	863	TYR	3.7
1	A	763	SER	3.6
1	A	599	THR	3.5
1	A	657	GLY	3.5
1	A	637	HIS	3.5
1	B	637	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	658	GLN	3.4
1	B	856	TYR	3.4
1	B	762	THR	3.3
1	A	520	LEU	3.1
1	A	522	ASP	3.1
1	A	736	MET	3.1
1	A	762	THR	3.0
1	A	658	GLN	3.0
1	A	564	GLY	3.0
1	B	739	PHE	3.0
1	A	759	VAL	3.0
1	B	563	ILE	3.0
1	B	763	SER	3.0
1	A	497	LYS	3.0
1	B	495	GLU	2.9
1	A	563	ILE	2.9
1	B	636	LEU	2.9
1	B	765	SER	2.9
1	B	733	ILE	2.9
1	B	740	SER	2.8
1	B	565	GLN	2.8
1	B	654	ILE	2.8
1	B	678	GLU	2.8
1	A	636	LEU	2.7
1	B	735	LYS	2.7
1	A	664	PRO	2.7
1	B	524	ASN	2.7
1	B	760	ARG	2.6
1	A	559	SER	2.6
1	A	739	PHE	2.6
1	A	733	ILE	2.6
1	B	745	LEU	2.5
1	B	738	SER	2.5
1	A	655	GLU	2.5
1	A	859	ASP	2.5
1	A	818	ALA	2.4
1	B	817	PHE	2.4
1	A	807	ARG	2.4
1	B	605	SER	2.3
1	A	524	ASN	2.3
1	B	599	THR	2.3
1	A	735	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	566	LYS	2.3
1	A	595	LEU	2.3
1	B	525	GLN	2.3
1	B	655	GLU	2.3
1	B	726	LYS	2.3
1	B	785	ILE	2.2
1	B	562	GLN	2.2
1	A	824	ASP	2.2
1	B	611	PHE	2.2
1	B	560	GLY	2.2
1	A	855	PRO	2.2
1	B	841	LYS	2.2
1	A	558	ILE	2.2
1	A	785	ILE	2.2
1	B	741	GLN	2.2
1	B	705	PHE	2.2
1	B	558	ILE	2.2
1	A	605	SER	2.1
1	A	755	LYS	2.1
1	A	817	PHE	2.1
1	B	595	LEU	2.1
1	A	645	LYS	2.1
1	A	681	ARG	2.1
1	A	758	ALA	2.1
1	A	566	LYS	2.0
1	A	838	TYR	2.0
1	B	612	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 monosaccharides 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,

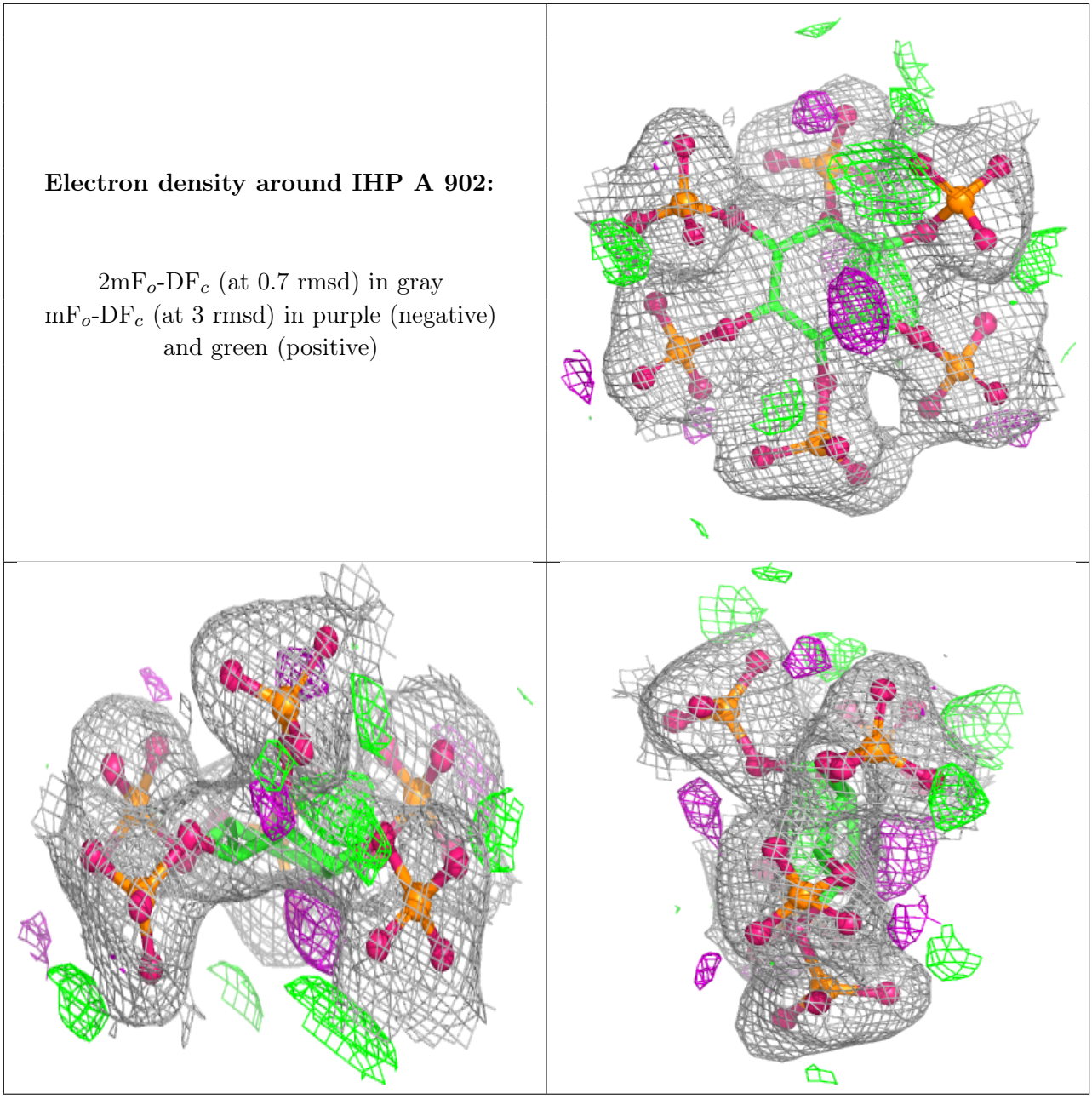
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	906	4/4	0.77	0.15	65,70,70,72	0
4	EDO	B	903	4/4	0.82	0.17	61,67,68,71	0
4	EDO	B	904	4/4	0.85	0.19	68,72,72,78	0
4	EDO	A	903	4/4	0.85	0.13	66,70,74,78	0
4	EDO	B	905	4/4	0.88	0.13	71,72,74,78	0
4	EDO	A	904	4/4	0.88	0.12	56,63,64,64	0
3	IHP	A	902	36/36	0.96	0.07	28,36,43,47	0
3	IHP	B	902	36/36	0.96	0.07	28,36,42,44	0
5	CL	A	905	1/1	0.98	0.04	41,41,41,41	0
2	ZN	B	901	1/1	1.00	0.02	31,31,31,31	0
2	ZN	A	901	1/1	1.00	0.02	30,30,30,30	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.

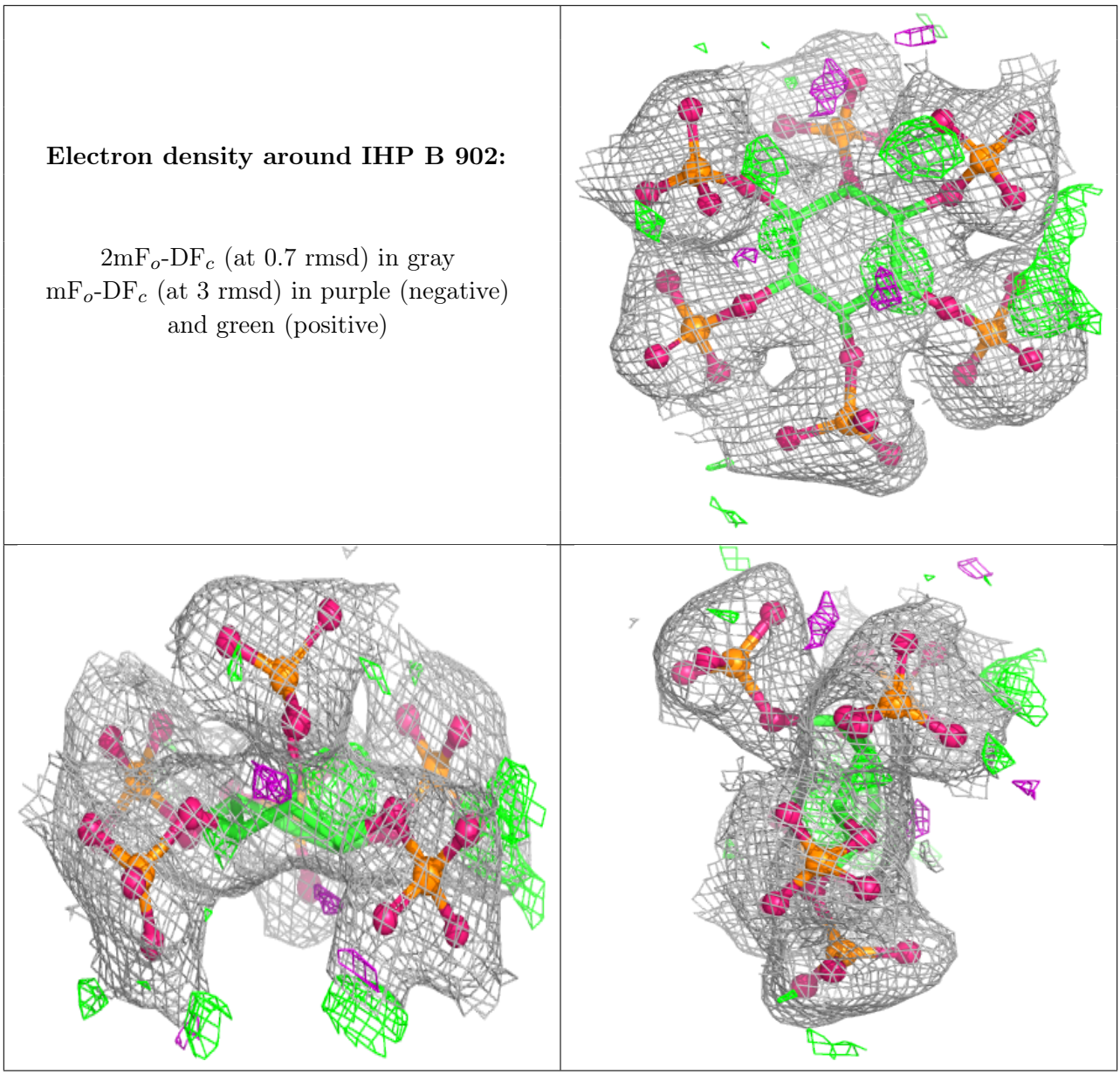
Electron density around IHP A 902:

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



Electron density around IHP B 902:

$2mF_o$-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.