



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:57 AM UTC

PDB ID : 9D5J / pdb_00009d5j
Title : Human Adenosine Deaminase Acting on dsRNA (ADAR2-RD) bound to dsRNA containing deoxyinosine at the -1 position of the guide strand
Authors : Fisher, A.J.; Cheng, J.; Manjunath, A.; Campbell, K.
Deposited on : 2024-08-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

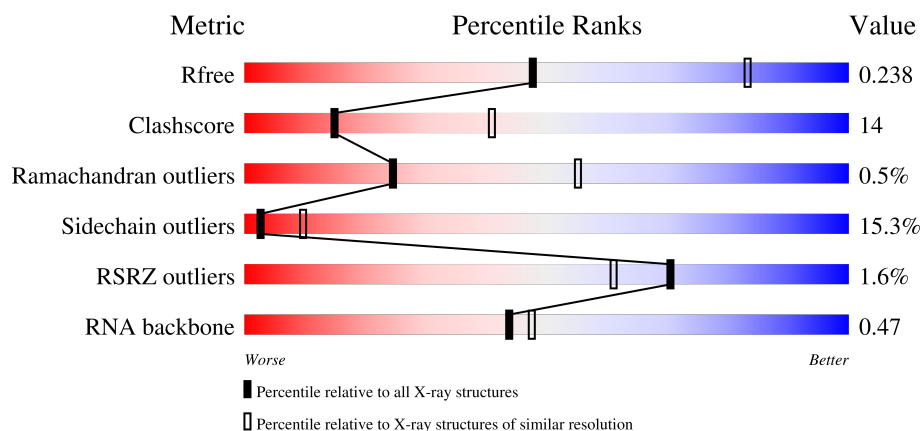
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	 46% 29% 21% 3%
1	B	487	 56% 31% 6% 7% 3%
2	C	32	 38% 53% 6% 3%
3	D	32	 62% 34% 4%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8019 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 Isoform 4 of Double-stranded RNA-specific editase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3019	1904	550	554	11			
1	B	454	Total	C	N	O	S	0	0	0
			3540	2235	639	653	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	488	GLN	GLU	engineered mutation	UNP P78563
B	488	GLN	GLU	engineered mutation	UNP P78563

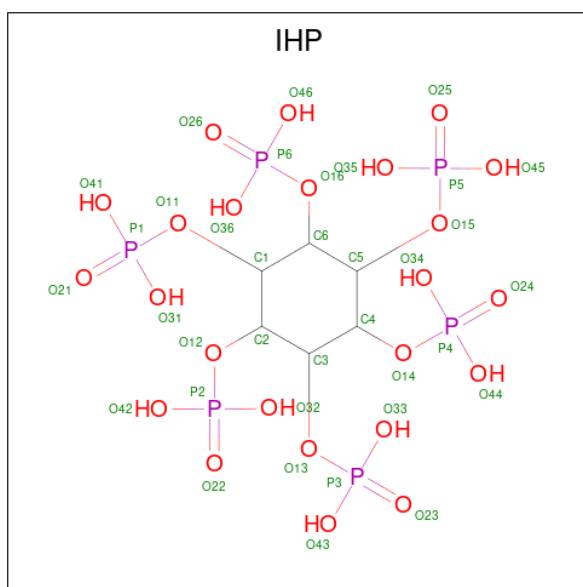
- Molecule 2 is a RNA chain called RNA Top Strand Containing 8-azanebularine (8AZ).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	32	Total	C	N	O	P	0	0	0
			685	305	126	223	31			

- Molecule 3 is DNA/RNA hybrid called RNA Bottom Strand containing deoxyinosine complementary to a guanosine adjacent to the target site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	32	Total	C	N	O	P	0	0	0
			674	303	121	219	31			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).

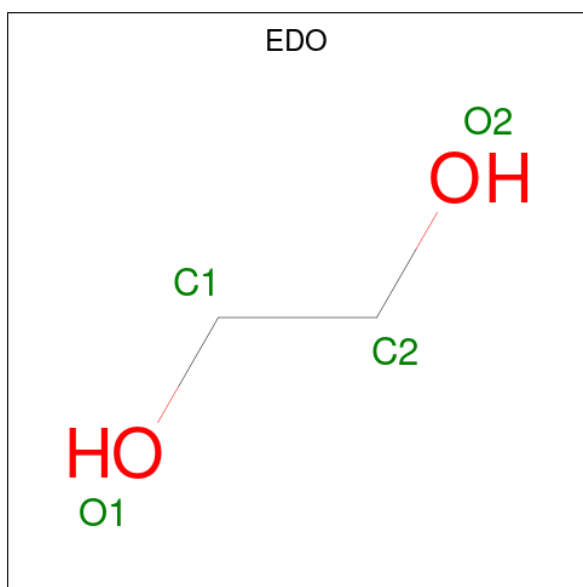


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			36	6	24	6		
4	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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

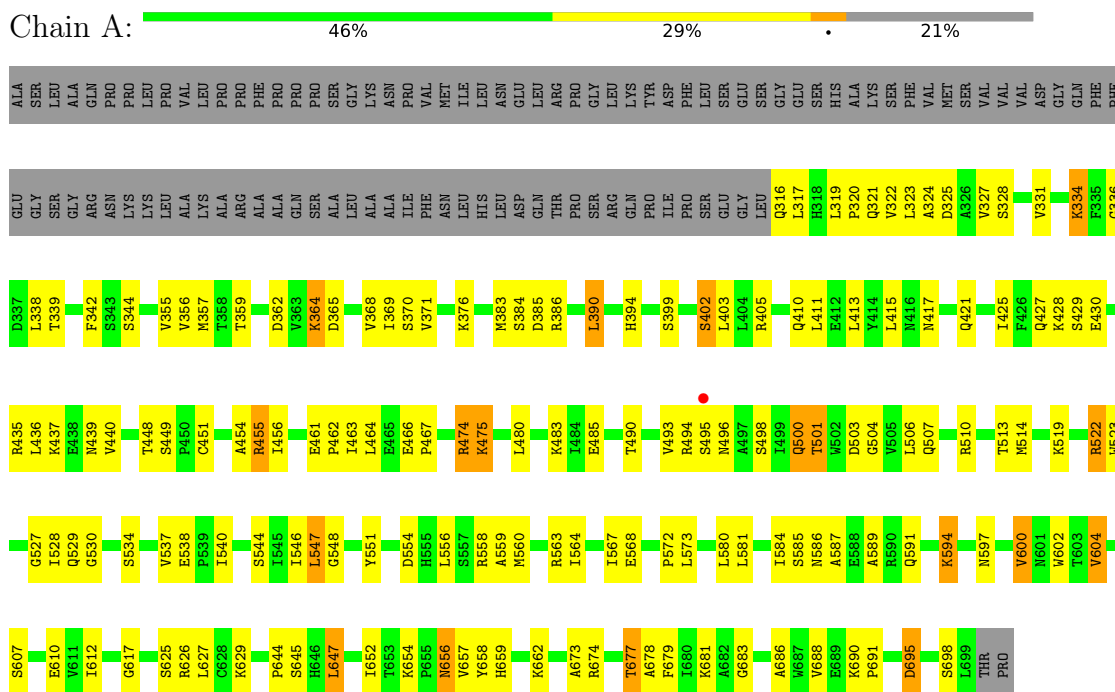
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	B	2	Total	O	0	0
			2	2		
7	C	3	Total	O	0	0
			3	3		
7	D	1	Total	O	0	0
			1	1		

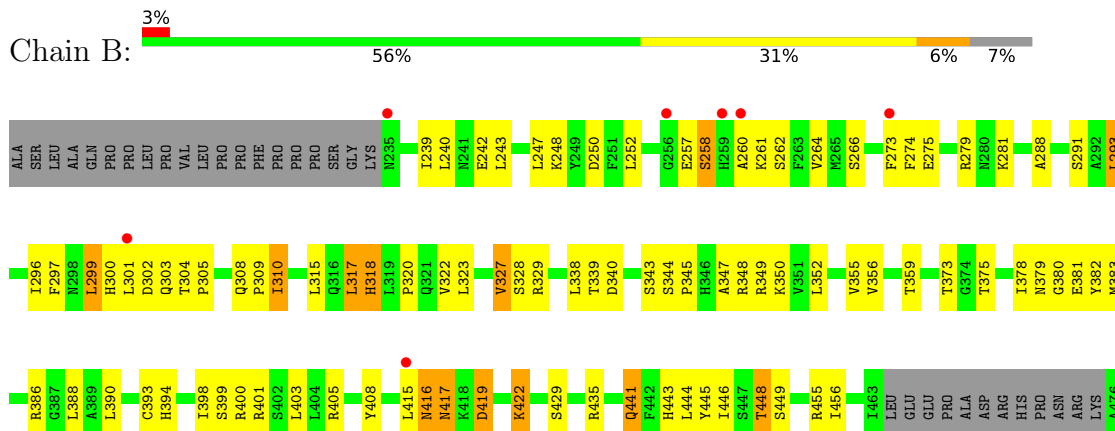
3 Residue-property plots

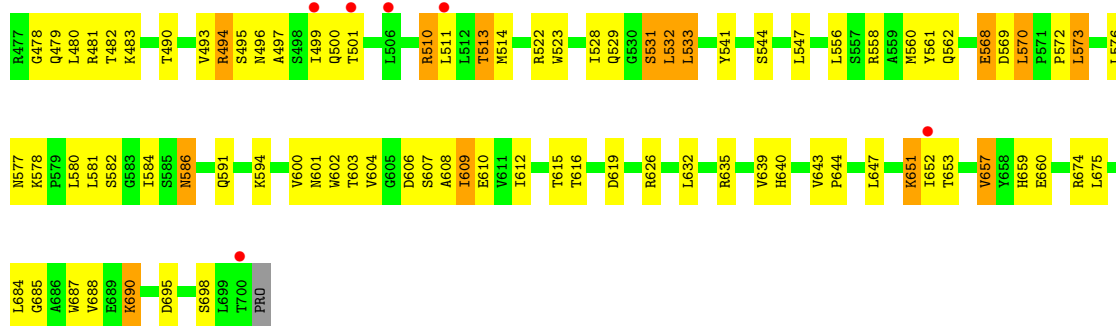
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Isoform 4 of Double-stranded RNA-specific editase 1



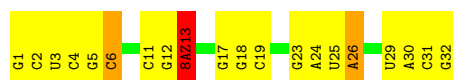
• Molecule 1: Isoform 4 of Double-stranded RNA-specific editase 1





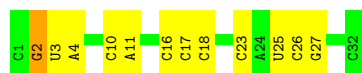
• Molecule 2: RNA Top Strand Containing 8-azanebularine (8AZ)

Chain C: 38% 53% 6% •



• Molecule 3: RNA Bottom Strand containing deoxyinosine complementary to a guanosine adjacent to the target site

Chain D: 62% 34% •



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.69Å 63.13Å 141.78Å 90.00° 118.23° 90.00°	Depositor
Resolution (Å)	49.60 – 2.80 49.60 – 2.81	Depositor EDS
% Data completeness (in resolution range)	65.0 (49.60-2.80) 64.9 (49.60-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.188 , 0.235 0.191 , 0.238	Depositor DCC
R_{free} test set	1091 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8019	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, ZN, 8AZ, EDO

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	0.47	0/3081	0.69	0/4164
1	B	0.38	0/3610	0.56	1/4876 (0.0%)
2	C	0.38	0/740	0.56	0/1151
3	D	0.34	0/727	0.55	0/1128
All	All	0.41	0/8158	0.61	1/11319 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	SER	CB-CA-C	-5.44	110.32	116.63

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	3019	0	3051	91	1
1	B	3540	0	3567	104	0
2	C	685	0	337	17	1
3	D	674	0	349	7	0
4	A	36	0	6	4	0
4	B	36	0	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	6	0	0
6	C	4	0	6	2	0
6	D	4	0	6	0	0
7	A	9	0	0	0	0
7	B	2	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
All	All	8019	0	7334	210	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 14.

All (210) 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:569:ASP:O	1:B:674:ARG:NH1	2.12	0.81
1:A:410:GLN:HG2	1:A:425:ILE:HG12	1.62	0.80
1:A:461:GLU:HG3	1:A:462:PRO:HD2	1.64	0.76
1:B:558:ARG:HA	1:B:562:GLN:HB2	1.69	0.74
1:B:380:GLY:HA2	1:B:383:MET:HE3	1.72	0.72
1:B:569:ASP:HB2	1:B:674:ARG:HD2	1.72	0.71
1:B:522:ARG:HA	1:B:675:LEU:HD11	1.73	0.71
1:B:400:ARG:HD3	1:B:523:TRP:CE2	2.27	0.69
1:B:383:MET:HE1	1:B:511:LEU:HD22	1.75	0.68
1:A:405:ARG:NH1	1:A:626:ARG:HD2	2.09	0.67
1:B:657:VAL:HG22	1:B:660:GLU:HG2	1.75	0.67
3:D:3:U:H2'	3:D:4:A:C8	2.30	0.66
1:B:279:ARG:NH2	2:C:17:G:OP1	2.30	0.65
1:B:257:GLU:N	1:B:260:ALA:O	2.30	0.64
1:A:430:GLU:OE1	1:A:435:ARG:NH1	2.32	0.63
1:A:324:ALA:HA	1:A:546:ILE:HG12	1.81	0.63
1:A:474:ARG:NH2	3:D:25:U:OP2	2.32	0.62
1:A:357:MET:HB2	1:A:369:ILE:CD1	2.29	0.62
1:B:532:LEU:HD12	1:B:532:LEU:H	1.64	0.62
1:A:410:GLN:HE21	1:A:425:ILE:HG23	1.65	0.62
1:B:340:ASP:O	1:B:343:SER:OG	2.11	0.62
1:A:644:PRO:HG2	1:A:647:LEU:HB2	1.81	0.61
1:B:586:ASN:OD1	1:B:586:ASN:N	2.33	0.61
1:B:561:TYR:HB2	1:B:576:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ARG:O	1:A:563:ARG:HG3	2.01	0.60
1:B:456:ILE:HG13	1:B:481:ARG:NH1	2.16	0.60
1:B:495:SER:HB2	1:B:685:GLY:HA2	1.84	0.59
1:B:252:LEU:HD11	1:B:266:SER:HB3	1.84	0.58
1:B:281:LYS:HE2	2:C:18:G:H5'	1.84	0.58
1:A:369:ILE:HG21	1:A:403:LEU:HD13	1.84	0.58
1:A:319:LEU:HD12	1:A:320:PRO:HD2	1.85	0.58
1:B:513:THR:HA	1:B:690:LYS:NZ	2.18	0.58
1:A:503:ASP:HB2	1:B:455:ARG:HD2	1.86	0.58
1:B:419:ASP:O	1:B:422:LYS:HG3	2.05	0.57
1:A:673:ALA:O	1:A:677:THR:HG23	2.04	0.57
1:B:601:ASN:ND2	1:B:610:GLU:HB3	2.19	0.57
1:A:356:VAL:HG12	1:A:368:VAL:HG22	1.85	0.57
1:B:494:ARG:HD3	1:B:494:ARG:N	2.19	0.57
1:A:514:MET:HE1	1:A:688:VAL:HB	1.85	0.57
1:A:602:TRP:CH2	1:A:604:VAL:HA	2.40	0.56
1:B:482:THR:HG23	1:B:493:VAL:HG12	1.88	0.56
1:B:601:ASN:HD21	1:B:610:GLU:HB3	1.70	0.56
1:A:394:HIS:CE1	1:A:483:LYS:HD3	2.41	0.56
1:B:511:LEU:HD21	1:B:690:LYS:HD3	1.88	0.56
2:C:11:C:O2'	2:C:12:G:H5'	2.06	0.55
1:A:463:ILE:O	1:A:466:GLU:N	2.39	0.55
2:C:23:G:H2'	2:C:24:A:C8	2.42	0.55
2:C:1:G:N3	6:C:101:EDO:H22	2.22	0.55
3:D:26:C:H2'	3:D:27:G:H8	1.71	0.55
1:A:548:GLY:HA2	1:A:584:ILE:HD13	1.88	0.55
1:B:556:LEU:O	1:B:560:MET:HG2	2.07	0.54
1:A:357:MET:HB2	1:A:369:ILE:HD13	1.90	0.53
1:B:544:SER:HB3	1:B:580:LEU:HD23	1.90	0.53
1:A:529:GLN:H	1:A:529:GLN:CD	2.17	0.53
1:B:514:MET:HE3	1:B:688:VAL:HB	1.89	0.53
1:B:408:TYR:CE1	1:B:533:LEU:HG	2.43	0.53
1:B:640:HIS:CE1	1:B:653:THR:HA	2.44	0.53
1:A:334:LYS:O	1:A:338:LEU:HG	2.08	0.53
1:A:656:ASN:OD1	1:A:656:ASN:N	2.31	0.53
1:A:629:LYS:HE3	4:A:801:IHP:O42	2.09	0.53
1:B:275:GLU:OE2	1:B:329:ARG:NH1	2.42	0.52
1:B:323:LEU:O	1:B:327:VAL:HG13	2.09	0.52
2:C:3:U:H2'	2:C:4:C:C6	2.44	0.52
3:D:26:C:H2'	3:D:27:G:C8	2.45	0.52
1:B:288:ALA:O	1:B:291:SER:OG	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LYS:HE3	1:A:647:LEU:HD21	1.91	0.52
1:B:602:TRP:CH2	1:B:604:VAL:HA	2.45	0.52
1:A:370:SER:HB2	1:A:402:SER:HB3	1.91	0.52
1:B:383:MET:SD	1:B:511:LEU:HD13	2.50	0.52
1:A:355:VAL:HG11	1:A:403:LEU:HD22	1.92	0.52
1:A:455:ARG:HD3	2:C:13:8AZ:OP1	2.09	0.52
1:B:639:VAL:O	1:B:643:VAL:HG23	2.09	0.52
1:A:519:LYS:NZ	4:A:801:IHP:O46	2.43	0.51
1:A:537:VAL:HG12	1:A:538:GLU:O	2.10	0.51
1:B:252:LEU:HB2	1:B:264:VAL:HG13	1.91	0.51
1:B:690:LYS:HD2	4:B:801:IHP:O36	2.10	0.51
2:C:1:G:O2'	6:C:101:EDO:H21	2.11	0.51
1:B:513:THR:HA	1:B:690:LYS:HZ2	1.73	0.51
1:B:659:HIS:HB2	1:B:695:ASP:HB3	1.92	0.51
1:A:417:ASN:O	1:A:421:GLN:HG3	2.11	0.51
1:A:494:ARG:C	1:A:496:ASN:H	2.19	0.51
1:A:554:ASP:OD1	1:A:554:ASP:N	2.42	0.50
1:A:514:MET:HE1	1:A:688:VAL:H	1.75	0.50
1:B:400:ARG:HD3	1:B:523:TRP:CZ2	2.47	0.50
1:A:567:ILE:HG13	1:A:678:ALA:HB2	1.93	0.50
1:B:309:PRO:HD2	1:B:581:LEU:HB2	1.93	0.50
1:B:378:ILE:HD11	1:B:382:TYR:O	2.11	0.50
1:B:600:VAL:HG21	1:B:609:ILE:HD12	1.94	0.49
1:A:500:GLN:HG3	1:A:691:PRO:HD3	1.94	0.49
1:A:451:CYS:N	2:C:13:8AZ:O6	2.35	0.49
2:C:3:U:H2'	2:C:4:C:H6	1.78	0.49
1:A:357:MET:HB2	1:A:369:ILE:HD11	1.95	0.49
3:D:3:U:H2'	3:D:4:A:H8	1.77	0.49
1:A:369:ILE:O	1:A:604:VAL:N	2.46	0.49
1:A:503:ASP:OD2	1:B:490:THR:OG1	2.28	0.48
1:A:551:TYR:CE2	1:A:556:LEU:HD23	2.49	0.48
1:A:572:PRO:O	1:A:573:LEU:HB2	2.12	0.48
1:A:323:LEU:O	1:A:327:VAL:HG13	2.14	0.48
1:A:480:LEU:HD21	1:A:679:PHE:CD2	2.48	0.48
2:C:30:A:H2'	2:C:31:C:O4'	2.14	0.48
1:B:261:LYS:O	1:B:279:ARG:HA	2.14	0.48
1:B:448:THR:OG1	1:B:449:SER:N	2.46	0.48
1:A:455:ARG:HG2	1:A:456:ILE:N	2.27	0.48
1:B:448:THR:O	1:B:547:LEU:HD22	2.13	0.48
1:B:568:GLU:CD	1:B:569:ASP:H	2.22	0.48
1:B:510:ARG:H	1:B:510:ARG:NE	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:SER:C	1:A:627:LEU:H	2.22	0.47
1:B:281:LYS:NZ	2:C:19:C:OP1	2.42	0.47
1:A:376:LYS:HD2	1:A:597:ASN:HA	1.96	0.47
1:A:594:LYS:HA	1:A:594:LYS:HD3	1.49	0.47
1:B:529:GLN:HB2	1:B:533:LEU:HB3	1.96	0.47
1:B:514:MET:HG3	1:B:687:TRP:CE2	2.50	0.47
1:B:496:ASN:O	1:B:496:ASN:ND2	2.48	0.47
1:B:612:ILE:HA	1:B:619:ASP:HA	1.96	0.47
1:B:408:TYR:CZ	1:B:533:LEU:HG	2.49	0.47
1:A:658:TYR:HB3	1:A:695:ASP:O	2.15	0.46
1:A:610:GLU:CD	1:A:612:ILE:HD11	2.40	0.46
1:A:647:LEU:HD23	1:A:647:LEU:HA	1.77	0.46
1:A:514:MET:HE2	1:A:514:MET:HB2	1.57	0.46
1:B:345:PRO:O	1:B:348:ARG:HG2	2.15	0.46
1:B:405:ARG:HH22	1:B:606:ASP:CG	2.24	0.46
1:B:594:LYS:HD2	1:B:594:LYS:HA	1.74	0.46
1:B:478:GLY:O	1:B:684:LEU:HD13	2.16	0.46
1:B:607:SER:OG	1:B:608:ALA:N	2.48	0.46
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.82	0.46
2:C:12:G:H2'	2:C:12:G:N3	2.30	0.46
1:B:394:HIS:CE1	1:B:483:LYS:HD3	2.50	0.46
1:B:373:THR:OG1	1:B:600:VAL:HG12	2.16	0.45
1:A:485:GLU:O	1:A:510:ARG:HD2	2.16	0.45
1:B:494:ARG:HH11	1:B:494:ARG:H	1.63	0.45
1:B:338:LEU:HB3	1:B:609:ILE:CG2	2.47	0.45
2:C:25:U:H2'	2:C:26:A:C8	2.52	0.45
1:A:390:LEU:H	1:A:617:GLY:HA3	1.82	0.45
1:A:437:LYS:O	1:A:440:VAL:HG12	2.17	0.45
1:A:448:THR:OG1	1:A:455:ARG:NH2	2.50	0.45
1:A:454:ALA:HB2	1:A:559:ALA:HB3	1.98	0.45
1:B:355:VAL:HG21	1:B:403:LEU:HD22	1.98	0.45
1:A:522:ARG:NH1	4:A:801:IHP:O23	2.50	0.45
1:B:401:ARG:NH2	4:B:801:IHP:O22	2.47	0.44
1:B:429:SER:HA	1:B:435:ARG:HG2	1.99	0.44
1:A:523:TRP:HA	1:A:527:GLY:O	2.18	0.44
2:C:23:G:H2'	2:C:24:A:H8	1.81	0.44
1:B:310:ILE:HD11	1:B:320:PRO:HG2	1.99	0.44
1:A:359:THR:HA	1:A:439:ASN:O	2.17	0.44
1:B:317:LEU:HD23	1:B:441:GLN:OE1	2.18	0.44
1:B:635:ARG:O	1:B:639:VAL:HG23	2.18	0.44
1:A:544:SER:HA	1:A:580:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:CD1	1:A:320:PRO:HD2	2.48	0.43
1:A:501:THR:HG1	1:A:504:GLY:H	1.65	0.43
1:B:541:TYR:HB3	1:B:577:ASN:ND2	2.33	0.43
1:B:239:ILE:O	1:B:243:LEU:HG	2.17	0.43
1:A:600:VAL:HA	1:A:610:GLU:O	2.18	0.43
1:B:242:GLU:HG3	1:B:243:LEU:N	2.33	0.43
1:A:339:THR:HB	1:A:344:SER:HB3	1.99	0.43
1:B:441:GLN:HB2	1:B:443:HIS:HE2	1.82	0.43
3:D:2:G:H2'	3:D:3:U:C6	2.52	0.43
1:A:336:GLY:HA3	1:A:342:PHE:CE1	2.53	0.43
1:A:475:LYS:HD2	1:A:475:LYS:HA	1.84	0.43
1:A:559:ALA:C	1:A:560:MET:HE2	2.43	0.43
1:B:393:CYS:HA	1:B:398:ILE:HD11	1.99	0.43
1:A:493:VAL:HG11	1:A:686:ALA:O	2.18	0.43
1:A:449:SER:HA	1:A:547:LEU:HD13	2.01	0.43
1:A:658:TYR:CZ	1:A:662:LYS:HE3	2.54	0.43
1:A:589:ALA:O	1:A:591:GLN:NE2	2.52	0.42
1:B:570:LEU:HD13	1:B:570:LEU:HA	1.72	0.42
1:B:651:LYS:HA	1:B:651:LYS:HD3	1.71	0.42
1:A:390:LEU:HD12	1:A:390:LEU:HA	1.74	0.42
1:B:382:TYR:CE2	1:B:616:THR:HG22	2.53	0.42
1:B:444:LEU:HD12	1:B:445:TYR:N	2.34	0.42
2:C:24:A:H2'	2:C:25:U:H6	1.85	0.42
1:B:441:GLN:HB2	1:B:443:HIS:NE2	2.35	0.42
1:A:584:ILE:HD11	1:A:587:ALA:HA	2.01	0.42
1:A:327:VAL:O	1:A:331:VAL:HG23	2.19	0.42
1:B:274:PHE:HB3	1:B:291:SER:OG	2.19	0.42
1:A:528:ILE:HG23	1:A:540:ILE:O	2.20	0.42
1:B:400:ARG:NH1	1:B:528:ILE:O	2.50	0.42
1:A:690:LYS:HE2	4:A:801:IHP:O36	2.20	0.42
1:B:449:SER:HB3	1:B:455:ARG:HG3	2.02	0.42
1:B:657:VAL:HG22	1:B:660:GLU:CG	2.45	0.42
1:A:385:ASP:OD1	1:A:386:ARG:HG3	2.20	0.41
1:B:328:SER:OG	1:B:584:ILE:HG21	2.20	0.41
1:B:339:THR:HG21	1:B:347:ALA:HB2	2.02	0.41
1:B:378:ILE:HG23	1:B:383:MET:HE2	2.02	0.41
1:A:514:MET:CE	1:A:688:VAL:H	2.33	0.41
2:C:5:G:O2'	2:C:6:C:H5'	2.20	0.41
1:A:430:GLU:H	1:A:430:GLU:CD	2.23	0.41
1:B:499:ILE:HG12	1:B:500:GLN:H	1.85	0.41
1:A:325:ASP:OD1	1:A:585:SER:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LYS:C	1:A:683:GLY:H	2.28	0.41
1:B:300:HIS:CG	1:B:301:LEU:N	2.88	0.41
1:B:304:THR:N	1:B:305:PRO:HD2	2.35	0.41
1:A:316:GLN:OE1	1:A:364:LYS:NZ	2.54	0.41
1:B:531:SER:HB2	4:B:801:IHP:O43	2.21	0.41
1:A:429:SER:HB2	1:A:435:ARG:HB3	2.03	0.41
1:B:303:GLN:HG3	1:B:305:PRO:HG2	2.03	0.41
1:A:483:LYS:HE2	1:A:513:THR:HG22	2.02	0.41
1:B:338:LEU:HD22	1:B:609:ILE:HG23	2.02	0.41
1:B:444:LEU:HD12	1:B:445:TYR:H	1.86	0.41
1:B:643:VAL:HG12	1:B:644:PRO:O	2.21	0.41
1:A:530:GLY:O	1:A:534:SER:HB3	2.21	0.41
1:A:625:SER:C	1:A:627:LEU:N	2.79	0.41
1:B:529:GLN:CD	1:B:529:GLN:H	2.29	0.41
1:B:258:SER:HB3	3:D:18:C:O2'	2.21	0.40
1:B:299:LEU:HD21	1:B:302:ASP:OD2	2.21	0.40
1:B:602:TRP:HA	1:B:626:ARG:NH2	2.36	0.40
1:A:362:ASP:HB3	1:A:365:ASP:OD1	2.20	0.40
1:B:572:PRO:O	1:B:573:LEU:HB2	2.22	0.40
1:B:416:ASN:O	1:B:417:ASN:C	2.62	0.40
1:A:436:LEU:HD13	1:A:440:VAL:HG13	2.03	0.40
1:B:293:LEU:HA	1:B:297:PHE:HD1	1.86	0.40

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)
1:A:410:GLN:NE2	2:C:32:G:O2'[4_445]	2.17	0.03

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	382/487 (78%)	348 (91%)	32 (8%)	2 (0%)	24	55
1	B	450/487 (92%)	403 (90%)	45 (10%)	2 (0%)	30	60
All	All	832/974 (85%)	751 (90%)	77 (9%)	4 (0%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	B	497	ALA
1	B	318	HIS
1	A	467	PRO

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	329/415 (79%)	283 (86%)	46 (14%)	3	12
1	B	384/415 (92%)	321 (84%)	63 (16%)	2	8
All	All	713/830 (86%)	604 (85%)	109 (15%)	3	10

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	LEU
1	A	321	GLN
1	A	328	SER
1	A	334	LYS
1	A	364	LYS
1	A	371	VAL
1	A	383	MET
1	A	384	SER
1	A	390	LEU
1	A	399	SER
1	A	402	SER
1	A	411	LEU

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Mol	Chain	Res	Type
1	A	413	LEU
1	A	415	LEU
1	A	427	GLN
1	A	455	ARG
1	A	464	LEU
1	A	474	ARG
1	A	475	LYS
1	A	490	THR
1	A	495	SER
1	A	498	SER
1	A	500	GLN
1	A	501	THR
1	A	507	GLN
1	A	522	ARG
1	A	547	LEU
1	A	564	ILE
1	A	568	GLU
1	A	581	LEU
1	A	586	ASN
1	A	594	LYS
1	A	600	VAL
1	A	604	VAL
1	A	607	SER
1	A	645	SER
1	A	647	LEU
1	A	652	ILE
1	A	654	LYS
1	A	656	ASN
1	A	657	VAL
1	A	659	HIS
1	A	674	ARG
1	A	677	THR
1	A	695	ASP
1	A	698	SER
1	B	240	LEU
1	B	247	LEU
1	B	248	LYS
1	B	250	ASP
1	B	262	SER
1	B	273	PHE
1	B	293	LEU
1	B	296	ILE

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Mol	Chain	Res	Type
1	B	299	LEU
1	B	308	GLN
1	B	310	ILE
1	B	315	LEU
1	B	317	LEU
1	B	318	HIS
1	B	322	VAL
1	B	327	VAL
1	B	344	SER
1	B	349	ARG
1	B	350	LYS
1	B	352	LEU
1	B	356	VAL
1	B	359	THR
1	B	375	THR
1	B	379	ASN
1	B	381	GLU
1	B	386	ARG
1	B	388	LEU
1	B	390	LEU
1	B	399	SER
1	B	415	LEU
1	B	416	ASN
1	B	417	ASN
1	B	419	ASP
1	B	422	LYS
1	B	441	GLN
1	B	446	ILE
1	B	448	THR
1	B	479	GLN
1	B	480	LEU
1	B	494	ARG
1	B	501	THR
1	B	510	ARG
1	B	513	THR
1	B	531	SER
1	B	532	LEU
1	B	533	LEU
1	B	568	GLU
1	B	570	LEU
1	B	573	LEU
1	B	578	LYS

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Mol	Chain	Res	Type
1	B	582	SER
1	B	586	ASN
1	B	591	GLN
1	B	603	THR
1	B	609	ILE
1	B	615	THR
1	B	632	LEU
1	B	647	LEU
1	B	651	LYS
1	B	652	ILE
1	B	657	VAL
1	B	690	LYS
1	B	698	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	A	427	GLN
1	A	586	ASN
1	A	591	GLN
1	B	321	GLN
1	B	391	ASN
1	B	496	ASN
1	B	630	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	31/32 (96%)	5 (16%)	0
3	D	29/32 (90%)	6 (20%)	0
All	All	60/64 (93%)	11 (18%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	C
2	C	6	C
2	C	13	8AZ
2	C	26	A

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Mol	Chain	Res	Type
2	C	29	U
3	D	2	G
3	D	10	C
3	D	11	A
3	D	16	C
3	D	17	C
3	D	23	C

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	8AZ	C	13	2,5	18,24,25	2.81	4 (22%)	19,35,38	2.09	4 (21%)

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	8AZ	C	13	2,5	-	3/7/35/36	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	13	8AZ	C2-N1	8.23	1.48	1.34
2	C	13	8AZ	N7-N8	6.63	1.42	1.32
2	C	13	8AZ	N9-N8	4.67	1.41	1.35
2	C	13	8AZ	C2-N3	2.29	1.34	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	8AZ	C5-C4-N3	-5.77	118.58	127.24
2	C	13	8AZ	C1'-N9-N8	-3.87	113.46	119.91
2	C	13	8AZ	C2-N3-C4	3.66	117.96	111.53
2	C	13	8AZ	C5-C4-N9	2.86	106.42	104.60

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	13	8AZ	O4'-C4'-C5'-O5'
2	C	13	8AZ	C3'-C4'-C5'-O5'
2	C	13	8AZ	O4'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	13	8AZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	EDO	D	101	-	3,3,3	0.32	0	2,2,2	0.08	0
6	EDO	C	101	-	3,3,3	0.32	0	2,2,2	0.33	0
4	IHP	A	801	-	36,36,36	0.97	3 (8%)	60,60,60	0.89	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	803	-	3,3,3	0.43	0	2,2,2	0.18	0
4	IHP	B	801	-	36,36,36	0.95	1 (2%)	60,60,60	0.74	1 (1%)

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	EDO	D	101	-	-	0/1/1/1	-
6	EDO	C	101	-	-	1/1/1/1	-
4	IHP	A	801	-	-	4/30/54/54	0/1/1/1
6	EDO	A	803	-	-	0/1/1/1	-
4	IHP	B	801	-	-	7/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	IHP	P5-O15	2.76	1.64	1.59
4	B	801	IHP	P4-O14	2.73	1.64	1.59
4	A	801	IHP	P3-O13	2.56	1.64	1.59
4	A	801	IHP	P1-O11	2.53	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	IHP	P4-O14-C4	2.54	130.22	123.43
4	A	801	IHP	O16-P6-O26	-2.09	101.88	109.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	IHP	C4-C5-O15-P5
6	C	101	EDO	O1-C1-C2-O2
4	A	801	IHP	C6-C5-O15-P5
4	B	801	IHP	C1-O11-P1-O41
4	B	801	IHP	C3-O13-P3-O33
4	B	801	IHP	C1-O11-P1-O21
4	B	801	IHP	C2-O12-P2-O22

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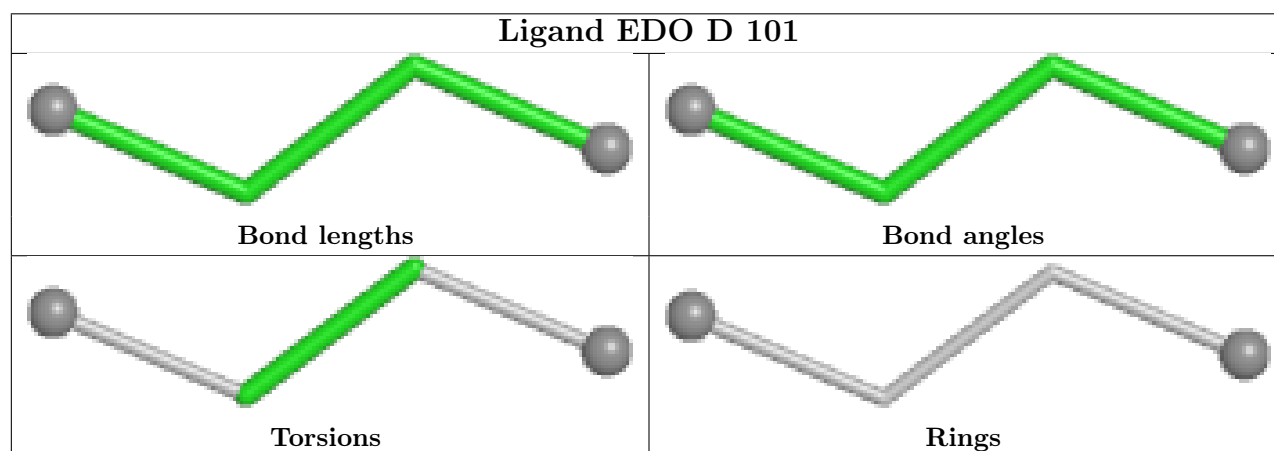
Mol	Chain	Res	Type	Atoms
4	A	801	IHP	C2-C3-O13-P3
4	B	801	IHP	C1-O11-P1-O31
4	B	801	IHP	C2-O12-P2-O42
4	B	801	IHP	C4-O14-P4-O44
4	A	801	IHP	C1-O11-P1-O21

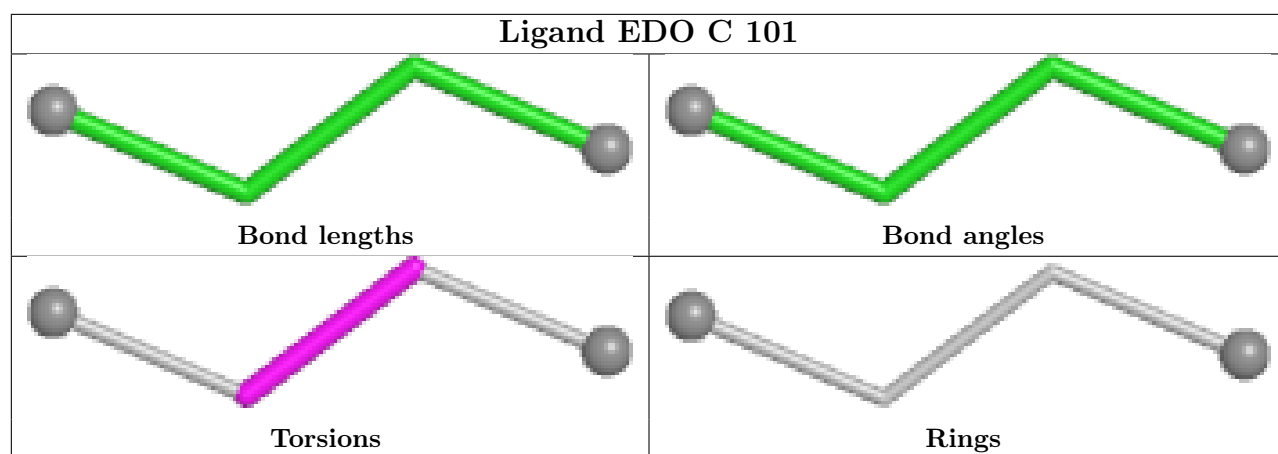
There are no ring outliers.

3 monomers are involved in 9 short contacts:

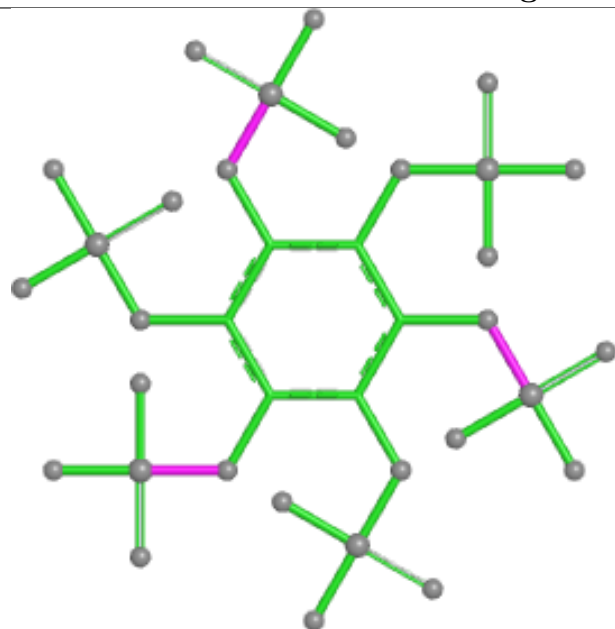
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	101	EDO	2	0
4	A	801	IHP	4	0
4	B	801	IHP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

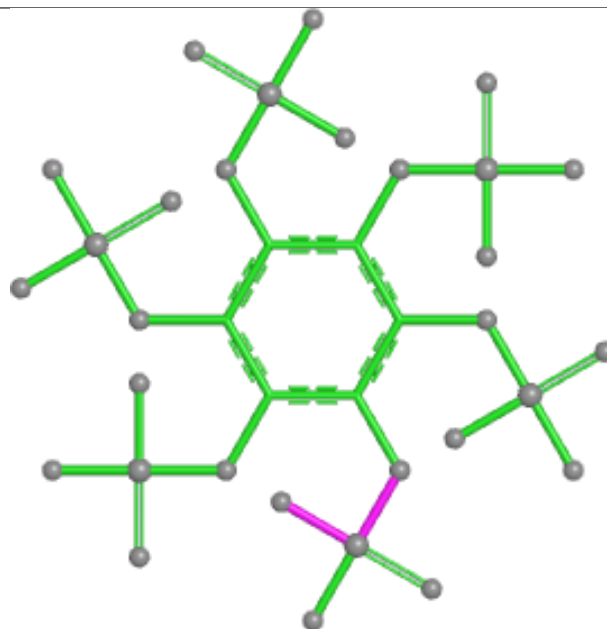




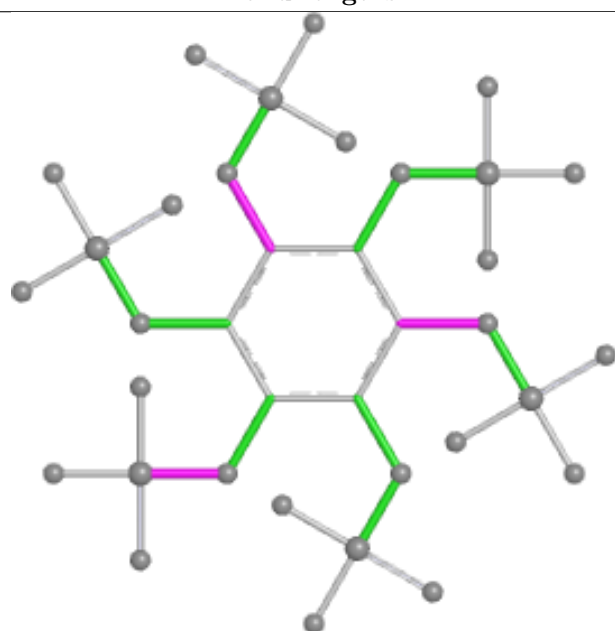
Ligand IHP A 801



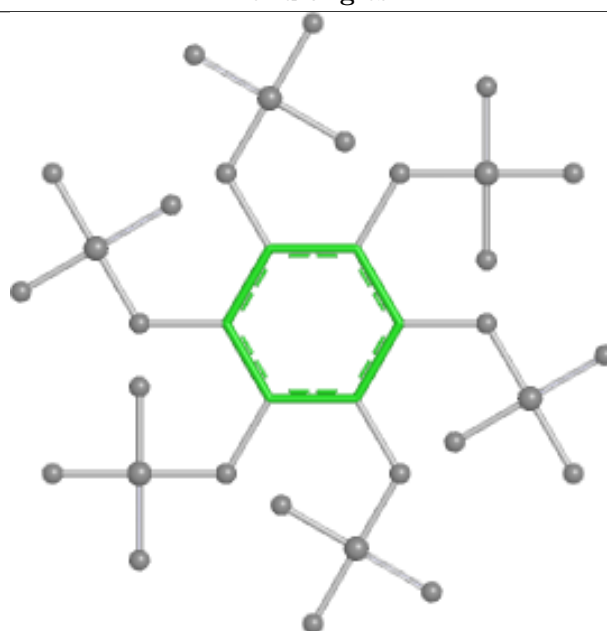
Bond lengths



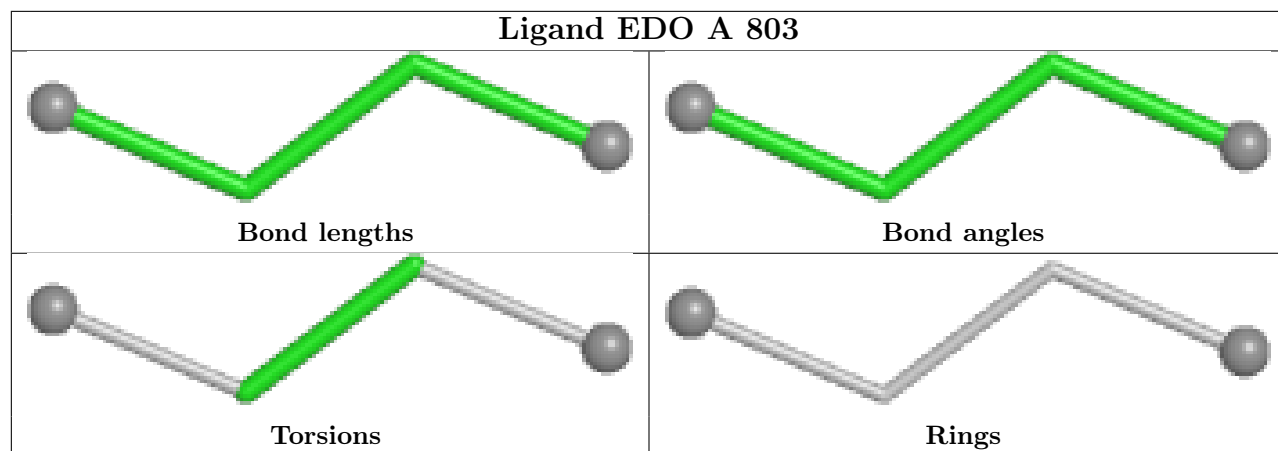
Bond angles

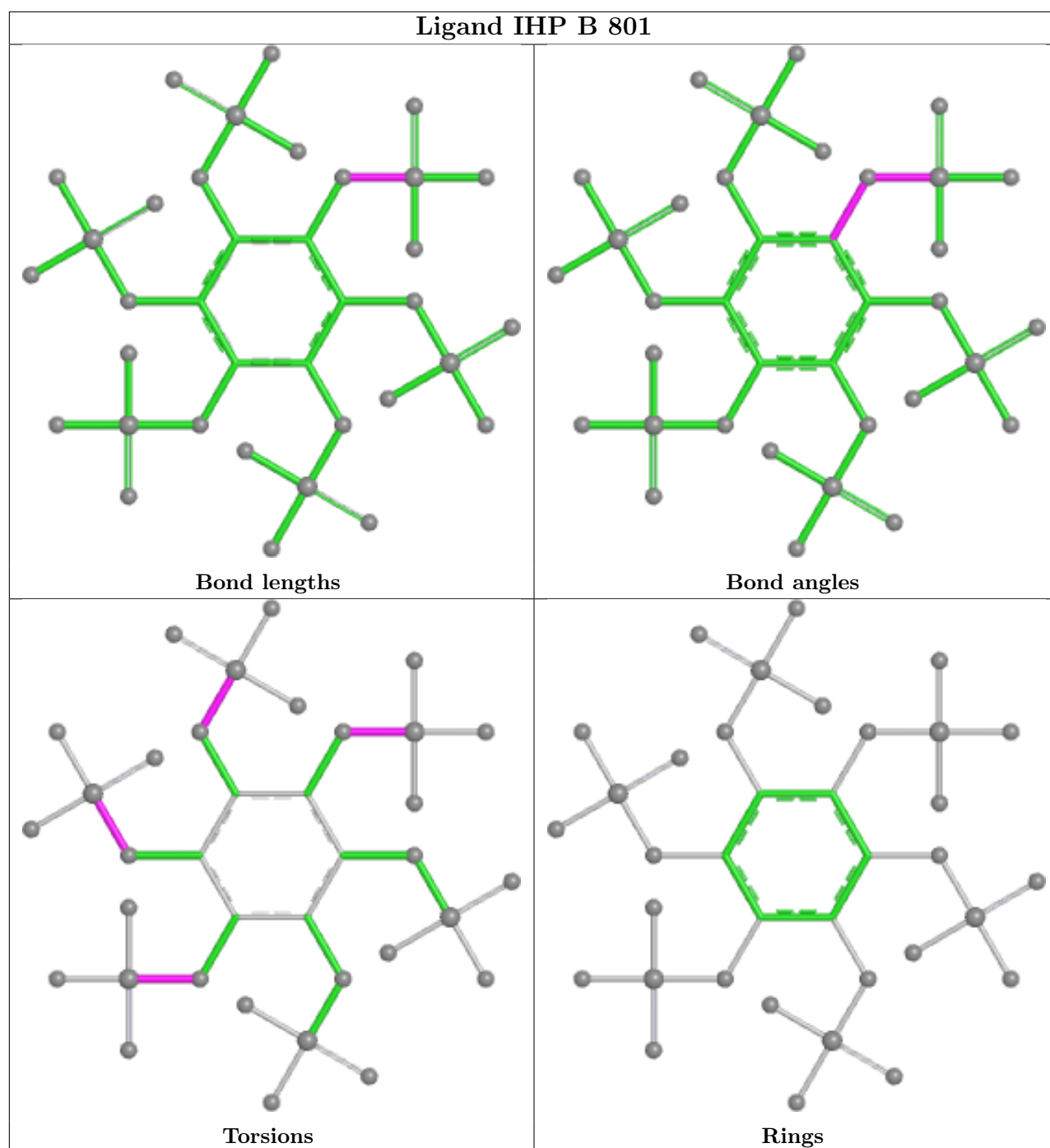


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/487 (78%)	-0.40	1 (0%) 90 86	28, 47, 92, 136	0
1	B	454/487 (93%)	-0.00	13 (2%) 53 43	45, 76, 152, 204	0
2	C	31/32 (96%)	-0.60	0 100 100	42, 78, 134, 139	0
3	D	31/32 (96%)	-0.64	0 100 100	38, 81, 127, 133	0
All	All	900/1038 (86%)	-0.21	14 (1%) 70 61	28, 62, 141, 204	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	HIS	3.5
1	B	499	ILE	2.7
1	B	415	LEU	2.5
1	B	501	THR	2.5
1	B	700	THR	2.4
1	B	256	GLY	2.3
1	B	273	PHE	2.3
1	B	301	LEU	2.3
1	B	260	ALA	2.2
1	B	506	LEU	2.2
1	A	495	SER	2.1
1	B	511	LEU	2.1
1	B	235	ASN	2.0
1	B	652	ILE	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	8AZ	C	13	22/23	0.96	0.07	35,38,42,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

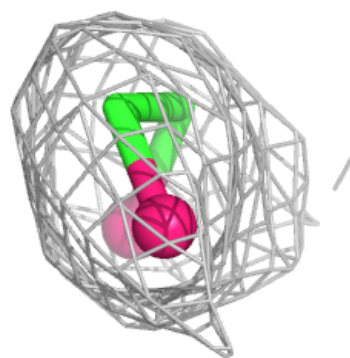
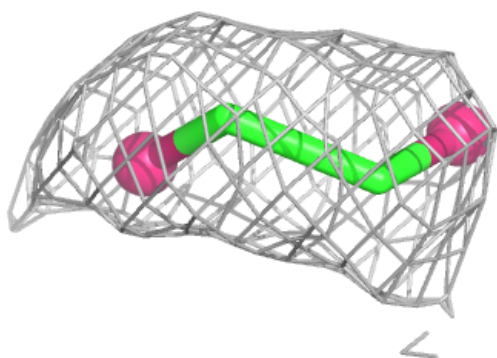
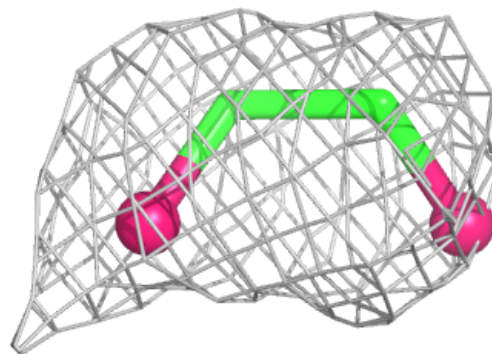
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	D	101	4/4	0.83	0.12	47,52,58,61	0
6	EDO	C	101	4/4	0.84	0.15	66,70,77,82	0
6	EDO	A	803	4/4	0.89	0.10	46,49,54,58	0
4	IHP	B	801	36/36	0.95	0.06	47,70,82,84	0
4	IHP	A	801	36/36	0.98	0.05	28,36,42,47	0
5	ZN	B	802	1/1	0.99	0.02	55,55,55,55	0
5	ZN	A	802	1/1	0.99	0.05	42,42,42,42	0

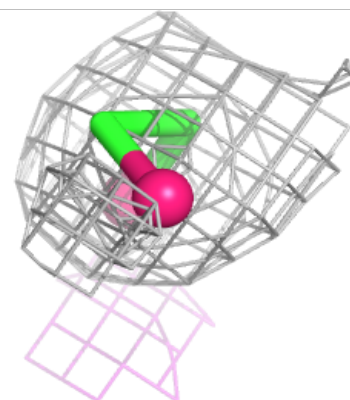
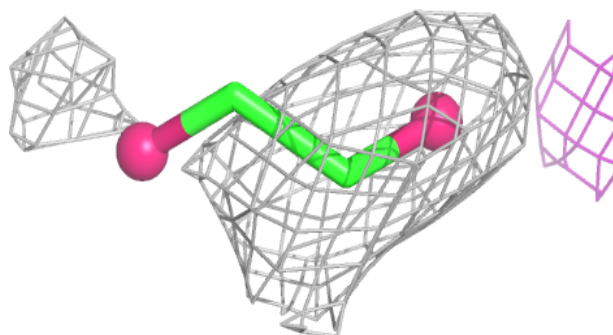
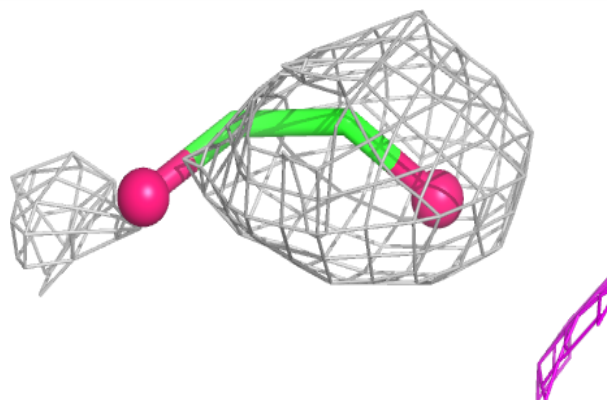
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EDO D 101:

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

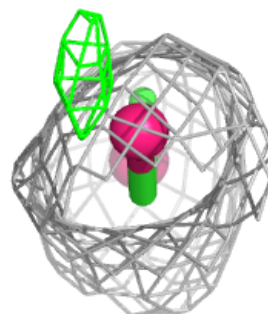
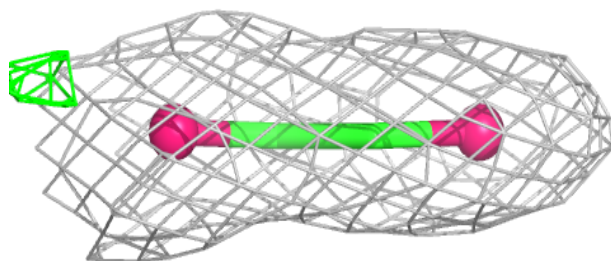
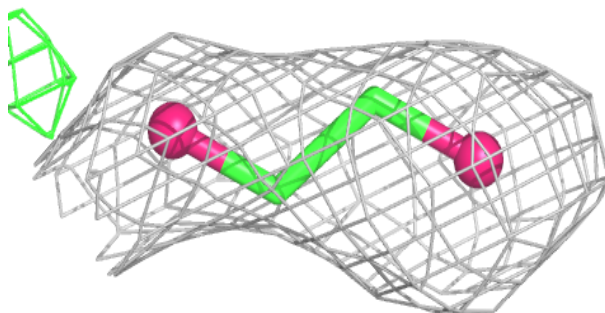
**Electron density around EDO C 101:**

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



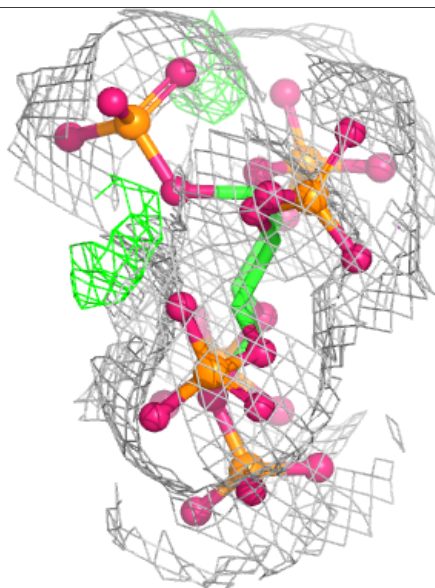
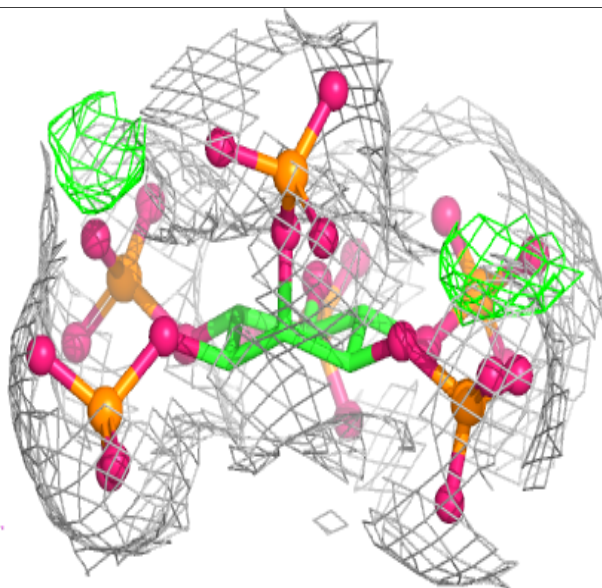
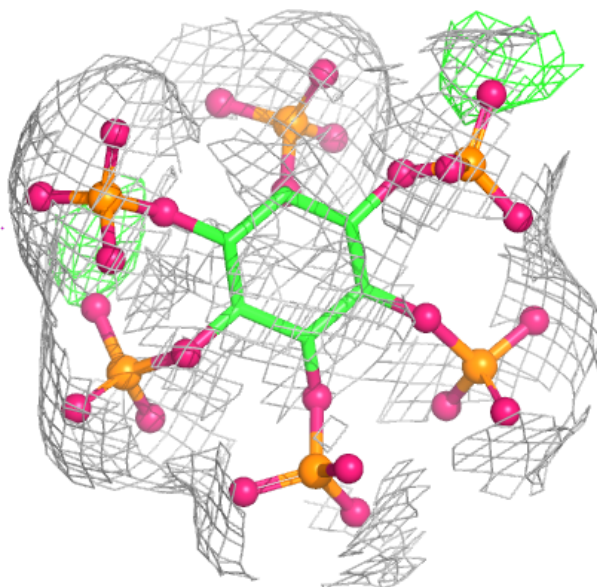
Electron density around EDO A 803:

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



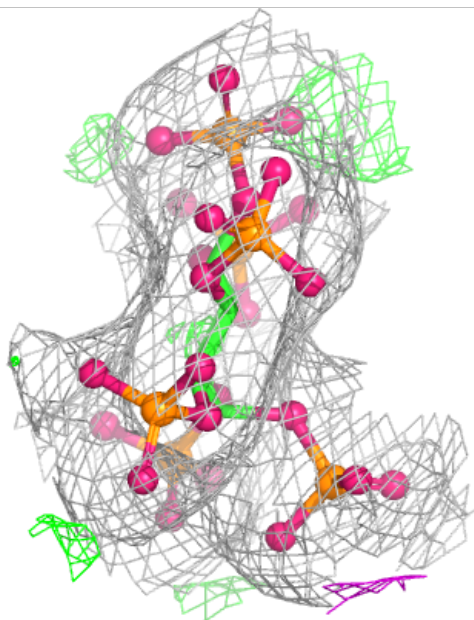
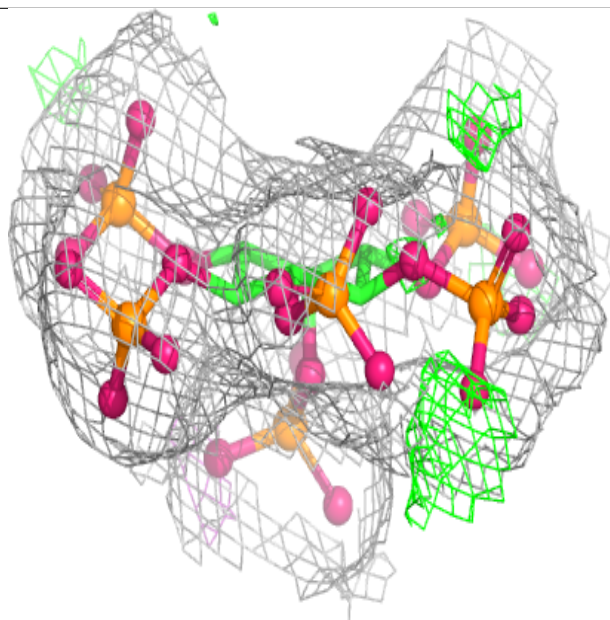
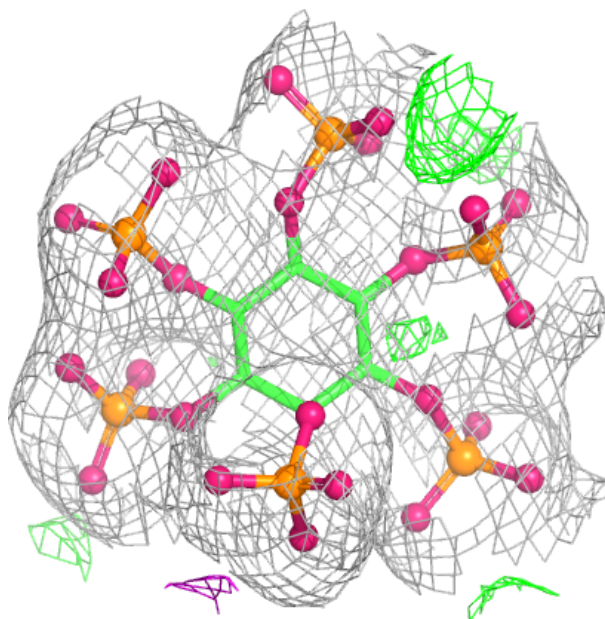
Electron density around IHP B 801:

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



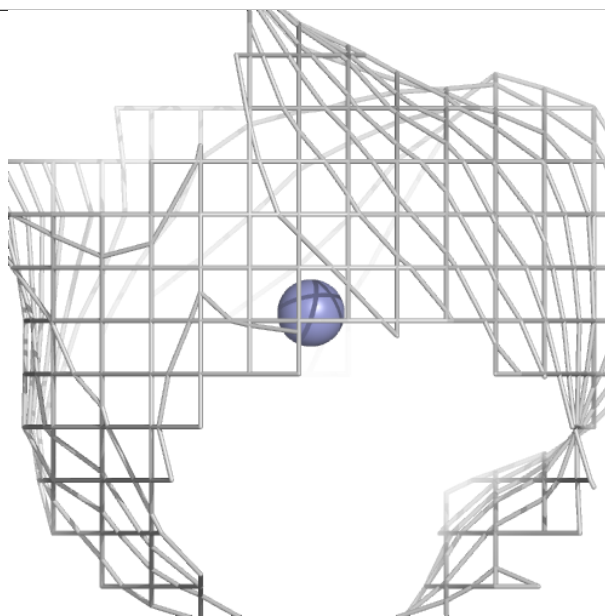
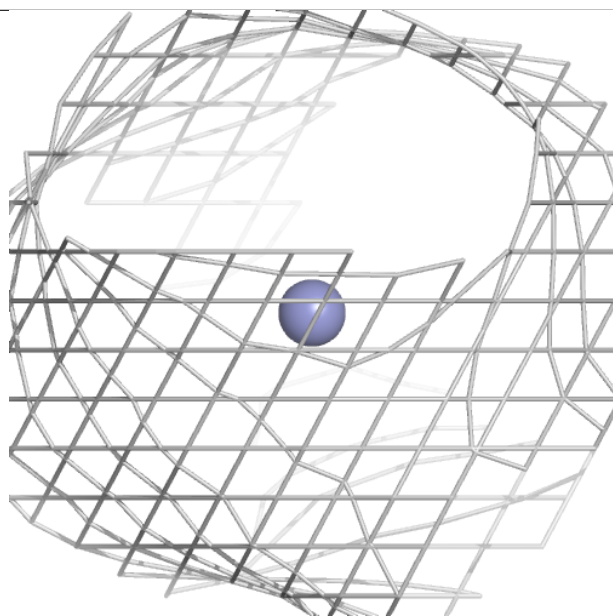
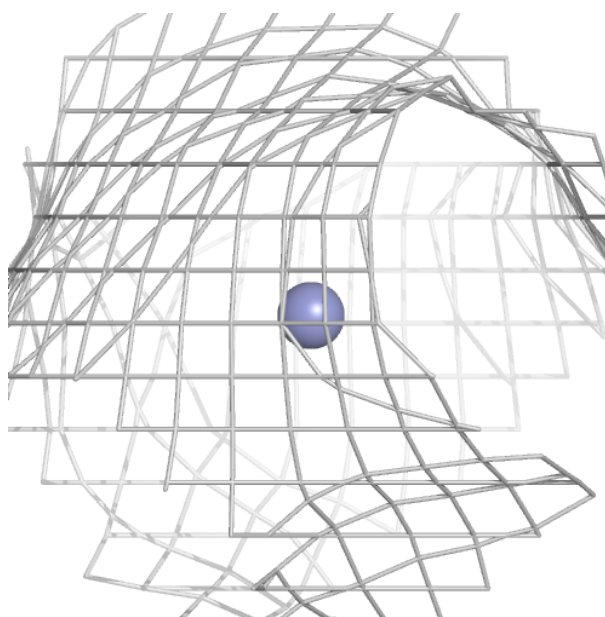
Electron density around IHP A 801:

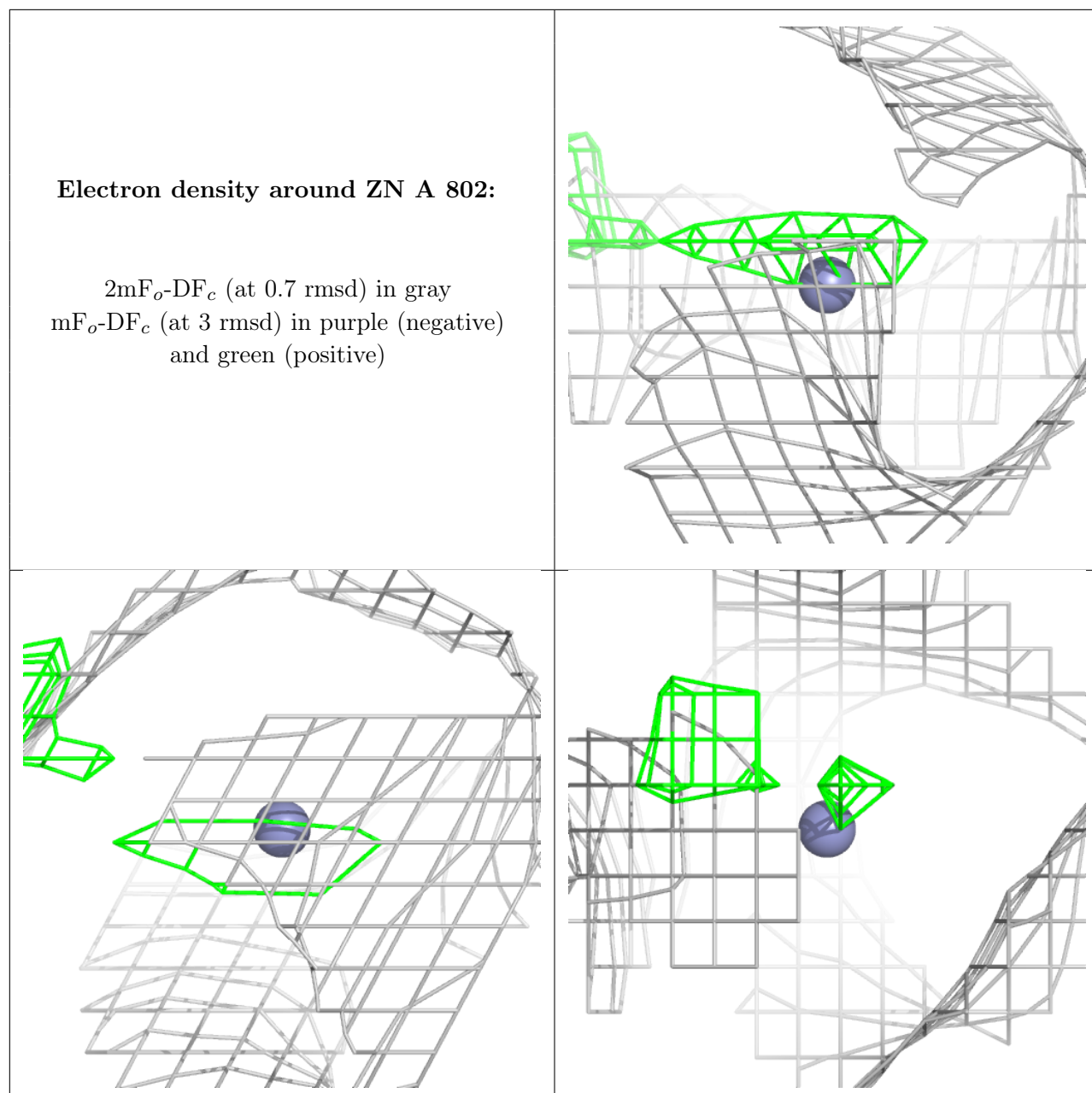
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 802:

$2mF_o-DF_c$ (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.