



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2022 – 06:33 PM JST

PDB ID : 7XEB
Title : Collagenase from Grimontia (Vibrio) hollisae 1706B complexed with Gly-Pro-Hyp
Authors : Ikeuchi, T.; Yasumoto, M.; Takita, T.; Mizutani, K.; Mikami, B.; Tanaka, K.; Hattori, S.; Yasukawa, K.
Deposited on : 2022-03-30
Resolution : 2.39 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

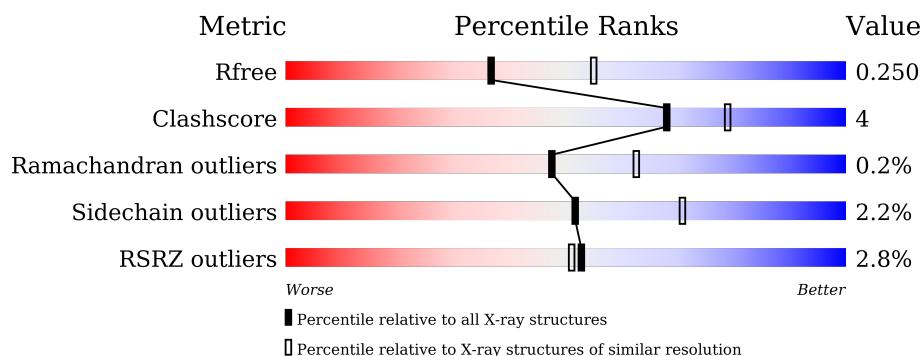
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	559	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
1	B	559	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 85%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
2	C	3	<div> <div style="width: 33%; height: 10px; background-color: green;"></div> <div style="width: 33%; height: 10px; background-color: yellow;"></div> <div style="width: 33%; height: 10px; background-color: orange;"></div> </div>
2	D	3	<div> <div style="width: 33%; height: 10px; background-color: green;"></div> <div style="width: 67%; height: 10px; background-color: yellow;"></div> </div>
2	G	3	<div> <div style="width: 33%; height: 10px; background-color: red;"></div> <div style="width: 67%; height: 10px; background-color: green;"></div> <div style="width: 33%; height: 10px; background-color: orange;"></div> </div>
2	H	3	<div> <div style="width: 33%; height: 10px; background-color: green;"></div> <div style="width: 67%; height: 10px; background-color: yellow;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	E	6	
3	F	6	
3	I	6	
3	J	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HYP	G	3	-	-	X	-
6	EDO	A	709	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8890 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 Microbial collagenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4218	2669	708	824	17			
1	B	533	Total	C	N	O	S	0	5	0
			4249	2691	714	825	19			

- Molecule 2 is a protein called GLY-PRO-HYP peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			20	12	3	5			
2	D	3	Total	C	N	O	0	0	0
			20	12	3	5			
2	G	3	Total	C	N	O	0	0	0
			20	12	3	5			
2	H	3	Total	C	N	O	0	0	0
			20	12	3	5			

- Molecule 3 is a protein called GLY-PRO-HYP-GLY-PRO-HYP peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			39	24	6	9			
3	F	6	Total	C	N	O	0	0	0
			39	24	6	9			
3	I	6	Total	C	N	O	0	0	0
			39	24	6	9			
3	J	6	Total	C	N	O	0	0	0
			39	24	6	9			

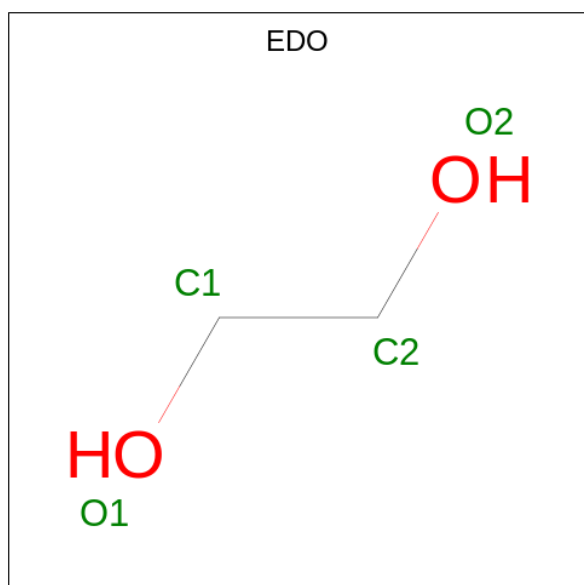
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		
5	B	4	Total	Ca	0	0
			4	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

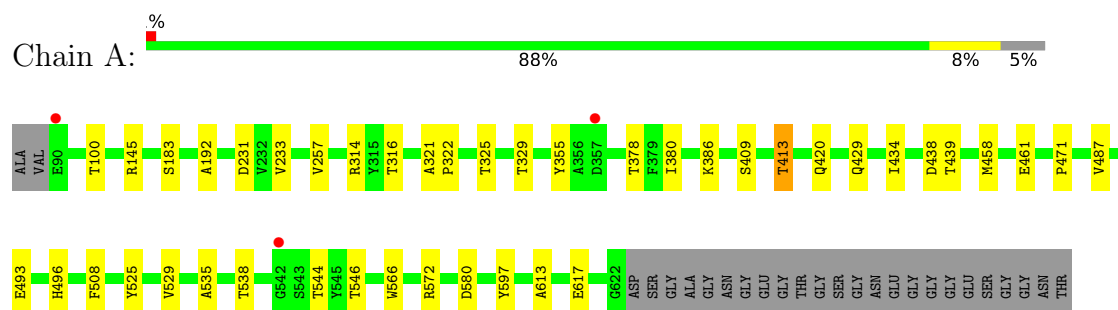
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	105	Total 105	O 105	0	0
7	B	48	Total 48	O 48	0	0
7	D	2	Total 2	O 2	0	0
7	E	1	Total 1	O 1	0	0
7	H	1	Total 1	O 1	0	0

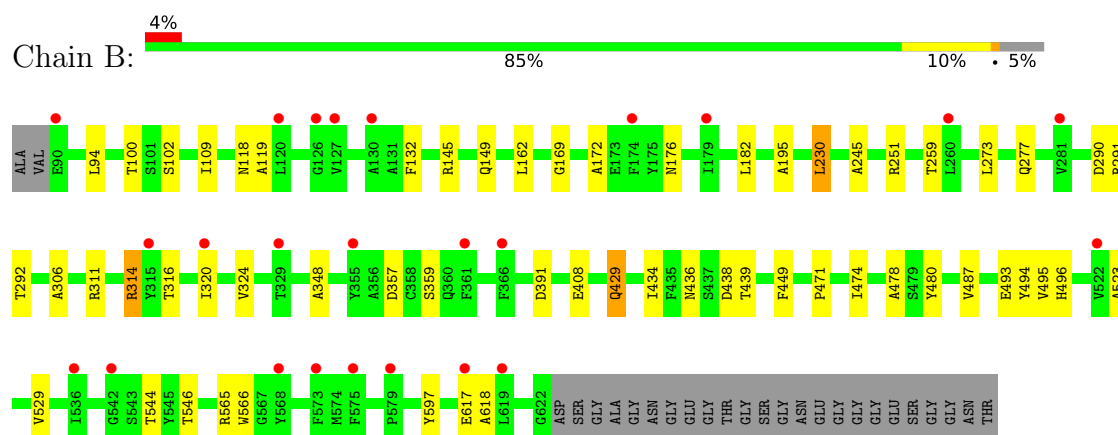
3 Residue-property plots

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: Microbial collagenase



- Molecule 1: Microbial collagenase



- Molecule 2: GLY-PRO-HYP peptide



- Molecule 2: GLY-PRO-HYP peptide



- Molecule 2: GLY-PRO-HYP peptide



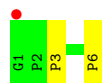
- Molecule 2: GLY-PRO-HYP peptide



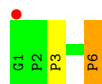
- Molecule 3: GLY-PRO-HYP-GLY-PRO-HYP peptide



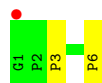
- Molecule 3: GLY-PRO-HYP-GLY-PRO-HYP peptide



- Molecule 3: GLY-PRO-HYP-GLY-PRO-HYP peptide



- Molecule 3: GLY-PRO-HYP-GLY-PRO-HYP peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.97Å 75.55Å 130.55Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	45.41 – 2.39 45.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.41-2.39) 98.5 (45.41-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.255 0.204 , 0.250	Depositor DCC
R_{free} test set	2703 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8890	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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

5.1 Standard geometry

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

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	0.45	0/4329	0.60	0/5901
1	B	0.40	0/4376	0.59	1/5963 (0.0%)
2	C	0.70	0/11	1.48	0/14
2	D	0.48	0/11	0.90	0/14
2	G	0.41	0/11	0.92	0/14
2	H	0.32	0/11	0.44	0/14
3	E	0.39	0/22	0.55	0/28
3	F	0.29	0/22	0.60	0/28
3	I	0.27	0/22	0.49	0/28
3	J	0.29	0/22	0.65	0/28
All	All	0.42	0/8837	0.60	1/12032 (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	314	ARG	CB-CA-C	-10.16	90.08	110.40

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	4218	0	3891	23	0
1	B	4249	0	3934	29	0
2	C	20	0	19	4	0
2	D	20	0	19	2	0
2	G	20	0	19	6	0
2	H	20	0	19	6	0
3	E	39	0	36	1	0
3	F	39	0	36	0	0
3	I	39	0	36	1	0
3	J	39	0	36	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	20	0	30	8	0
7	A	105	0	0	0	0
7	B	48	0	0	1	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
7	H	1	0	0	0	0
All	All	8890	0	8075	63	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 4.

All (63) 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)
2:G:3:HYP:C	2:H:1:GLY:N	2.41	0.83
2:G:3:HYP:C	2:H:1:GLY:H1	2.07	0.68
2:G:3:HYP:OXT	2:H:1:GLY:HA2	1.97	0.64
2:C:3:HYP:OXT	2:D:1:GLY:N	2.30	0.64
2:G:3:HYP:C	2:H:1:GLY:H2	2.11	0.64
1:A:461:GLU:HB2	6:A:709:EDO:H21	1.82	0.61
2:G:3:HYP:OXT	2:H:1:GLY:CA	2.49	0.61
1:A:525:TYR:CE1	1:A:572:ARG:HG3	2.38	0.58
1:A:508:PHE:HB2	6:A:709:EDO:C1	2.35	0.57
1:B:306:ALA:HB1	1:B:348:ALA:HB2	1.87	0.57
1:A:409:SER:O	1:A:413:THR:HG23	2.04	0.56
1:A:613:ALA:O	1:A:617:GLU:HG2	2.07	0.55
1:B:230:LEU:HD23	1:B:277:GLN:HG3	1.88	0.55
1:B:434:ILE:HD13	1:B:487:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:HYP:C	2:D:1:GLY:N	2.72	0.53
2:G:3:HYP:OXT	2:H:1:GLY:N	2.42	0.53
1:B:94:LEU:HD13	1:B:119:ALA:HB3	1.92	0.52
1:B:311:ARG:O	1:B:314:ARG:HG3	2.09	0.52
1:A:438:ASP:OD1	1:A:439:THR:N	2.43	0.52
1:B:438:ASP:OD1	1:B:439:THR:N	2.43	0.51
1:A:508:PHE:CD1	6:A:709:EDO:H11	2.46	0.51
1:B:109:ILE:HG21	1:B:162:LEU:HD23	1.92	0.51
1:A:314:ARG:HB3	1:A:355:TYR:HB3	1.94	0.48
1:B:408:GLU:HB2	1:B:494:TYR:OH	2.13	0.48
1:B:617:GLU:HG3	1:B:618:ALA:N	2.29	0.47
6:A:709:EDO:H22	2:C:2:PRO:HD2	1.97	0.47
1:B:544:THR:HA	1:B:566:TRP:CZ2	2.49	0.47
1:A:325:THR:O	1:A:329:THR:HG23	2.14	0.47
1:B:357:ASP:OD2	1:B:359:SER:OG	2.26	0.46
1:B:493:GLU:O	1:B:496:HIS:HB2	2.15	0.46
1:B:172:ALA:O	1:B:176:ASN:HB3	2.16	0.45
1:B:565[B]:ARG:NH1	7:B:805:HOH:O	2.48	0.45
1:A:544:THR:HA	1:A:566:TRP:CZ2	2.51	0.45
1:B:118:ASN:OD1	3:I:6:HYP:HD22	2.16	0.45
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.76	0.45
1:A:580:ASP:OD1	1:A:580:ASP:N	2.47	0.45
1:B:495:VAL:HG11	1:B:523:ALA:HA	1.98	0.45
1:A:461:GLU:OE1	6:A:709:EDO:H12	2.18	0.44
1:A:233:VAL:HG22	1:A:257:VAL:HB	1.98	0.44
1:A:429:GLN:O	1:A:471:PRO:HD2	2.18	0.44
1:A:493:GLU:O	1:A:496:HIS:HB2	2.18	0.44
1:B:145[B]:ARG:HB3	1:B:145[B]:ARG:NH1	2.33	0.44
3:E:2:PRO:HA	3:E:3:HYP:HD23	1.88	0.44
6:A:709:EDO:H22	2:C:2:PRO:CD	2.47	0.43
1:B:478:ALA:HB1	1:B:480:TYR:CZ	2.54	0.43
1:B:495:VAL:CG1	1:B:523:ALA:HA	2.49	0.43
1:A:378:THR:HG23	1:A:386:LYS:HE3	2.01	0.42
1:A:461:GLU:HB2	6:A:709:EDO:C2	2.49	0.42
1:B:290:ASP:OD1	1:B:292:THR:OG1	2.30	0.42
1:A:508:PHE:HB2	6:A:709:EDO:H11	2.02	0.42
1:B:320:ILE:O	1:B:324:VAL:HG23	2.19	0.42
1:B:132:PHE:CD1	1:B:169:GLY:HA2	2.54	0.42
1:B:429:GLN:O	1:B:471:PRO:HD2	2.21	0.41
1:B:449:PHE:CD2	1:B:474:ILE:HG12	2.55	0.41
1:A:434:ILE:HD13	1:A:487:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:HB2	1:A:192:ALA:HA	2.02	0.41
1:A:321:ALA:HB3	1:A:322:PRO:HD3	2.03	0.41
1:A:380:ILE:HD13	1:A:386:LYS:HG3	2.03	0.41
1:B:145[A]:ARG:HG3	1:B:195:ALA:HB2	2.02	0.41
1:B:391:ASP:HB3	1:B:436:ASN:OD1	2.21	0.41
1:A:535:ALA:O	1:A:538:THR:HG22	2.20	0.41
1:B:245:ALA:O	1:B:251:ARG:NH1	2.44	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	531/559 (95%)	516 (97%)	14 (3%)	1 (0%)	47	62
1	B	536/559 (96%)	520 (97%)	15 (3%)	1 (0%)	47	62
2	C	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
2	G	1/3 (33%)	1 (100%)	0	0	100	100
2	H	1/3 (33%)	1 (100%)	0	0	100	100
3	E	3/6 (50%)	3 (100%)	0	0	100	100
3	F	3/6 (50%)	3 (100%)	0	0	100	100
3	I	3/6 (50%)	3 (100%)	0	0	100	100
3	J	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	1083/1154 (94%)	1051 (97%)	30 (3%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	529	VAL
1	A	529	VAL

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	429/442 (97%)	420 (98%)	9 (2%)	53	72
1	B	434/442 (98%)	424 (98%)	10 (2%)	50	70
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
2	G	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
3	E	2/2 (100%)	2 (100%)	0	100	100
3	F	2/2 (100%)	2 (100%)	0	100	100
3	I	2/2 (100%)	2 (100%)	0	100	100
3	J	2/2 (100%)	2 (100%)	0	100	100
All	All	875/896 (98%)	856 (98%)	19 (2%)	52	71

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	THR
1	A	183	SER
1	A	231	ASP
1	A	316	THR
1	A	413	THR
1	A	420	GLN
1	A	458	MET
1	A	546	THR
1	A	597	TYR
1	B	100	THR
1	B	102	SER
1	B	230	LEU

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Mol	Chain	Res	Type
1	B	259	THR
1	B	273	LEU
1	B	291	ARG
1	B	316	THR
1	B	429	GLN
1	B	546	THR
1	B	597	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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
3	HYP	F	6	3	9,9,9	1.17	1 (11%)	10,12,12	1.22	1 (10%)
3	HYP	I	6	3	9,9,9	1.18	1 (11%)	10,12,12	1.78	4 (40%)
2	HYP	D	3	2	9,9,9	1.26	0	10,12,12	1.47	1 (10%)
3	HYP	E	6	3	9,9,9	1.17	0	10,12,12	1.74	3 (30%)
3	HYP	E	3	3	6,8,9	0.89	0	5,10,12	2.11	3 (60%)
3	HYP	J	3	3	6,8,9	0.80	0	5,10,12	2.25	2 (40%)
3	HYP	J	6	3	9,9,9	1.34	1 (11%)	10,12,12	1.78	2 (20%)
2	HYP	G	3	2,4	9,9,9	1.13	0	10,12,12	1.44	2 (20%)
3	HYP	F	3	3	6,8,9	1.06	0	5,10,12	2.10	1 (20%)
2	HYP	H	3	2	9,9,9	1.51	2 (22%)	10,12,12	1.60	2 (20%)
3	HYP	I	3	3	6,8,9	0.85	0	5,10,12	1.74	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HYP	C	3	2,4	9,9,9	1.04	0	10,12,12	1.49	2 (20%)

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
3	HYP	F	6	3	-	2/4/13/13	0/1/1/1
3	HYP	I	6	3	-	3/4/13/13	0/1/1/1
2	HYP	D	3	2	-	0/4/13/13	0/1/1/1
3	HYP	E	6	3	-	2/4/13/13	0/1/1/1
3	HYP	E	3	3	-	0/0/11/13	0/1/1/1
3	HYP	J	3	3	-	0/0/11/13	0/1/1/1
3	HYP	J	6	3	-	2/4/13/13	0/1/1/1
2	HYP	G	3	2,4	-	4/4/13/13	0/1/1/1
3	HYP	F	3	3	-	0/0/11/13	0/1/1/1
2	HYP	H	3	2	-	3/4/13/13	0/1/1/1
3	HYP	I	3	3	-	0/0/11/13	0/1/1/1
2	HYP	C	3	2,4	-	4/4/13/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	HYP	CA-C	2.88	1.60	1.52
3	J	6	HYP	CD-CG	2.51	1.59	1.53
3	I	6	HYP	CA-C	2.23	1.58	1.52
2	H	3	HYP	CD-CG	2.22	1.59	1.53
3	F	6	HYP	CA-C	2.03	1.57	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	3	HYP	CB-CG-CD	-3.70	98.72	103.27
3	F	3	HYP	CB-CG-CD	-3.66	98.78	103.27
3	E	3	HYP	CB-CG-CD	-3.06	99.51	103.27
3	E	6	HYP	CG-CB-CA	3.01	107.77	103.96
3	I	6	HYP	CB-CG-CD	-2.95	99.64	103.27
2	D	3	HYP	CG-CB-CA	2.90	107.62	103.96
3	J	6	HYP	OD1-CG-CD	2.89	116.67	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	6	HYP	O-C-CA	-2.89	112.76	122.26
2	C	3	HYP	CG-CB-CA	2.74	107.43	103.96
3	I	6	HYP	O-C-CA	-2.68	113.45	122.26
2	H	3	HYP	OD1-CG-CD	2.68	116.20	110.35
2	G	3	HYP	O-C-CA	-2.56	113.85	122.26
3	J	6	HYP	O-C-CA	-2.47	114.15	122.26
3	J	3	HYP	OD1-CG-CB	2.42	116.01	110.03
2	H	3	HYP	O-C-CA	-2.38	114.43	122.26
2	G	3	HYP	OD1-CG-CB	2.24	115.58	110.03
3	I	6	HYP	OD1-CG-CB	2.24	115.58	110.03
2	C	3	HYP	CB-CA-N	2.24	110.58	106.22
3	E	3	HYP	OD1-CG-CB	2.18	115.41	110.03
3	I	3	HYP	OD1-CG-CB	2.17	115.39	110.03
3	F	6	HYP	OD1-CG-CB	2.16	115.37	110.03
3	E	3	HYP	CG-CB-CA	-2.10	101.32	103.96
3	I	3	HYP	CB-CG-CD	-2.09	100.70	103.27
3	E	6	HYP	OXT-C-CA	2.07	120.28	113.40
3	I	6	HYP	C-CA-N	2.01	114.67	106.73

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	HYP	O-C-CA-N
2	C	3	HYP	OXT-C-CA-N
2	G	3	HYP	O-C-CA-N
2	G	3	HYP	OXT-C-CA-N
2	G	3	HYP	O-C-CA-CB
2	G	3	HYP	OXT-C-CA-CB
3	E	6	HYP	O-C-CA-N
3	E	6	HYP	OXT-C-CA-N
3	F	6	HYP	O-C-CA-N
3	F	6	HYP	OXT-C-CA-N
2	C	3	HYP	O-C-CA-CB
2	C	3	HYP	OXT-C-CA-CB
3	I	6	HYP	O-C-CA-CB
2	H	3	HYP	O-C-CA-N
2	H	3	HYP	OXT-C-CA-N
3	I	6	HYP	O-C-CA-N
3	I	6	HYP	OXT-C-CA-N
3	J	6	HYP	O-C-CA-N
3	J	6	HYP	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	H	3	HYP	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	6	HYP	1	0
3	E	3	HYP	1	0
2	G	3	HYP	6	0
2	C	3	HYP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 10 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	A	707	-	3,3,3	0.68	0	2,2,2	0.15	0
6	EDO	A	706	-	3,3,3	0.15	0	2,2,2	0.24	0
6	EDO	A	710	-	3,3,3	0.50	0	2,2,2	0.39	0
6	EDO	A	709	-	3,3,3	0.55	0	2,2,2	0.68	0
6	EDO	A	708	-	3,3,3	0.54	0	2,2,2	0.84	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
6	EDO	A	707	-	-	0/1/1/1	-
6	EDO	A	706	-	-	1/1/1/1	-
6	EDO	A	710	-	-	1/1/1/1	-
6	EDO	A	709	-	-	0/1/1/1	-
6	EDO	A	708	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	708	EDO	O1-C1-C2-O2
6	A	706	EDO	O1-C1-C2-O2
6	A	710	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	709	EDO	8	0

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	533/559 (95%)	0.35	3 (0%) 89 88	25, 39, 59, 93	0
1	B	533/559 (95%)	0.56	24 (4%) 33 31	36, 51, 71, 97	0
2	C	2/3 (66%)	1.29	0 100 100	45, 45, 45, 54	0
2	D	2/3 (66%)	0.37	0 100 100	40, 40, 40, 41	0
2	G	2/3 (66%)	2.63	1 (50%) 0 0	58, 58, 58, 61	0
2	H	2/3 (66%)	0.45	0 100 100	55, 55, 55, 56	0
3	E	4/6 (66%)	0.12	0 100 100	42, 43, 46, 47	0
3	F	4/6 (66%)	0.70	1 (25%) 0 0	48, 53, 67, 77	0
3	I	4/6 (66%)	0.96	1 (25%) 0 0	46, 55, 58, 65	0
3	J	4/6 (66%)	1.78	1 (25%) 0 0	63, 69, 80, 85	0
All	All	1090/1154 (94%)	0.47	31 (2%) 53 51	25, 46, 68, 97	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1	GLY	5.2
1	B	90	GLU	5.0
1	A	90	GLU	4.4
1	B	573	PHE	4.1
1	B	617	GLU	3.5
2	G	1	GLY	3.5
1	B	619	LEU	3.2
1	B	361	PHE	3.0
1	B	355	TYR	2.9
1	B	579	PRO	2.8
1	B	320	ILE	2.8
1	B	126	GLY	2.7
3	F	1	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	2.5
1	B	281	VAL	2.5
1	B	315	TYR	2.4
1	B	536	ILE	2.4
1	A	542	GLY	2.3
1	B	575	PHE	2.3
1	B	260	LEU	2.3
1	A	357	ASP	2.2
1	B	120	LEU	2.2
1	B	568	TYR	2.2
1	B	174	PHE	2.2
1	B	366	PHE	2.1
1	B	179	ILE	2.1
1	B	542	GLY	2.1
1	B	127	VAL	2.1
1	B	329	THR	2.1
1	B	522	VAL	2.1
3	I	1	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HYP	G	3	9/9	0.77	0.31	55,59,62,62	9
2	HYP	H	3	9/9	0.86	0.20	53,58,63,64	0
2	HYP	C	3	9/9	0.88	0.25	40,43,45,48	9
3	HYP	I	6	9/9	0.88	0.15	48,57,67,68	0
3	HYP	J	3	8/9	0.90	0.18	63,68,73,75	0
3	HYP	J	6	9/9	0.91	0.18	52,55,74,75	0
3	HYP	F	6	9/9	0.92	0.15	41,46,56,67	0
3	HYP	E	6	9/9	0.93	0.13	44,50,58,63	0
3	HYP	F	3	8/9	0.93	0.15	51,56,59,59	0
3	HYP	I	3	8/9	0.94	0.15	40,47,54,55	0
2	HYP	D	3	9/9	0.94	0.14	42,44,49,50	0
3	HYP	E	3	8/9	0.97	0.13	36,44,51,51	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

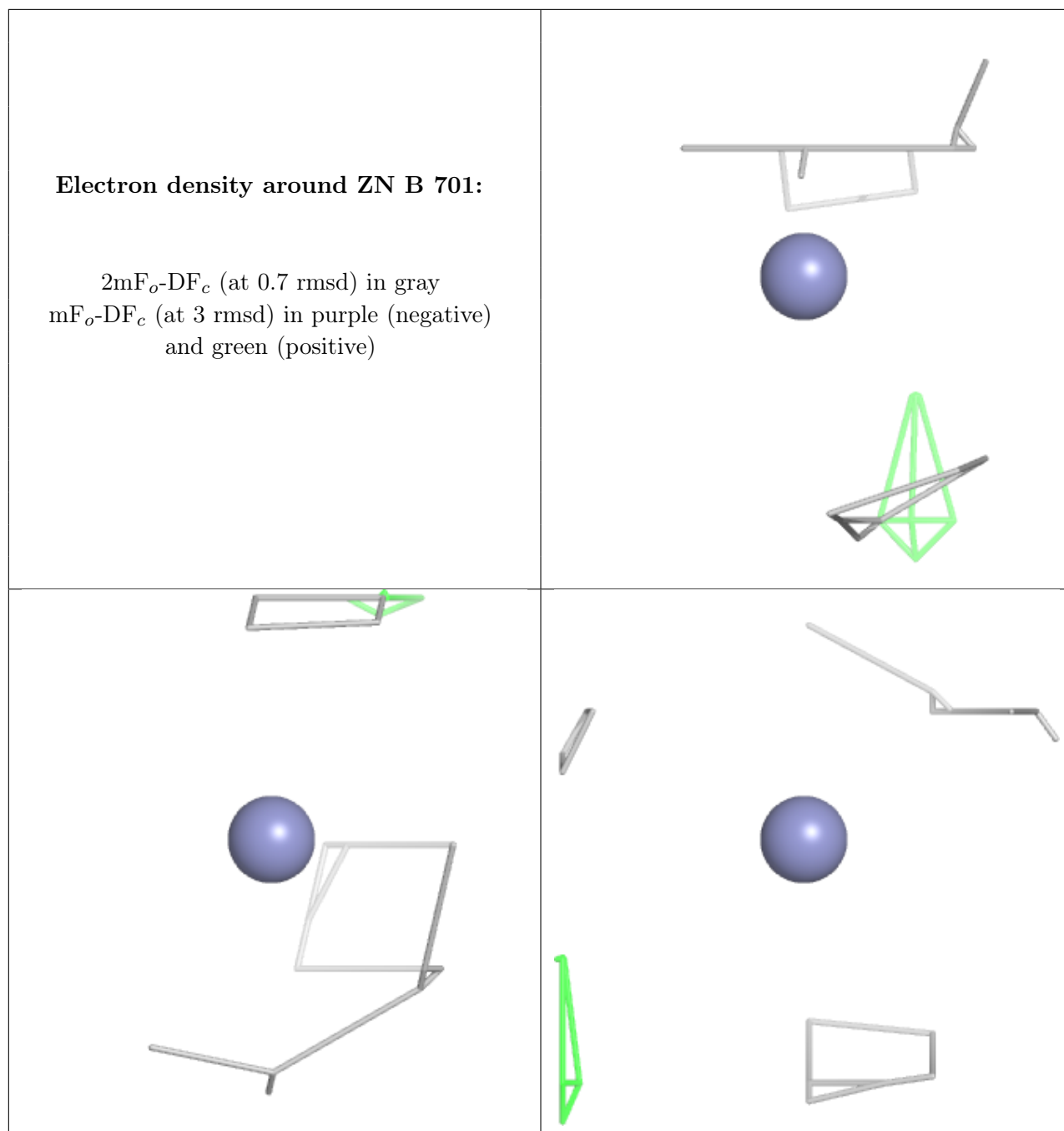
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

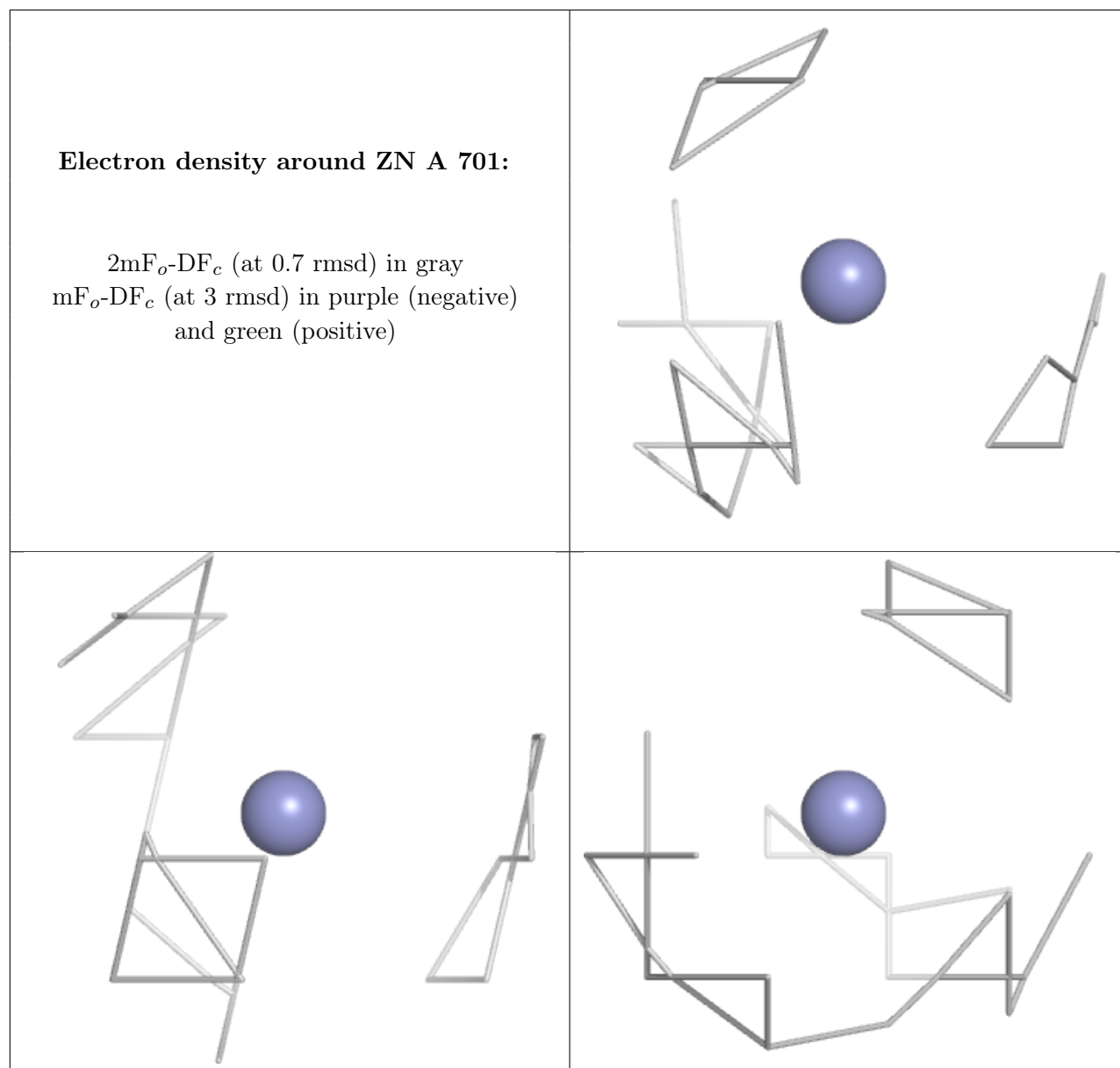
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	A	707	4/4	0.75	0.27	46,48,51,53	0
6	EDO	A	709	4/4	0.86	0.29	34,39,40,44	0
6	EDO	A	710	4/4	0.88	0.24	43,44,46,53	0
6	EDO	A	706	4/4	0.92	0.23	42,44,44,47	0
6	EDO	A	708	4/4	0.93	0.21	28,29,34,38	0
5	CA	B	705	1/1	0.95	0.14	78,78,78,78	0
5	CA	B	703	1/1	0.95	0.10	55,55,55,55	0
5	CA	B	704	1/1	0.95	0.06	60,60,60,60	0
5	CA	A	704	1/1	0.97	0.08	53,53,53,53	0
5	CA	A	705	1/1	0.98	0.07	71,71,71,71	0
5	CA	B	702	1/1	0.98	0.12	37,37,37,37	0
5	CA	A	702	1/1	0.98	0.17	30,30,30,30	0
5	CA	A	703	1/1	0.98	0.12	41,41,41,41	0
4	ZN	B	701	1/1	0.98	0.05	69,69,69,69	0
4	ZN	A	701	1/1	0.99	0.07	51,51,51,51	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 ZN B 701:

$2mF_o-DF_c$ (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.