



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:35 PM UTC

PDB ID : 8HFD / pdb_00008hfd
Title : Crystal structure of allantoinase from E. coli BL21
Authors : Lin, E.S.; Huang, H.Y.; Yang, P.C.; Liu, H.W.; Huang, C.Y.
Deposited on : 2022-11-10
Resolution : 2.07 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
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

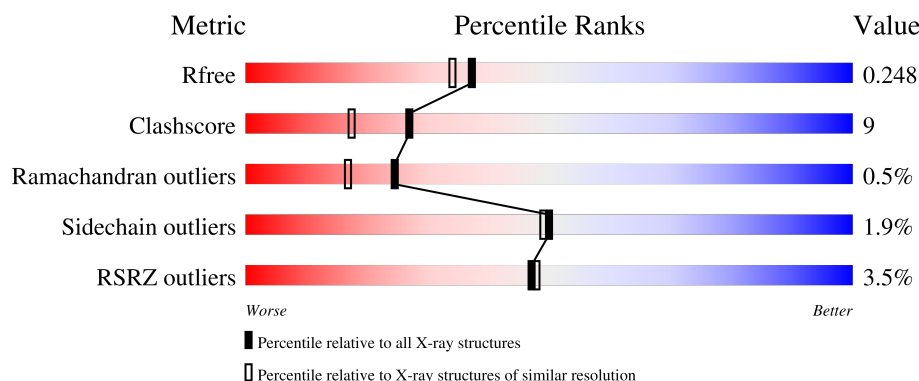
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

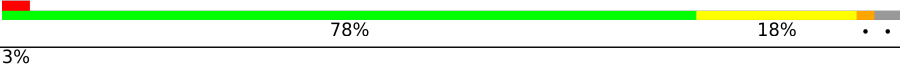
The reported resolution of this entry is 2.07 Å.

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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	459	
1	B	459	
1	C	459	
1	D	459	

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	PEG	C	501	-	-	X	-
2	PEG	D	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14819 atoms, of which 60 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 Allantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3473	2179	604	666	24			
1	B	447	Total	C	N	O	S	0	0	0
			3437	2160	596	658	23			
1	C	448	Total	C	N	O	S	0	0	0
			3448	2166	600	659	23			
1	D	445	Total	C	N	O	S	0	0	0
			3425	2152	594	656	23			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	HIS	-	expression tag	UNP A0A1V3VVF3
A	455	HIS	-	expression tag	UNP A0A1V3VVF3
A	456	HIS	-	expression tag	UNP A0A1V3VVF3
A	457	HIS	-	expression tag	UNP A0A1V3VVF3
A	458	HIS	-	expression tag	UNP A0A1V3VVF3
A	459	HIS	-	expression tag	UNP A0A1V3VVF3
B	454	HIS	-	expression tag	UNP A0A1V3VVF3
B	455	HIS	-	expression tag	UNP A0A1V3VVF3
B	456	HIS	-	expression tag	UNP A0A1V3VVF3
B	457	HIS	-	expression tag	UNP A0A1V3VVF3
B	458	HIS	-	expression tag	UNP A0A1V3VVF3
B	459	HIS	-	expression tag	UNP A0A1V3VVF3
C	454	HIS	-	expression tag	UNP A0A1V3VVF3
C	455	HIS	-	expression tag	UNP A0A1V3VVF3
C	456	HIS	-	expression tag	UNP A0A1V3VVF3
C	457	HIS	-	expression tag	UNP A0A1V3VVF3
C	458	HIS	-	expression tag	UNP A0A1V3VVF3
C	459	HIS	-	expression tag	UNP A0A1V3VVF3
D	454	HIS	-	expression tag	UNP A0A1V3VVF3
D	455	HIS	-	expression tag	UNP A0A1V3VVF3
D	456	HIS	-	expression tag	UNP A0A1V3VVF3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	457	HIS	-	expression tag	UNP A0A1V3VVF3
D	458	HIS	-	expression tag	UNP A0A1V3VVF3
D	459	HIS	-	expression tag	UNP A0A1V3VVF3

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0

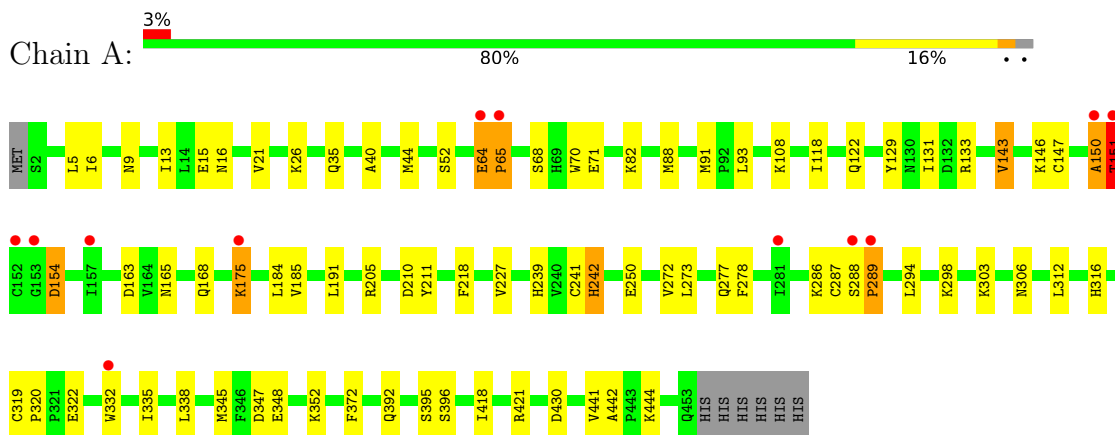
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	264	Total 264	O 264	0	0
4	B	245	Total 245	O 245	0	0
4	C	222	Total 222	O 222	0	0
4	D	195	Total 195	O 195	0	0

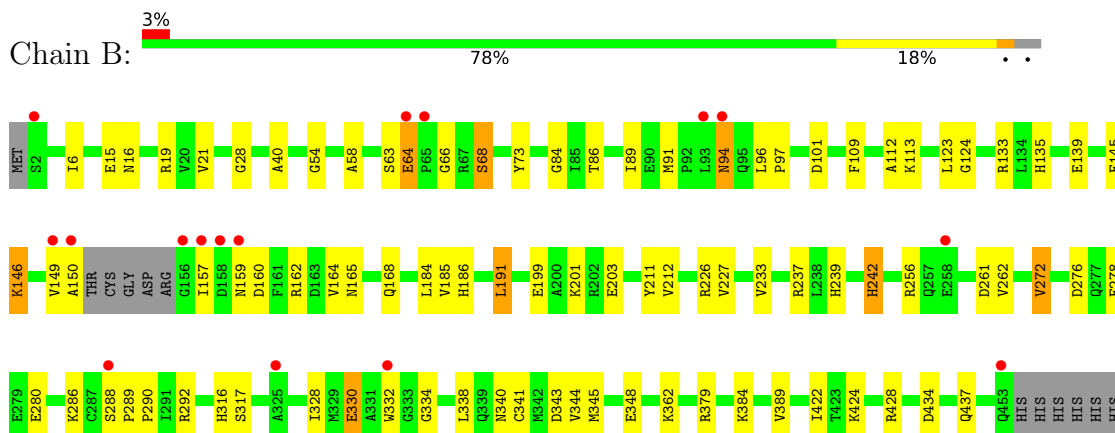
3 Residue-property plots

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.

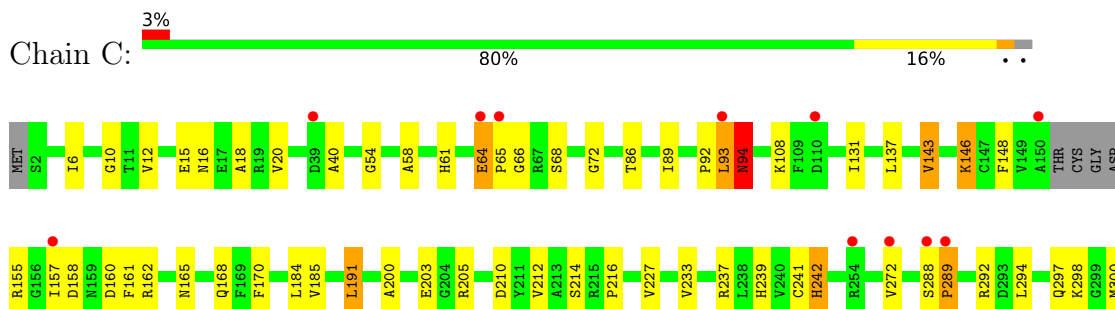
• Molecule 1: Allantoinase



• Molecule 1: Allantoinase



• Molecule 1: Allantoinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.16Å 77.14Å 144.85Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	29.92 – 2.07 29.92 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.92-2.07) 99.0 (29.92-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.92 (at 2.06Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.205 , 0.249 0.209 , 0.248	Depositor DCC
R_{free} test set	1997 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14819	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.63% 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: KCX, PEG, 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	0.53	0/3525	0.80	6/4765 (0.1%)
1	B	0.49	0/3488	0.71	3/4714 (0.1%)
1	C	0.41	0/3499	0.65	3/4728 (0.1%)
1	D	0.43	0/3476	0.66	1/4698 (0.0%)
All	All	0.47	0/13988	0.71	13/18905 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	PRO	N-CA-C	-12.91	94.94	110.70
1	C	289	PRO	N-CA-C	-10.74	97.60	110.70
1	B	64	GLU	N-CA-C	9.94	125.97	112.55
1	A	65	PRO	CB-CA-C	7.78	118.48	111.40
1	A	65	PRO	N-CA-C	-7.38	98.11	110.21
1	C	94	ASN	CB-CA-C	6.28	122.92	110.42
1	C	289	PRO	CB-CA-C	6.23	118.53	110.92
1	B	64	GLU	CB-CA-C	-5.91	102.74	113.49
1	D	94	ASN	CB-CA-C	5.61	121.58	110.42
1	B	94	ASN	CB-CA-C	5.41	121.18	110.42
1	A	150	ALA	N-CA-C	-5.09	100.60	108.90
1	A	289	PRO	CB-CA-C	5.09	117.12	110.92
1	A	151	THR	N-CA-C	-5.03	105.24	111.33

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	3473	0	3417	60	0
1	B	3437	0	3384	66	0
1	C	3448	0	3398	69	0
1	D	3425	0	3371	65	0
2	A	14	20	20	4	0
2	B	7	10	10	1	0
2	C	7	10	10	8	0
2	D	14	20	20	8	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	264	0	0	7	0
4	B	245	0	0	5	0
4	C	222	0	0	5	0
4	D	195	0	0	3	0
All	All	14759	60	13630	252	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 9.

All (252) 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:D:63:SER:HA	1:D:95:GLN:HG3	1.52	0.92
1:B:15:GLU:OE1	1:D:16:ASN:HB3	1.70	0.90
1:C:64:GLU:HG3	1:C:72:GLY:HA2	1.56	0.88
1:B:288:SER:HB3	1:B:289:PRO:HD3	1.57	0.86
1:D:306:ASN:HD21	2:D:502:PEG:H21	1.38	0.86
1:D:288:SER:HB3	1:D:289:PRO:HD3	1.60	0.84
1:C:434:ASP:HB3	1:C:437:GLN:HG3	1.60	0.83
1:B:109:PHE:O	1:B:113:LYS:HE3	1.81	0.80
1:C:272:VAL:HG22	1:C:348:GLU:HG3	1.64	0.79
1:A:306:ASN:HD21	2:A:502:PEG:H12	1.47	0.79
1:B:91:MET:SD	1:B:146:KCX:HG2	2.25	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASP:HB3	1:B:422:ILE:CD1	2.15	0.76
1:A:294:LEU:HG	1:A:298:LYS:HE3	1.68	0.74
1:C:292:ARG:HG2	2:C:501:PEG:H41	1.68	0.73
1:A:288:SER:HB3	1:A:289:PRO:HD3	1.69	0.73
1:A:150:ALA:O	1:A:165:ASN:HA	1.90	0.72
1:C:237:ARG:HD2	4:C:705:HOH:O	1.90	0.71
1:C:131:ILE:HD11	1:C:168:GLN:HB3	1.74	0.69
1:D:306:ASN:HD21	2:D:502:PEG:H41	1.58	0.68
1:A:91:MET:SD	1:A:146:KCX:HG2	2.35	0.67
1:C:292:ARG:CG	2:C:501:PEG:H41	2.24	0.67
1:C:272:VAL:CG2	1:C:348:GLU:HG3	2.24	0.67
1:B:272:VAL:HG22	1:B:348:GLU:HG3	1.76	0.66
1:C:212:VAL:CG1	2:C:501:PEG:H42	2.25	0.66
1:D:167:TRP:CZ2	1:D:171:LYS:HD3	2.31	0.66
1:B:272:VAL:CG2	1:B:348:GLU:HG3	2.25	0.66
1:D:306:ASN:ND2	2:D:502:PEG:H21	2.09	0.66
1:A:319:CYS:HG	1:A:332:TRP:CD1	2.14	0.66
1:D:306:ASN:ND2	2:D:502:PEG:H41	2.12	0.65
1:B:15:GLU:HG2	1:B:362:LYS:NZ	2.11	0.65
1:A:430:ASP:HB2	1:A:444:LYS:HE2	1.80	0.64
1:C:64:GLU:HG3	1:C:72:GLY:CA	2.28	0.64
1:A:9:ASN:HB3	4:A:605:HOH:O	1.99	0.63
1:C:319:CYS:HG	1:C:332:TRP:CD1	2.17	0.63
1:A:306:ASN:ND2	2:A:502:PEG:H31	2.15	0.62
1:B:276:ASP:O	1:B:280:GLU:HG3	2.00	0.61
1:A:65:PRO:HG3	1:A:108:LYS:HG3	1.81	0.61
1:B:54:GLY:HA2	1:B:389:VAL:HG23	1.83	0.61
1:D:64:GLU:O	1:D:65:PRO:C	2.44	0.61
1:C:158:ASP:HA	1:C:162:ARG:HH12	1.67	0.60
1:C:64:GLU:O	1:C:65:PRO:C	2.43	0.60
1:B:162:ARG:NH1	4:B:601:HOH:O	2.33	0.60
1:D:272:VAL:HG22	1:D:348:GLU:HG3	1.85	0.59
1:D:294:LEU:O	1:D:298:LYS:HG2	2.02	0.59
1:C:92:PRO:HD2	1:C:93:LEU:HD23	1.85	0.59
1:A:16:ASN:HB3	1:C:15:GLU:OE2	2.03	0.58
1:A:64:GLU:O	1:A:68:SER:HB3	2.03	0.58
1:B:362:LYS:HD2	4:B:765:HOH:O	2.03	0.58
1:C:143:VAL:CG1	1:C:372:PHE:HB3	2.33	0.58
1:C:157:ILE:HB	1:C:160:ASP:HB2	1.86	0.58
1:C:288:SER:HB3	1:C:289:PRO:HD3	1.86	0.58
1:C:292:ARG:HG2	2:C:501:PEG:C4	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ARG:HD2	4:D:645:HOH:O	2.03	0.58
1:C:170:PHE:HE1	1:C:233:VAL:HG12	1.69	0.57
1:D:201:LYS:HZ1	1:D:330:GLU:CD	2.12	0.57
1:B:288:SER:HB3	1:B:289:PRO:CD	2.31	0.57
1:D:91:MET:SD	1:D:146:KCX:HG2	2.44	0.57
1:A:347:ASP:O	1:A:352:LYS:HG3	2.05	0.56
1:C:143:VAL:HG11	1:C:372:PHE:HB3	1.88	0.56
1:B:343:ASP:HB3	1:B:422:ILE:HD13	1.86	0.56
1:A:191:LEU:HD21	1:B:165:ASN:CG	2.30	0.56
1:D:171:LYS:HE3	1:D:175:LYS:HE2	1.87	0.55
1:B:317:SER:O	1:B:332:TRP:HZ3	1.89	0.55
1:C:200:ALA:HB3	1:C:329:MET:HE2	1.88	0.55
1:B:211:TYR:CE1	1:B:286:LYS:HE3	2.42	0.55
1:B:15:GLU:HG2	1:B:362:LYS:HZ1	1.72	0.55
1:B:149:VAL:O	1:B:150:ALA:C	2.49	0.55
1:A:133:ARG:HD3	4:A:792:HOH:O	2.06	0.54
1:C:316:HIS:CG	1:C:338:LEU:HB2	2.43	0.54
1:A:316:HIS:CG	1:A:338:LEU:HB2	2.42	0.54
1:D:141:GLY:HA2	4:D:655:HOH:O	2.07	0.54
1:D:185:VAL:HG11	1:D:227:VAL:HG21	1.89	0.54
1:B:237:ARG:HD3	1:B:261:ASP:OD2	2.08	0.53
1:C:58:ALA:HA	1:C:89:ILE:HB	1.90	0.53
1:C:294:LEU:O	1:C:298:LYS:HG2	2.07	0.53
1:B:199:GLU:O	1:B:203:GLU:HG3	2.09	0.53
1:A:146:KCX:HG3	1:A:184:LEU:HB2	1.89	0.53
1:D:64:GLU:HB3	1:D:65:PRO:HD3	1.90	0.53
1:A:131:ILE:HD11	1:A:168:GLN:HB3	1.91	0.53
1:A:5:LEU:HD11	1:A:44:MET:HG3	1.91	0.52
1:A:306:ASN:HD21	2:A:502:PEG:H31	1.72	0.52
1:D:316:HIS:CG	1:D:338:LEU:HB2	2.43	0.52
1:D:288:SER:HB3	1:D:289:PRO:CD	2.36	0.52
1:B:316:HIS:CG	1:B:338:LEU:HB2	2.45	0.52
1:D:29:LYS:HE2	1:D:376:GLN:NE2	2.25	0.52
1:D:207:THR:OG1	1:D:210:ASP:OD2	2.27	0.52
1:D:434:ASP:HB3	1:D:437:GLN:HB2	1.93	0.51
1:B:201:LYS:HE3	1:B:330:GLU:OE2	2.10	0.51
1:D:256:ARG:HG2	1:D:262:VAL:HG13	1.92	0.51
1:D:292:ARG:HG2	2:D:501:PEG:H11	1.92	0.51
1:C:328:ILE:HD13	4:C:652:HOH:O	2.09	0.51
1:A:185:VAL:HG11	1:A:227:VAL:HG21	1.92	0.51
1:A:322:GLU:HB2	4:A:627:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:CG2	1:B:226:ARG:HH12	2.24	0.51
1:C:157:ILE:HG22	1:C:158:ASP:O	2.12	0.50
1:D:272:VAL:CG2	1:D:348:GLU:HG3	2.40	0.50
1:D:97:PRO:HA	1:D:159:ASN:HB2	1.93	0.50
1:C:158:ASP:HA	1:C:162:ARG:NH1	2.26	0.50
1:B:341:CYS:O	1:B:345:MET:HB2	2.12	0.50
1:A:6:ILE:HG13	1:A:40:ALA:HB2	1.93	0.50
1:A:146:KCX:HD3	1:A:147:CYS:N	2.27	0.50
1:C:292:ARG:HB3	2:C:501:PEG:H41	1.93	0.49
1:D:256:ARG:CG	1:D:262:VAL:HG13	2.42	0.49
1:A:13:ILE:HD12	1:A:52:SER:HB2	1.94	0.49
1:B:64:GLU:O	1:B:68:SER:CB	2.61	0.49
1:B:58:ALA:HA	1:B:89:ILE:HB	1.94	0.49
1:B:63:SER:OG	1:B:94:ASN:HB2	2.12	0.49
1:D:129:TYR:O	1:D:133:ARG:NH1	2.43	0.49
1:B:97:PRO:HB3	1:B:159:ASN:CG	2.38	0.49
1:C:61:HIS:CE1	1:C:93:LEU:HG	2.48	0.49
1:C:54:GLY:HA3	1:C:86:THR:OG1	2.13	0.48
1:C:65:PRO:HG3	1:C:108:LYS:HG3	1.95	0.48
1:D:58:ALA:HA	1:D:89:ILE:HB	1.94	0.48
1:C:292:ARG:CB	2:C:501:PEG:H41	2.42	0.48
1:A:441:VAL:HG23	1:A:442:ALA:O	2.13	0.48
1:D:217:VAL:HG23	2:D:501:PEG:H22	1.95	0.48
1:B:157:ILE:HB	1:B:160:ASP:HB2	1.95	0.48
1:B:84:GLY:O	1:B:389:VAL:HG21	2.14	0.48
1:C:430:ASP:OD2	1:C:444:LYS:NZ	2.46	0.48
1:A:16:ASN:HB2	4:A:631:HOH:O	2.14	0.48
1:B:101:ASP:OD2	1:B:133:ARG:NH1	2.41	0.48
1:C:319:CYS:SG	1:C:332:TRP:CD1	3.07	0.48
1:B:6:ILE:HG13	1:B:40:ALA:HB2	1.95	0.47
1:B:135:HIS:O	1:B:139:GLU:HG3	2.14	0.47
1:C:312:LEU:HD13	1:C:345:MET:HE2	1.95	0.47
1:A:184:LEU:HG	1:A:239:HIS:HB3	1.95	0.47
1:A:319:CYS:HB2	1:A:320:PRO:HD2	1.96	0.47
1:B:185:VAL:HG11	1:B:227:VAL:HG11	1.96	0.47
1:A:312:LEU:CD1	1:A:345:MET:HE2	2.45	0.47
1:A:175:LYS:HA	1:A:175:LYS:HD2	1.70	0.47
1:D:24:ALA:HB2	1:D:37:LEU:HD13	1.97	0.47
1:D:63:SER:OG	1:D:94:ASN:HB2	2.14	0.47
1:C:304:LEU:HD13	1:C:355:MET:HE1	1.97	0.47
2:A:501:PEG:H11	4:A:655:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:VAL:HG22	1:B:290:PRO:HB2	1.95	0.46
1:D:206:VAL:HG12	1:D:329:MET:HG3	1.97	0.46
1:A:272:VAL:HG22	1:A:348:GLU:HG3	1.97	0.46
1:D:171:LYS:O	1:D:175:LYS:HD2	2.14	0.46
1:A:165:ASN:CG	1:B:191:LEU:HD11	2.41	0.46
1:D:146:KCX:HD3	1:D:147:CYS:N	2.30	0.46
1:B:184:LEU:HG	1:B:239:HIS:HB3	1.98	0.46
1:C:203:GLU:HB3	4:C:607:HOH:O	2.14	0.46
1:D:317:SER:O	1:D:332:TRP:HZ3	1.98	0.46
1:D:142:VAL:HG13	1:D:144:GLY:H	1.81	0.46
1:B:66:GLY:HA3	1:B:96:LEU:HB2	1.98	0.45
1:D:65:PRO:CG	1:D:108:LYS:HG3	2.47	0.45
1:A:392:GLN:HG2	1:A:395:SER:HB3	1.97	0.45
1:C:165:ASN:CG	1:D:191:LEU:HD21	2.41	0.45
1:A:88:MET:HG2	1:A:118:ILE:HD11	1.97	0.45
1:A:211:TYR:CE1	1:A:286:LYS:HE3	2.52	0.45
1:C:191:LEU:HD11	1:D:165:ASN:CG	2.41	0.45
1:D:287:CYS:HB3	1:D:335:ILE:HG12	1.99	0.45
1:A:218:PHE:CD2	1:B:233:VAL:HG11	2.51	0.45
1:C:241:CYS:O	1:C:242:HIS:C	2.59	0.45
1:B:292:ARG:HD3	2:B:501:PEG:H21	1.99	0.45
1:D:212:VAL:HG22	1:D:290:PRO:HB2	1.98	0.45
1:A:287:CYS:HB3	1:A:335:ILE:HG12	1.99	0.45
1:B:19:ARG:HG3	1:B:21:VAL:HG13	1.98	0.45
1:C:214:SER:C	1:C:216:PRO:HD3	2.42	0.44
1:A:21:VAL:HA	1:A:35:GLN:HE22	1.83	0.44
1:A:129:TYR:O	1:A:133:ARG:NH1	2.51	0.44
1:C:10:GLY:O	1:C:20:VAL:HA	2.17	0.44
1:C:184:LEU:HG	1:C:239:HIS:HB3	2.00	0.44
2:D:501:PEG:H32	4:D:619:HOH:O	2.16	0.44
1:B:54:GLY:HA3	1:B:86:THR:OG1	2.18	0.44
1:D:67:ARG:HD2	1:D:94:ASN:O	2.18	0.44
1:A:278:PHE:CZ	1:A:286:LYS:HA	2.53	0.44
1:B:256:ARG:HG3	1:B:262:VAL:HG13	1.99	0.44
1:D:65:PRO:HG2	1:D:108:LYS:HG3	1.99	0.44
1:D:131:ILE:HD11	1:D:168:GLN:HB3	2.00	0.44
1:C:389:VAL:HG21	1:C:422:ILE:HD12	1.98	0.44
1:D:215:ARG:HB2	1:D:290:PRO:HG3	1.98	0.44
1:A:151:THR:HG21	1:B:226:ARG:HH12	1.83	0.44
1:D:54:GLY:HA3	1:D:86:THR:OG1	2.17	0.44
1:D:389:VAL:HG11	1:D:422:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:CG1	1:A:372:PHE:HB3	2.48	0.43
1:C:212:VAL:HG12	2:C:501:PEG:H42	1.99	0.43
1:B:15:GLU:HG2	1:B:362:LYS:HZ3	1.79	0.43
1:A:250:GLU:HG3	1:A:303:LYS:HE3	1.99	0.43
1:C:93:LEU:O	1:C:94:ASN:HB2	2.18	0.43
1:D:87:THR:OG1	1:D:377:LYS:HE3	2.18	0.43
1:A:184:LEU:HD12	1:A:184:LEU:N	2.33	0.43
1:C:12:VAL:O	1:C:18:ALA:HA	2.19	0.43
1:D:358:PRO:O	1:D:362:LYS:HG2	2.18	0.43
1:B:124:GLY:O	1:B:145:PHE:HA	2.18	0.43
1:B:242:HIS:O	1:B:242:HIS:ND1	2.49	0.43
1:A:396:SER:HA	1:A:418:ILE:O	2.18	0.43
1:D:241:CYS:O	1:D:242:HIS:C	2.61	0.43
1:C:58:ALA:HB3	1:C:313:VAL:HG11	2.01	0.43
1:C:64:GLU:O	1:C:66:GLY:N	2.51	0.43
1:C:205:ARG:HB3	1:C:210:ASP:CG	2.43	0.43
1:A:205:ARG:HB3	1:A:210:ASP:CG	2.44	0.43
1:B:157:ILE:HG22	1:B:159:ASN:H	1.84	0.43
1:D:306:ASN:HD21	2:D:502:PEG:C4	2.28	0.43
1:A:273:LEU:HA	1:A:277:GLN:OE1	2.19	0.42
1:C:212:VAL:HG11	2:C:501:PEG:H42	1.98	0.42
1:B:164:VAL:HB	1:B:168:GLN:HB2	2.02	0.42
1:D:278:PHE:CD1	1:D:278:PHE:C	2.98	0.42
1:A:288:SER:HB3	1:A:289:PRO:CD	2.45	0.42
1:A:319:CYS:SG	1:A:332:TRP:CD1	3.11	0.42
1:D:242:HIS:O	1:D:242:HIS:ND1	2.51	0.42
1:D:375:GLN:HE21	1:D:375:GLN:HB2	1.48	0.42
1:A:154:ASP:HB2	1:A:163:ASP:OD2	2.20	0.42
1:C:319:CYS:HB2	1:C:320:PRO:HD2	2.01	0.42
1:C:143:VAL:HG13	1:C:372:PHE:HB3	2.01	0.42
1:D:135:HIS:O	1:D:139:GLU:HG3	2.19	0.42
1:A:143:VAL:HG22	1:A:372:PHE:O	2.20	0.42
1:B:73:TYR:CE2	1:B:112:ALA:HB2	2.54	0.42
1:B:424:LYS:NZ	4:B:620:HOH:O	2.53	0.42
1:D:396:SER:OG	1:D:419:GLY:HA2	2.20	0.42
1:B:332:TRP:CZ3	1:B:334:GLY:HA3	2.55	0.42
1:C:61:HIS:HB2	1:C:316:HIS:O	2.19	0.42
1:D:65:PRO:CD	1:D:108:LYS:HG3	2.50	0.42
1:D:131:ILE:HD11	1:D:168:GLN:HG2	2.01	0.42
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.92	0.42
1:D:205:ARG:HB3	1:D:210:ASP:CG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TRP:CD1	1:A:320:PRO:HD3	2.55	0.42
1:A:218:PHE:CG	1:B:233:VAL:HG11	2.54	0.42
1:B:97:PRO:HB3	1:B:159:ASN:ND2	2.34	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.94	0.41
1:B:28:GLY:HA2	1:B:428:ARG:C	2.45	0.41
1:C:6:ILE:HG13	1:C:40:ALA:HB2	2.02	0.41
1:C:64:GLU:HG2	1:C:68:SER:CB	2.50	0.41
1:C:148:PHE:CD1	1:C:161:PHE:HE2	2.39	0.41
1:B:186:HIS:HE1	1:B:288:SER:HB3	1.86	0.41
1:C:184:LEU:HD11	1:C:372:PHE:HE1	1.85	0.41
1:D:124:GLY:O	1:D:145:PHE:HA	2.20	0.41
1:A:241:CYS:O	1:A:242:HIS:C	2.63	0.41
1:C:16:ASN:HB2	4:C:693:HOH:O	2.19	0.41
1:B:89:ILE:HG22	1:B:123:LEU:HG	2.02	0.41
1:B:278:PHE:CD1	1:B:278:PHE:C	2.99	0.41
1:B:328:ILE:HG13	4:B:723:HOH:O	2.20	0.41
1:C:15:GLU:CD	1:C:379:ARG:HE	2.29	0.41
1:D:24:ALA:HB3	1:D:32:ALA:HB3	2.03	0.41
1:B:340:ASN:O	1:B:344:VAL:HB	2.21	0.41
1:B:379:ARG:HG3	1:B:384:LYS:HG3	2.02	0.41
1:C:242:HIS:O	1:C:242:HIS:ND1	2.52	0.41
1:A:421:ARG:HD2	4:A:607:HOH:O	2.19	0.40
1:B:422:ILE:N	1:B:422:ILE:HD12	2.36	0.40
1:B:434:ASP:CG	1:B:437:GLN:HE21	2.29	0.40
1:C:61:HIS:HE1	1:C:93:LEU:HG	1.85	0.40
1:C:146:KCX:HZ	1:C:146:KCX:HG2	1.66	0.40
1:C:64:GLU:HG2	1:C:68:SER:HB2	2.03	0.40
1:C:185:VAL:HG11	1:C:227:VAL:HG21	2.03	0.40
1:A:93:LEU:HD23	1:A:93:LEU:H	1.86	0.40
1:A:82:LYS:NZ	4:A:606:HOH:O	2.47	0.40
1:A:108:LYS:NZ	1:A:122:GLN:OE1	2.54	0.40
1:B:113:LYS:HE2	1:B:113:LYS:HA	2.02	0.40
1:C:300:MET:HE3	1:C:300:MET:HB3	1.94	0.40
1:B:16:ASN:HB2	4:B:686:HOH:O	2.21	0.40
1:C:297:GLN:HB2	4:C:634:HOH:O	2.21	0.40
1:D:149:VAL:HG12	1:D:150:ALA:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/459 (98%)	435 (97%)	12 (3%)	2 (0%)	30	23
1	B	442/459 (96%)	429 (97%)	12 (3%)	1 (0%)	43	38
1	C	443/459 (96%)	428 (97%)	13 (3%)	2 (0%)	24	17
1	D	440/459 (96%)	427 (97%)	10 (2%)	3 (1%)	18	10
All	All	1774/1836 (97%)	1719 (97%)	47 (3%)	8 (0%)	24	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	B	242	HIS
1	C	94	ASN
1	C	242	HIS
1	D	242	HIS
1	D	94	ASN
1	A	71	GLU
1	D	64	GLU

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	369/376 (98%)	362 (98%)	7 (2%)	50	49
1	B	365/376 (97%)	361 (99%)	4 (1%)	65	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	366/376 (97%)	357 (98%)	9 (2%)	42	38
1	D	364/376 (97%)	356 (98%)	8 (2%)	45	43
All	All	1464/1504 (97%)	1436 (98%)	28 (2%)	50	49

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	26	LYS
1	A	64	GLU
1	A	143	VAL
1	A	151	THR
1	A	154	ASP
1	A	175	LYS
1	B	68	SER
1	B	191	LEU
1	B	272	VAL
1	B	330	GLU
1	C	64	GLU
1	C	93	LEU
1	C	143	VAL
1	C	155	ARG
1	C	191	LEU
1	C	304	LEU
1	C	311	CYS
1	C	332	TRP
1	C	453	GLN
1	D	142	VAL
1	D	158	ASP
1	D	159	ASN
1	D	227	VAL
1	D	366	THR
1	D	375	GLN
1	D	389	VAL
1	D	452	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	375	GLN
1	B	181	GLN
1	B	392	GLN
1	B	437	GLN
1	B	451	HIS
1	B	452	GLN
1	C	9	ASN
1	C	35	GLN
1	C	69	HIS
1	C	296	ASN
1	C	297	GLN
1	C	401	ASN
1	D	181	GLN
1	D	306	ASN
1	D	340	ASN
1	D	375	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	KCX	C	146	1,3	10,11,12	1.11	1 (10%)	6,12,14	1.09	1 (16%)
1	KCX	B	146	1,3	10,11,12	1.06	1 (10%)	6,12,14	1.63	1 (16%)
1	KCX	D	146	1,3	10,11,12	2.18	1 (10%)	6,12,14	3.01	1 (16%)
1	KCX	A	146	1,3	10,11,12	0.48	0	6,12,14	0.31	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
1	KCX	C	146	1,3	-	4/9/10/12	-
1	KCX	B	146	1,3	-	2/9/10/12	-
1	KCX	D	146	1,3	-	6/9/10/12	-
1	KCX	A	146	1,3	-	5/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	KCX	OQ1-CX	6.55	1.33	1.21
1	B	146	KCX	CE-NZ	2.35	1.51	1.46
1	C	146	KCX	CE-NZ	2.21	1.51	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	KCX	OQ1-CX-NZ	-7.36	113.74	124.92
1	B	146	KCX	OQ1-CX-NZ	-3.89	119.01	124.92
1	C	146	KCX	OQ1-CX-NZ	-2.42	121.25	124.92

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	146	KCX	N-CA-CB-CG
1	A	146	KCX	C-CA-CB-CG
1	A	146	KCX	OQ1-CX-NZ-CE
1	A	146	KCX	OQ2-CX-NZ-CE
1	B	146	KCX	N-CA-CB-CG
1	B	146	KCX	C-CA-CB-CG
1	C	146	KCX	C-CA-CB-CG
1	D	146	KCX	N-CA-CB-CG
1	D	146	KCX	C-CA-CB-CG
1	D	146	KCX	OQ1-CX-NZ-CE
1	D	146	KCX	OQ2-CX-NZ-CE
1	C	146	KCX	CA-CB-CG-CD
1	C	146	KCX	CG-CD-CE-NZ
1	D	146	KCX	CE-CD-CG-CB
1	D	146	KCX	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	A	146	KCX	CE-CD-CG-CB
1	C	146	KCX	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	146	KCX	1	0
1	B	146	KCX	1	0
1	D	146	KCX	2	0
1	A	146	KCX	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
2	PEG	B	501	-	6,6,6	0.17	0	5,5,5	0.13	0
2	PEG	A	502	-	6,6,6	0.10	0	5,5,5	0.10	0
2	PEG	A	501	-	6,6,6	0.26	0	5,5,5	0.23	0
2	PEG	C	501	-	6,6,6	0.36	0	5,5,5	0.64	0
2	PEG	D	501	-	6,6,6	0.14	0	5,5,5	0.17	0
2	PEG	D	502	-	6,6,6	0.12	0	5,5,5	0.08	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
2	PEG	B	501	-	-	1/4/4/4	-
2	PEG	A	502	-	-	1/4/4/4	-
2	PEG	A	501	-	-	3/4/4/4	-
2	PEG	C	501	-	-	3/4/4/4	-
2	PEG	D	501	-	-	2/4/4/4	-
2	PEG	D	502	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	PEG	O2-C3-C4-O4
2	A	501	PEG	O1-C1-C2-O2
2	D	502	PEG	O2-C3-C4-O4
2	A	502	PEG	O2-C3-C4-O4
2	A	501	PEG	O2-C3-C4-O4
2	C	501	PEG	O1-C1-C2-O2
2	D	502	PEG	O1-C1-C2-O2
2	B	501	PEG	O2-C3-C4-O4
2	D	501	PEG	C4-C3-O2-C2
2	D	502	PEG	C4-C3-O2-C2
2	D	501	PEG	O2-C3-C4-O4
2	A	501	PEG	C4-C3-O2-C2
2	C	501	PEG	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PEG	1	0
2	A	502	PEG	3	0
2	A	501	PEG	1	0
2	C	501	PEG	8	0
2	D	501	PEG	3	0
2	D	502	PEG	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	451/459 (98%)	0.18	12 (2%) 56 58	21, 28, 41, 68	0
1	B	446/459 (97%)	0.22	16 (3%) 46 47	19, 27, 41, 76	0
1	C	447/459 (97%)	0.32	14 (3%) 51 52	23, 31, 44, 61	0
1	D	444/459 (96%)	0.37	21 (4%) 36 36	23, 31, 45, 68	0
All	All	1788/1836 (97%)	0.27	63 (3%) 47 48	19, 30, 44, 76	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	288	SER	8.5
1	A	288	SER	8.3
1	B	150	ALA	6.4
1	D	288	SER	5.4
1	A	151	THR	5.4
1	B	288	SER	5.4
1	C	64	GLU	4.5
1	A	153	GLY	4.3
1	A	150	ALA	4.1
1	B	156	GLY	3.9
1	A	65	PRO	3.9
1	A	157	ILE	3.9
1	C	332	TRP	3.7
1	D	150	ALA	3.7
1	C	93	LEU	3.6
1	D	93	LEU	3.6
1	A	332	TRP	3.5
1	D	65	PRO	3.5
1	B	157	ILE	3.5
1	D	64	GLU	3.4
1	A	289	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	93	LEU	3.3
1	D	452	GLN	3.2
1	C	65	PRO	3.2
1	D	94	ASN	3.2
1	B	65	PRO	3.1
1	D	149	VAL	3.0
1	D	66	GLY	3.0
1	D	289	PRO	3.0
1	D	107	LEU	2.9
1	B	149	VAL	2.8
1	C	150	ALA	2.8
1	C	289	PRO	2.7
1	B	2	SER	2.7
1	C	157	ILE	2.7
1	B	258	GLU	2.6
1	B	325	ALA	2.6
1	B	159	ASN	2.6
1	A	64	GLU	2.6
1	B	94	ASN	2.6
1	B	453	GLN	2.6
1	C	110	ASP	2.5
1	D	96	LEU	2.5
1	C	254	ARG	2.5
1	D	39	ASP	2.4
1	D	332	TRP	2.4
1	D	402	ASP	2.3
1	C	272	VAL	2.3
1	B	64	GLU	2.2
1	A	281	ILE	2.2
1	D	159	ASN	2.2
1	B	158	ASP	2.2
1	B	332	TRP	2.2
1	C	39	ASP	2.2
1	D	110	ASP	2.2
1	A	152	CYS	2.2
1	D	97	PRO	2.1
1	A	175	LYS	2.1
1	D	42	GLU	2.1
1	C	402	ASP	2.1
1	C	328	ILE	2.1
1	D	2	SER	2.1
1	D	258	GLU	2.0

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
1	KCX	D	146	12/13	0.77	0.21	26,32,40,40	0
1	KCX	A	146	12/13	0.84	0.15	18,24,30,34	0
1	KCX	B	146	12/13	0.90	0.11	22,27,30,35	0
1	KCX	C	146	12/13	0.95	0.07	21,29,33,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

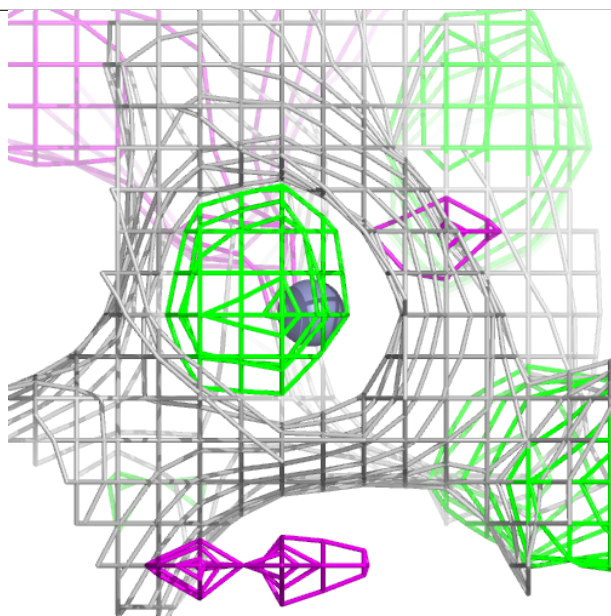
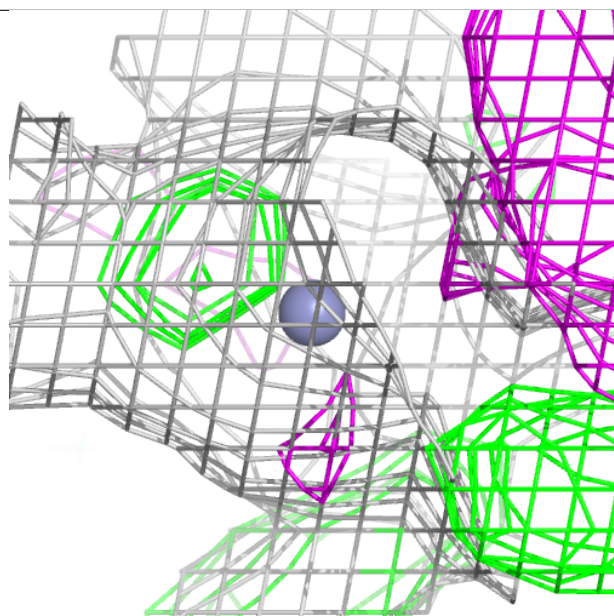
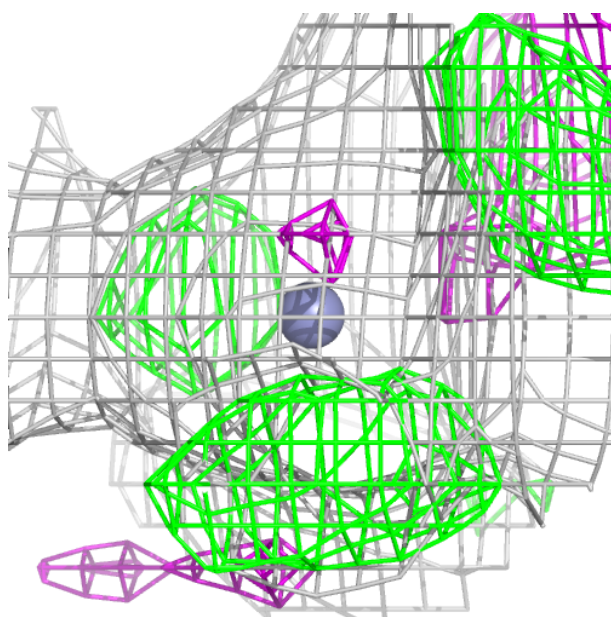
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEG	B	501	7/7	0.80	0.16	24,37,46,51	0
2	PEG	D	502	7/7	0.82	0.21	20,20,20,20	0
2	PEG	C	501	7/7	0.84	0.15	28,40,53,58	0
2	PEG	A	501	7/7	0.84	0.18	19,45,56,67	0
2	PEG	D	501	7/7	0.88	0.16	19,42,51,53	0
2	PEG	A	502	7/7	0.88	0.20	20,20,20,20	0
3	ZN	D	503	1/1	0.92	0.07	36,36,36,36	0
3	ZN	D	504	1/1	0.94	0.07	36,36,36,36	0
3	ZN	C	502	1/1	0.98	0.03	31,31,31,31	0
3	ZN	B	503	1/1	0.99	0.01	30,30,30,30	0
3	ZN	A	503	1/1	0.99	0.05	25,25,25,25	0
3	ZN	C	503	1/1	0.99	0.03	35,35,35,35	0
3	ZN	A	504	1/1	0.99	0.02	30,30,30,30	0
3	ZN	B	502	1/1	0.99	0.02	26,26,26,26	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.

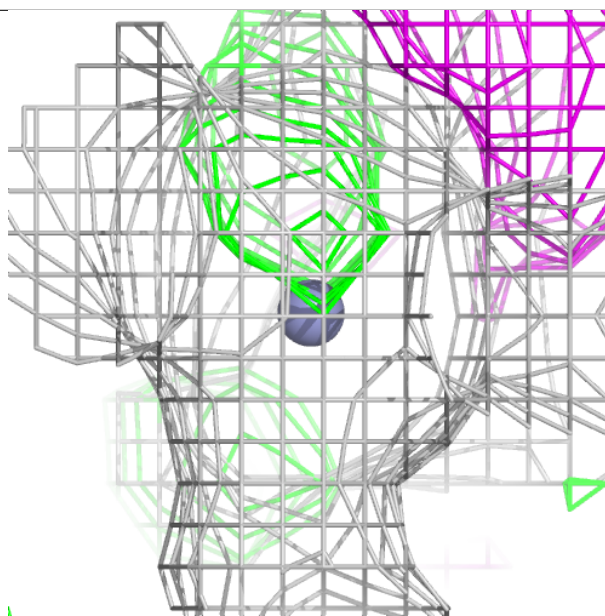
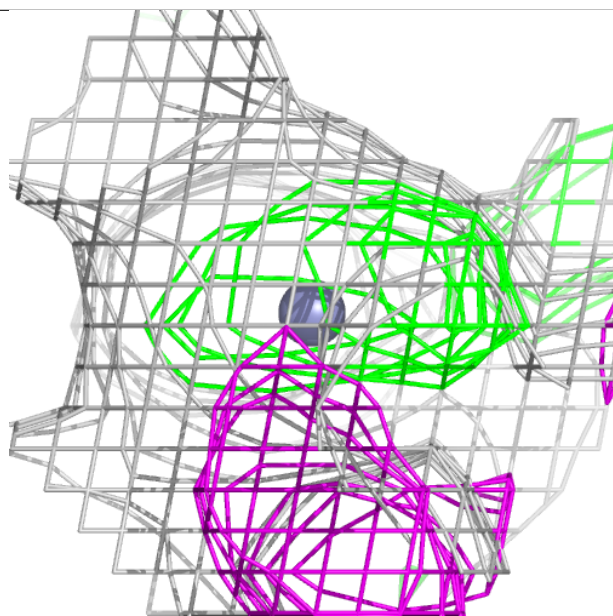
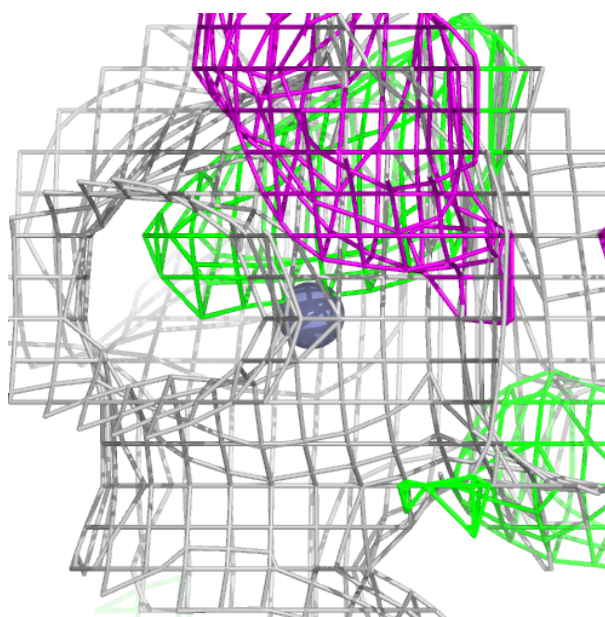
Electron density around ZN D 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



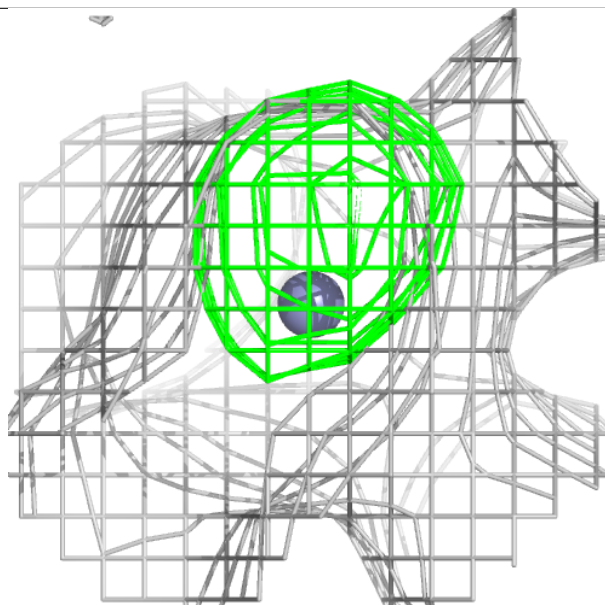
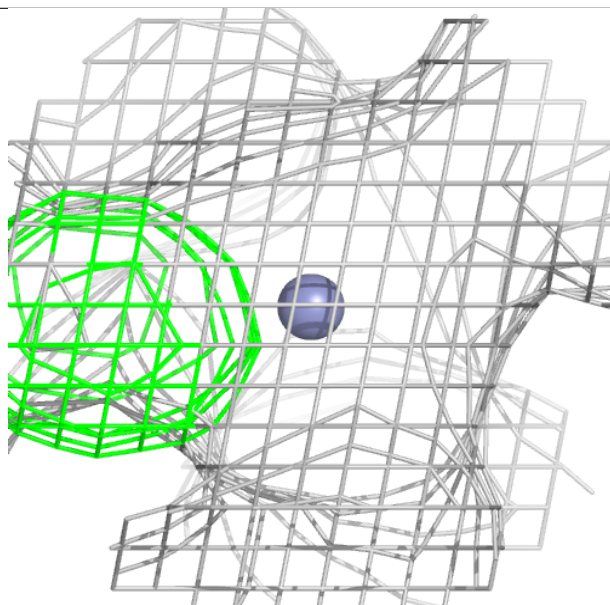
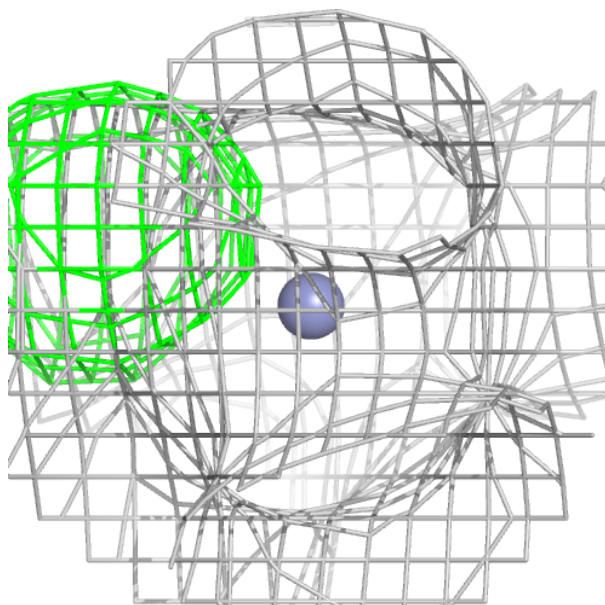
Electron density around ZN D 504:

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and green (positive)



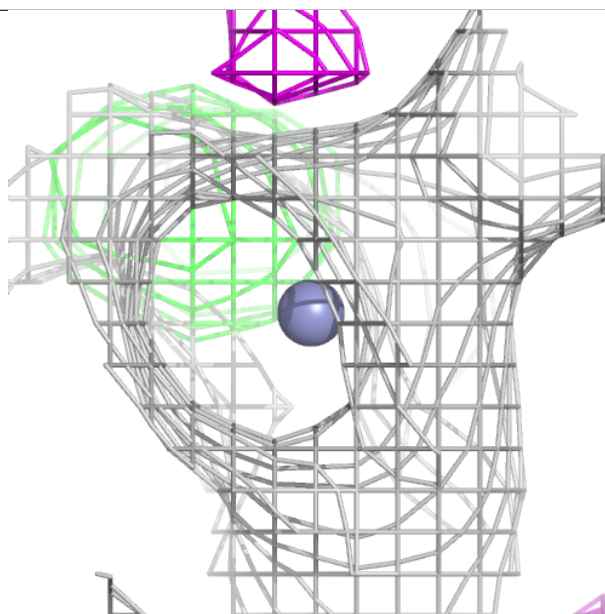
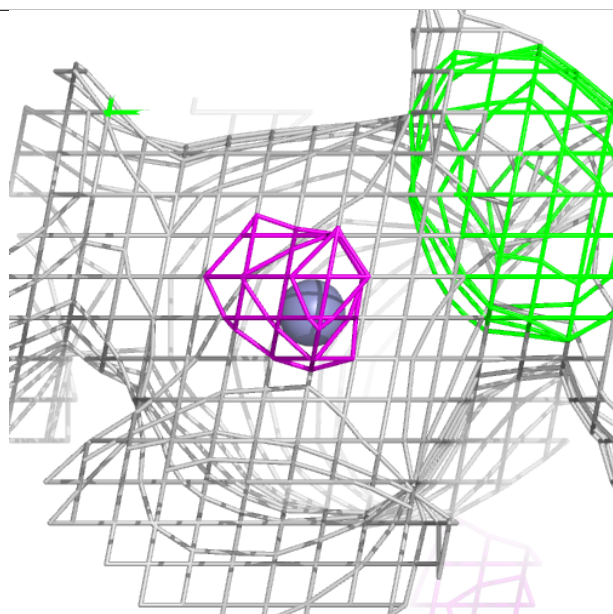
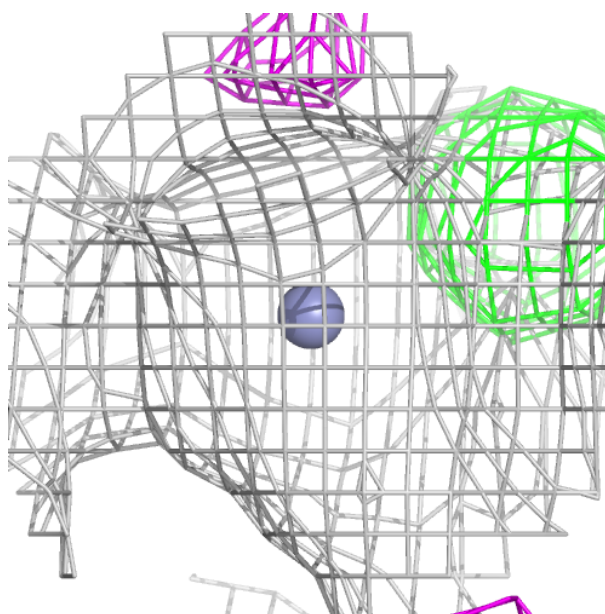
Electron density around ZN C 502:

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and green (positive)



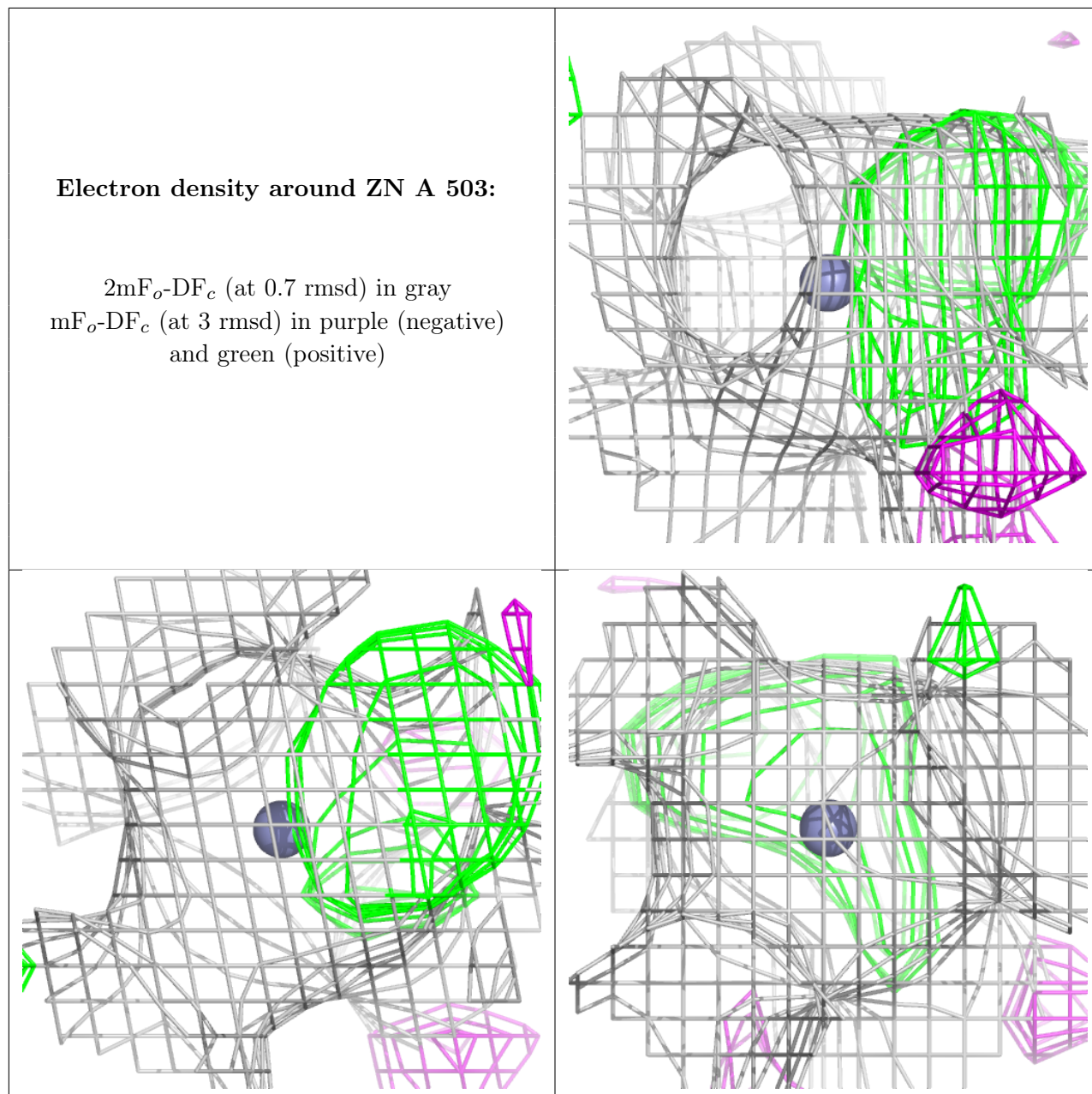
Electron density around ZN B 503:

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and green (positive)



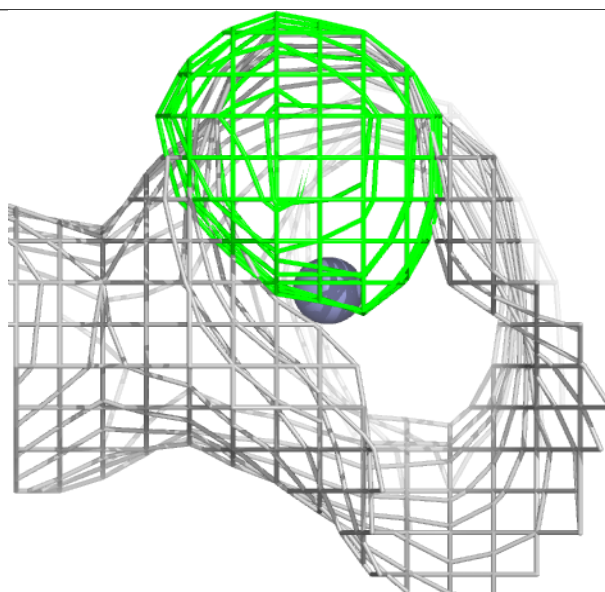
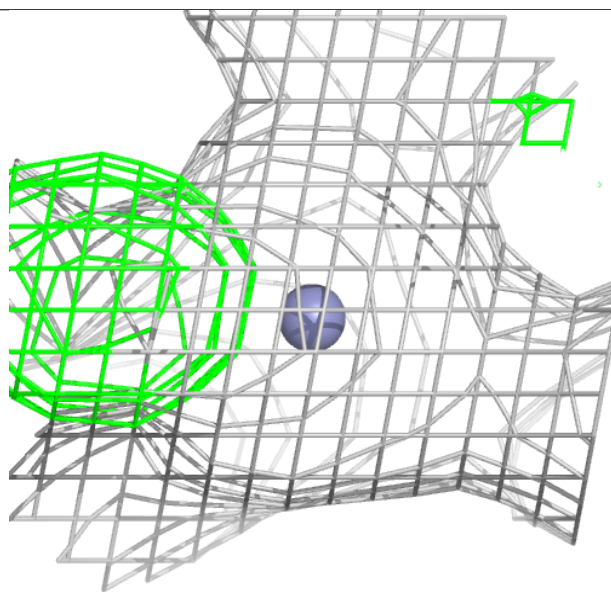
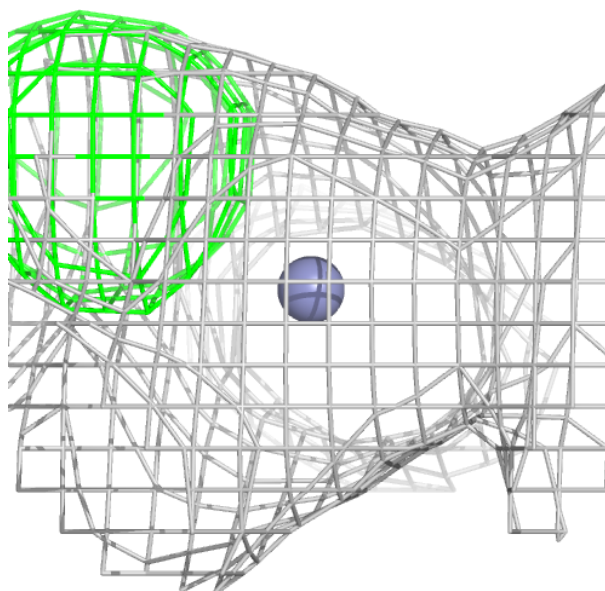
Electron density around ZN A 503:

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and green (positive)



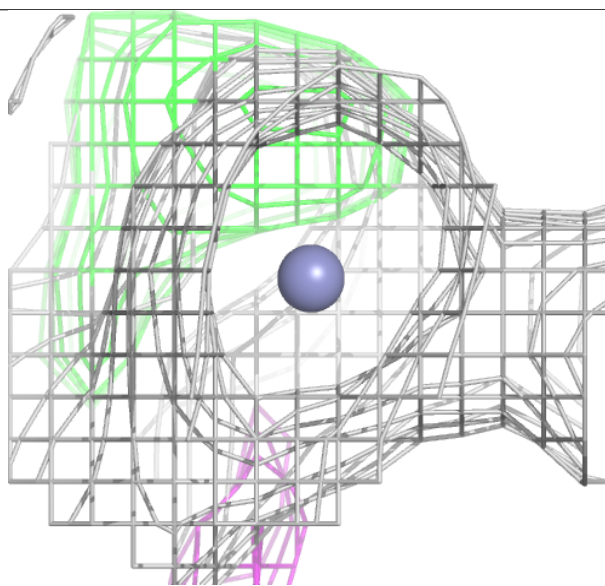
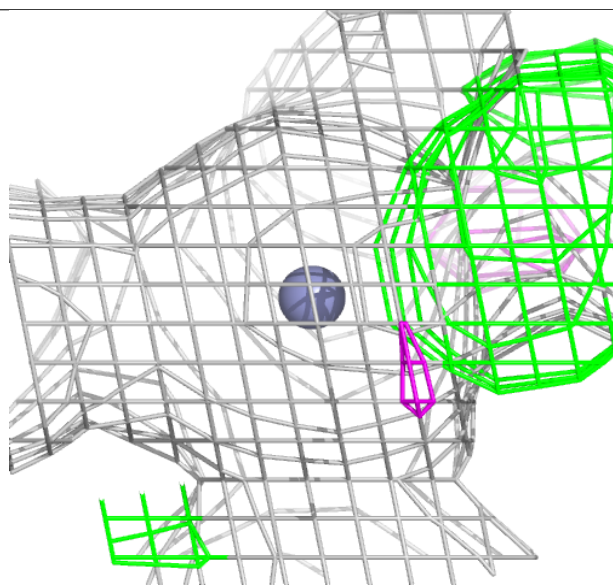
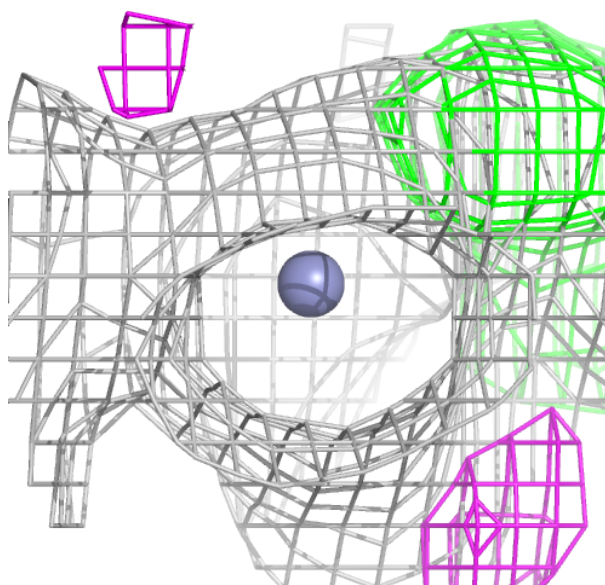
Electron density around ZN C 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



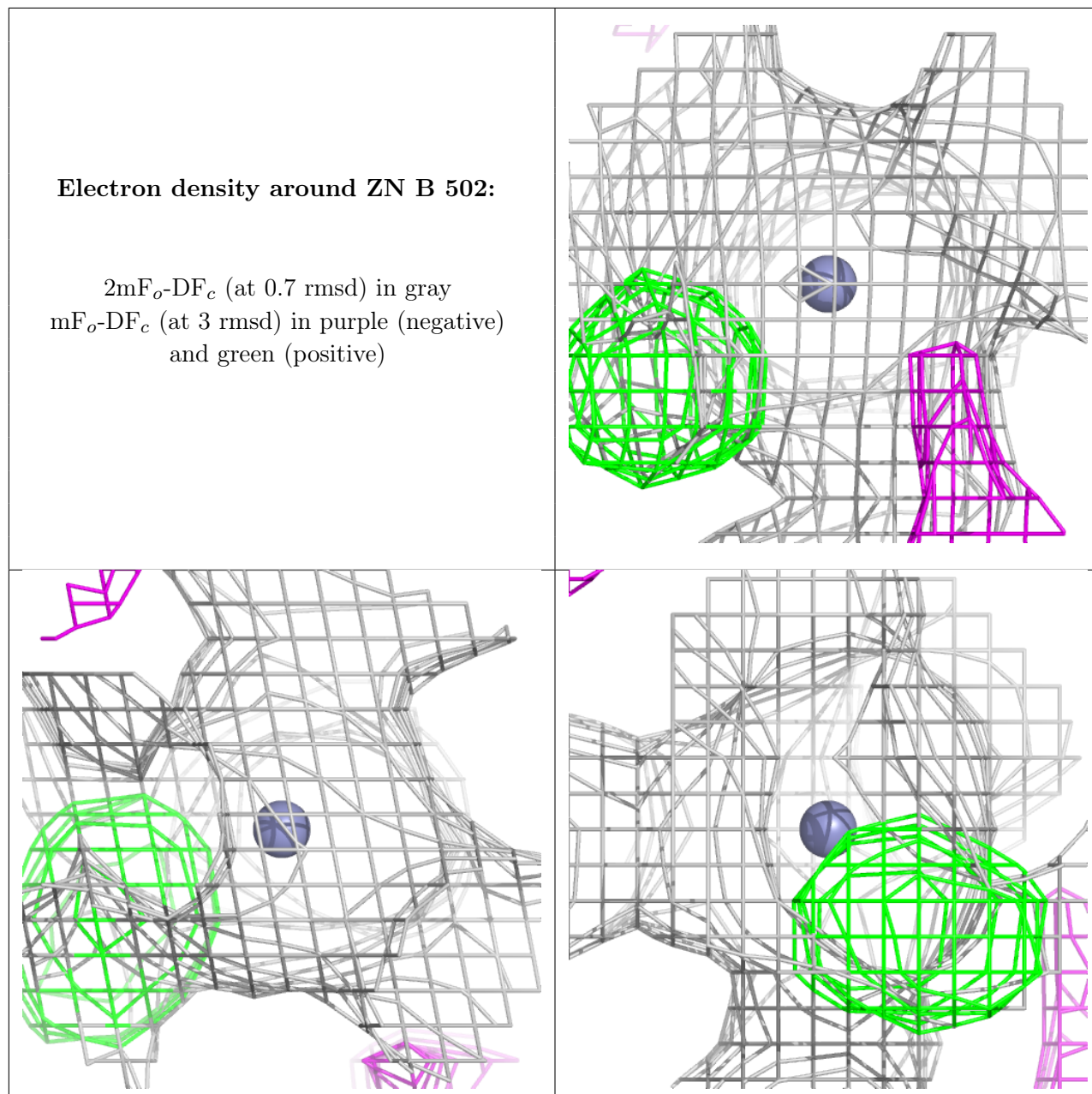
Electron density around ZN A 504:

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and green (positive)



Electron density around ZN B 502:

$2mF_o-DF_c$ (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.