



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:14 PM UTC

PDB ID : 8YAF / pdb_00008yaf
Title : SOD1, Nanobody1 and Nanobody2 complex
Authors : Cheng, S.
Deposited on : 2024-02-09
Resolution : 3.28 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
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

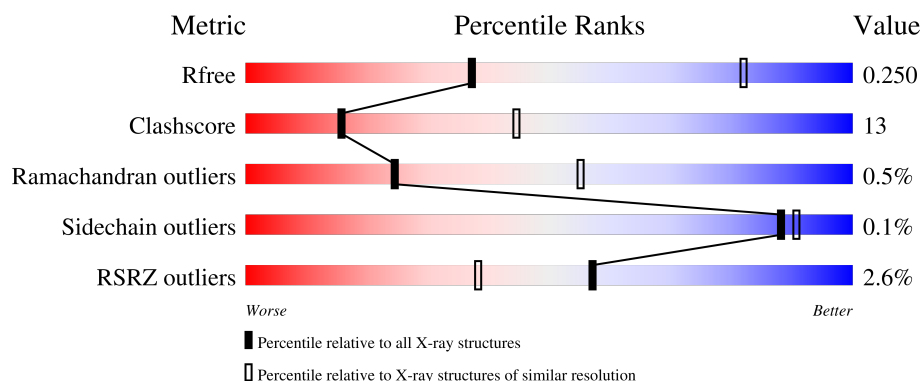
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	153	80% 19% .
1	D	153	82% 17% .
1	H	153	89% 11% .
1	L	153	82% 16% .
1	P	153	82% 18% .

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Mol	Chain	Length	Quality of chain
1	T	153	 3% 89% 11%
2	B	118	 % 60% 36% .
2	E	118	 65% 32% .
2	I	118	 % 74% 23% . .
2	M	118	 74% 23% . .
2	Q	118	 % 72% 25% .
2	U	118	 % 59% 38% .
3	C	131	 73% 27%
3	F	131	 18% 63% 36% .
3	J	131	 % 71% 28% .
3	N	131	 8% 69% 30% .
3	R	131	 3% 73% 26% .
3	V	131	 4% 64% 34% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17762 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	2	0	0
			1100	674	201	221	4			
1	D	153	Total	C	N	O	S	6	0	0
			1110	679	203	224	4			
1	H	153	Total	C	N	O	S	4	0	0
			1110	679	203	224	4			
1	L	153	Total	C	N	O	S	4	0	0
			1110	679	203	224	4			
1	P	153	Total	C	N	O	S	4	0	0
			1110	679	203	224	4			
1	T	153	Total	C	N	O	S	3	0	0
			1110	679	203	224	4			

- Molecule 2 is a protein called NB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	114	Total	C	N	O	S	0	0	0
			859	536	150	168	5			
2	E	115	Total	C	N	O	S	0	0	0
			865	539	151	170	5			
2	I	115	Total	C	N	O	S	0	0	0
			865	539	151	170	5			
2	M	115	Total	C	N	O	S	0	0	0
			865	539	151	170	5			
2	Q	115	Total	C	N	O	S	0	0	0
			865	539	151	170	5			
2	U	115	Total	C	N	O	S	0	0	0
			865	539	151	170	5			

- Molecule 3 is a protein called NB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			987	609	174	198	6			
3	F	131	Total	C	N	O	S	0	0	0
			987	609	174	198	6			
3	J	131	Total	C	N	O	S	0	0	0
			987	609	174	198	6			
3	N	131	Total	C	N	O	S	0	0	0
			987	609	174	198	6			
3	R	131	Total	C	N	O	S	0	0	0
			987	609	174	198	6			
3	V	131	Total	C	N	O	S	0	0	0
			987	609	174	198	6			

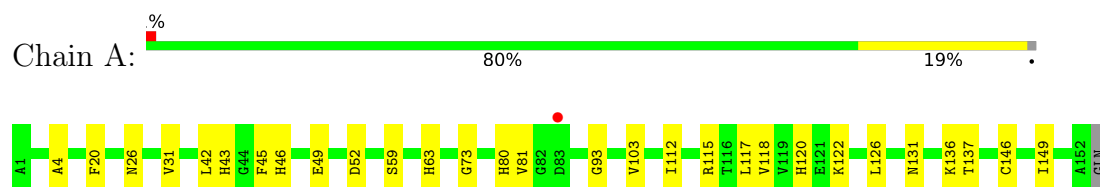
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	1	0
			1	1		
4	D	1	Total	Zn	1	0
			1	1		
4	H	1	Total	Zn	1	0
			1	1		
4	L	1	Total	Zn	1	0
			1	1		
4	P	1	Total	Zn	1	0
			1	1		
4	T	1	Total	Zn	1	0
			1	1		

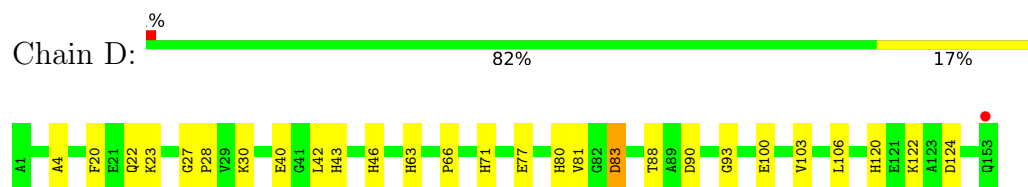
3 Residue-property plots [i](#)

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

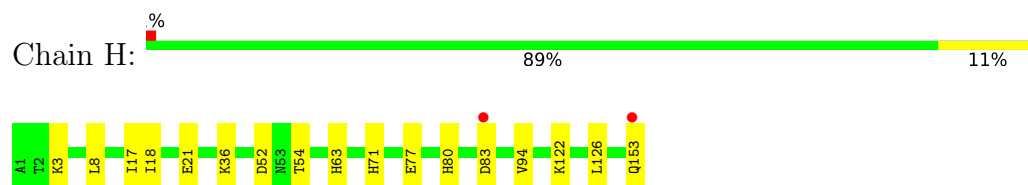
- Molecule 1: Superoxide dismutase [Cu-Zn]



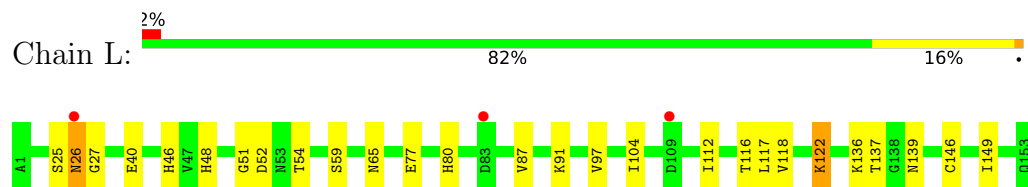
- Molecule 1: Superoxide dismutase [Cu-Zn]



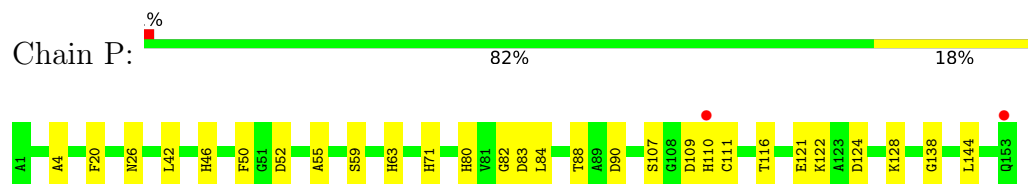
- Molecule 1: Superoxide dismutase [Cu-Zn]



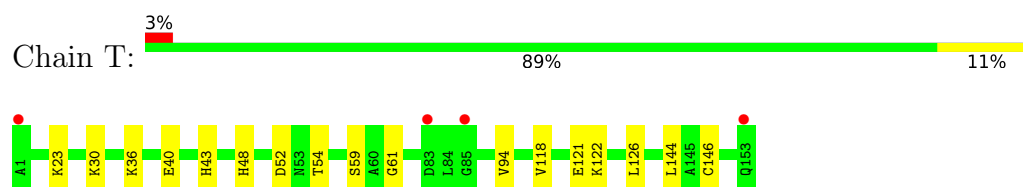
- Molecule 1: Superoxide dismutase [Cu-Zn]



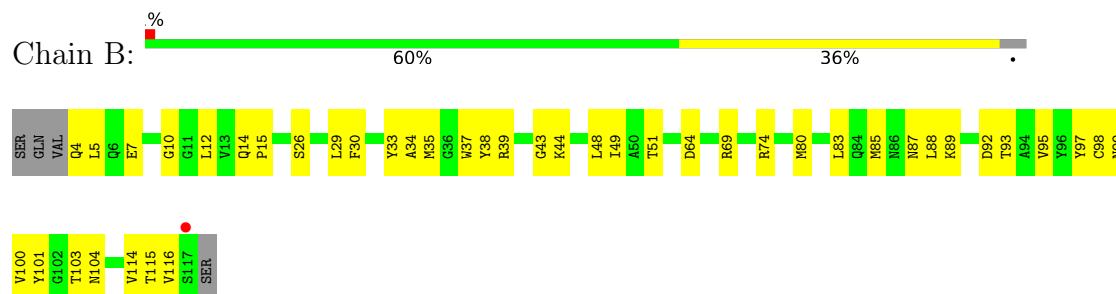
- Molecule 1: Superoxide dismutase [Cu-Zn]



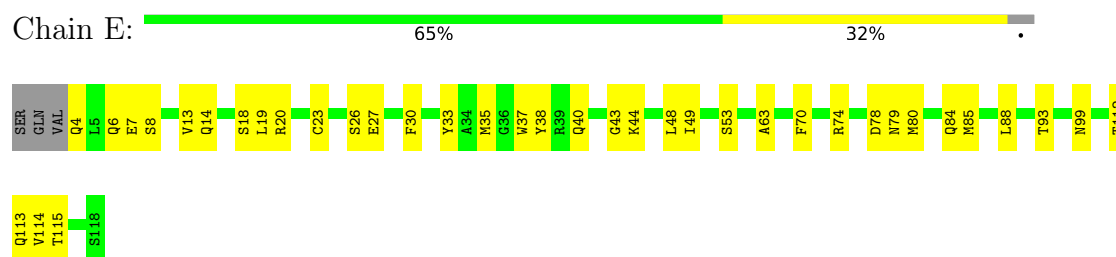
- Molecule 1: Superoxide dismutase [Cu-Zn]



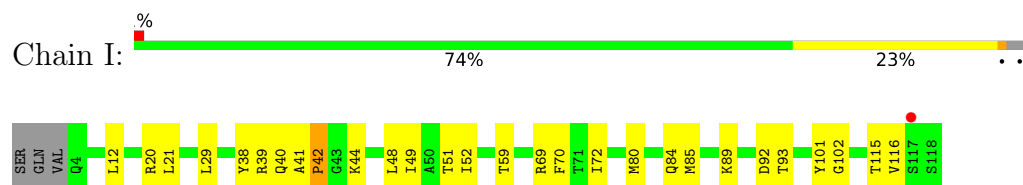
- Molecule 2: NB1



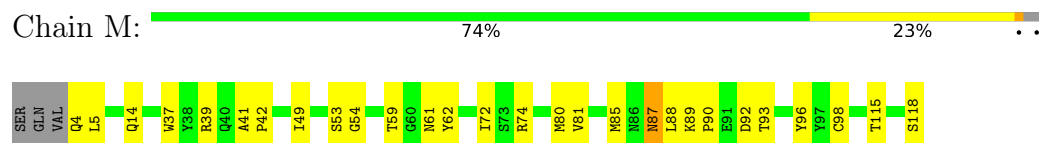
- Molecule 2: NB1



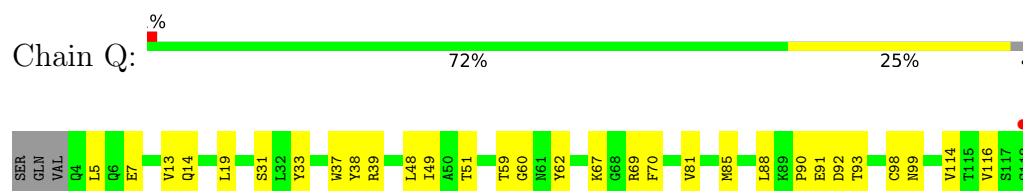
- Molecule 2: NB1



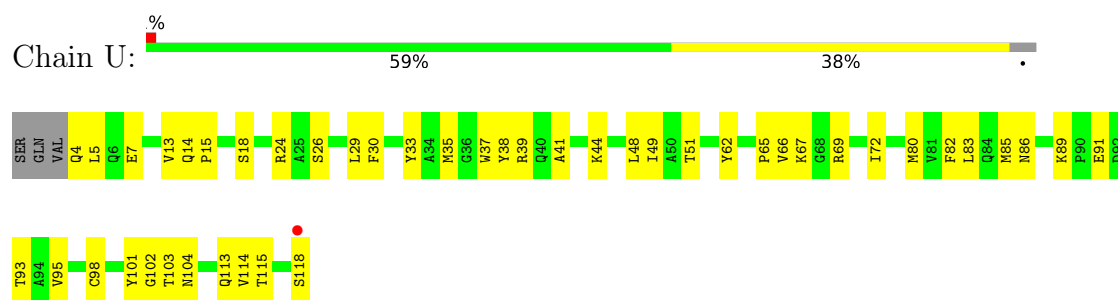
- Molecule 2: NB1



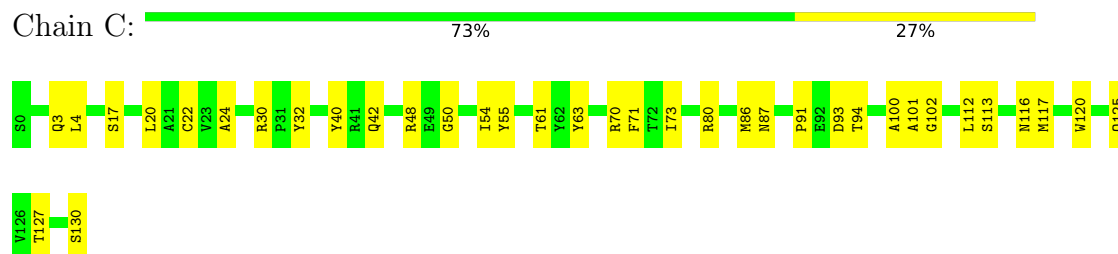
- Molecule 2: NB1



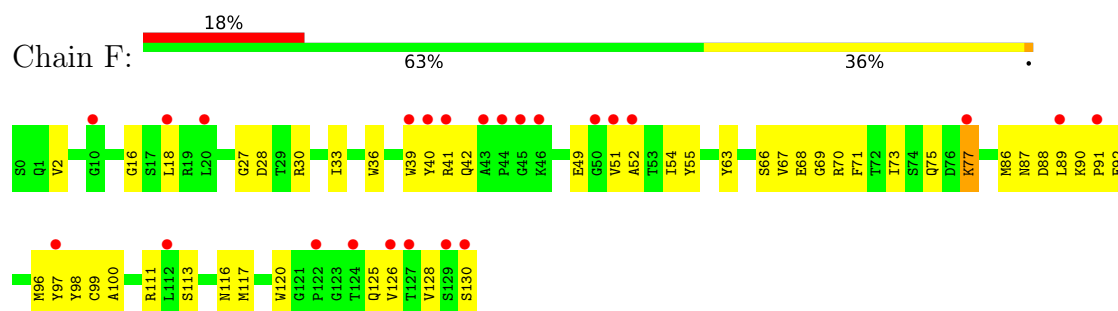
- Molecule 2: NB1



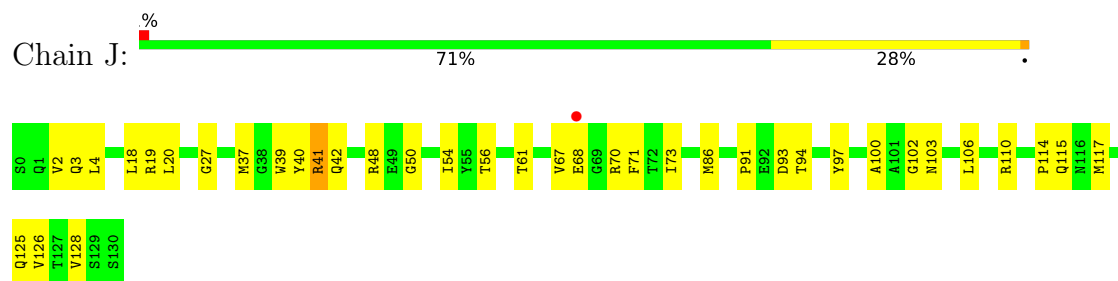
• Molecule 3: NB2



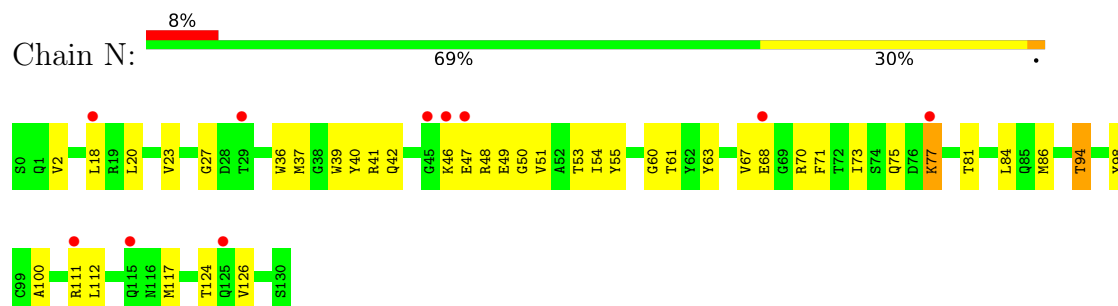
• Molecule 3: NB2



• Molecule 3: NB2

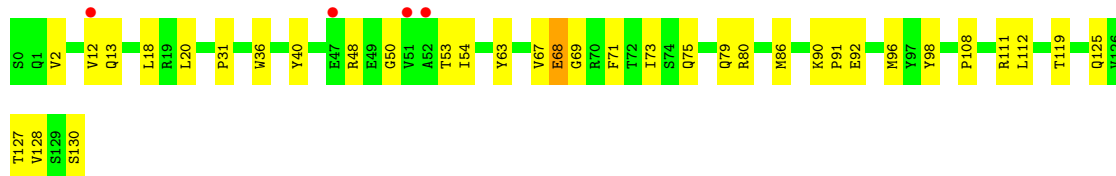


• Molecule 3: NB2



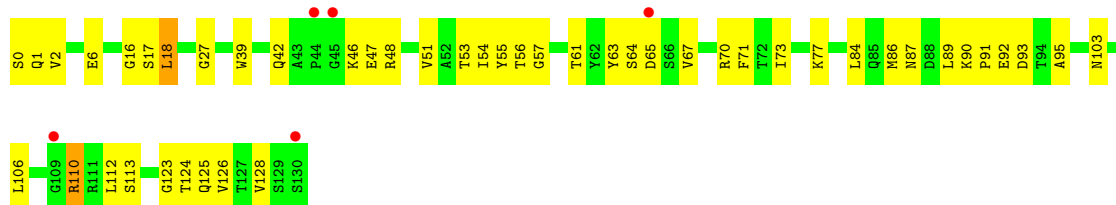
● Molecule 3: NB2

Chain R:  3% 73% 26%



● Molecule 3: NB2

Chain V:  4% 64% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.95Å 218.89Å 122.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.68 – 3.28 81.68 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.8 (81.68-3.28) 99.8 (81.68-3.28)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.26Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.200 , 0.249 0.200 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17762	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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: 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	0.44	0/1118	0.67	0/1508
1	D	0.50	0/1128	0.79	3/1520 (0.2%)
1	H	0.46	0/1128	0.73	0/1520
1	L	0.48	0/1128	0.72	1/1520 (0.1%)
1	P	0.49	0/1128	0.77	0/1520
1	T	0.47	0/1128	0.73	0/1520
2	B	0.49	0/877	0.75	0/1190
2	E	0.48	0/883	0.67	0/1198
2	I	0.51	0/883	0.74	1/1198 (0.1%)
2	M	0.44	0/883	0.66	0/1198
2	Q	0.50	0/883	0.71	0/1198
2	U	0.45	0/883	0.73	0/1198
3	C	0.49	0/1009	0.76	0/1369
3	F	0.35	0/1009	0.56	1/1369 (0.1%)
3	J	0.53	0/1009	0.87	0/1369
3	N	0.38	0/1009	0.67	1/1369 (0.1%)
3	R	0.61	2/1009 (0.2%)	1.00	4/1369 (0.3%)
3	V	0.46	0/1009	0.66	0/1369
All	All	0.48	2/18104 (0.0%)	0.74	11/24502 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	31	PRO	CB-CG	-10.58	0.96	1.49
3	R	31	PRO	CG-CD	-7.83	1.24	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	31	PRO	CA-CB-CG	-18.23	69.86	104.50
3	R	31	PRO	N-CD-CG	-18.09	76.07	103.20
3	R	31	PRO	CB-CG-CD	10.32	139.14	106.10
3	R	31	PRO	CA-N-CD	-7.99	100.82	112.00
1	D	28	PRO	N-CD-CG	-7.53	91.91	103.20
3	N	77	LYS	CD-CE-NZ	-7.43	88.13	111.90
1	D	28	PRO	CA-CB-CG	-6.66	91.84	104.50
2	I	42	PRO	CA-N-CD	-5.70	104.02	112.00
1	L	122	LYS	CB-CA-C	-5.67	107.32	114.40
3	F	77	LYS	CD-CE-NZ	5.24	128.67	111.90
1	D	83	ASP	OD1-CG-OD2	-5.18	110.47	122.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	41	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1100	0	1069	18	0
1	D	1110	0	1077	26	0
1	H	1110	0	1077	19	0
1	L	1110	0	1077	24	0
1	P	1110	0	1077	30	0
1	T	1110	0	1077	10	0
2	B	859	0	827	30	0
2	E	865	0	832	34	0
2	I	865	0	832	21	0
2	M	865	0	832	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	865	0	832	24	0
2	U	865	0	832	32	0
3	C	987	0	938	26	0
3	F	987	0	938	41	0
3	J	987	0	938	36	1
3	N	987	0	938	29	1
3	R	987	0	938	26	0
3	V	987	0	938	37	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	H	1	0	0	0	0
4	L	1	0	0	0	0
4	P	1	0	0	0	0
4	T	1	0	0	0	0
All	All	17762	0	17069	463	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 13.

All (463) 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:HIS:ND1	1:D:83:ASP:OD1	1.91	1.03
1:D:80:HIS:ND1	1:D:83:ASP:OD2	1.98	0.96
2:B:93:THR:HG23	2:B:115:THR:HA	1.49	0.94
2:U:93:THR:HG23	2:U:115:THR:HA	1.50	0.93
3:C:94:THR:HG23	3:C:127:THR:HA	1.53	0.89
2:E:4:GLN:HE21	2:E:26:SER:CB	1.89	0.85
3:N:54:ILE:HD13	3:N:75:GLN:HG2	1.56	0.85
1:H:71:HIS:ND1	1:H:83:ASP:OD2	2.10	0.84
2:E:85:MET:HE2	2:E:88:LEU:HD21	1.60	0.82
2:I:39:ARG:HG2	2:I:49:ILE:HG13	1.61	0.82
3:J:54:ILE:HG13	3:J:61:THR:HG22	1.60	0.82
3:J:102:GLY:HA3	3:J:117:MET:HE3	1.60	0.81
1:D:81:VAL:HG13	1:D:103:VAL:HG12	1.62	0.81
2:M:93:THR:HG23	2:M:115:THR:HA	1.61	0.81
2:E:93:THR:HG23	2:E:115:THR:HA	1.64	0.79
1:P:80:HIS:ND1	1:P:83:ASP:OD2	2.15	0.79
3:R:54:ILE:HD13	3:R:75:GLN:HG2	1.66	0.78
3:C:24:ALA:HB3	3:C:80:ARG:HG2	1.68	0.76
2:I:21:LEU:HD13	2:I:85:MET:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:THR:HG22	3:J:128:VAL:H	1.51	0.75
1:D:93:GLY:HA3	3:F:55:TYR:HE2	1.50	0.74
1:D:71:HIS:ND1	1:D:83:ASP:OD2	2.21	0.73
2:B:43:GLY:C	2:B:44:LYS:HE2	2.13	0.72
2:M:39:ARG:HG2	2:M:49:ILE:HG13	1.72	0.70
3:V:70:ARG:NH2	3:V:93:ASP:OD2	2.24	0.70
3:F:54:ILE:HD13	3:F:75:GLN:HG2	1.75	0.69
3:C:101:ALA:C	3:C:117:MET:HE3	2.17	0.69
2:I:93:THR:HG23	2:I:115:THR:HA	1.73	0.69
3:N:111:ARG:HH11	3:N:112:LEU:HB2	1.58	0.69
2:I:69:ARG:NH2	2:I:92:ASP:OD2	2.27	0.68
3:J:91:PRO:O	3:J:94:THR:HG23	1.94	0.68
1:A:81:VAL:HG13	1:A:103:VAL:HG12	1.76	0.67
1:D:80:HIS:ND1	1:D:83:ASP:CG	2.53	0.67
2:Q:85:MET:HE2	2:Q:88:LEU:HD21	1.76	0.67
3:N:71:PHE:CZ	3:N:86:MET:HE3	2.29	0.67
3:R:91:PRO:HA	3:R:128:VAL:HB	1.76	0.67
3:V:91:PRO:HA	3:V:128:VAL:HB	1.76	0.67
3:C:70:ARG:NH2	3:C:93:ASP:OD2	2.28	0.66
3:F:41:ARG:HG3	3:F:97:TYR:CZ	2.29	0.66
2:U:89:LYS:HB2	2:U:91:GLU:OE1	1.96	0.66
2:U:89:LYS:CB	2:U:91:GLU:OE1	2.44	0.66
1:P:52:ASP:O	1:P:59:SER:OG	2.11	0.65
3:R:96:MET:HE2	3:R:125:GLN:HB2	1.77	0.65
2:M:87:ASN:O	2:M:87:ASN:ND2	2.30	0.65
2:Q:7:GLU:N	2:Q:7:GLU:OE1	2.30	0.65
3:J:2:VAL:HG22	3:J:27:GLY:HA3	1.78	0.64
1:A:80:HIS:HE1	1:A:136:LYS:O	1.79	0.64
3:J:106:LEU:HD23	3:J:110:ARG:O	1.97	0.64
2:M:85:MET:HE2	2:M:88:LEU:HD21	1.79	0.64
3:J:20:LEU:HD13	3:J:86:MET:HE3	1.79	0.63
2:Q:90:PRO:O	2:Q:93:THR:HG23	1.98	0.63
1:P:90:ASP:OD1	1:P:90:ASP:N	2.31	0.63
3:J:102:GLY:N	3:J:117:MET:HE2	2.14	0.63
1:L:122:LYS:HB3	2:M:53:SER:HB2	1.80	0.63
2:M:39:ARG:HB3	2:M:96:TYR:CE2	2.34	0.63
1:H:17:ILE:HD13	1:L:54:THR:HG22	1.80	0.63
2:U:5:LEU:HD21	2:U:29:LEU:HD23	1.81	0.63
3:F:88:ASP:OD1	3:F:90:LYS:NZ	2.32	0.63
2:Q:37:TRP:HE1	2:Q:81:VAL:HG12	1.62	0.63
2:B:38:TYR:CE1	2:B:48:LEU:HD13	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:26:ASN:HA	1:P:26:ASN:HA	1.81	0.62
3:V:47:GLU:HG3	3:V:48:ARG:H	1.64	0.62
1:H:77:GLU:CD	1:H:77:GLU:H	2.06	0.62
2:M:4:GLN:O	2:M:5:LEU:HD23	1.99	0.62
3:R:36:TRP:CE2	3:R:111:ARG:HD3	2.34	0.62
3:J:103:ASN:O	3:J:106:LEU:HD13	2.00	0.62
1:P:50:PHE:O	1:P:116:THR:OG1	2.18	0.62
1:P:63:HIS:HD2	1:P:80:HIS:CE1	2.18	0.61
1:D:4:ALA:HB3	1:D:20:PHE:HB2	1.82	0.61
1:H:71:HIS:CE1	1:H:83:ASP:CG	2.79	0.61
3:J:94:THR:HG22	3:J:128:VAL:N	2.15	0.61
2:Q:93:THR:HG22	2:Q:116:VAL:H	1.64	0.61
3:F:91:PRO:HG3	3:F:130:SER:HB2	1.83	0.61
3:F:28:ASP:OD2	3:F:33:ILE:HG13	2.00	0.61
2:U:83:LEU:HD23	2:U:85:MET:HE2	1.83	0.61
3:V:2:VAL:HG22	3:V:27:GLY:HA3	1.81	0.61
2:I:41:ALA:HB1	2:I:42:PRO:HD3	1.82	0.60
1:P:71:HIS:ND1	1:P:80:HIS:CE1	2.69	0.60
1:P:63:HIS:CD2	1:P:80:HIS:CE1	2.90	0.60
3:J:102:GLY:HA3	3:J:117:MET:CE	2.31	0.60
1:P:42:LEU:HD23	1:P:88:THR:HG23	1.83	0.60
2:B:37:TRP:O	2:B:49:ILE:HG22	2.02	0.59
2:M:90:PRO:O	2:M:93:THR:OG1	2.17	0.59
3:C:102:GLY:N	3:C:117:MET:HE3	2.17	0.59
3:N:20:LEU:HD12	3:N:84:LEU:HD23	1.85	0.59
3:F:71:PHE:CE1	3:F:86:MET:HG2	2.37	0.59
1:A:112:ILE:HA	1:A:115:ARG:HG3	1.84	0.59
3:F:91:PRO:HA	3:F:128:VAL:HB	1.85	0.58
1:D:93:GLY:HA3	3:F:55:TYR:CE2	2.35	0.58
3:V:56:THR:O	3:V:77:LYS:HE2	2.03	0.58
2:U:37:TRP:O	2:U:49:ILE:HG22	2.02	0.58
2:E:30:PHE:HA	2:E:35:MET:HE3	1.85	0.58
3:F:39:TRP:CE3	3:F:99:CYS:HB2	2.38	0.58
1:T:36:LYS:HD3	1:T:94:VAL:HG22	1.86	0.58
3:R:48:ARG:HG2	3:R:48:ARG:HH11	1.69	0.58
3:R:63:TYR:CE1	3:R:73:ILE:HG22	2.38	0.58
3:F:28:ASP:OD2	3:F:30:ARG:NH1	2.37	0.58
3:F:40:TYR:HE1	3:F:117:MET:HE2	1.69	0.58
1:A:49:GLU:O	1:A:115:ARG:HD3	2.04	0.58
3:C:42:GLN:HB2	3:C:48:ARG:HG2	1.86	0.58
2:U:51:THR:HB	2:U:101:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:21:LEU:CD1	2:I:85:MET:HE3	2.31	0.57
2:Q:91:GLU:OE1	2:Q:91:GLU:N	2.31	0.57
3:C:63:TYR:CE2	3:C:73:ILE:HG22	2.39	0.57
3:F:96:MET:HG3	3:F:125:GLN:HG3	1.86	0.57
1:H:63:HIS:CE1	1:H:71:HIS:CE1	2.92	0.57
1:P:4:ALA:HB3	1:P:20:PHE:HB2	1.87	0.57
1:L:118:VAL:HG22	1:L:146:CYS:HB3	1.85	0.57
2:U:4:GLN:HG3	2:U:26:SER:HB3	1.87	0.57
3:F:63:TYR:CE1	3:F:73:ILE:HG22	2.39	0.56
1:A:131:ASN:HA	2:B:64:ASP:OD2	2.05	0.56
2:E:4:GLN:NE2	2:E:26:SER:CB	2.65	0.56
3:F:41:ARG:NH1	3:F:49:GLU:OE2	2.39	0.56
3:R:96:MET:CE	3:R:125:GLN:HB2	2.35	0.56
3:C:54:ILE:HG13	3:C:61:THR:HG22	1.87	0.56
2:U:38:TYR:CE2	2:U:48:LEU:HD13	2.41	0.56
2:U:41:ALA:HB3	2:U:44:LYS:HD2	1.88	0.56
3:F:100:ALA:HB2	3:F:120:TRP:CE3	2.41	0.56
1:A:93:GLY:HA3	3:C:55:TYR:CE2	2.41	0.55
3:J:37:MET:HE2	3:J:56:THR:HG21	1.88	0.55
1:L:91:LYS:HE2	3:N:60:GLY:HA2	1.88	0.55
3:F:40:TYR:CE1	3:F:117:MET:HE2	2.41	0.55
3:V:67:VAL:HG11	3:V:71:PHE:HB2	1.88	0.55
1:P:55:ALA:HB3	1:P:59:SER:HB3	1.88	0.55
2:U:83:LEU:HD23	2:U:85:MET:CE	2.36	0.55
2:E:18:SER:O	2:E:19:LEU:HD12	2.05	0.55
1:P:71:HIS:CE1	1:P:83:ASP:OD1	2.59	0.55
2:B:10:GLY:O	2:E:14:GLN:NE2	2.40	0.55
3:N:46:LYS:HG2	3:N:47:GLU:N	2.21	0.55
3:V:6:GLU:OE1	3:V:6:GLU:N	2.37	0.55
2:M:89:LYS:N	2:M:92:ASP:OD2	2.40	0.55
3:F:113:SER:OG	3:F:116:ASN:OD1	2.21	0.55
3:N:42:GLN:OE1	3:N:48:ARG:NH1	2.32	0.55
3:J:100:ALA:HB1	3:J:117:MET:HG2	1.88	0.55
2:B:38:TYR:HE2	2:B:99:ASN:HB3	1.72	0.55
1:P:63:HIS:HD2	1:P:80:HIS:HE1	1.55	0.55
1:D:42:LEU:CD2	1:D:88:THR:HG22	2.37	0.54
2:E:38:TYR:CE2	2:E:48:LEU:HD13	2.42	0.54
2:M:37:TRP:HE1	2:M:81:VAL:HG12	1.71	0.54
3:V:53:THR:HB	3:V:112:LEU:HD21	1.89	0.54
2:E:38:TYR:HE1	2:E:99:ASN:HB3	1.71	0.54
3:N:51:VAL:HG21	3:N:71:PHE:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:46:HIS:O	1:L:117:LEU:HD12	2.07	0.54
3:J:102:GLY:CA	3:J:117:MET:HE3	2.34	0.54
1:D:80:HIS:CE1	1:D:83:ASP:OD2	2.61	0.54
3:J:70:ARG:NH2	3:J:93:ASP:OD2	2.41	0.53
1:H:71:HIS:HB2	1:H:80:HIS:CE1	2.44	0.53
2:E:13:VAL:HG21	2:E:19:LEU:CD1	2.38	0.53
3:R:67:VAL:HG11	3:R:71:PHE:CG	2.43	0.53
1:D:93:GLY:CA	3:F:55:TYR:HE2	2.19	0.53
3:F:28:ASP:OD1	3:F:30:ARG:HD3	2.08	0.53
3:R:71:PHE:CE1	3:R:86:MET:HG2	2.44	0.53
3:J:125:GLN:HG3	3:J:126:VAL:N	2.23	0.53
2:E:4:GLN:NE2	2:E:26:SER:OG	2.34	0.53
3:N:39:TRP:HD1	3:N:73:ILE:HD12	1.73	0.53
3:V:125:GLN:HG3	3:V:126:VAL:N	2.24	0.53
1:D:23:LYS:HZ2	1:D:30:LYS:HE3	1.75	0.52
1:T:48:HIS:HD2	1:T:61:GLY:O	1.91	0.52
3:F:67:VAL:HG13	3:F:70:ARG:HB2	1.91	0.52
2:U:89:LYS:HB3	2:U:91:GLU:OE1	2.09	0.52
2:M:14:GLN:HB3	2:M:118:SER:HB3	1.91	0.52
3:V:67:VAL:HG11	3:V:71:PHE:CG	2.44	0.52
3:V:71:PHE:CE1	3:V:86:MET:HB3	2.44	0.52
3:J:100:ALA:CB	3:J:117:MET:HG2	2.39	0.52
2:U:80:MET:HE2	2:U:82:PHE:CZ	2.45	0.52
3:F:18:LEU:HD23	3:F:126:VAL:HG13	1.92	0.52
3:C:100:ALA:HB2	3:C:120:TRP:CE3	2.45	0.52
2:I:38:TYR:CE2	2:I:48:LEU:HD13	2.45	0.52
3:F:90:LYS:HB3	3:F:92:GLU:OE1	2.10	0.51
1:P:121:GLU:HB2	1:P:144:LEU:CD1	2.40	0.51
2:E:40:GLN:NE2	2:E:44:LYS:O	2.41	0.51
1:H:3:LYS:NZ	1:H:153:GLN:HB2	2.25	0.51
3:J:41:ARG:HG3	3:J:97:TYR:CZ	2.45	0.51
2:E:27:GLU:HA	2:E:79:ASN:OD1	2.11	0.51
2:I:39:ARG:HG2	2:I:49:ILE:CG1	2.37	0.51
3:N:71:PHE:CE2	3:N:86:MET:HE3	2.45	0.51
2:B:35:MET:HE2	2:B:100:VAL:HG12	1.92	0.51
2:U:62:TYR:O	2:U:67:LYS:NZ	2.44	0.51
2:Q:69:ARG:NH2	2:Q:92:ASP:OD2	2.43	0.51
2:Q:93:THR:HG22	2:Q:116:VAL:N	2.24	0.51
2:B:14:GLN:HG3	2:B:15:PRO:HD2	1.92	0.51
3:C:20:LEU:HG	3:C:86:MET:HE3	1.92	0.51
1:H:71:HIS:ND1	1:H:83:ASP:CG	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:O	1:A:149:ILE:HG13	2.11	0.51
3:J:86:MET:HE1	3:J:126:VAL:HG21	1.92	0.51
1:L:26:ASN:HA	1:P:26:ASN:HB2	1.93	0.51
3:J:40:TYR:HA	3:J:50:GLY:HA2	1.93	0.51
1:D:23:LYS:HD3	1:D:23:LYS:N	2.26	0.50
2:U:93:THR:HA	2:U:114:VAL:O	2.11	0.50
3:R:12:VAL:HG22	3:R:13:GLN:H	1.76	0.50
2:E:44:LYS:HE3	2:E:44:LYS:HA	1.93	0.50
1:D:22:GLN:HE21	1:D:27:GLY:H	1.58	0.50
1:D:122:LYS:HB3	2:E:53:SER:OG	2.10	0.50
1:H:71:HIS:CE1	1:H:83:ASP:OD1	2.65	0.50
3:J:67:VAL:HG11	3:J:71:PHE:HB2	1.94	0.50
2:M:41:ALA:HB1	2:M:42:PRO:HD2	1.94	0.50
3:R:20:LEU:CD1	3:R:86:MET:HE2	2.42	0.50
3:V:42:GLN:C	3:V:95:ALA:HB1	2.37	0.50
2:Q:38:TYR:HE1	2:Q:99:ASN:HB3	1.76	0.50
3:C:30:ARG:HD2	3:C:32:TYR:OH	2.11	0.50
1:P:46:HIS:ND1	1:P:63:HIS:HE1	2.09	0.50
3:V:39:TRP:O	3:V:51:VAL:HG22	2.12	0.50
2:Q:93:THR:CG2	2:Q:116:VAL:H	2.24	0.50
2:E:33:TYR:HD2	2:E:74:ARG:NH1	2.10	0.50
1:L:52:ASP:O	1:L:59:SER:HB2	2.12	0.50
3:C:113:SER:OG	3:C:116:ASN:OD1	2.26	0.49
3:N:23:VAL:HG22	3:N:81:THR:OG1	2.12	0.49
1:P:82:GLY:O	1:P:84:LEU:HD12	2.12	0.49
3:R:108:PRO:HG3	3:R:111:ARG:NH2	2.28	0.49
3:V:17:SER:O	3:V:18:LEU:HB2	2.11	0.49
1:H:17:ILE:O	1:H:18:ILE:HD13	2.12	0.49
3:V:0:SER:OG	3:V:1:GLN:N	2.43	0.49
3:J:71:PHE:CE1	3:J:86:MET:HB3	2.48	0.49
3:J:102:GLY:N	3:J:117:MET:CE	2.75	0.49
3:F:67:VAL:HG11	3:F:71:PHE:CG	2.48	0.49
2:E:70:PHE:CE2	2:E:85:MET:HE3	2.48	0.49
2:B:12:LEU:HD12	2:B:115:THR:HB	1.94	0.49
3:F:41:ARG:HB3	3:F:49:GLU:HB3	1.95	0.48
3:V:86:MET:HE2	3:V:89:LEU:HD21	1.95	0.48
3:N:67:VAL:HG11	3:N:71:PHE:CG	2.48	0.48
3:R:40:TYR:HA	3:R:50:GLY:HA2	1.95	0.48
3:V:90:LYS:HB3	3:V:92:GLU:OE1	2.13	0.48
3:R:125:GLN:HG2	3:R:127:THR:HG23	1.94	0.48
3:F:86:MET:HB3	3:F:89:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:LEU:HG	3:C:86:MET:CE	2.44	0.48
1:L:40:GLU:OE1	1:L:91:LYS:HA	2.13	0.48
2:U:13:VAL:HG12	2:U:14:GLN:O	2.13	0.48
1:H:126:LEU:HG	2:I:102:GLY:HA2	1.96	0.48
3:N:40:TYR:OH	3:N:117:MET:HE3	2.13	0.48
1:A:45:PHE:CZ	1:A:117:LEU:HD21	2.49	0.48
2:B:103:THR:OG1	2:B:104:ASN:N	2.44	0.48
1:A:52:ASP:O	1:A:59:SER:HB2	2.14	0.47
3:F:63:TYR:HE1	3:F:73:ILE:HG22	1.78	0.47
1:H:52:ASP:OD1	1:H:54:THR:HG23	2.13	0.47
1:P:63:HIS:CD2	1:P:71:HIS:ND1	2.82	0.47
1:T:52:ASP:OD1	1:T:54:THR:HG23	2.14	0.47
2:U:7:GLU:N	2:U:7:GLU:OE1	2.47	0.47
2:E:13:VAL:HG12	2:E:14:GLN:O	2.14	0.47
1:P:71:HIS:CE1	1:P:83:ASP:CG	2.92	0.47
2:B:39:ARG:O	2:B:39:ARG:HG3	2.13	0.47
2:M:39:ARG:HG2	2:M:49:ILE:CG1	2.42	0.47
1:P:122:LYS:HD3	2:Q:59:THR:HB	1.97	0.47
3:V:16:GLY:O	3:V:89:LEU:HD12	2.13	0.47
3:V:103:ASN:O	3:V:106:LEU:HG	2.13	0.47
3:N:37:MET:O	3:N:53:THR:HA	2.14	0.47
1:P:46:HIS:CG	1:P:63:HIS:CE1	3.02	0.47
3:C:112:LEU:HD23	3:C:112:LEU:HA	1.59	0.47
1:D:66:PRO:HD2	1:D:81:VAL:HG23	1.97	0.47
3:F:36:TRP:CD2	3:F:111:ARG:HG2	2.49	0.47
1:P:124:ASP:OD1	1:P:138:GLY:HA3	2.14	0.47
3:R:71:PHE:CZ	3:R:86:MET:HG2	2.49	0.47
2:B:7:GLU:N	2:B:7:GLU:OE1	2.48	0.47
2:E:113:GLN:HG3	2:E:114:VAL:N	2.29	0.47
1:L:122:LYS:HD2	2:M:59:THR:HB	1.96	0.47
2:Q:5:LEU:HD22	2:Q:98:CYS:O	2.15	0.47
1:A:20:PHE:HD2	1:A:31:VAL:HG22	1.80	0.47
3:N:68:GLU:C	3:N:70:ARG:H	2.23	0.47
2:U:4:GLN:HG3	2:U:26:SER:CB	2.44	0.47
2:U:18:SER:HB2	2:U:86:ASN:HA	1.97	0.47
1:A:4:ALA:HB3	1:A:20:PHE:HB2	1.96	0.47
3:R:68:GLU:OE1	3:R:69:GLY:N	2.48	0.47
3:R:53:THR:HG22	3:R:112:LEU:HG	1.96	0.47
2:B:4:GLN:HG3	2:B:26:SER:HB2	1.97	0.46
2:B:51:THR:HB	2:B:101:TYR:CE1	2.50	0.46
3:N:41:ARG:NH1	3:N:49:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:40:GLU:HG2	2:U:33:TYR:CE2	2.50	0.46
3:V:54:ILE:HB	3:V:73:ILE:HG12	1.96	0.46
1:D:40:GLU:HG3	1:D:90:ASP:O	2.16	0.46
3:F:51:VAL:HG23	3:F:52:ALA:H	1.80	0.46
3:F:68:GLU:HB3	3:F:69:GLY:H	1.55	0.46
1:L:87:VAL:HG11	1:L:97:VAL:HG22	1.97	0.46
2:Q:39:ARG:O	2:Q:39:ARG:HG2	2.13	0.46
1:H:63:HIS:ND1	1:H:71:HIS:CE1	2.84	0.46
3:J:20:LEU:HD23	3:J:39:TRP:CZ3	2.51	0.46
2:Q:39:ARG:HD2	2:Q:49:ILE:HD13	1.98	0.46
3:C:71:PHE:CZ	3:C:86:MET:HB3	2.51	0.46
1:D:22:GLN:HB3	1:D:106:LEU:HD12	1.98	0.46
3:F:2:VAL:HG22	3:F:27:GLY:HA3	1.97	0.46
2:M:5:LEU:HD13	2:M:98:CYS:O	2.16	0.46
3:J:3:GLN:C	3:J:4:LEU:HD23	2.41	0.46
2:E:78:ASP:O	2:E:79:ASN:HB2	2.14	0.46
3:F:39:TRP:CZ3	3:F:99:CYS:HB2	2.50	0.46
2:I:52:ILE:HB	2:I:72:ILE:HG12	1.98	0.46
2:M:37:TRP:CD2	2:M:98:CYS:HB2	2.51	0.46
3:N:18:LEU:HD23	3:N:126:VAL:HG13	1.97	0.46
3:N:51:VAL:HG21	3:N:71:PHE:HD2	1.80	0.46
2:E:70:PHE:CZ	2:E:85:MET:HE3	2.50	0.46
2:U:15:PRO:HD2	2:U:118:SER:HB3	1.97	0.46
1:A:43:HIS:HA	1:A:122:LYS:O	2.16	0.46
3:V:90:LYS:HB3	3:V:92:GLU:CD	2.40	0.46
3:J:19:ARG:HG3	3:J:19:ARG:HH11	1.81	0.45
3:V:67:VAL:HG11	3:V:71:PHE:CB	2.46	0.45
2:B:35:MET:CE	2:B:100:VAL:HG12	2.47	0.45
3:N:54:ILE:HG13	3:N:61:THR:HG22	1.99	0.45
2:B:30:PHE:HA	2:B:35:MET:HE3	1.98	0.45
2:E:7:GLU:OE1	2:E:7:GLU:N	2.50	0.45
2:M:49:ILE:HD13	2:M:49:ILE:HA	1.77	0.45
1:P:71:HIS:ND1	1:P:83:ASP:OD2	2.49	0.45
2:B:89:LYS:C	2:B:116:VAL:HG11	2.42	0.45
3:N:2:VAL:HG23	3:N:27:GLY:HA3	1.97	0.45
2:Q:37:TRP:O	2:Q:49:ILE:HG22	2.17	0.45
3:V:0:SER:O	3:V:27:GLY:HA2	2.17	0.45
1:D:71:HIS:ND1	1:D:83:ASP:CG	2.75	0.45
2:I:20:ARG:HD2	2:I:84:GLN:OE1	2.17	0.45
3:N:63:TYR:CE2	3:N:73:ILE:HG22	2.51	0.45
3:V:54:ILE:HG13	3:V:61:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:112:LEU:HD23	3:V:112:LEU:HA	1.73	0.45
3:F:96:MET:HA	3:F:125:GLN:HA	1.99	0.45
1:A:20:PHE:CD2	1:A:31:VAL:HG22	2.51	0.45
2:B:5:LEU:HD13	2:B:98:CYS:O	2.17	0.45
3:F:42:GLN:HB3	3:F:98:TYR:HE1	1.82	0.45
3:R:67:VAL:HG11	3:R:71:PHE:HB2	1.98	0.45
1:H:122:LYS:HB2	1:H:122:LYS:HE3	1.69	0.45
1:L:51:GLY:HA2	1:L:116:THR:OG1	2.17	0.45
1:L:80:HIS:HE1	1:L:136:LYS:O	2.00	0.45
3:N:36:TRP:CH2	3:N:55:TYR:HB2	2.52	0.45
3:R:91:PRO:HG3	3:R:130:SER:HB2	1.99	0.45
1:P:63:HIS:NE2	1:P:71:HIS:CE1	2.85	0.44
1:T:126:LEU:HD11	2:U:102:GLY:HA2	1.98	0.44
2:U:103:THR:OG1	2:U:104:ASN:N	2.51	0.44
2:E:70:PHE:N	2:E:70:PHE:CD1	2.85	0.44
2:Q:70:PHE:CE1	2:Q:85:MET:HB3	2.53	0.44
3:C:4:LEU:HB3	3:C:22:CYS:SG	2.57	0.44
2:E:38:TYR:CE1	2:E:99:ASN:HB3	2.52	0.44
2:Q:93:THR:HA	2:Q:114:VAL:O	2.17	0.44
2:U:4:GLN:O	2:U:5:LEU:HD23	2.18	0.44
3:J:67:VAL:HG11	3:J:71:PHE:CG	2.53	0.44
2:U:66:VAL:HA	2:U:69:ARG:NH1	2.31	0.44
3:V:39:TRP:CD1	3:V:84:LEU:HB2	2.52	0.44
1:D:30:LYS:HE2	1:D:100:GLU:OE2	2.17	0.44
2:U:65:PRO:O	2:U:69:ARG:NH1	2.50	0.44
1:A:73:GLY:HA3	1:A:126:LEU:HG	2.00	0.44
1:A:118:VAL:HG22	1:A:146:CYS:HB3	2.00	0.44
2:B:80:MET:HE2	2:B:80:MET:HB3	1.69	0.44
1:H:8:LEU:HD11	1:H:18:ILE:HG12	2.00	0.44
3:R:18:LEU:HA	3:R:18:LEU:HD12	1.79	0.44
3:R:96:MET:HE2	3:R:125:GLN:CB	2.44	0.44
2:U:62:TYR:CE1	2:U:72:ILE:HG22	2.53	0.44
3:F:16:GLY:O	3:F:87:ASN:HA	2.18	0.43
1:D:43:HIS:HA	1:D:122:LYS:O	2.18	0.43
3:J:102:GLY:CA	3:J:117:MET:CE	2.94	0.43
2:Q:31:SER:HA	2:Q:33:TYR:CE2	2.53	0.43
3:F:41:ARG:HG3	3:F:97:TYR:CE1	2.54	0.43
3:J:37:MET:CE	3:J:56:THR:HG21	2.49	0.43
2:U:39:ARG:HD2	2:U:49:ILE:HD13	2.00	0.43
2:B:51:THR:HB	2:B:101:TYR:CZ	2.53	0.43
2:B:33:TYR:HD2	2:B:74:ARG:NH1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:HIS:ND1	1:D:120:HIS:CD2	2.86	0.43
1:H:71:HIS:HB2	1:H:80:HIS:HE1	1.84	0.43
1:T:52:ASP:HB3	1:T:59:SER:O	2.19	0.43
1:D:66:PRO:HD2	1:D:81:VAL:CG2	2.49	0.43
1:H:122:LYS:HD3	2:I:59:THR:HB	2.00	0.43
2:I:89:LYS:C	2:I:116:VAL:HG11	2.44	0.43
1:P:20:PHE:CD1	1:P:20:PHE:N	2.87	0.43
1:P:80:HIS:CG	1:P:83:ASP:OD2	2.72	0.43
3:V:47:GLU:HG3	3:V:48:ARG:N	2.32	0.43
3:V:55:TYR:CE2	3:V:57:GLY:HA3	2.53	0.43
2:I:40:GLN:NE2	2:I:44:LYS:O	2.47	0.43
2:M:4:GLN:C	2:M:5:LEU:HD23	2.43	0.43
2:M:62:TYR:CE1	2:M:72:ILE:HG22	2.53	0.43
1:T:23:LYS:HE2	1:T:30:LYS:HE3	2.00	0.43
2:I:41:ALA:HB3	2:I:44:LYS:HD3	2.01	0.43
3:J:114:PRO:HD2	3:J:115:GLN:NE2	2.33	0.43
1:L:48:HIS:CD2	1:L:118:VAL:HB	2.53	0.43
3:N:86:MET:HE2	3:N:86:MET:HB3	1.96	0.43
3:R:96:MET:HB3	3:R:98:TYR:CE1	2.54	0.43
2:E:20:ARG:HD2	2:E:84:GLN:OE1	2.19	0.42
2:I:29:LEU:HD23	2:I:29:LEU:HA	1.71	0.42
2:Q:51:THR:O	2:Q:60:GLY:HA2	2.20	0.42
3:C:17:SER:OG	3:C:87:ASN:HB3	2.20	0.42
3:C:91:PRO:HG3	3:C:130:SER:HB3	2.01	0.42
1:L:26:ASN:HA	1:P:26:ASN:CB	2.49	0.42
3:V:39:TRP:HD1	3:V:73:ILE:HD12	1.83	0.42
2:B:37:TRP:CG	2:B:83:LEU:HD22	2.54	0.42
2:E:6:GLN:O	2:E:23:CYS:HA	2.19	0.42
2:U:95:VAL:HG22	2:U:113:GLN:OE1	2.20	0.42
3:V:63:TYR:CE1	3:V:73:ILE:HG22	2.53	0.42
1:A:46:HIS:ND1	1:A:120:HIS:CD2	2.87	0.42
3:F:89:LEU:HB3	3:F:128:VAL:HG11	2.02	0.42
3:J:71:PHE:CD1	3:J:86:MET:HA	2.54	0.42
3:C:40:TYR:HA	3:C:50:GLY:HA2	2.02	0.42
3:F:51:VAL:HG23	3:F:52:ALA:N	2.34	0.42
3:V:46:LYS:HA	3:V:46:LYS:HD3	1.82	0.42
3:J:20:LEU:HD22	3:J:86:MET:CE	2.49	0.42
2:M:88:LEU:HD23	2:M:88:LEU:HA	1.89	0.42
3:N:111:ARG:NH1	3:N:112:LEU:HB2	2.29	0.42
3:R:63:TYR:HE1	3:R:73:ILE:HG22	1.85	0.42
3:V:53:THR:HB	3:V:112:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:MET:HE1	2:B:114:VAL:HG11	2.01	0.42
2:B:95:VAL:HG12	2:B:97:TYR:CE1	2.54	0.42
3:C:71:PHE:CE1	3:C:86:MET:HB3	2.55	0.42
3:F:77:LYS:H	3:F:77:LYS:HG3	1.47	0.42
3:F:77:LYS:HE2	3:F:77:LYS:HB2	1.86	0.42
1:P:124:ASP:HA	1:P:138:GLY:O	2.19	0.42
3:N:94:THR:HG23	3:N:94:THR:O	2.19	0.42
2:U:5:LEU:HD13	2:U:98:CYS:O	2.20	0.42
2:U:24:ARG:HD3	2:U:24:ARG:C	2.45	0.42
2:E:49:ILE:HD12	2:E:63:ALA:HB3	2.01	0.42
1:H:3:LYS:HG2	1:H:21:GLU:HG3	2.02	0.42
1:H:36:LYS:HG2	1:H:94:VAL:HG22	2.02	0.42
3:V:17:SER:HA	3:V:87:ASN:HA	2.00	0.42
2:B:37:TRP:CD1	2:B:83:LEU:HB2	2.55	0.41
3:F:71:PHE:CZ	3:F:86:MET:HG2	2.55	0.41
2:I:12:LEU:HD23	2:I:115:THR:HB	2.02	0.41
2:U:30:PHE:HA	2:U:35:MET:HE3	2.02	0.41
1:L:65:ASN:ND2	1:L:80:HIS:CD2	2.88	0.41
2:Q:62:TYR:HB2	2:Q:67:LYS:HG2	2.02	0.41
1:T:121:GLU:HB2	1:T:144:LEU:HD21	2.01	0.41
3:C:63:TYR:CZ	3:C:73:ILE:HG22	2.56	0.41
2:E:70:PHE:HA	2:E:84:GLN:O	2.20	0.41
2:I:69:ARG:HH22	2:I:92:ASP:CG	2.28	0.41
3:J:42:GLN:OE1	3:J:48:ARG:NH1	2.44	0.41
1:L:65:ASN:ND2	1:L:80:HIS:HD2	2.19	0.41
1:A:63:HIS:CE1	1:A:137:THR:HA	2.56	0.41
1:D:77:GLU:O	1:D:77:GLU:HG2	2.20	0.41
3:N:49:GLU:HB3	3:N:50:GLY:H	1.67	0.41
1:A:42:LEU:HD12	2:B:34:ALA:HB3	2.01	0.41
2:B:29:LEU:HA	2:B:29:LEU:HD23	1.75	0.41
2:E:80:MET:HB3	2:E:80:MET:HE2	1.55	0.41
1:L:137:THR:HG23	1:L:139:ASN:H	1.86	0.41
1:T:43:HIS:HA	1:T:122:LYS:O	2.20	0.41
2:E:37:TRP:O	2:E:49:ILE:HG22	2.20	0.41
3:J:67:VAL:HG11	3:J:71:PHE:CB	2.51	0.41
1:L:122:LYS:NZ	2:M:61:ASN:OD1	2.54	0.41
2:M:54:GLY:O	2:M:74:ARG:NH2	2.50	0.41
3:V:64:SER:OG	3:V:65:ASP:N	2.53	0.41
2:E:43:GLY:C	2:E:44:LYS:HD2	2.45	0.41
2:I:70:PHE:CE1	2:I:85:MET:HB3	2.56	0.41
1:L:77:GLU:O	1:L:77:GLU:HG2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:110:ARG:HA	3:V:113:SER:OG	2.21	0.41
3:C:3:GLN:OE1	3:V:124:THR:OG1	2.35	0.41
3:C:100:ALA:HB1	3:C:117:MET:HG2	2.02	0.41
3:C:125:GLN:HE21	3:C:127:THR:HG22	1.86	0.41
1:D:71:HIS:HE2	1:D:124:ASP:CG	2.28	0.41
2:E:70:PHE:N	2:E:70:PHE:HD1	2.19	0.41
3:J:18:LEU:HA	3:J:18:LEU:HD23	1.69	0.41
1:L:25:SER:O	1:L:27:GLY:N	2.54	0.41
2:M:80:MET:HE2	2:M:80:MET:HB3	1.68	0.41
3:R:90:LYS:HB3	3:R:92:GLU:OE1	2.21	0.41
2:B:69:ARG:NH2	2:B:92:ASP:OD2	2.53	0.41
1:D:23:LYS:N	1:D:23:LYS:CD	2.84	0.41
3:N:98:TYR:CD1	3:N:98:TYR:N	2.89	0.41
2:Q:13:VAL:HG12	2:Q:14:GLN:O	2.21	0.41
1:T:118:VAL:HG22	1:T:146:CYS:HB3	2.02	0.41
3:V:6:GLU:CD	3:V:123:GLY:H	2.29	0.41
2:E:23:CYS:C	2:E:80:MET:HE3	2.46	0.40
2:I:80:MET:HE3	2:I:80:MET:HB3	1.85	0.40
1:L:112:ILE:HD12	1:L:149:ILE:HD13	2.03	0.40
3:N:77:LYS:HD3	3:N:77:LYS:N	2.35	0.40
3:R:2:VAL:O	3:R:119:THR:HG21	2.21	0.40
3:R:79:GLN:O	3:R:80:ARG:HG2	2.21	0.40
2:I:51:THR:HB	2:I:101:TYR:CE1	2.57	0.40
3:J:54:ILE:HB	3:J:73:ILE:HD13	2.04	0.40
1:P:128:LYS:O	2:Q:48:LEU:HB3	2.21	0.40
2:Q:13:VAL:HG21	2:Q:19:LEU:HG	2.03	0.40
2:B:88:LEU:HA	2:B:88:LEU:HD23	1.80	0.40
2:E:8:SER:CA	2:E:112:THR:HG21	2.51	0.40
1:L:104:ILE:O	1:L:104:ILE:HG13	2.22	0.40
1:P:109:ASP:C	1:P:111:CYS:H	2.29	0.40
2:Q:70:PHE:CZ	2:Q:85:MET:HE3	2.56	0.40
3:C:54:ILE:HD13	3:C:54:ILE:HG21	1.82	0.40
1:L:25:SER:C	1:L:27:GLY:H	2.30	0.40
3:N:100:ALA:HB1	3:N:117:MET:HG3	2.03	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)
3:J:3:GLN:OE1	3:N:124:THR:OG1[2_555]	2.10	0.10

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	150/153 (98%)	140 (93%)	9 (6%)	1 (1%)	18	48
1	D	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
1	H	151/153 (99%)	139 (92%)	12 (8%)	0	100	100
1	L	151/153 (99%)	139 (92%)	11 (7%)	1 (1%)	18	48
1	P	151/153 (99%)	136 (90%)	13 (9%)	2 (1%)	9	35
1	T	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
2	B	112/118 (95%)	104 (93%)	7 (6%)	1 (1%)	14	43
2	E	113/118 (96%)	104 (92%)	9 (8%)	0	100	100
2	I	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
2	M	113/118 (96%)	101 (89%)	11 (10%)	1 (1%)	14	43
2	Q	113/118 (96%)	105 (93%)	8 (7%)	0	100	100
2	U	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
3	C	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
3	F	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
3	J	129/131 (98%)	117 (91%)	11 (8%)	1 (1%)	16	44
3	N	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	16	44
3	R	129/131 (98%)	119 (92%)	9 (7%)	1 (1%)	16	44
3	V	129/131 (98%)	118 (92%)	9 (7%)	2 (2%)	7	31
All	All	2356/2412 (98%)	2173 (92%)	172 (7%)	11 (0%)	24	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	68	GLU
1	L	26	ASN
3	N	94	THR
2	B	87	ASN

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Mol	Chain	Res	Type
3	V	18	LEU
1	P	107	SER
3	V	110	ARG
2	M	87	ASN
1	P	110	HIS
3	R	68	GLU
1	A	26	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	117/118 (99%)	117 (100%)	0	100	100
1	D	118/118 (100%)	118 (100%)	0	100	100
1	H	118/118 (100%)	118 (100%)	0	100	100
1	L	118/118 (100%)	118 (100%)	0	100	100
1	P	118/118 (100%)	118 (100%)	0	100	100
1	T	118/118 (100%)	118 (100%)	0	100	100
2	B	90/94 (96%)	90 (100%)	0	100	100
2	E	91/94 (97%)	91 (100%)	0	100	100
2	I	91/94 (97%)	91 (100%)	0	100	100
2	M	91/94 (97%)	91 (100%)	0	100	100
2	Q	91/94 (97%)	91 (100%)	0	100	100
2	U	91/94 (97%)	91 (100%)	0	100	100
3	C	102/102 (100%)	102 (100%)	0	100	100
3	F	102/102 (100%)	101 (99%)	1 (1%)	68	77
3	J	102/102 (100%)	102 (100%)	0	100	100
3	N	102/102 (100%)	102 (100%)	0	100	100
3	R	102/102 (100%)	102 (100%)	0	100	100
3	V	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1864/1884 (99%)	1863 (100%)	1 (0%)	88 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	66	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
2	B	61	ASN
2	B	79	ASN
3	C	1	GLN
3	C	79	GLN
1	D	53	ASN
2	E	4	GLN
2	E	6	GLN
2	E	61	ASN
1	H	153	GLN
2	I	45	GLN
2	I	61	ASN
3	J	115	GLN
1	L	53	ASN
3	N	115	GLN
1	P	63	HIS
2	Q	113	GLN
1	T	48	HIS
2	U	4	GLN
2	U	75	ASN
2	U	86	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	152/153 (99%)	-0.21	1 (0%) 84 70	49, 60, 75, 88	2 (1%)
1	D	153/153 (100%)	-0.14	1 (0%) 84 70	46, 59, 80, 91	4 (2%)
1	H	153/153 (100%)	-0.24	2 (1%) 75 56	44, 56, 73, 98	3 (1%)
1	L	153/153 (100%)	-0.02	3 (1%) 65 46	52, 63, 79, 98	4 (2%)
1	P	153/153 (100%)	-0.06	2 (1%) 75 56	48, 57, 77, 95	3 (1%)
1	T	153/153 (100%)	-0.17	4 (2%) 57 38	47, 59, 79, 93	1 (0%)
2	B	114/118 (96%)	0.14	1 (0%) 81 65	52, 63, 90, 98	0
2	E	115/118 (97%)	0.08	0 100 100	51, 62, 84, 102	0
2	I	115/118 (97%)	0.02	1 (0%) 81 65	46, 57, 79, 98	0
2	M	115/118 (97%)	0.27	0 100 100	56, 68, 93, 104	0
2	Q	115/118 (97%)	0.11	1 (0%) 81 65	44, 61, 81, 96	0
2	U	115/118 (97%)	0.09	1 (0%) 81 65	50, 63, 87, 110	0
3	C	131/131 (100%)	-0.14	0 100 100	49, 58, 78, 87	0
3	F	131/131 (100%)	1.09	24 (18%) 3 3	68, 125, 160, 177	0
3	J	131/131 (100%)	-0.09	1 (0%) 82 68	43, 56, 78, 103	0
3	N	131/131 (100%)	0.66	10 (7%) 20 15	64, 93, 134, 145	0
3	R	131/131 (100%)	0.53	4 (3%) 51 34	60, 94, 124, 136	0
3	V	131/131 (100%)	0.34	5 (3%) 44 30	52, 74, 112, 124	0
All	All	2392/2412 (99%)	0.11	61 (2%) 57 38	43, 63, 118, 177	17 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	43	ALA	4.7
3	J	68	GLU	4.3
3	R	47	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	P	110	HIS	3.5
3	V	65	ASP	3.3
3	F	41	ARG	3.2
3	F	46	LYS	3.2
2	U	118	SER	3.1
3	F	77	LYS	3.0
1	T	83	ASP	3.0
3	N	45	GLY	2.9
3	F	44	PRO	2.9
2	B	117	SER	2.9
1	H	83	ASP	2.9
2	Q	118	SER	2.9
3	F	51	VAL	2.8
3	F	127	THR	2.8
3	V	109	GLY	2.7
3	N	115	GLN	2.7
1	L	26	ASN	2.7
1	T	153	GLN	2.6
3	N	18	LEU	2.6
3	F	52	ALA	2.6
3	V	45	GLY	2.6
3	F	45	GLY	2.5
3	V	130	SER	2.5
3	F	50	GLY	2.5
3	F	112	LEU	2.5
3	F	39	TRP	2.4
3	F	97	TYR	2.4
3	N	46	LYS	2.4
1	A	83	ASP	2.4
1	L	83	ASP	2.4
3	N	111	ARG	2.4
3	N	29	THR	2.4
3	N	125	GLN	2.4
3	F	89	LEU	2.4
3	F	40	TYR	2.3
3	R	52	ALA	2.3
3	F	124	THR	2.3
1	D	153	GLN	2.3
3	F	130	SER	2.3
2	I	117	SER	2.3
3	R	12	VAL	2.3
1	P	153	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	18	LEU	2.2
3	F	122	PRO	2.2
3	F	129	SER	2.2
3	F	20	LEU	2.2
3	V	44	PRO	2.2
3	N	68	GLU	2.1
3	F	10	GLY	2.1
3	F	126	VAL	2.1
1	T	1	ALA	2.1
3	F	91	PRO	2.1
3	R	51	VAL	2.1
1	L	109	ASP	2.1
1	H	153	GLN	2.1
1	T	85	GLY	2.1
3	N	77	LYS	2.0
3	N	47	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

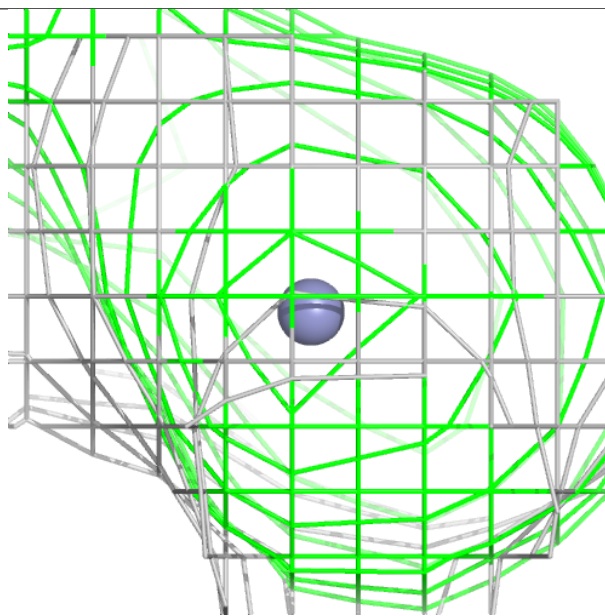
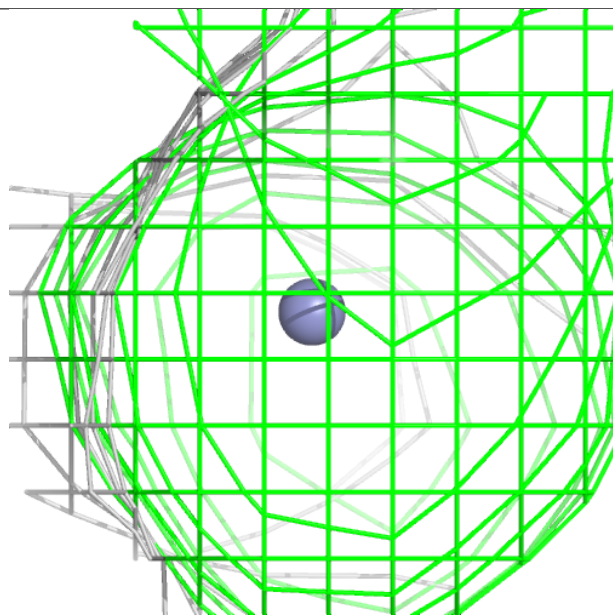
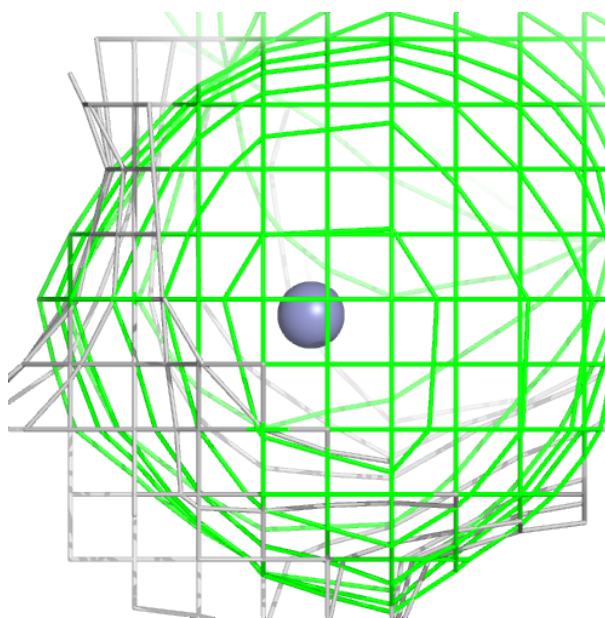
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	A	201	1/1	-	-	61,61,61,61	1
4	ZN	D	201	1/1	-	-	104,104,104,104	1
4	ZN	H	201	1/1	-	-	88,88,88,88	1
4	ZN	L	201	1/1	-	-	59,59,59,59	1
4	ZN	P	201	1/1	-	-	68,68,68,68	1
4	ZN	T	201	1/1	-	-	103,103,103,103	1

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.

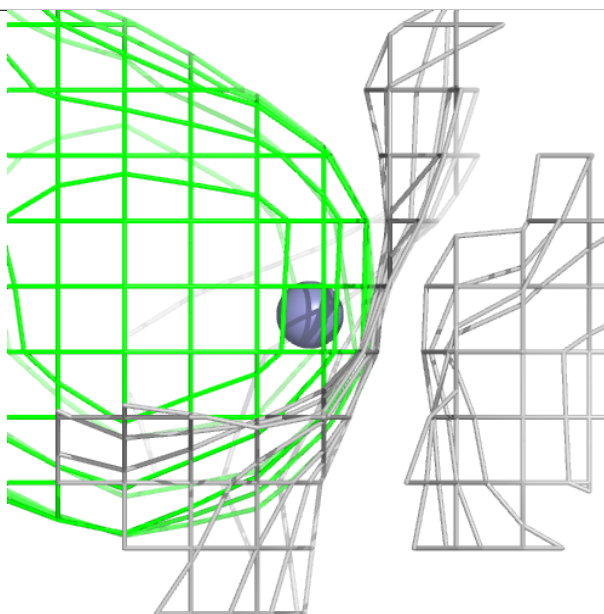
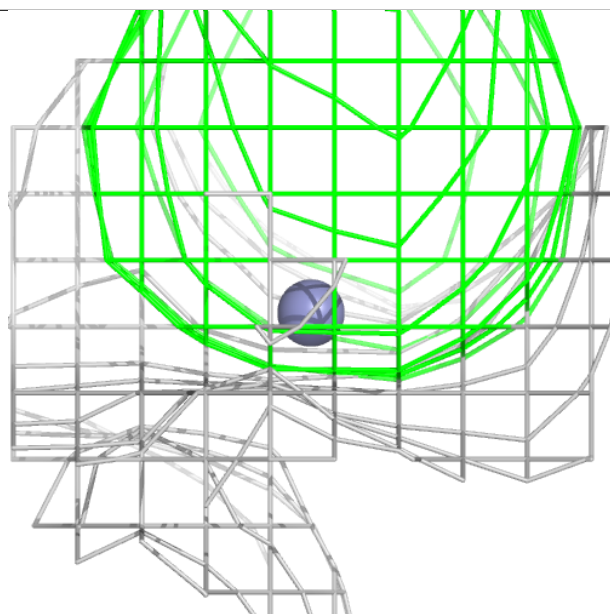
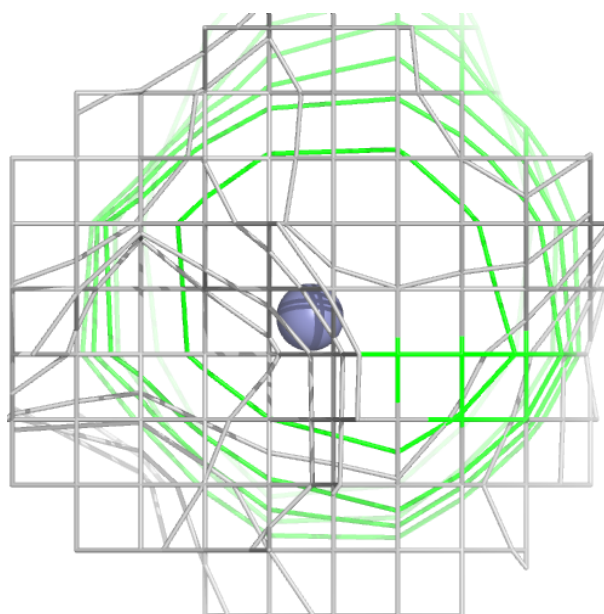
Electron density around ZN A 201:

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



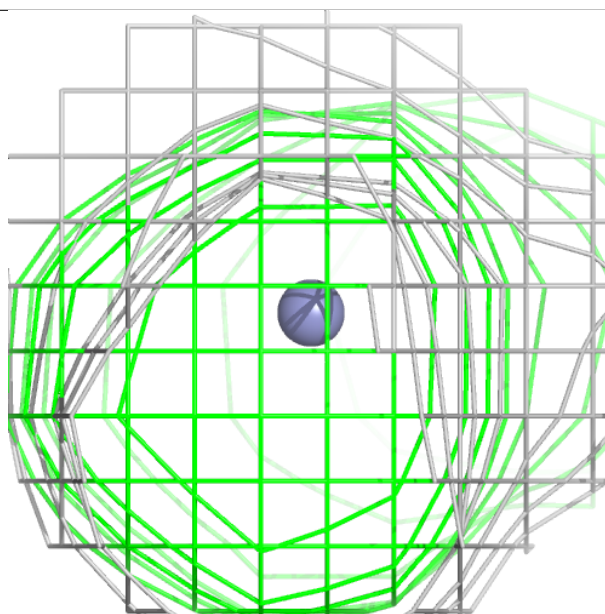
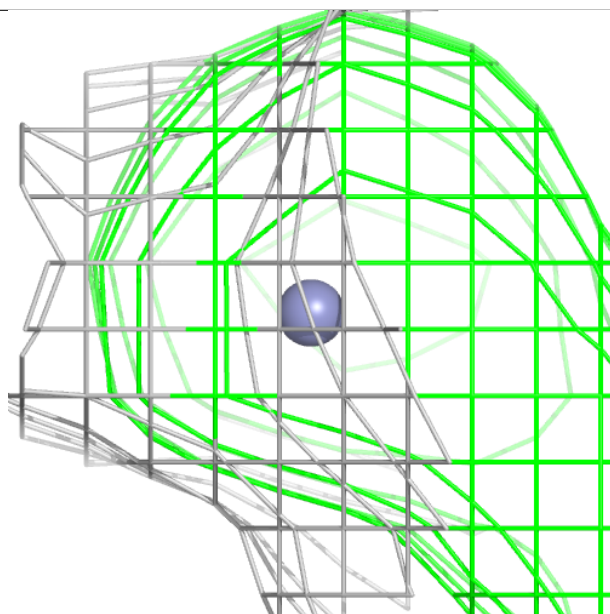
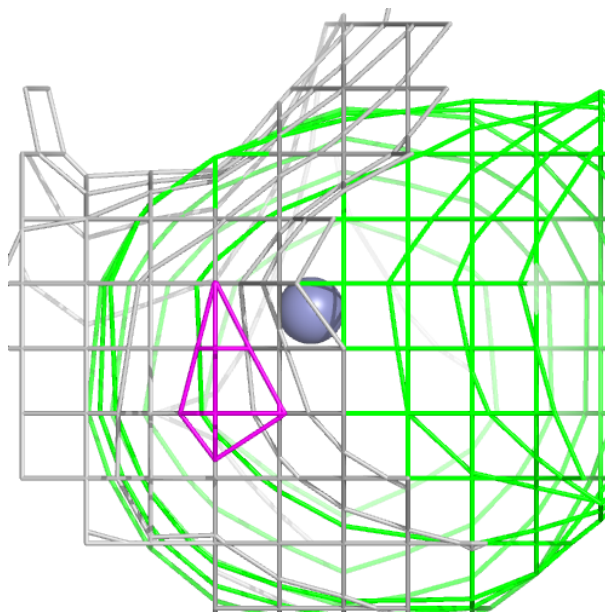
Electron density around ZN D 201:

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



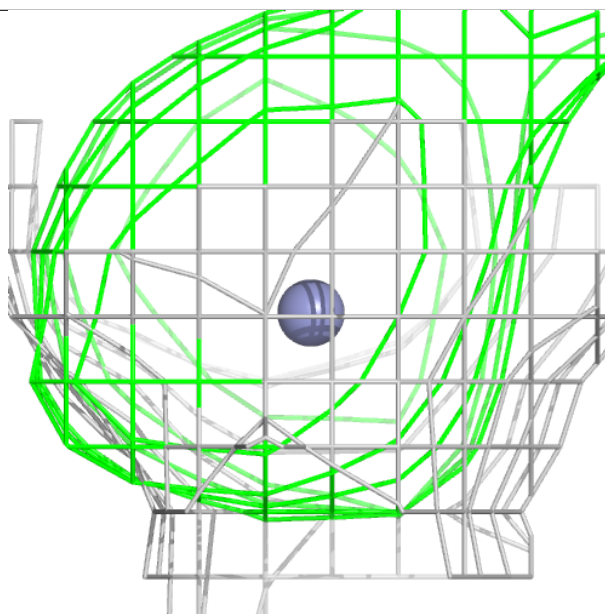
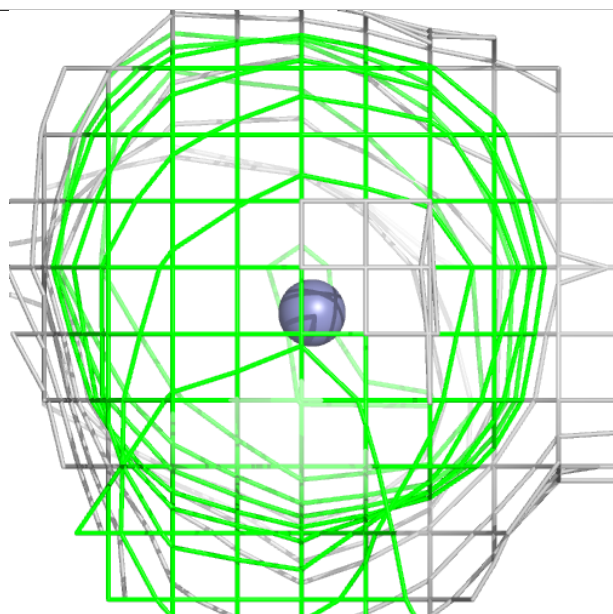
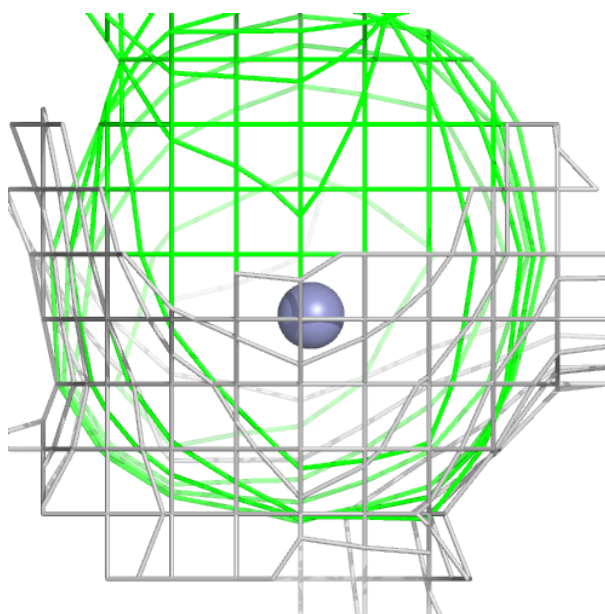
Electron density around ZN H 201:

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



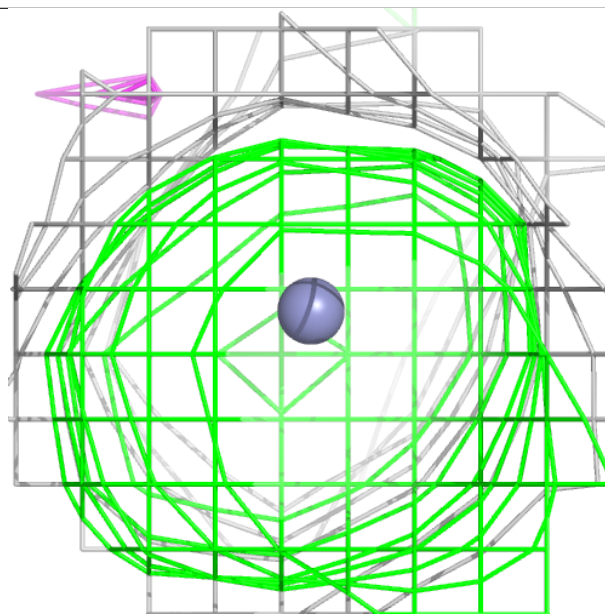
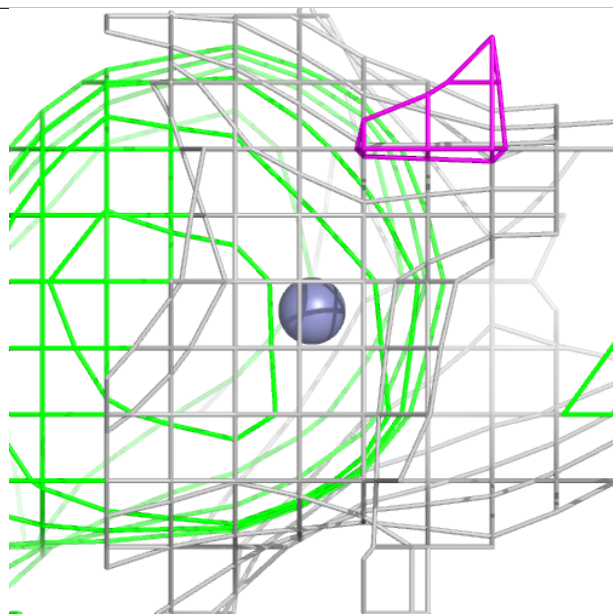
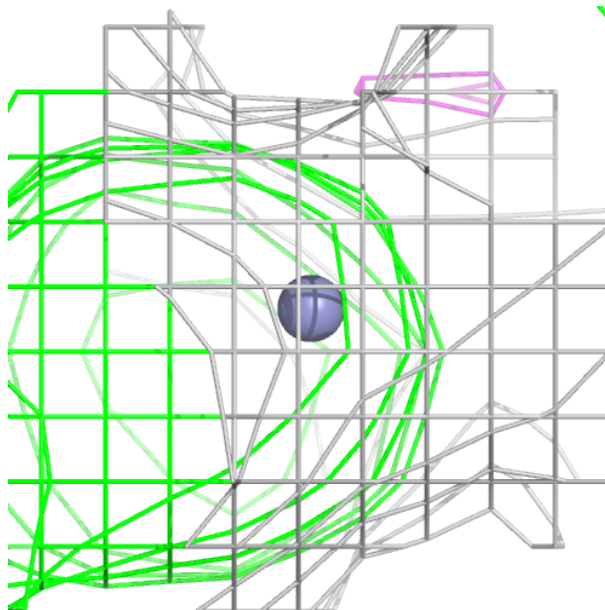
Electron density around ZN L 201:

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



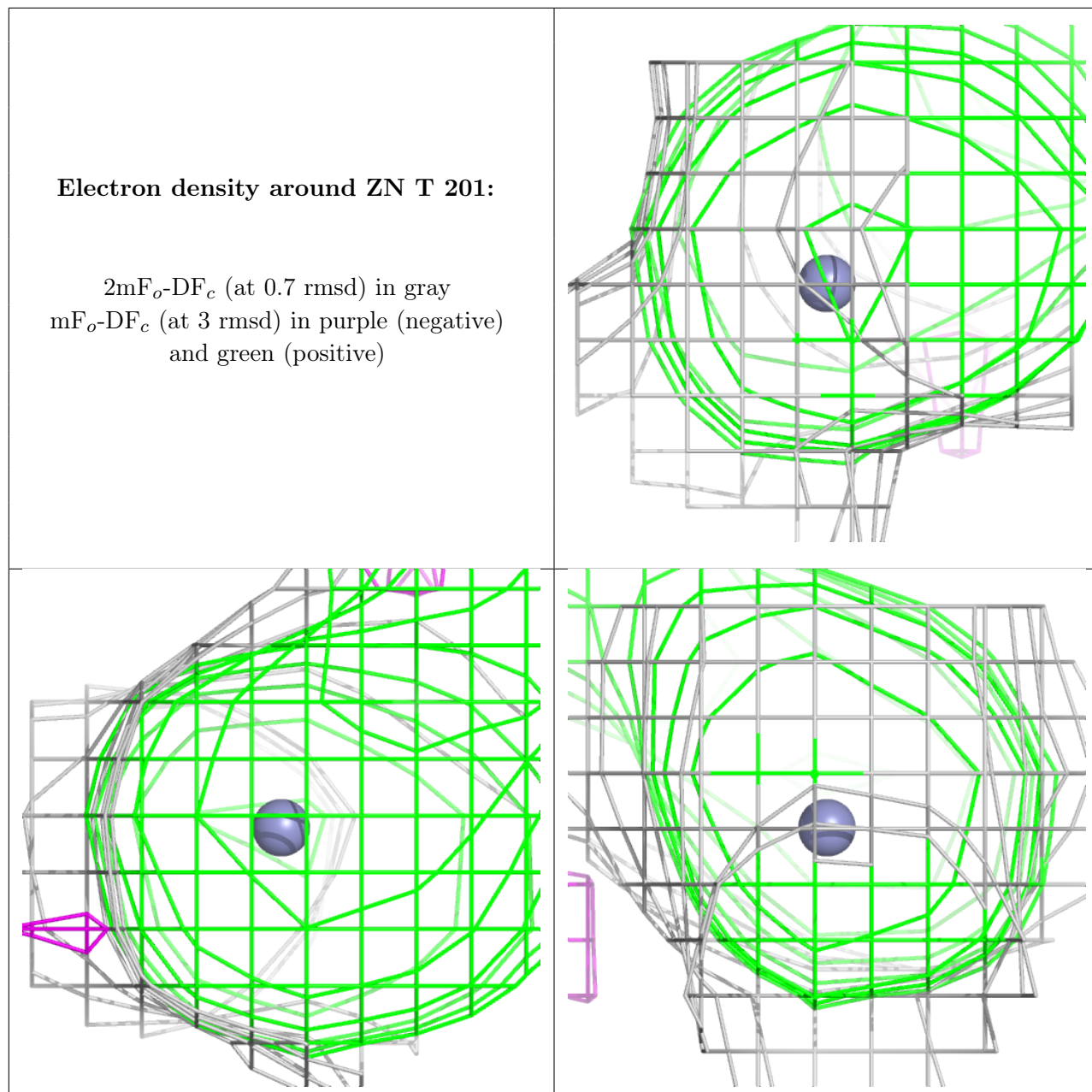
Electron density around ZN P 201:

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



Electron density around ZN T 201:

$2mF_o-DF_c$ (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.