wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 01:10 PM EDT

PDB ID	:	7RPV
Title	:	Crystal structure of affinity-enhancing and catalytically inactive ACE2 in complex with SARS-CoV-2 RBD
Authors	:	Chen, Y.; Tolbert, D.W.; Pazgier, M.
Deposited on	:	2021-08-04
Resolution	:	3.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

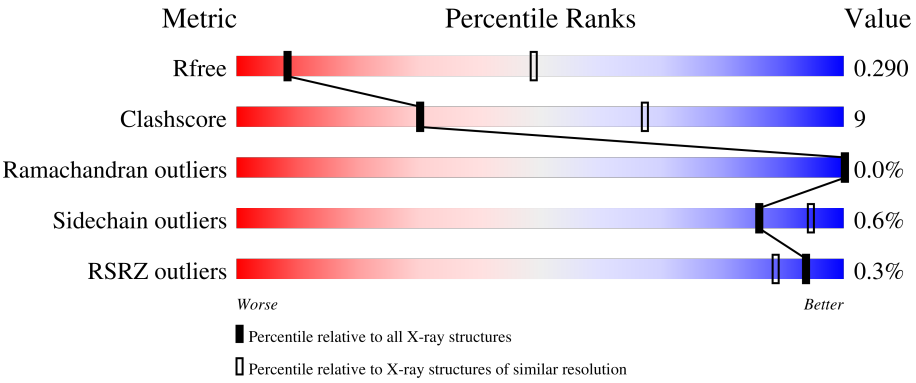
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	597	% 76% 24%
1	B	597	77% 22% .
1	C	597	81% 19%
1	D	597	79% 20%
2	E	218	% 76% 10% 14%

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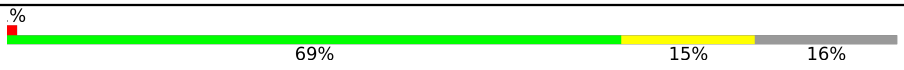
Mol	Chain	Length	Quality of chain
2	F	218	
2	G	218	
2	H	218	

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
3	NAG	A	1003	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25688 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4871	3120	801	922	28			
1	B	597	Total	C	N	O	S	0	0	0
			4871	3120	801	922	28			
1	C	595	Total	C	N	O	S	0	0	0
			4857	3113	799	917	28			
1	D	596	Total	C	N	O	S	0	0	0
			4862	3116	800	918	28			

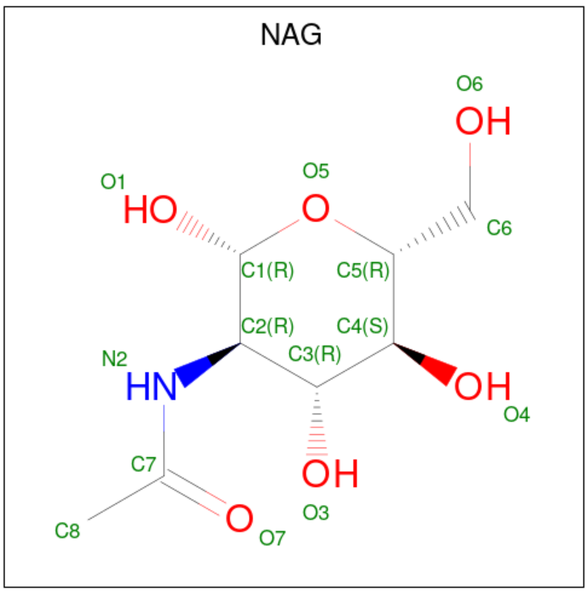
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	PHE	LEU	engineered mutation	UNP Q9BYF1
A	82	TYR	MET	engineered mutation	UNP Q9BYF1
A	325	TYR	GLN	engineered mutation	UNP Q9BYF1
A	374	ALA	HIS	engineered mutation	UNP Q9BYF1
A	378	ALA	HIS	engineered mutation	UNP Q9BYF1
B	79	PHE	LEU	engineered mutation	UNP Q9BYF1
B	82	TYR	MET	engineered mutation	UNP Q9BYF1
B	325	TYR	GLN	engineered mutation	UNP Q9BYF1
B	374	ALA	HIS	engineered mutation	UNP Q9BYF1
B	378	ALA	HIS	engineered mutation	UNP Q9BYF1
C	79	PHE	LEU	engineered mutation	UNP Q9BYF1
C	82	TYR	MET	engineered mutation	UNP Q9BYF1
C	325	TYR	GLN	engineered mutation	UNP Q9BYF1
C	374	ALA	HIS	engineered mutation	UNP Q9BYF1
C	378	ALA	HIS	engineered mutation	UNP Q9BYF1
D	79	PHE	LEU	engineered mutation	UNP Q9BYF1
D	82	TYR	MET	engineered mutation	UNP Q9BYF1
D	325	TYR	GLN	engineered mutation	UNP Q9BYF1
D	374	ALA	HIS	engineered mutation	UNP Q9BYF1
D	378	ALA	HIS	engineered mutation	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	187	Total C N O S 1487 953 247 279 8	0	0	0
2	F	184	Total C N O S 1463 939 243 273 8	0	0	0
2	G	184	Total C N O S 1465 940 243 274 8	0	0	0
2	H	185	Total C N O S 1469 942 244 275 8	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- 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 1 1	0	0

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

- Molecule 5 is water.

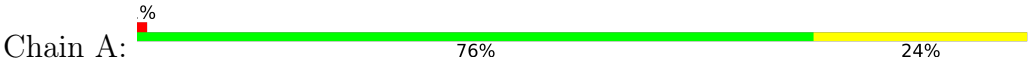
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total O 3 3	0	0

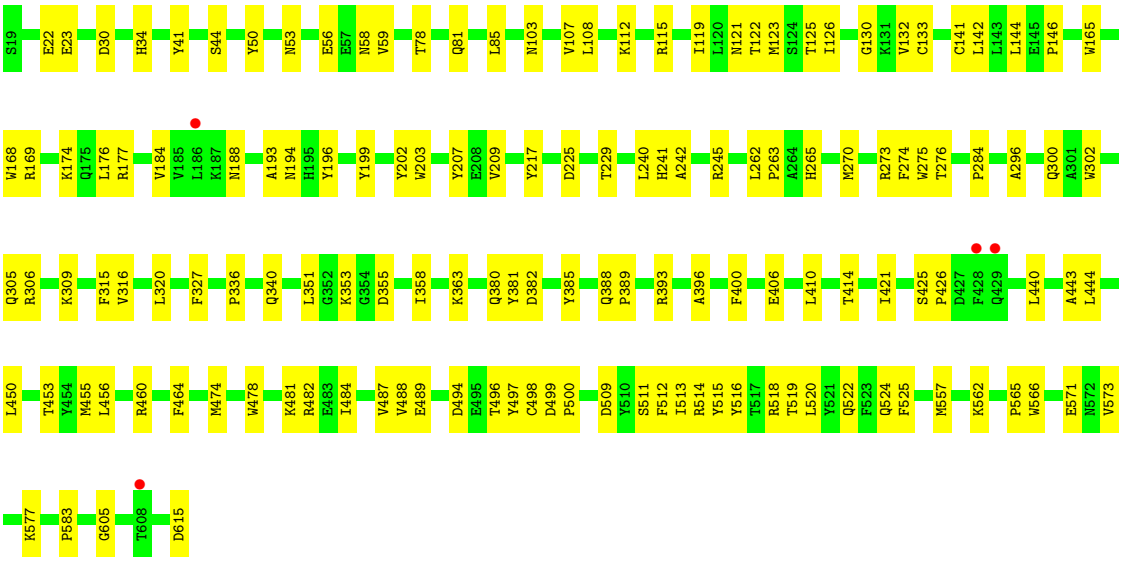
3 Residue-property plots (i)

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

• Molecule 1: Processed angiotensin-converting enzyme 2

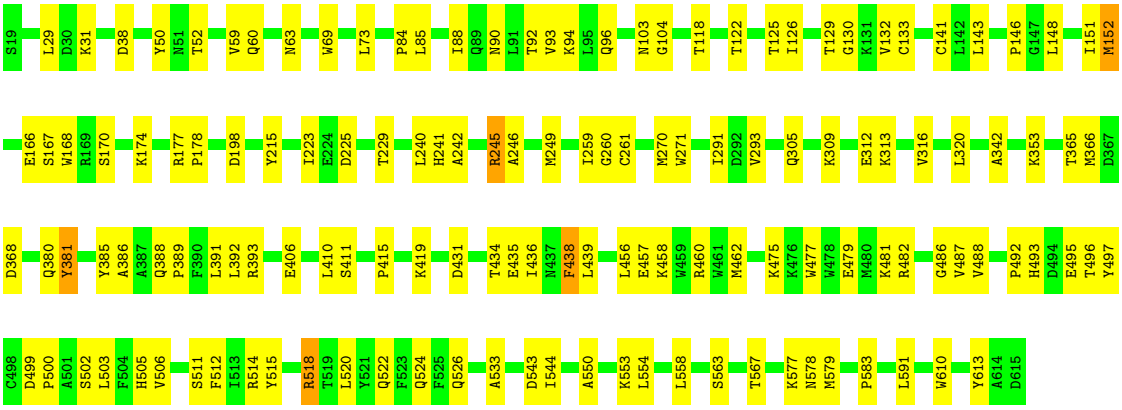
Chain A:





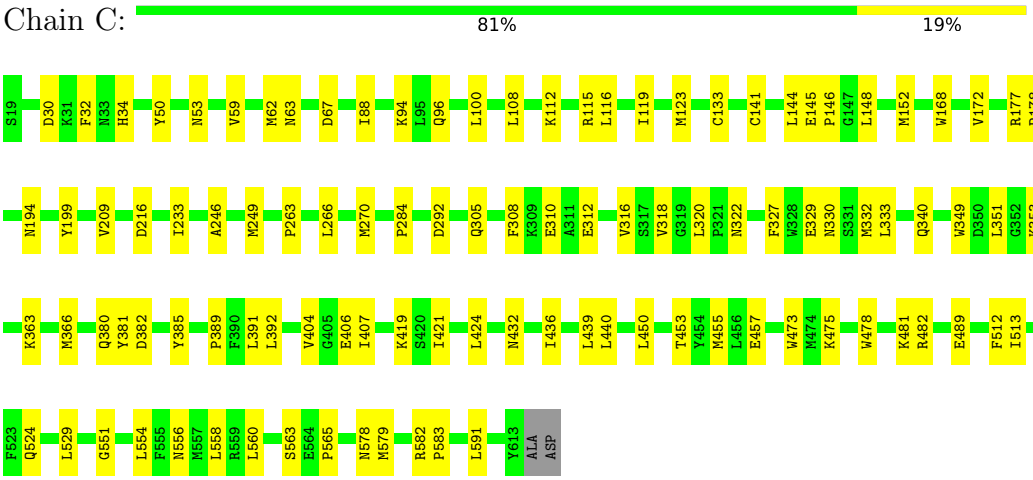
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain B:



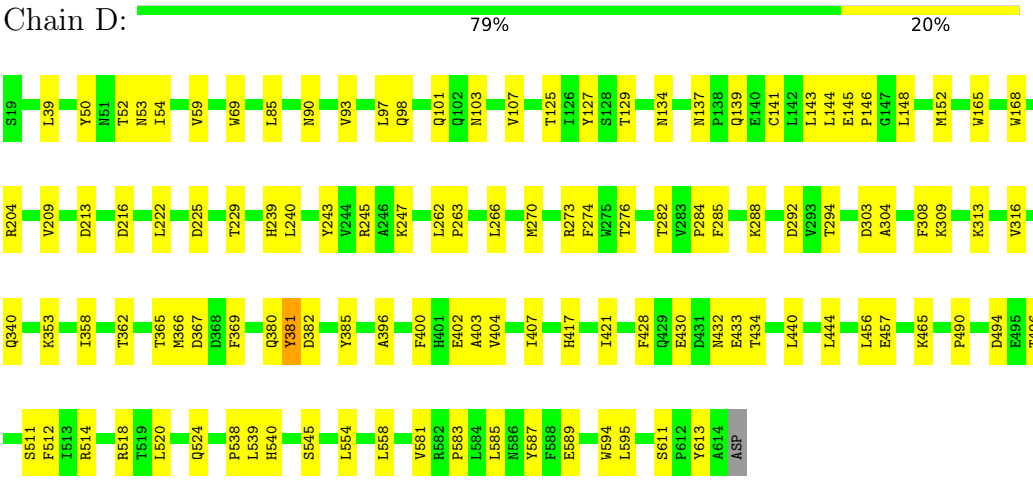
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain C:



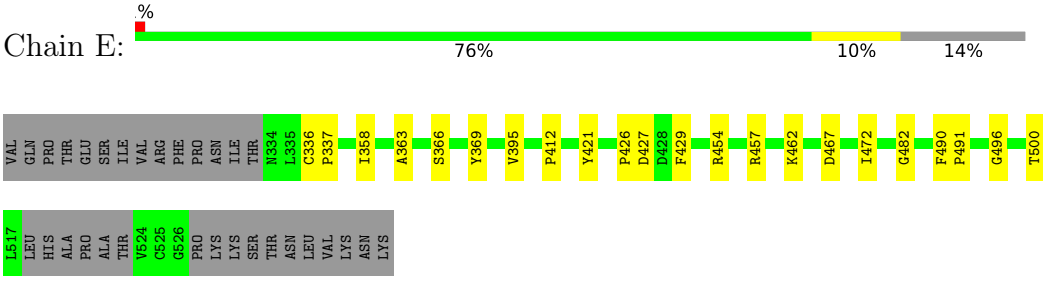
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain D:



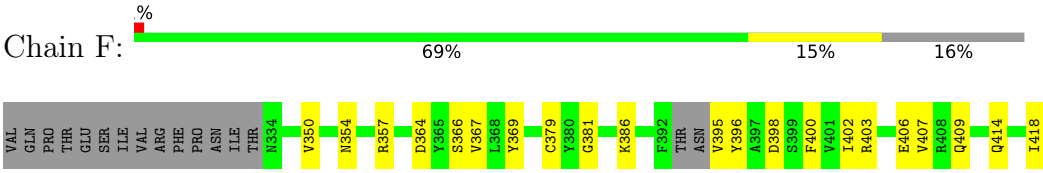
• Molecule 2: Spike protein S1

Chain E:



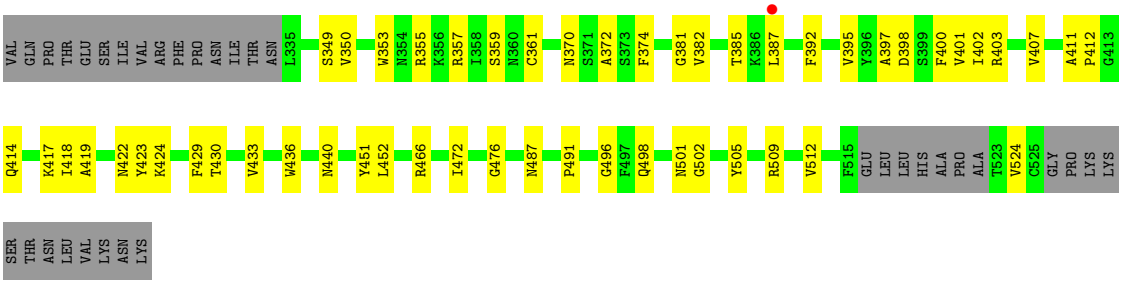
• Molecule 2: Spike protein S1

Chain F:



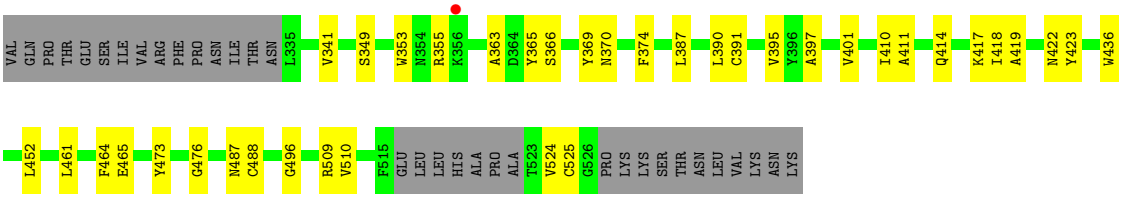
• Molecule 2: Spike protein S1

Chain G:



• Molecule 2: Spike protein S1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.67Å 136.31Å 132.67Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	47.92 – 3.54 47.92 – 3.54	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.92-3.54) 97.0 (47.92-3.54)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.243 , 0.292 0.244 , 0.290	Depositor DCC
R_{free} test set	2662 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	98.5	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.055 for -h,-l,-k 0.040 for -h,l,k 0.064 for k,h,-l 0.034 for -k,-h,-l 0.047 for l,k,-h 0.034 for l,h,k 0.055 for k,l,h 0.039 for k,-l,-h 0.059 for -l,-h,k 0.048 for h,-k,-l 0.317 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	25688	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.30	0/5009	0.49	0/6806
1	B	0.27	0/5009	0.48	0/6806
1	C	0.26	0/4995	0.45	0/6788
1	D	0.27	0/5000	0.47	0/6795
2	E	0.27	0/1527	0.50	0/2074
2	F	0.28	0/1502	0.51	0/2039
2	G	0.31	0/1505	0.55	0/2045
2	H	0.30	0/1509	0.52	0/2050
All	All	0.28	0/26056	0.48	0/35403

There are no bond length outliers.

There are no bond angle outliers.

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	4871	0	4631	116	0
1	B	4871	0	4633	99	0
1	C	4857	0	4622	70	0
1	D	4862	0	4627	81	0
2	E	1487	0	1403	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1463	0	1381	23	0
2	G	1465	0	1384	45	0
2	H	1469	0	1387	26	0
3	A	84	0	78	8	0
3	B	84	0	78	0	0
3	C	84	0	78	2	0
3	D	84	0	78	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	D	3	0	0	0	0
All	All	25688	0	24380	464	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.

The worst 5 of 464 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CE1	1:A:59:VAL:HB	1.86	1.10
1:A:50:TYR:HE1	1:A:59:VAL:CB	1.66	1.08
1:A:50:TYR:HE1	1:A:59:VAL:HB	0.95	1.07
1:A:50:TYR:CD1	1:A:59:VAL:HA	1.93	1.02
1:A:50:TYR:CE1	1:A:59:VAL:CB	2.42	1.01

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	595/597 (100%)	572 (96%)	23 (4%)	0	100	100
1	B	595/597 (100%)	573 (96%)	21 (4%)	1 (0%)	47	80
1	C	593/597 (99%)	579 (98%)	14 (2%)	0	100	100
1	D	594/597 (100%)	581 (98%)	13 (2%)	0	100	100
2	E	183/218 (84%)	172 (94%)	11 (6%)	0	100	100
2	F	178/218 (82%)	171 (96%)	7 (4%)	0	100	100
2	G	180/218 (83%)	170 (94%)	10 (6%)	0	100	100
2	H	181/218 (83%)	168 (93%)	13 (7%)	0	100	100
All	All	3099/3260 (95%)	2986 (96%)	112 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	PRO

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	525/525 (100%)	524 (100%)	1 (0%)	93	98
1	B	525/525 (100%)	517 (98%)	8 (2%)	65	84
1	C	524/525 (100%)	521 (99%)	3 (1%)	86	94
1	D	524/525 (100%)	520 (99%)	4 (1%)	81	92
2	E	162/191 (85%)	162 (100%)	0	100	100
2	F	159/191 (83%)	159 (100%)	0	100	100
2	G	160/191 (84%)	160 (100%)	0	100	100
2	H	160/191 (84%)	160 (100%)	0	100	100
All	All	2739/2864 (96%)	2723 (99%)	16 (1%)	86	94

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	381	TYR
1	D	213	ASP
1	B	518	ARG
1	D	141	CYS
1	B	438	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	B	24	GLN
1	B	195	HIS
1	B	380	GLN
1	D	340	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\#\|Z\|>2$
3	NAG	C	1005	1	14,14,15	0.41	0	17,19,21	0.52	0
3	NAG	C	1002	1	14,14,15	0.40	0	17,19,21	0.87	2 (11%)
3	NAG	D	1004	1	14,14,15	0.50	0	17,19,21	1.02	1 (5%)
3	NAG	B	1004	1	14,14,15	0.36	0	17,19,21	1.07	1 (5%)
3	NAG	A	1003	1	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
3	NAG	C	1001	1	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	B	1005	1	14,14,15	1.14	2 (14%)	17,19,21	2.53	5 (29%)
3	NAG	D	1002	1	14,14,15	0.36	0	17,19,21	0.53	0
3	NAG	D	1006	1	14,14,15	0.54	0	17,19,21	0.66	1 (5%)
3	NAG	B	1002	1	14,14,15	0.17	0	17,19,21	0.50	0
3	NAG	A	1006	1	14,14,15	0.30	0	17,19,21	0.64	1 (5%)
3	NAG	D	1003	1	14,14,15	1.58	2 (14%)	17,19,21	1.76	2 (11%)
3	NAG	C	1004	1	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	D	1001	1	14,14,15	0.37	0	17,19,21	0.63	0
3	NAG	B	1001	1	14,14,15	1.13	2 (14%)	17,19,21	0.86	1 (5%)
3	NAG	A	1005	1	14,14,15	0.55	0	17,19,21	0.54	0
3	NAG	A	1002	1	14,14,15	0.29	0	17,19,21	1.15	1 (5%)
3	NAG	D	1005	1	14,14,15	0.17	0	17,19,21	0.67	1 (5%)
3	NAG	B	1006	1	14,14,15	0.21	0	17,19,21	0.68	1 (5%)
3	NAG	A	1001	1	14,14,15	1.27	2 (14%)	17,19,21	0.78	0
3	NAG	A	1004	1	14,14,15	1.05	1 (7%)	17,19,21	1.22	1 (5%)
3	NAG	C	1003	1	14,14,15	0.44	0	17,19,21	1.38	2 (11%)
3	NAG	C	1006	1	14,14,15	0.37	0	17,19,21	0.60	1 (5%)
3	NAG	B	1003	1	14,14,15	0.30	0	17,19,21	0.69	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
3	NAG	C	1005	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
3	NAG	D	1004	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1004	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1003	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1001	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1005	1	-	3/6/23/26	0/1/1/1
3	NAG	D	1002	1	-	2/6/23/26	0/1/1/1
3	NAG	D	1006	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1002	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1006	1	-	4/6/23/26	0/1/1/1
3	NAG	D	1003	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1004	1	-	3/6/23/26	0/1/1/1
3	NAG	D	1001	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1001	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
3	NAG	D	1005	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1006	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1001	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1004	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1003	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1006	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1003	1	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1003	NAG	O5-C1	-4.66	1.36	1.43
3	A	1001	NAG	O5-C1	-4.21	1.37	1.43
3	B	1005	NAG	C1-C2	3.60	1.57	1.52
3	B	1001	NAG	O5-C1	-3.51	1.38	1.43
3	A	1004	NAG	C1-C2	3.43	1.57	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1005	NAG	C2-N2-C7	7.81	134.02	122.90
3	D	1003	NAG	C2-N2-C7	4.95	129.95	122.90
3	B	1005	NAG	C1-O5-C5	4.67	118.52	112.19
3	C	1003	NAG	C2-N2-C7	4.52	129.34	122.90
3	D	1003	NAG	C1-C2-N2	4.05	117.41	110.49

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	NAG	C8-C7-N2-C2
3	A	1002	NAG	O7-C7-N2-C2
3	B	1005	NAG	C1-C2-N2-C7
3	C	1002	NAG	C8-C7-N2-C2
3	C	1002	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1004	NAG	1	0
3	A	1003	NAG	8	0
3	D	1003	NAG	4	0
3	C	1004	NAG	1	0
3	D	1005	NAG	1	0
3	C	1003	NAG	1	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	597/597 (100%)	-0.35	4 (0%) 87 79	90, 129, 181, 232	0
1	B	597/597 (100%)	-0.37	0 100 100	85, 126, 180, 238	0
1	C	595/597 (99%)	-0.39	0 100 100	71, 103, 144, 173	0
1	D	596/597 (99%)	-0.37	0 100 100	68, 105, 147, 222	0
2	E	187/218 (85%)	-0.31	2 (1%) 80 69	82, 117, 160, 201	0
2	F	184/218 (84%)	-0.29	2 (1%) 80 69	73, 119, 175, 238	0
2	G	184/218 (84%)	-0.36	1 (0%) 91 84	84, 136, 222, 279	0
2	H	185/218 (84%)	-0.23	1 (0%) 91 84	89, 136, 198, 246	0
All	All	3125/3260 (95%)	-0.35	10 (0%) 94 89	68, 118, 174, 279	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	PHE	3.1
2	E	515	PHE	3.1
2	G	387	LEU	2.8
2	H	356	LYS	2.7
1	A	608	THR	2.6

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

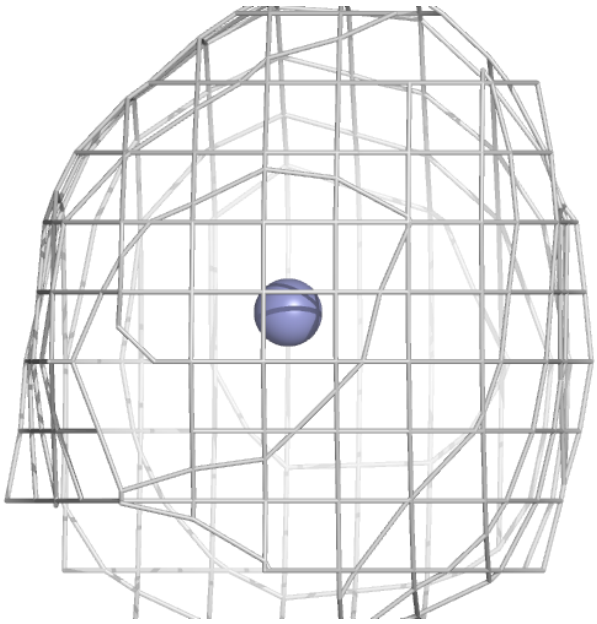
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

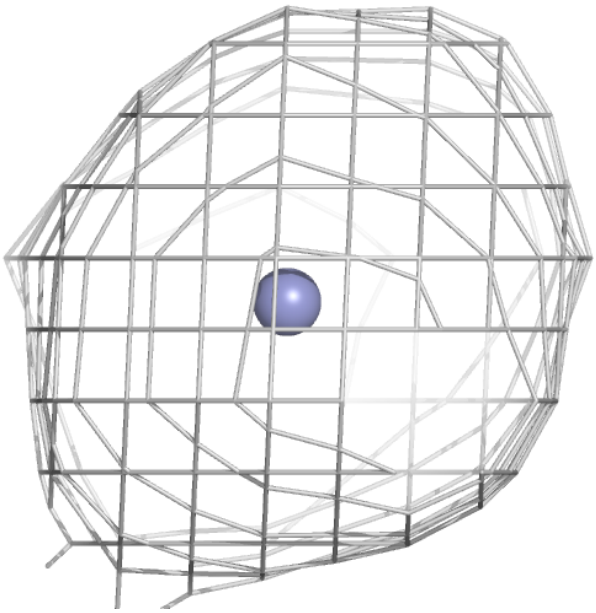
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	1005	14/15	0.75	0.32	123,155,173,187	0
3	NAG	D	1005	14/15	0.82	0.27	115,151,161,162	0
3	NAG	B	1002	14/15	0.83	0.22	126,145,158,167	0
3	NAG	B	1003	14/15	0.85	0.47	130,147,162,172	0
3	NAG	D	1002	14/15	0.86	0.21	109,122,137,138	0
3	NAG	D	1003	14/15	0.86	0.26	125,142,149,153	0
3	NAG	A	1005	14/15	0.86	0.28	130,144,158,163	0
4	ZN	C	1007	1/1	0.88	0.14	115,115,115,115	0
3	NAG	B	1001	14/15	0.89	0.31	129,139,168,177	0
3	NAG	C	1003	14/15	0.89	0.29	116,129,139,140	0
3	NAG	B	1004	14/15	0.90	0.16	102,120,137,147	0
3	NAG	C	1005	14/15	0.90	0.18	115,139,154,156	0
3	NAG	A	1006	14/15	0.90	0.24	121,131,140,149	0
3	NAG	A	1001	14/15	0.91	0.31	129,141,161,163	0
3	NAG	C	1001	14/15	0.91	0.20	133,140,160,171	0
4	ZN	A	1007	1/1	0.92	0.05	142,142,142,142	0
3	NAG	C	1002	14/15	0.92	0.17	75,81,90,97	0
3	NAG	A	1004	14/15	0.93	0.15	102,119,144,154	0
3	NAG	A	1002	14/15	0.93	0.17	75,81,90,97	0
3	NAG	B	1006	14/15	0.93	0.29	117,132,151,167	0
3	NAG	A	1003	14/15	0.93	0.30	75,81,90,97	0
3	NAG	C	1006	14/15	0.94	0.17	106,120,125,139	0
3	NAG	D	1006	14/15	0.94	0.22	106,119,128,130	0
3	NAG	D	1001	14/15	0.94	0.16	75,81,90,97	0
3	NAG	D	1004	14/15	0.94	0.21	102,111,126,142	0
3	NAG	C	1004	14/15	0.95	0.17	102,107,135,142	0
4	ZN	D	1007	1/1	0.95	0.20	112,112,112,112	0
4	ZN	B	1007	1/1	0.96	0.12	103,103,103,103	0

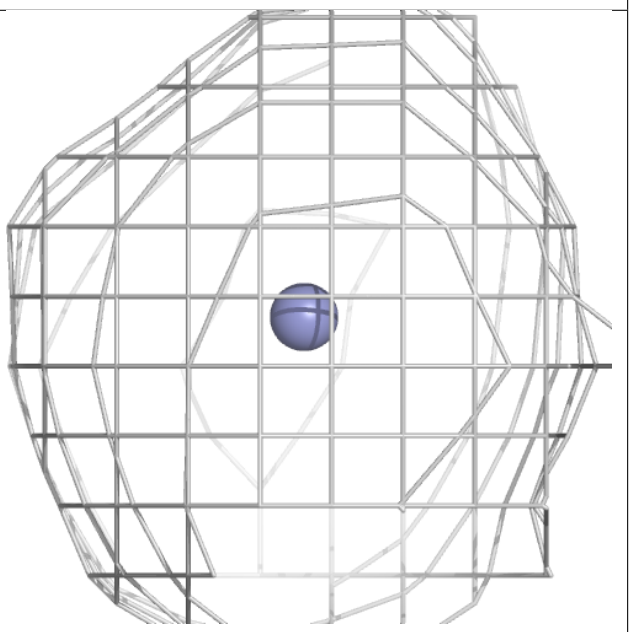
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN C 1007:

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

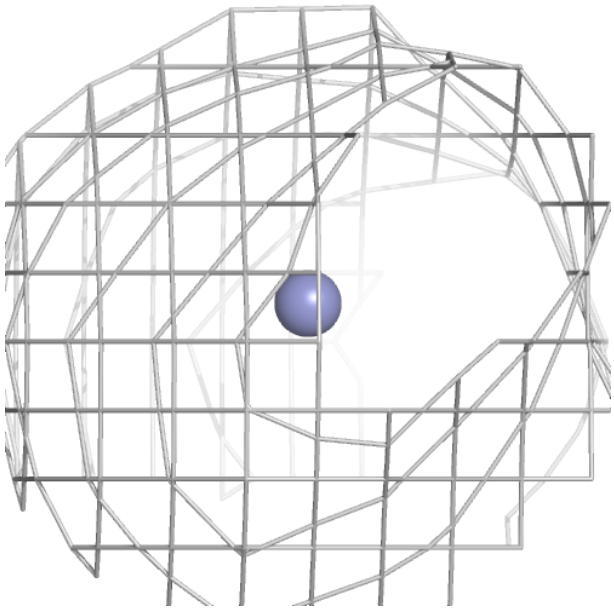


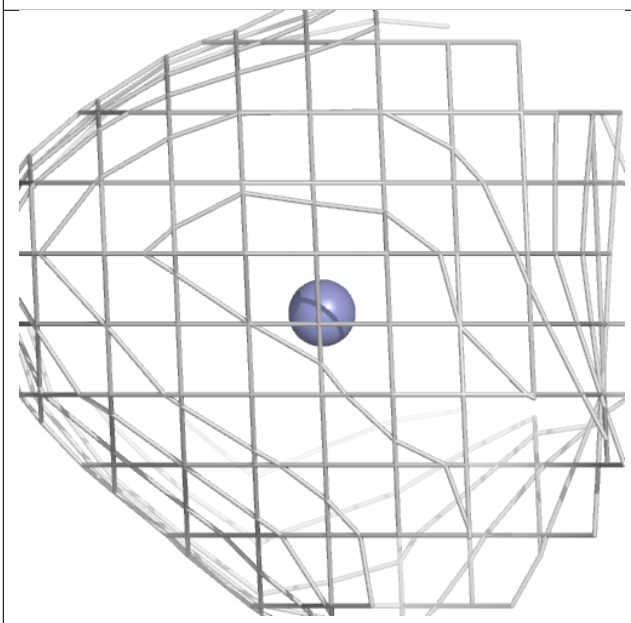


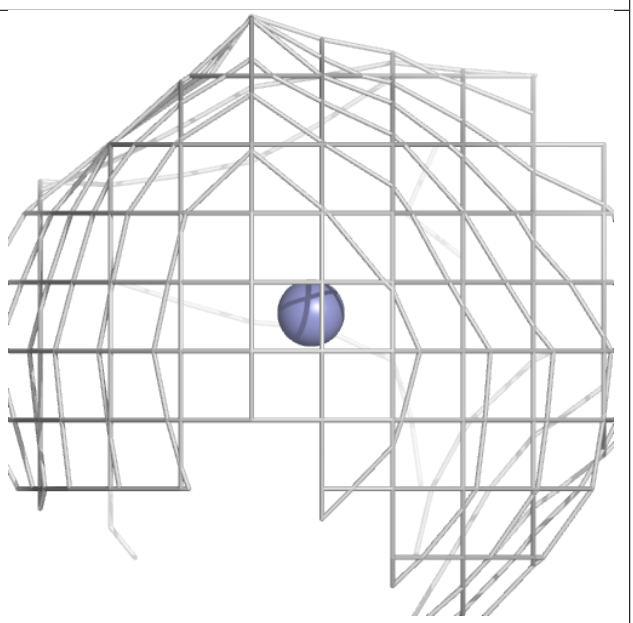


Electron density around ZN A 1007:

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

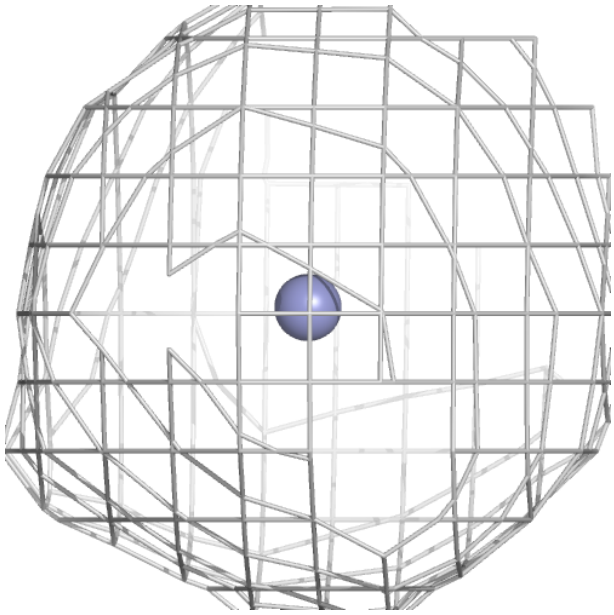


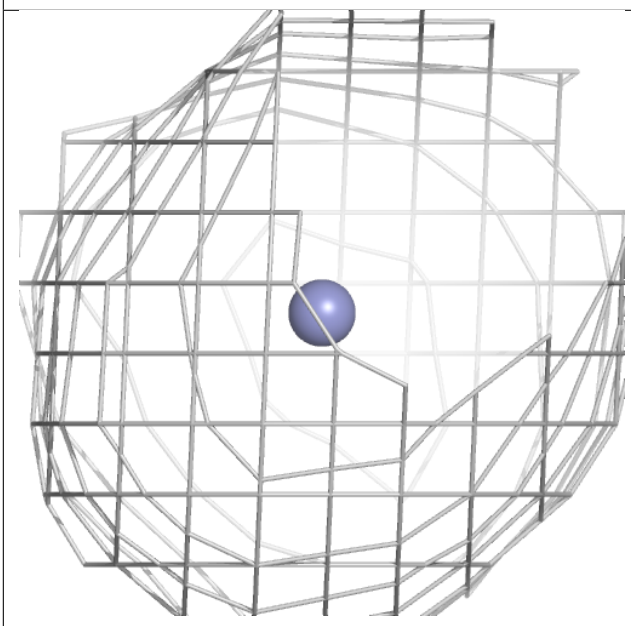


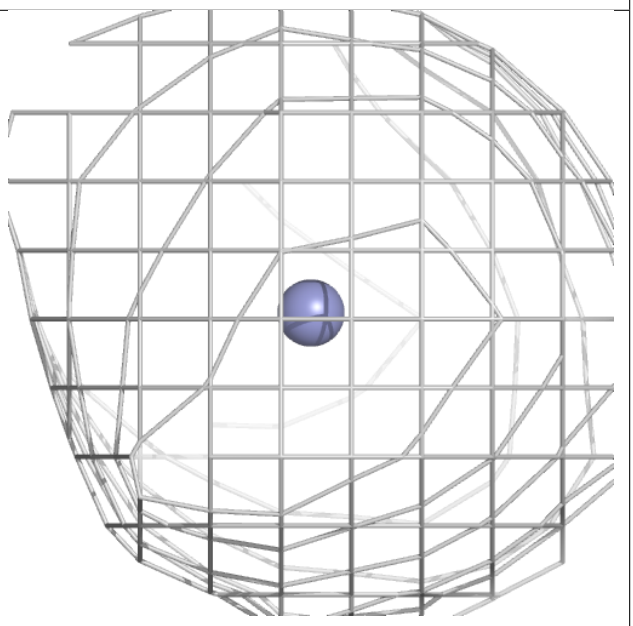


Electron density around ZN D 1007:

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

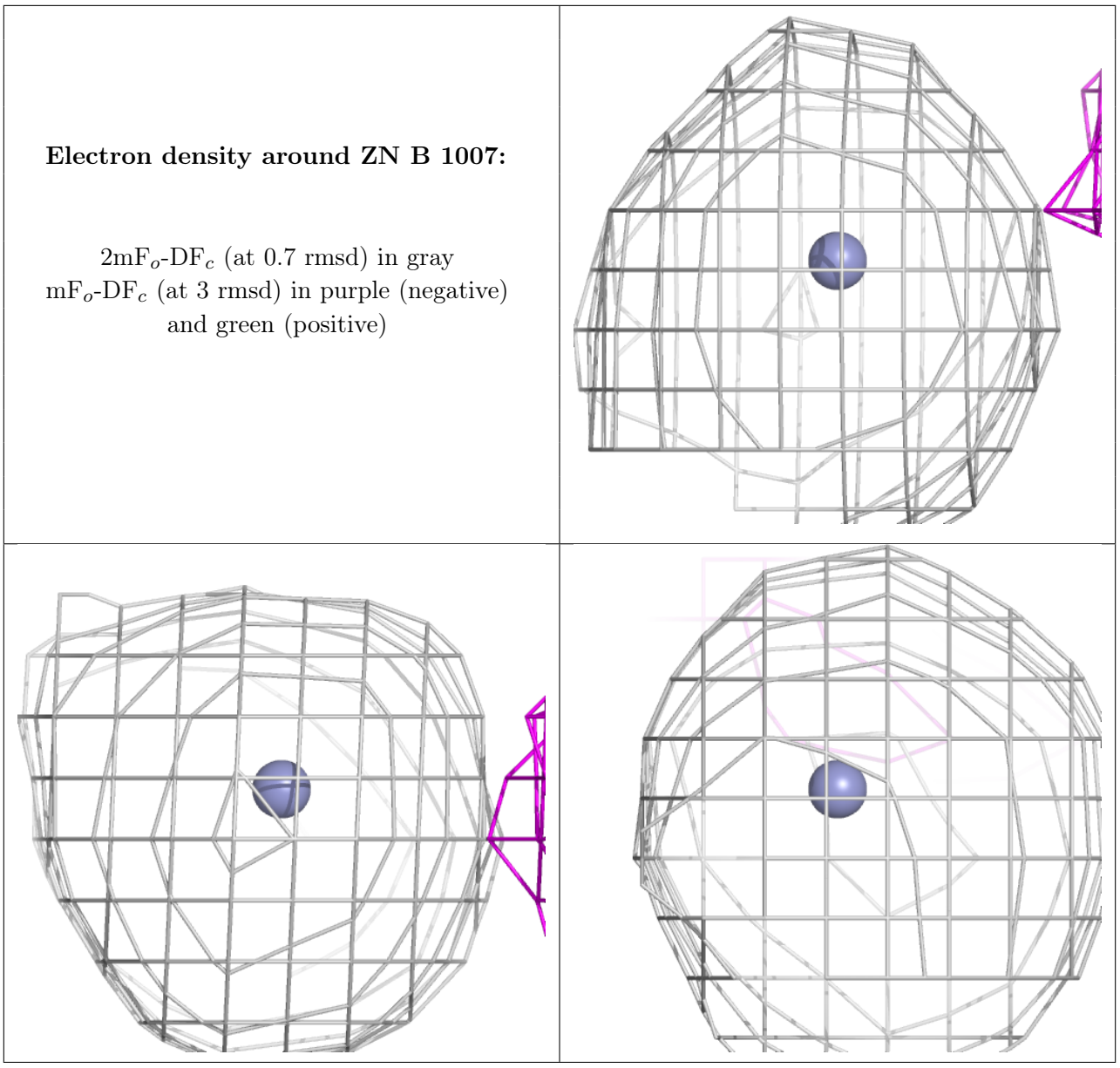






Electron density around ZN B 1007:

$2mF_o$-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 (i)

There are no such residues in this entry.