



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:20 AM UTC

PDB ID : 8OPR / pdb_00008opr
Title : Structure of the EA1 surface layer of Bacillus anthracis
Authors : Sogues, A.; Remaut, H.
Deposited on : 2023-04-07
Resolution : 1.81 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

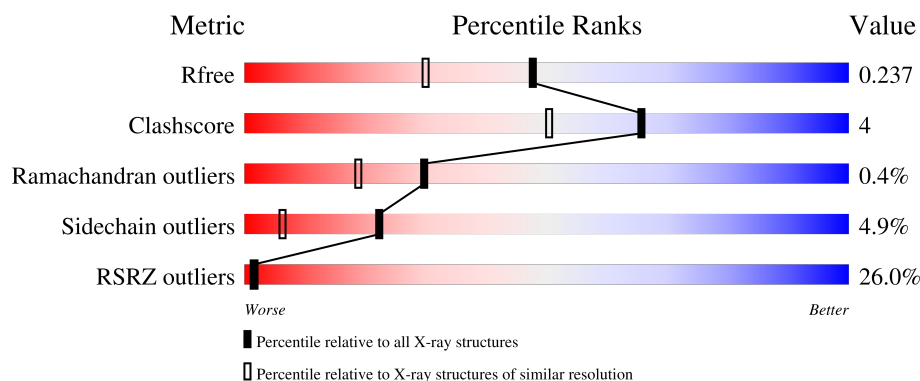
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	665	9% 88% 9% ...
2	B	127	43% 76% 16% 6%
3	C	133	89% 76% 16% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7588 atoms, of which 15 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 S-layer protein EA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			4793	3009	800	983	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MET	-	initiating methionine	UNP P94217
A	199	HIS	-	expression tag	UNP P94217
A	200	HIS	-	expression tag	UNP P94217
A	201	HIS	-	expression tag	UNP P94217
A	202	HIS	-	expression tag	UNP P94217
A	203	HIS	-	expression tag	UNP P94217
A	204	HIS	-	expression tag	UNP P94217
A	205	ILE	-	expression tag	UNP P94217
A	206	THR	-	expression tag	UNP P94217
A	207	SER	-	expression tag	UNP P94217
A	208	LEU	-	expression tag	UNP P94217
A	209	TYR	-	expression tag	UNP P94217
A	210	LYS	-	expression tag	UNP P94217
A	211	LYS	-	expression tag	UNP P94217
A	212	GLY	-	expression tag	UNP P94217
A	213	GLN	-	expression tag	UNP P94217
A	214	MET	-	expression tag	UNP P94217
A	827	LEU	THR	conflict	UNP P94217

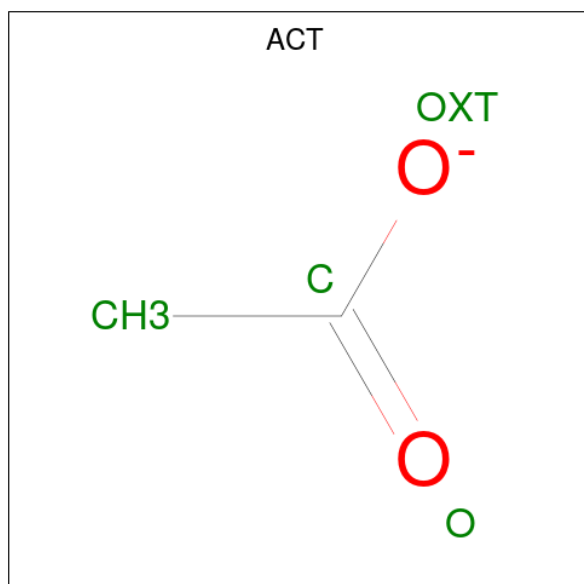
- Molecule 2 is a protein called Nanobody 643.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			897	555	159	180	3			

- Molecule 3 is a protein called Nanobody 632.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			980	615	175	186	4			

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

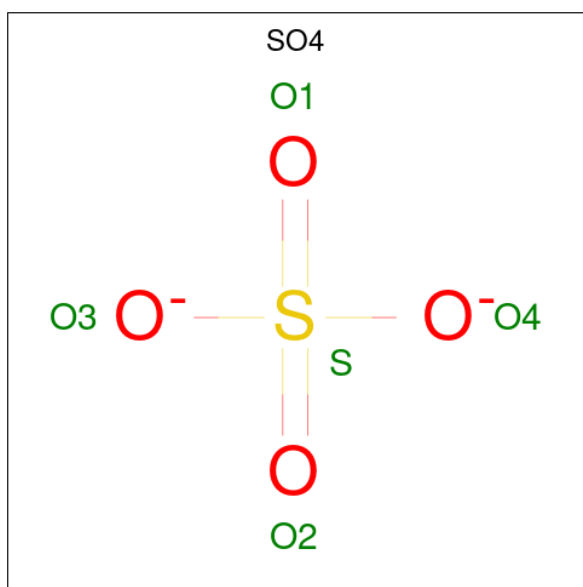


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	3	0
			7	2	3	2		
4	A	1	Total	C	H	O	3	0
			7	2	3	2		
4	A	1	Total	C	H	O	3	0
			7	2	3	2		
4	A	1	Total	C	H	O	3	0
			7	2	3	2		
4	A	1	Total	C	H	O	3	0
			7	2	3	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca	0	0
			3	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

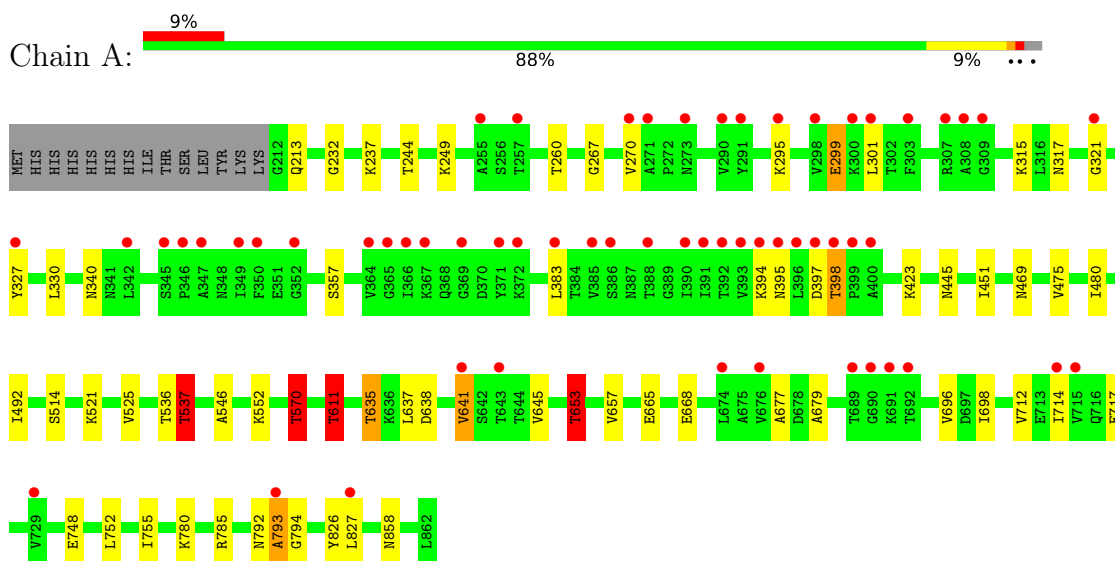
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	795	Total	O	0	0
			795	795		
7	B	46	Total	O	0	0
			46	46		
7	C	19	Total	O	0	0
			19	19		

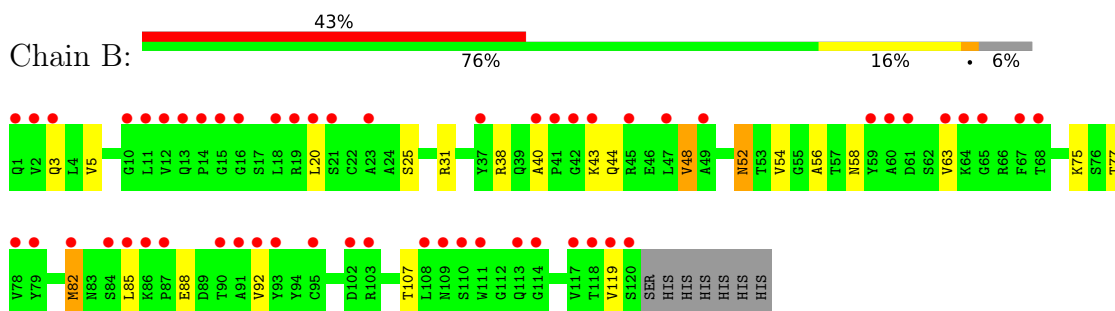
3 Residue-property plots [i](#)

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.

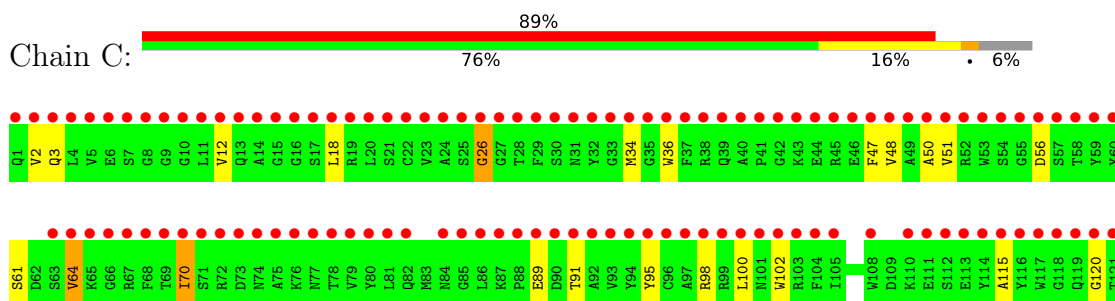
• Molecule 1: S-layer protein EA1



• Molecule 2: Nanobody 643



• Molecule 3: Nanobody 632



Q122	Q123	T124	V125	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.93Å 74.30Å 87.65Å 107.85° 101.14° 112.42°	Depositor
Resolution (Å)	63.37 – 1.81 63.37 – 1.81	Depositor EDS
% Data completeness (in resolution range)	53.0 (63.37-1.81) 53.1 (63.37-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.81Å)	Xtriage
Refinement program	BUSTER 2.10.4 (3-FEB-2022)	Depositor
R, R_{free}	0.204 , 0.243 0.199 , 0.237	Depositor DCC
R_{free} test set	3807 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7588	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: ACT, CA, SO4

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	0.80	3/4848 (0.1%)	1.02	10/6589 (0.2%)
2	B	0.63	0/912	0.92	1/1238 (0.1%)
3	C	0.55	0/1003	0.92	0/1356
All	All	0.74	3/6763 (0.0%)	0.99	11/9183 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	752	LEU	CA-C	7.36	1.57	1.53
1	A	492	ILE	CG1-CD1	-6.03	1.28	1.51
1	A	793	ALA	CA-C	5.15	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	826	TYR	CA-C-N	13.33	140.87	122.34
1	A	826	TYR	C-N-CA	13.33	140.87	122.34
1	A	570	THR	N-CA-CB	-8.98	98.22	111.51
1	A	653	THR	N-CA-CB	-7.55	99.56	110.36
1	A	611	THR	N-CA-CB	-6.37	101.03	110.85
2	B	5	VAL	N-CA-C	5.61	114.81	106.85
1	A	570	THR	CB-CA-C	5.47	120.86	111.45
1	A	445	ASN	N-CA-C	-5.16	107.12	113.41
1	A	537	THR	N-CA-CB	-5.01	102.97	111.69
1	A	792	ASN	CA-C-N	5.00	131.09	121.54
1	A	792	ASN	C-N-CA	5.00	131.09	121.54

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	4793	0	4817	31	0
2	B	897	0	865	9	0
3	C	980	0	931	13	0
4	A	20	15	15	2	0
5	A	3	0	0	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
7	A	795	0	0	2	0
7	B	46	0	0	0	0
7	C	19	0	0	0	0
All	All	7573	15	6628	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (50) 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:546:ALA:H	1:A:570:THR:HG22	1.35	0.91
1:A:653:THR:HG21	7:A:1077:HOH:O	1.81	0.80
1:A:536:THR:OG1	1:A:570:THR:HG21	1.82	0.80
1:A:514:SER:HB3	1:A:537:THR:HG22	1.69	0.74
1:A:611:THR:HG23	7:A:1077:HOH:O	1.92	0.69
2:B:75:LYS:HB2	2:B:77:THR:HG22	1.75	0.68
1:A:315:LYS:HZ2	1:A:321:GLY:H	1.45	0.64
2:B:48:VAL:HG23	2:B:63:VAL:HG21	1.79	0.64
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.83	0.61
1:A:827:LEU:HD21	1:A:858:ASN:HB3	1.82	0.61
1:A:611:THR:HG21	1:A:657:VAL:HG11	1.85	0.59
1:A:315:LYS:NZ	1:A:321:GLY:H	2.01	0.58
1:A:327:TYR:HA	1:A:330:LEU:HD12	1.85	0.57
3:C:34:MET:HE1	3:C:98:ARG:HG3	1.87	0.57
3:C:2:VAL:HG22	3:C:26:GLY:HA3	1.89	0.54
3:C:36:TRP:HD1	3:C:70:ILE:CD1	2.21	0.53
1:A:340:ASN:HD21	3:C:102:TRP:H	1.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:MET:HG2	2:B:85:LEU:HD21	1.92	0.51
2:B:3:GLN:HB2	2:B:25:SER:HB3	1.94	0.50
2:B:75:LYS:HB2	2:B:77:THR:CG2	2.39	0.49
3:C:100:LEU:HB2	3:C:115:ALA:HB2	1.94	0.49
1:A:213:GLN:HG3	1:A:237:LYS:HD2	1.94	0.49
1:A:394:LYS:HG2	1:A:395:ASN:H	1.79	0.48
1:A:398:THR:HG23	1:A:451:ILE:HG12	1.96	0.48
1:A:244:THR:HG22	1:A:249:LYS:HG2	1.96	0.47
1:A:785:ARG:HD3	1:A:794:GLY:O	2.14	0.47
1:A:475:VAL:HG22	1:A:480:ILE:HG22	1.96	0.47
1:A:357:SER:HA	4:A:902:ACT:H2	1.97	0.45
2:B:52:ASN:HD21	2:B:54:VAL:HG22	1.82	0.45
3:C:61:SER:HB3	3:C:64:VAL:HG12	1.98	0.45
1:A:677:ALA:HB3	1:A:696:VAL:HG11	2.00	0.44
1:A:267:GLY:O	2:B:52:ASN:HB2	2.18	0.44
1:A:525:VAL:HA	1:A:611:THR:HG22	2.00	0.44
1:A:637:LEU:HB3	1:A:714:ILE:HD13	2.00	0.43
3:C:51:VAL:HB	3:C:70:ILE:HG12	1.99	0.43
3:C:95:TYR:HA	3:C:120:GLY:HA2	2.01	0.43
1:A:295:LYS:HG2	1:A:317:ASN:HA	2.01	0.42
3:C:91:THR:HG23	3:C:124:THR:HA	2.01	0.42
3:C:12:VAL:HG11	3:C:18:LEU:HB2	2.01	0.42
1:A:340:ASN:HD21	3:C:102:TRP:N	2.16	0.42
1:A:679:ALA:HB2	1:A:698:ILE:HD12	2.02	0.42
1:A:469:ASN:HB3	4:A:901:ACT:H1	2.01	0.41
1:A:638:ASP:HB3	1:A:641:VAL:CG1	2.51	0.41
1:A:635:THR:HG21	1:A:645:VAL:HG21	2.03	0.41
2:B:52:ASN:ND2	2:B:56:ALA:H	2.19	0.41
1:A:299:GLU:HB3	1:A:301:LEU:HG	2.02	0.41
1:A:232:GLY:O	1:A:260:THR:HA	2.22	0.40
3:C:47:PHE:HE1	3:C:50:ALA:HB2	1.86	0.40
1:A:748:GLU:HB2	1:A:755:ILE:HB	2.02	0.40
3:C:36:TRP:CD1	3:C:70:ILE:CD1	3.04	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	649/665 (98%)	630 (97%)	17 (3%)	2 (0%)	36	26
2	B	118/127 (93%)	112 (95%)	6 (5%)	0	100	100
3	C	123/133 (92%)	116 (94%)	5 (4%)	2 (2%)	7	2
All	All	890/925 (96%)	858 (96%)	28 (3%)	4 (0%)	30	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	ASP
1	A	793	ALA
3	C	56	ASP
3	C	26	GLY

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	526/557 (94%)	508 (97%)	18 (3%)	32	14
2	B	95/104 (91%)	83 (87%)	12 (13%)	4	0
3	C	100/109 (92%)	95 (95%)	5 (5%)	22	6
All	All	721/770 (94%)	686 (95%)	35 (5%)	22	6

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	VAL
1	A	299	GLU
1	A	383	LEU
1	A	398	THR
1	A	423	LYS
1	A	521	LYS
1	A	537	THR
1	A	552	LYS
1	A	570	THR
1	A	611	THR
1	A	635	THR
1	A	641	VAL
1	A	653	THR
1	A	665	GLU
1	A	668	GLU
1	A	712	VAL
1	A	717	GLU
1	A	780	LYS
2	B	20	LEU
2	B	31	ARG
2	B	38	ARG
2	B	44	GLN
2	B	48	VAL
2	B	52	ASN
2	B	58	ASN
2	B	82	MET
2	B	88	GLU
2	B	92	VAL
2	B	107	THR
2	B	119	VAL
3	C	3	GLN
3	C	48	VAL
3	C	64	VAL
3	C	70	ILE
3	C	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	A	340	ASN
1	A	435	ASN
1	A	518	ASN

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Mol	Chain	Res	Type
1	A	640	ASN
1	A	699	HIS
1	A	760	ASN
1	A	850	GLN
1	A	858	ASN
2	B	32	ASN
2	B	52	ASN
3	C	13	GLN
3	C	77	ASN
3	C	101	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	A	910	-	4,4,4	0.29	0	6,6,6	0.44	0
4	ACT	A	904	-	3,3,3	1.03	0	3,3,3	1.61	1 (33%)
6	SO4	B	201	-	4,4,4	0.37	0	6,6,6	0.16	0
4	ACT	A	902	-	3,3,3	0.55	0	3,3,3	1.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	909	-	4,4,4	0.32	0	6,6,6	0.43	0
4	ACT	A	901	-	3,3,3	1.24	0	3,3,3	1.28	0
4	ACT	A	903	-	3,3,3	1.07	0	3,3,3	1.36	0
6	SO4	B	202	-	4,4,4	0.29	0	6,6,6	0.15	0
4	ACT	A	905	-	3,3,3	0.79	0	3,3,3	1.66	1 (33%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	905	ACT	OXT-C-O	2.35	130.73	122.03
4	A	904	ACT	OXT-C-O	2.11	129.85	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	ACT	1	0
4	A	901	ACT	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, 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	651/665 (97%)	0.42	59 (9%) 15 16	16, 36, 67, 85	0
2	B	120/127 (94%)	2.11	55 (45%) 0 0	40, 71, 109, 117	0
3	C	125/133 (93%)	3.94	119 (95%) 0 0	74, 132, 160, 168	0
All	All	896/925 (96%)	1.13	233 (26%) 1 2	16, 44, 139, 168	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	11	LEU	8.4
3	C	123	VAL	8.2
2	B	11	LEU	7.8
3	C	12	VAL	7.0
3	C	4	LEU	6.7
3	C	2	VAL	6.5
3	C	79	VAL	6.4
3	C	40	ALA	6.3
3	C	117	TRP	6.2
3	C	75	ALA	6.2
3	C	125	VAL	6.0
3	C	95	TYR	5.9
3	C	37	PHE	5.8
3	C	86	LEU	5.8
3	C	41	PRO	5.7
2	B	119	VAL	5.7
3	C	29	PHE	5.7
2	B	18	LEU	5.6
3	C	33	GLY	5.6
3	C	20	LEU	5.5
3	C	5	VAL	5.5
3	C	16	GLY	5.5
3	C	80	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
3	C	108	TRP	5.4
3	C	14	ALA	5.4
3	C	24	ALA	5.4
1	A	383	LEU	5.3
1	A	396	LEU	5.3
3	C	70	ILE	5.3
3	C	34	MET	5.3
2	B	12	VAL	5.2
3	C	53	TRP	5.2
3	C	18	LEU	5.1
3	C	3	GLN	5.1
3	C	47	PHE	5.1
3	C	64	VAL	5.0
3	C	32	TYR	5.0
3	C	10	GLY	4.9
3	C	94	TYR	4.8
3	C	88	PRO	4.8
3	C	59	TYR	4.8
3	C	51	VAL	4.8
3	C	116	TYR	4.7
3	C	119	GLN	4.6
1	A	399	PRO	4.6
3	C	55	GLY	4.6
3	C	23	VAL	4.6
1	A	827	LEU	4.6
1	A	398	THR	4.6
3	C	92	ALA	4.6
3	C	57	SER	4.5
2	B	120	SER	4.5
2	B	41	PRO	4.4
3	C	36	TRP	4.4
1	A	394	LYS	4.4
1	A	366	ILE	4.4
3	C	97	ALA	4.3
3	C	1	GLN	4.3
3	C	78	THR	4.2
2	B	13	GLN	4.2
3	C	91	THR	4.2
3	C	52	ARG	4.1
3	C	45	ARG	4.1
2	B	117	VAL	4.1
3	C	66	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
3	C	48	VAL	4.0
3	C	71	SER	4.0
3	C	28	THR	4.0
3	C	43	LYS	4.0
3	C	93	VAL	4.0
3	C	74	ASN	3.9
1	A	793	ALA	3.9
2	B	40	ALA	3.9
1	A	364	VAL	3.9
3	C	81	LEU	3.9
2	B	68	THR	3.9
3	C	114	TYR	3.8
2	B	43	LYS	3.8
1	A	365	GLY	3.7
3	C	87	LYS	3.7
3	C	31	ASN	3.7
3	C	17	SER	3.6
2	B	60	ALA	3.6
2	B	91	ALA	3.6
3	C	115	ALA	3.6
3	C	35	GLY	3.6
2	B	1	GLN	3.6
3	C	27	GLY	3.6
3	C	13	GLN	3.6
3	C	68	PHE	3.6
2	B	23	ALA	3.6
1	A	342	LEU	3.6
3	C	65	LYS	3.5
3	C	77	ASN	3.5
3	C	100	LEU	3.5
3	C	67	ARG	3.5
1	A	397	ASP	3.5
1	A	349	ILE	3.5
3	C	19	ARG	3.5
3	C	7	SER	3.4
3	C	42	GLY	3.4
3	C	120	GLY	3.4
3	C	60	TYR	3.4
2	B	59	TYR	3.4
3	C	85	GLY	3.4
2	B	95	CYS	3.3
3	C	38	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	690	GLY	3.3
3	C	122	GLN	3.3
2	B	16	GLY	3.3
3	C	98	ARG	3.3
3	C	50	ALA	3.3
3	C	69	THR	3.3
3	C	15	GLY	3.2
2	B	87	PRO	3.2
1	A	393	VAL	3.2
1	A	367	LYS	3.2
3	C	26	GLY	3.2
3	C	111	GLU	3.2
3	C	49	ALA	3.1
3	C	105	ILE	3.1
2	B	10	GLY	3.1
2	B	20	LEU	3.1
3	C	22	CYS	3.1
3	C	63	SER	3.1
3	C	124	THR	3.1
2	B	14	PRO	3.1
3	C	72	ARG	3.0
3	C	54	SER	3.0
1	A	388	THR	3.0
2	B	15	GLY	3.0
2	B	19	ARG	3.0
2	B	118	THR	3.0
1	A	321	GLY	3.0
3	C	73	ASP	3.0
3	C	90	ASP	3.0
3	C	8	GLY	3.0
3	C	6	GLU	3.0
3	C	112	SER	2.9
2	B	85	LEU	2.9
3	C	118	GLY	2.9
3	C	21	SER	2.9
1	A	715	VAL	2.9
3	C	121	THR	2.9
1	A	395	ASN	2.9
1	A	391	ILE	2.9
1	A	307	ARG	2.8
3	C	44	GLU	2.8
3	C	76	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	352	GLY	2.7
2	B	84	SER	2.7
2	B	42	GLY	2.7
3	C	56	ASP	2.7
1	A	390	ILE	2.7
1	A	729	VAL	2.7
2	B	82	MET	2.7
2	B	90	THR	2.7
1	A	301	LEU	2.7
1	A	290	VAL	2.7
2	B	63	VAL	2.6
1	A	392	THR	2.6
1	A	689	THR	2.6
1	A	691	LYS	2.6
3	C	25	SER	2.6
2	B	79	TYR	2.6
1	A	303	PHE	2.6
2	B	102	ASP	2.6
2	B	2	VAL	2.6
2	B	93	TYR	2.5
3	C	39	GLN	2.5
3	C	96	CYS	2.5
1	A	372	LYS	2.5
1	A	347	ALA	2.5
3	C	58	THR	2.5
2	B	114	GLY	2.5
2	B	109	ASN	2.5
2	B	113	GLN	2.5
1	A	308	ALA	2.5
1	A	692	THR	2.5
2	B	92	VAL	2.5
1	A	346	PRO	2.5
1	A	369	GLY	2.4
3	C	102	TRP	2.4
3	C	101	ASN	2.4
3	C	104	PHE	2.4
1	A	298	VAL	2.4
3	C	113	GLU	2.4
1	A	386	SER	2.4
1	A	291	TYR	2.4
2	B	49	ALA	2.4
3	C	89	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	273	ASN	2.4
2	B	65	GLY	2.4
1	A	385	VAL	2.3
1	A	641	VAL	2.3
3	C	30	SER	2.3
2	B	47	LEU	2.3
1	A	350	PHE	2.3
1	A	295	LYS	2.3
1	A	271	ALA	2.3
1	A	345	SER	2.3
2	B	61	ASP	2.3
3	C	84	ASN	2.3
2	B	86	LYS	2.3
2	B	108	LEU	2.3
2	B	111	TRP	2.2
3	C	9	GLY	2.2
3	C	82	GLN	2.2
1	A	309	GLY	2.2
1	A	400	ALA	2.2
1	A	327	TYR	2.1
1	A	371	TYR	2.1
3	C	46	GLU	2.1
1	A	300	LYS	2.1
3	C	110	LYS	2.1
1	A	257	THR	2.1
1	A	676	VAL	2.1
2	B	103	ARG	2.1
1	A	714	ILE	2.1
2	B	37	TYR	2.1
2	B	45	ARG	2.1
2	B	110	SER	2.1
2	B	78	VAL	2.1
1	A	674	LEU	2.1
1	A	255	ALA	2.1
1	A	643	THR	2.0
2	B	3	GLN	2.0
1	A	270	VAL	2.0
3	C	99	ARG	2.0
2	B	64	LYS	2.0
2	B	21	SER	2.0
2	B	67	PHE	2.0
3	C	103	ARG	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](#)

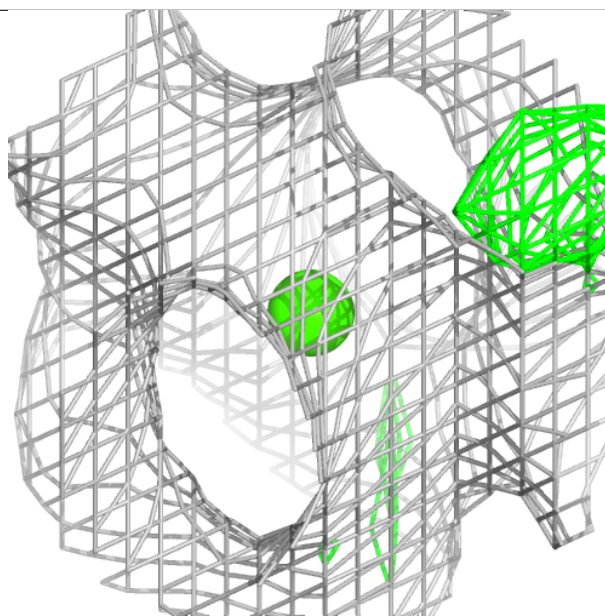
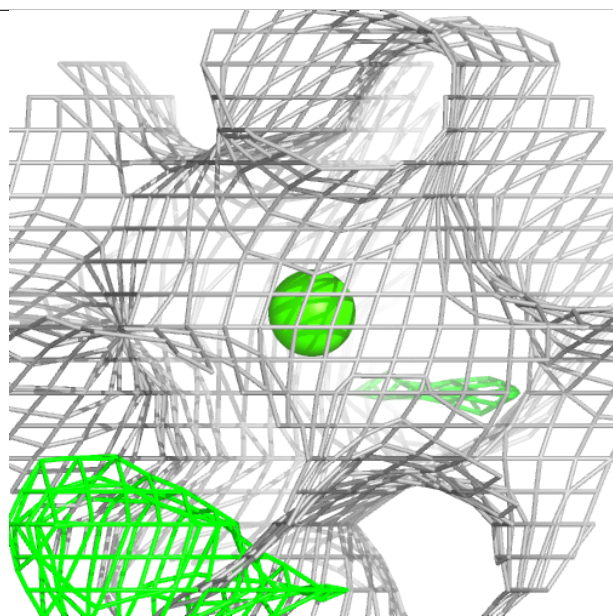
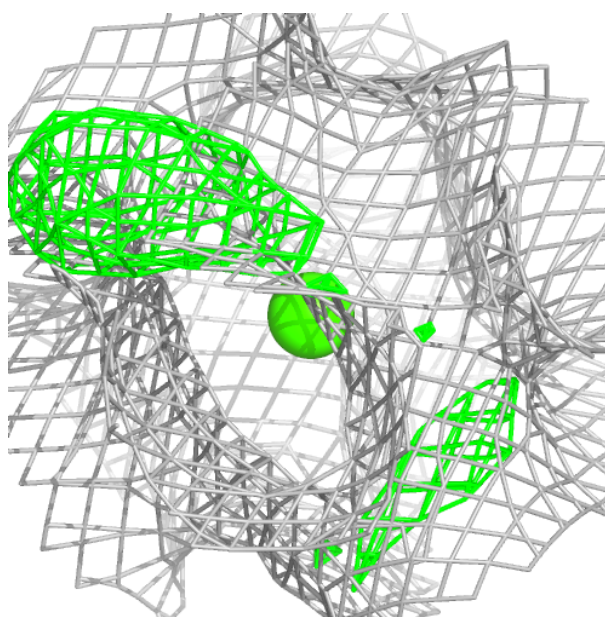
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	904	4/4	0.66	0.27	66,66,70,70	3
4	ACT	A	903	4/4	0.72	0.23	50,50,54,55	3
6	SO4	B	202	5/5	0.72	0.25	146,146,146,146	0
4	ACT	A	901	4/4	0.78	0.18	33,33,39,40	3
6	SO4	A	910	5/5	0.85	0.16	102,102,102,102	0
4	ACT	A	902	4/4	0.90	0.17	37,37,40,42	3
6	SO4	A	909	5/5	0.90	0.11	63,63,63,63	0
6	SO4	B	201	5/5	0.95	0.08	64,65,65,65	0
4	ACT	A	905	4/4	0.97	0.08	42,42,43,44	3
5	CA	A	908	1/1	0.98	0.03	29,29,29,29	0
5	CA	A	906	1/1	0.99	0.02	25,25,25,25	0
5	CA	A	907	1/1	1.00	0.02	38,38,38,38	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.

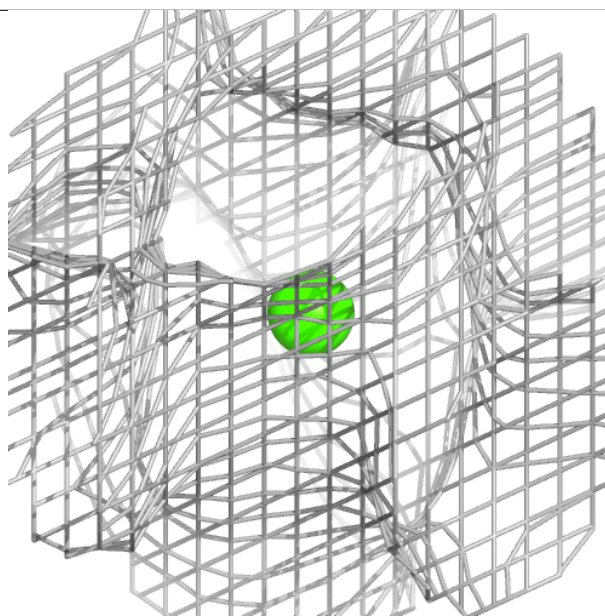
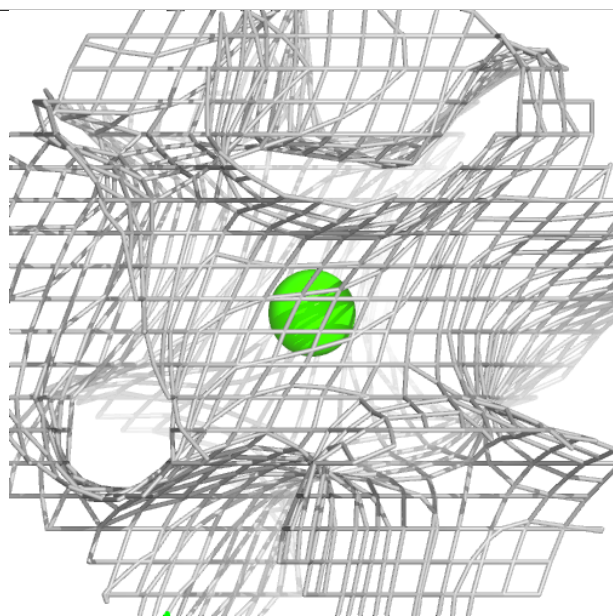
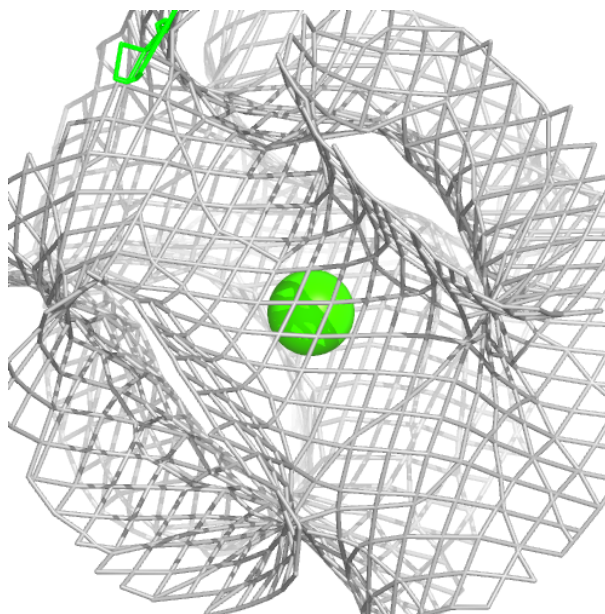
Electron density around CA A 908:

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



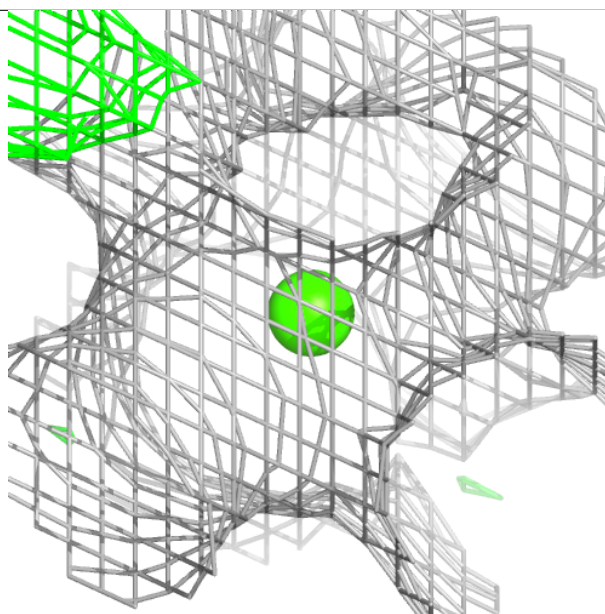
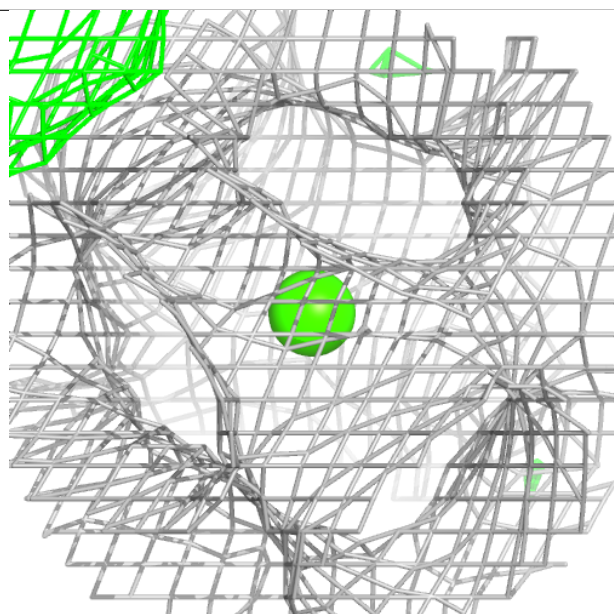
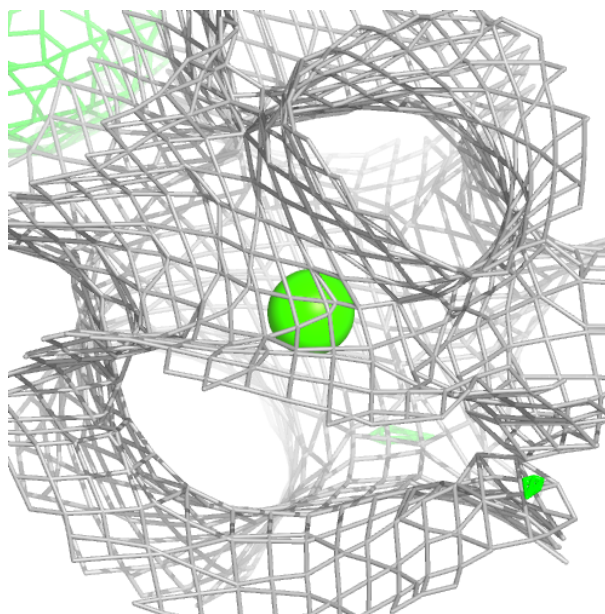
Electron density around CA A 906:

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



Electron density around CA A 907:

$2mF_o-DF_c$ (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.