



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:07 AM UTC

PDB ID : 6VS7 / pdb_00006vs7
Title : Sialic acid binding region of Streptococcus Sanguinis SK1 adhesin
Authors : Stubbs, H.E.; Iverson, T.M.
Deposited on : 2020-02-10
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

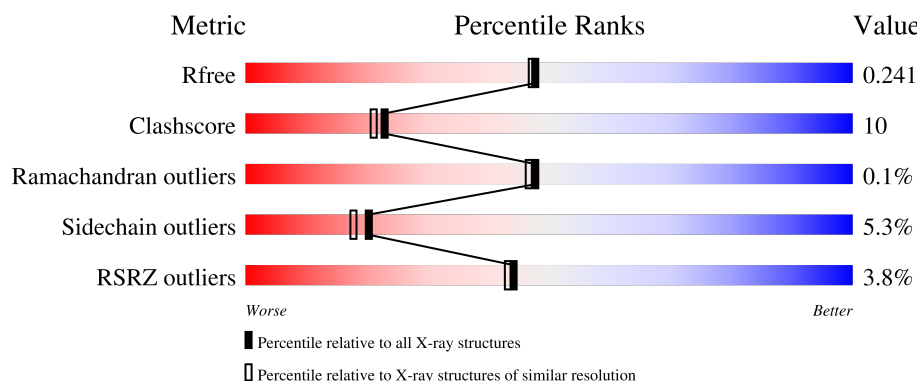
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	409	2% 78% 21% .
1	E	409	5% 76% 20% .

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
5	TRS	E	706	-	X	-	-
6	EDO	A	713	-	-	X	-
6	EDO	E	711	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7496 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.

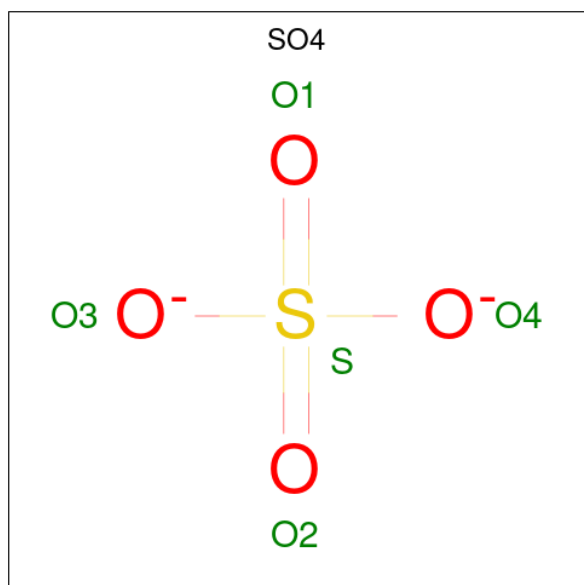
- Molecule 1 is a protein called Adhesin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	0	7	0
			3194	1985	555	654			
1	E	409	Total	C	N	O	0	15	0
			3265	2022	576	667			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		
2	E	4	Total	Ca	0	0
			4	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

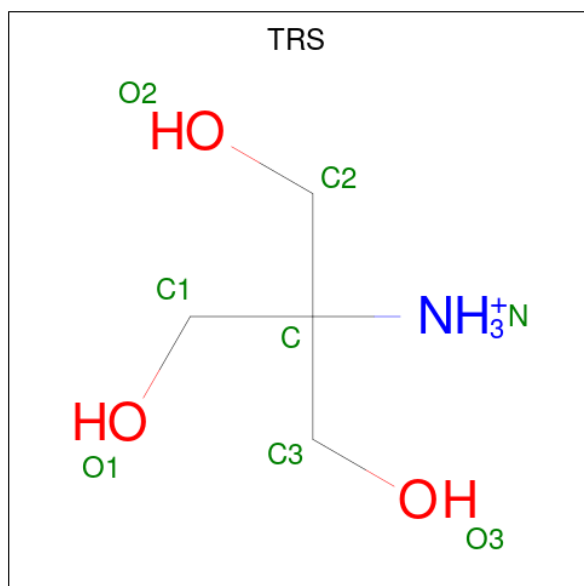


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0
5	E	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			6	3	3		

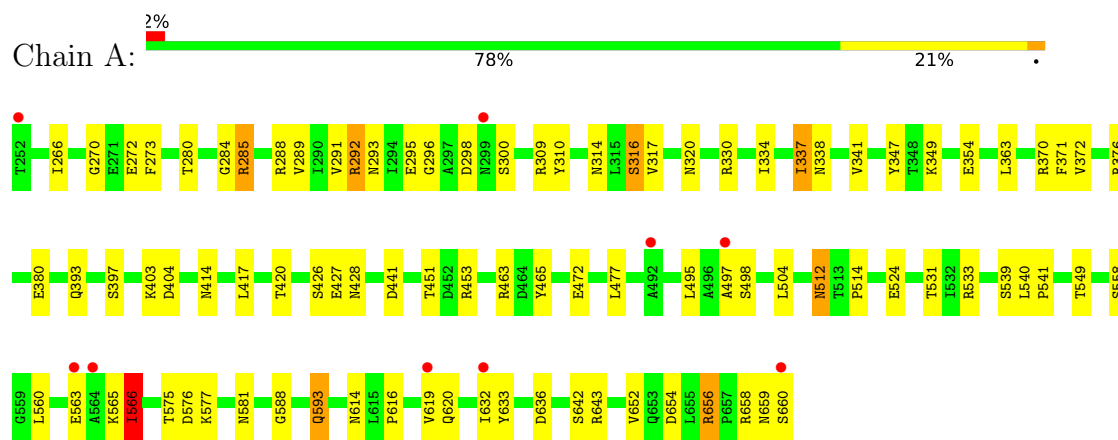
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	498	Total	O	0	0
			498	498		
8	E	447	Total	O	0	0
			447	447		

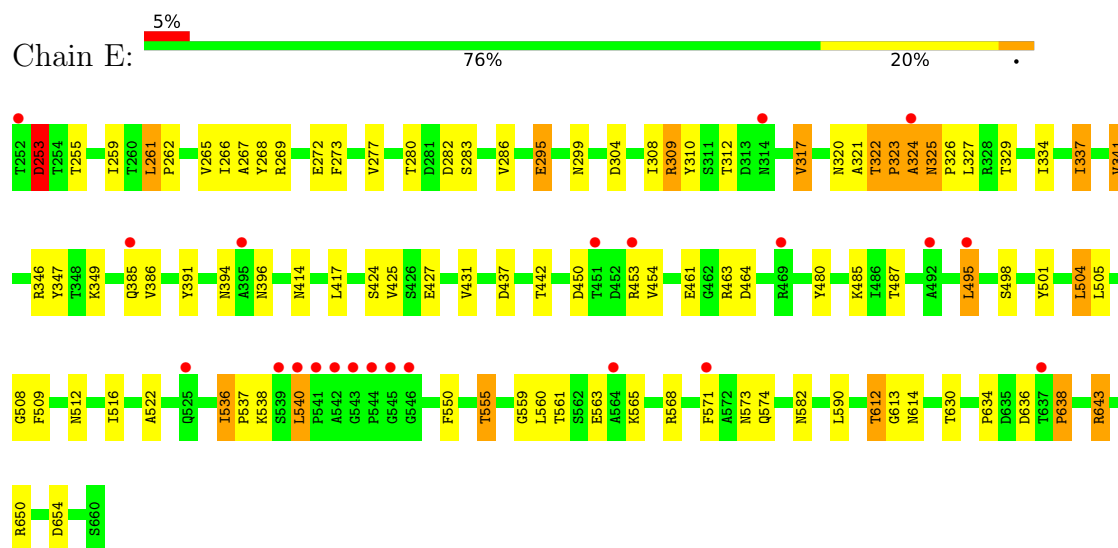
3 Residue-property plots

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

• Molecule 1: Adhesin



• Molecule 1: Adhesin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.21Å 269.86Å 47.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.00) 83.3 (50.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.98Å)	Xtriage
Refinement program	PHENIX v.1.17.1-3660	Depositor
R, R_{free}	0.211 , 0.240 0.211 , 0.241	Depositor DCC
R_{free} test set	3466 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7496	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.74% 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: SO4, GOL, TRS, EDO, MG, CA

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	0.92	18/3257 (0.6%)	0.73	5/4463 (0.1%)
1	E	0.95	22/3328 (0.7%)	0.74	7/4558 (0.2%)
All	All	0.93	40/6585 (0.6%)	0.73	12/9021 (0.1%)

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
1	E	0	1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	265	VAL	C-O	-7.21	1.16	1.24
1	A	293	ASN	C-O	-7.19	1.14	1.23
1	E	322	THR	C-O	-6.84	1.17	1.24
1	E	394	ASN	C-O	-6.84	1.15	1.23
1	A	588	GLY	C-O	-6.83	1.17	1.24
1	A	337	ILE	C-O	-6.71	1.16	1.24
1	E	574	GLN	C-O	-6.69	1.15	1.24
1	E	590	LEU	C-O	-6.34	1.16	1.24
1	E	324	ALA	N-CA	-6.08	1.38	1.46
1	E	310	TYR	C-O	-6.08	1.16	1.23
1	E	308	ILE	C-O	-6.05	1.17	1.24
1	E	259	ILE	C-O	-6.04	1.17	1.24
1	A	289	VAL	C-O	-5.87	1.17	1.24
1	A	531	THR	C-O	-5.83	1.17	1.24
1	A	338	ASN	C-O	-5.72	1.16	1.24
1	E	634	PRO	C-O	-5.71	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	VAL	C-O	-5.66	1.18	1.24
1	E	638	PRO	C-O	-5.62	1.17	1.24
1	A	291	VAL	C-O	-5.61	1.18	1.24
1	A	371	PHE	C-O	-5.57	1.16	1.23
1	E	427	GLU	C-O	-5.55	1.17	1.24
1	A	298	ASP	C-O	-5.53	1.17	1.24
1	A	512	ASN	C-O	-5.39	1.17	1.24
1	E	309	ARG	C-O	-5.28	1.17	1.23
1	E	255	THR	C-O	-5.25	1.18	1.24
1	A	404	ASP	C-O	-5.23	1.18	1.24
1	E	267	ALA	C-O	-5.21	1.17	1.24
1	A	316	SER	C-O	-5.20	1.17	1.23
1	A	280	THR	C-O	-5.15	1.17	1.23
1	E	273	PHE	C-O	-5.15	1.17	1.23
1	A	403	LYS	C-O	-5.13	1.18	1.24
1	E	268	TYR	C-O	-5.13	1.17	1.24
1	A	284	GLY	C-O	-5.09	1.17	1.24
1	E	654	ASP	C-O	-5.09	1.17	1.23
1	E	269	ARG	C-O	-5.08	1.17	1.23
1	A	273	PHE	C-O	-5.07	1.17	1.23
1	E	396	ASN	N-CA	-5.05	1.39	1.46
1	E	573	ASN	C-O	-5.05	1.17	1.23
1	E	295	GLU	C-O	-5.03	1.17	1.23
1	A	370	ARG	C-O	-5.00	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	253	ASP	N-CA-CB	14.35	134.75	110.49
1	E	325	ASN	N-CA-C	-9.96	91.82	108.75
1	E	324	ALA	N-CA-C	9.90	131.88	110.80
1	A	566	ILE	N-CA-C	6.76	118.78	108.71
1	E	261	LEU	N-CA-C	6.73	114.28	108.22
1	E	612	THR	N-CA-C	6.20	117.73	110.97
1	A	292	ARG	N-CA-C	5.53	117.20	108.96
1	E	322	THR	CA-C-N	5.33	126.50	119.84
1	E	322	THR	C-N-CA	5.33	126.50	119.84
1	A	285	ARG	N-CA-C	5.25	117.64	108.76
1	A	300	SER	N-CA-C	5.24	118.04	110.28
1	A	316	SER	N-CA-C	5.05	118.30	111.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	PRO	Peptide

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	3194	0	3105	63	2
1	E	3265	0	3168	58	3
2	A	4	0	0	0	0
2	E	4	0	0	0	0
3	A	20	0	0	1	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
5	A	8	0	12	0	1
5	E	8	0	12	5	0
6	A	20	0	30	8	0
6	E	20	0	30	7	0
7	E	6	0	8	0	0
8	A	498	0	0	25	3
8	E	447	0	0	29	5
All	All	7496	0	6365	134	8

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 10.

All (134) 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:575:THR:HG22	1:A:633:TYR:CE2	1.67	1.26
1:A:540:LEU:HA	8:A:801:HOH:O	1.40	1.20
1:A:575:THR:HG22	1:A:633:TYR:CD2	1.75	1.20
1:A:581:ASN:ND2	6:A:713:EDO:H11	1.53	1.19
1:A:581:ASN:HD21	6:A:713:EDO:C1	1.60	1.14
1:E:613:GLY:CA	8:E:802:HOH:O	1.95	1.13
1:E:613:GLY:C	8:E:802:HOH:O	1.95	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:714:EDO:H22	8:A:1160:HOH:O	1.52	1.10
1:A:658:ARG:C	8:A:803:HOH:O	1.97	1.04
1:E:613:GLY:HA2	8:E:802:HOH:O	1.56	1.01
1:A:541:PRO:HD3	8:A:801:HOH:O	1.57	1.00
1:A:575:THR:HG21	1:A:643:ARG:N	1.77	1.00
1:A:575:THR:CG2	1:A:633:TYR:CD2	2.46	0.99
1:A:539:SER:O	8:A:801:HOH:O	1.83	0.95
1:A:420:THR:OG1	8:A:802:HOH:O	1.83	0.95
6:E:711:EDO:O2	8:E:801:HOH:O	1.84	0.95
1:E:612:THR:O	8:E:802:HOH:O	1.85	0.94
1:A:659:ASN:O	8:A:803:HOH:O	1.87	0.92
6:E:711:EDO:O1	8:E:803:HOH:O	1.90	0.89
1:E:614:ASN:N	8:E:802:HOH:O	2.03	0.86
1:A:581:ASN:HD21	6:A:713:EDO:H11	0.73	0.86
1:E:283:SER:OG	8:E:805:HOH:O	1.95	0.82
1:E:346[B]:ARG:NH2	8:E:812:HOH:O	2.10	0.81
1:E:277[B]:VAL:HG22	1:E:329:THR:HB	1.62	0.81
1:E:461:GLU:HG3	1:E:565[A]:LYS:HB3	1.63	0.80
1:E:638:PRO:O	8:E:806:HOH:O	1.98	0.79
1:A:354:GLU:OE2	8:A:804:HOH:O	2.02	0.76
1:E:450:ASP:OD2	8:E:808:HOH:O	2.04	0.75
3:A:706:SO4:O4	8:A:805:HOH:O	2.04	0.75
1:A:576:ASP:OD2	8:A:807:HOH:O	2.06	0.74
1:E:442:THR:OG1	8:E:807:HOH:O	2.03	0.74
1:E:559:GLY:O	8:E:809:HOH:O	2.04	0.74
1:A:659:ASN:N	8:A:803:HOH:O	2.13	0.73
6:A:713:EDO:O2	8:A:806:HOH:O	2.05	0.73
5:E:706:TRS:O3	8:E:810:HOH:O	2.06	0.72
1:A:575:THR:CG2	1:A:633:TYR:HD2	2.03	0.72
1:A:593:GLN:O	1:A:593:GLN:HG3	1.89	0.71
6:E:711:EDO:C1	8:E:801:HOH:O	2.36	0.71
1:A:614:ASN:HB2	6:A:713:EDO:H12	1.73	0.70
1:A:658:ARG:CB	8:A:803:HOH:O	2.41	0.69
1:E:391:TYR:O	8:E:813:HOH:O	2.11	0.68
1:A:565:LYS:NZ	8:A:812:HOH:O	2.27	0.67
5:E:706:TRS:O1	8:E:811:HOH:O	2.08	0.67
1:E:272:GLU:HG2	1:E:334:ILE:HG12	1.77	0.67
1:E:253:ASP:N	8:E:824:HOH:O	2.27	0.66
1:A:427[A]:GLU:H	1:A:427[A]:GLU:CD	2.04	0.65
6:A:713:EDO:H22	8:A:1142:HOH:O	1.98	0.64
1:A:575:THR:HG22	1:A:633:TYR:HE2	1.49	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:TYR:HB3	1:E:349:LYS:HE2	1.80	0.63
1:A:541:PRO:CD	8:A:801:HOH:O	2.24	0.63
1:E:461:GLU:O	8:E:814:HOH:O	2.15	0.63
1:E:650[A]:ARG:NH1	8:E:828:HOH:O	2.32	0.62
1:E:286[A]:VAL:HG22	1:E:321:ALA:HB2	1.82	0.62
1:A:497:ALA:HA	8:A:904:HOH:O	2.02	0.60
1:A:549:THR:CG2	1:A:566:ILE:HD11	2.31	0.60
1:E:630:THR:OG1	8:E:815:HOH:O	2.16	0.60
1:E:463:ARG:HH22	6:E:711:EDO:H11	1.66	0.59
1:E:540[B]:LEU:HD22	1:E:571:PHE:HE2	1.68	0.59
1:A:512:ASN:ND2	1:A:514:PRO:HD3	2.19	0.58
1:A:575:THR:CG2	1:A:643:ARG:N	2.61	0.58
6:E:711:EDO:O1	8:E:801:HOH:O	1.84	0.58
1:A:285:ARG:HH21	1:A:316:SER:HB2	1.68	0.58
1:A:309:ARG:HD2	8:A:1034:HOH:O	2.04	0.58
1:A:288[A]:ARG:NH2	8:A:819:HOH:O	2.37	0.57
1:E:555:THR:HG23	8:E:877:HOH:O	2.04	0.57
1:A:295:GLU:HG3	1:A:296:GLY:N	2.19	0.57
1:A:453:ARG:NE	8:A:809:HOH:O	2.18	0.56
1:E:414:ASN:HB3	1:E:417:LEU:HG	1.88	0.55
1:A:347:TYR:HB3	1:A:349:LYS:HE2	1.89	0.55
1:A:575:THR:HG21	1:A:643:ARG:CA	2.37	0.55
1:E:540[B]:LEU:HD22	1:E:571:PHE:CE2	2.42	0.55
1:A:654:ASP:OD1	1:A:656:ARG:HD3	2.07	0.54
1:E:509:PHE:CZ	1:E:536:ILE:HD12	2.44	0.53
1:A:272:GLU:HG2	1:A:334:ILE:HG12	1.91	0.53
1:E:337:ILE:HD12	1:E:437:ASP:HA	1.92	0.52
1:E:464:ASP:OD1	1:E:568:ARG:HB2	2.09	0.52
1:E:501:TYR:CZ	1:E:505:LEU:HD11	2.45	0.52
1:A:575:THR:HG23	1:A:642:SER:OG	2.10	0.52
1:A:270:GLY:HA3	1:A:337:ILE:HD12	1.90	0.51
1:A:575:THR:HG21	1:A:643:ARG:H	1.71	0.51
1:A:566:ILE:O	1:A:566:ILE:HG23	2.11	0.50
1:A:575:THR:HG23	1:A:633:TYR:CD2	2.42	0.49
1:E:508:GLY:HA2	8:E:1078:HOH:O	2.12	0.49
1:E:509:PHE:HZ	1:E:536:ILE:HD12	1.77	0.49
1:E:325:ASN:OD1	5:E:706:TRS:H11	2.12	0.49
1:E:425:VAL:HG22	1:E:431:VAL:HG22	1.94	0.49
1:A:414:ASN:HB3	1:A:417:LEU:HG	1.95	0.48
1:A:317:VAL:HG22	1:A:320:ASN:HB3	1.96	0.48
1:A:453:ARG:NH2	8:A:809:HOH:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ASP:OD2	1:A:656:ARG:NH1	2.44	0.48
1:E:312:THR:HG21	1:E:327:LEU:HD21	1.96	0.48
1:A:317:VAL:CG2	1:A:320:ASN:HB3	2.43	0.47
5:E:706:TRS:N	8:E:817:HOH:O	2.24	0.47
1:A:577:LYS:HE3	8:A:1190:HOH:O	2.14	0.47
1:E:324:ALA:C	1:E:326:PRO:HD3	2.40	0.46
1:E:555:THR:HG22	1:E:561:THR:HG23	1.97	0.46
1:E:286[A]:VAL:HG23	1:E:327:LEU:HD22	1.96	0.46
1:A:472:GLU:CD	1:A:533:ARG:HE	2.24	0.46
1:E:504:LEU:HG	1:E:550:PHE:HZ	1.82	0.45
1:E:480:TYR:HA	1:E:522:ALA:HB1	1.99	0.45
1:A:524:GLU:OE1	8:A:810:HOH:O	2.21	0.45
1:E:463:ARG:HH12	6:E:711:EDO:H21	1.82	0.45
1:A:659:ASN:C	8:A:803:HOH:O	2.50	0.45
1:E:341:VAL:HG13	8:E:1112:HOH:O	2.17	0.45
1:E:501:TYR:CE2	1:E:505:LEU:HD11	2.52	0.45
1:E:537:PRO:HD2	1:E:540[A]:LEU:HD11	1.97	0.45
1:A:465:TYR:OH	1:A:477[A]:LEU:HD23	2.17	0.44
1:E:325:ASN:HB2	5:E:706:TRS:O1	2.18	0.44
1:A:636:ASP:OD1	1:A:643:ARG:HD2	2.18	0.44
1:A:397:SER:HA	1:A:427[B]:GLU:HG3	2.00	0.44
1:A:616:PRO:HB2	1:A:619[A]:VAL:HG23	1.99	0.43
1:A:560:LEU:HD23	1:A:560:LEU:HA	1.83	0.43
1:E:322:THR:HA	1:E:323:PRO:HD3	1.64	0.43
1:E:261:LEU:HB2	1:E:262:PRO:HD2	2.01	0.43
1:A:376:ARG:NH2	1:A:380:GLU:OE2	2.37	0.43
1:A:575:THR:HG21	1:A:643:ARG:C	2.44	0.43
1:E:464:ASP:OD2	1:E:568:ARG:NH2	2.52	0.43
1:E:337:ILE:HD13	1:E:337:ILE:HA	1.78	0.42
1:E:555:THR:HA	1:E:560:LEU:O	2.20	0.42
1:E:317:VAL:HG22	1:E:320:ASN:HB3	2.02	0.42
6:A:712:EDO:C1	8:A:814:HOH:O	2.67	0.42
6:E:712:EDO:H12	8:E:1097:HOH:O	2.20	0.42
1:E:424:SER:OG	8:E:804:HOH:O	1.90	0.42
1:E:636:ASP:OD1	1:E:643:ARG:HD2	2.19	0.42
1:E:485:LYS:HE3	1:E:487:THR:HG22	2.01	0.42
1:A:426:SER:OG	1:A:428:ASN:OD1	2.38	0.42
1:E:512:ASN:ND2	8:E:857:HOH:O	2.53	0.42
1:A:463:ARG:HD3	1:A:465:TYR:CZ	2.54	0.41
1:E:582:ASN:CG	1:E:650[B]:ARG:HD3	2.45	0.41
1:A:575:THR:CG2	1:A:642:SER:C	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:LEU:HD22	1:E:495:LEU:HA	1.58	0.41
1:E:563:GLU:O	1:E:565[A]:LYS:HG2	2.21	0.41
1:A:495:LEU:HA	1:A:498:SER:OG	2.21	0.41
1:A:310:TYR:HA	1:A:330:ARG:O	2.21	0.40

All (8) 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)
1:A:393:GLN:NE2	1:E:453[B]:ARG:NH1[1_554]	1.37	0.83
1:E:309:ARG:CD	5:A:710:TRS:N[4_455]	1.70	0.50
8:A:1104:HOH:O	8:E:990:HOH:O[4_554]	1.97	0.23
8:E:1076:HOH:O	8:E:1119:HOH:O[2_765]	1.97	0.23
8:A:1200:HOH:O	8:E:997:HOH:O[4_555]	1.99	0.21
8:A:1214:HOH:O	8:E:1048:HOH:O[4_555]	2.06	0.14
1:A:558:SER:O	1:E:453[A]:ARG:NH2[1_554]	2.17	0.03
8:E:989:HOH:O	8:E:1023:HOH:O[2_765]	2.17	0.03

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	414/409 (101%)	404 (98%)	10 (2%)	0	100	100
1	E	422/409 (103%)	408 (97%)	13 (3%)	1 (0%)	43	42
All	All	836/818 (102%)	812 (97%)	23 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	253	ASP

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	356/349 (102%)	338 (95%)	18 (5%)	21	19
1	E	364/349 (104%)	340 (93%)	24 (7%)	15	12
All	All	720/698 (103%)	678 (94%)	42 (6%)	20	15

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266[A]	ILE
1	A	266[B]	ILE
1	A	292	ARG
1	A	314	ASN
1	A	341	VAL
1	A	363	LEU
1	A	441	ASP
1	A	451	THR
1	A	504	LEU
1	A	563	GLU
1	A	566	ILE
1	A	593	GLN
1	A	620	GLN
1	A	632[A]	ILE
1	A	632[B]	ILE
1	A	652	VAL
1	A	656	ARG
1	A	660	SER
1	E	266	ILE
1	E	280	THR
1	E	282[A]	ASP
1	E	282[B]	ASP
1	E	295	GLU
1	E	299	ASN
1	E	304	ASP
1	E	317	VAL
1	E	337	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	341	VAL
1	E	385[A]	GLN
1	E	385[B]	GLN
1	E	386	VAL
1	E	454	VAL
1	E	495	LEU
1	E	498	SER
1	E	504	LEU
1	E	516	ILE
1	E	536	ILE
1	E	538	LYS
1	E	540[A]	LEU
1	E	540[B]	LEU
1	E	555	THR
1	E	643	ARG

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	447	GLN
1	A	581	ASN
1	A	582	ASN
1	A	614	ASN
1	E	512	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 10 are monoatomic - leaving 17 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	$\# Z > 2$
5	TRS	A	710	-	7,7,7	0.32	0	9,9,9	0.99	0
6	EDO	A	715	-	3,3,3	0.22	0	2,2,2	0.65	0
3	SO4	A	706	-	4,4,4	0.26	0	6,6,6	0.20	0
5	TRS	E	706	-	7,7,7	1.20	0	9,9,9	1.75	4 (44%)
6	EDO	A	714	-	3,3,3	0.62	0	2,2,2	1.48	0
6	EDO	E	709	-	3,3,3	0.42	0	2,2,2	0.43	0
3	SO4	A	708	-	4,4,4	0.32	0	6,6,6	0.35	0
6	EDO	E	708	-	3,3,3	0.36	0	2,2,2	0.57	0
6	EDO	A	713	-	3,3,3	0.33	0	2,2,2	0.78	0
3	SO4	A	707	-	4,4,4	0.27	0	6,6,6	0.29	0
6	EDO	A	712	-	3,3,3	0.20	0	2,2,2	1.31	0
3	SO4	A	705	-	4,4,4	0.26	0	6,6,6	0.15	0
6	EDO	E	712	-	3,3,3	0.37	0	2,2,2	0.77	0
7	GOL	E	707	-	5,5,5	0.89	0	5,5,5	1.14	0
6	EDO	E	710	-	3,3,3	0.26	0	2,2,2	0.71	0
6	EDO	E	711	-	3,3,3	0.36	0	2,2,2	0.76	0
6	EDO	A	711	-	3,3,3	0.36	0	2,2,2	0.70	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
5	TRS	A	710	-	-	0/9/9/9	-
6	EDO	A	715	-	-	0/1/1/1	-
5	TRS	E	706	-	-	7/9/9/9	-
6	EDO	A	714	-	-	1/1/1/1	-
6	EDO	E	709	-	-	0/1/1/1	-
6	EDO	E	708	-	-	0/1/1/1	-
6	EDO	A	713	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	712	-	-	0/1/1/1	-
6	EDO	E	712	-	-	0/1/1/1	-
7	GOL	E	707	-	-	4/4/4/4	-
6	EDO	E	710	-	-	0/1/1/1	-
6	EDO	E	711	-	-	0/1/1/1	-
6	EDO	A	711	-	-	0/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	706	TRS	C2-C-C1	-2.99	102.70	110.66
5	E	706	TRS	O2-C2-C	2.40	117.57	110.88
5	E	706	TRS	O3-C3-C	2.28	117.23	110.88
5	E	706	TRS	C2-C-N	2.21	113.81	108.17

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	706	TRS	C1-C-C2-O2
5	E	706	TRS	C3-C-C2-O2
7	E	707	GOL	O1-C1-C2-C3
7	E	707	GOL	C1-C2-C3-O3
7	E	707	GOL	O2-C2-C3-O3
6	A	714	EDO	O1-C1-C2-O2
5	E	706	TRS	N-C-C2-O2
5	E	706	TRS	C1-C-C3-O3
5	E	706	TRS	C2-C-C3-O3
7	E	707	GOL	O1-C1-C2-O2
5	E	706	TRS	C3-C-C1-O1
5	E	706	TRS	N-C-C3-O3

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	710	TRS	0	1
3	A	706	SO4	1	0
5	E	706	TRS	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	714	EDO	1	0
6	A	713	EDO	6	0
6	A	712	EDO	1	0
6	E	712	EDO	1	0
6	E	711	EDO	6	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	409/409 (100%)	0.19	9 (2%) 62 61	14, 32, 45, 63	7 (1%)
1	E	409/409 (100%)	0.42	22 (5%) 31 30	14, 34, 54, 115	15 (3%)
All	All	818/818 (100%)	0.30	31 (3%) 44 43	14, 33, 50, 115	22 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	540[A]	LEU	7.1
1	E	542	ALA	6.3
1	E	541	PRO	4.9
1	A	632[A]	ILE	4.8
1	E	451[A]	THR	4.5
1	E	525	GLN	4.2
1	E	453[A]	ARG	4.1
1	E	545	GLY	3.3
1	A	619[A]	VAL	3.3
1	E	543	GLY	3.1
1	E	324	ALA	2.9
1	E	252	THR	2.8
1	A	299	ASN	2.8
1	A	492	ALA	2.6
1	E	395	ALA	2.5
1	E	544	PRO	2.5
1	E	469	ARG	2.5
1	E	546	GLY	2.5
1	E	385[A]	GLN	2.4
1	E	495	LEU	2.4
1	E	314	ASN	2.4
1	E	564	ALA	2.3
1	E	539	SER	2.3
1	A	252	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	660	SER	2.3
1	A	497	ALA	2.3
1	A	564	ALA	2.3
1	E	492	ALA	2.2
1	A	563	GLU	2.2
1	E	637	THR	2.0
1	E	571	PHE	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
6	EDO	A	711	4/4	0.73	0.14	37,39,40,44	0
6	EDO	E	709	4/4	0.73	0.14	44,45,49,49	0
5	TRS	A	710	8/8	0.75	0.14	40,44,48,48	0
6	EDO	E	710	4/4	0.76	0.17	41,42,45,45	0
6	EDO	A	713	4/4	0.77	0.15	43,43,51,56	0
6	EDO	A	712	4/4	0.79	0.17	42,43,44,52	0
7	GOL	E	707	6/6	0.79	0.14	52,54,57,58	0
6	EDO	E	711	4/4	0.81	0.13	45,48,49,50	0
6	EDO	A	715	4/4	0.83	0.12	44,45,48,55	0
6	EDO	E	708	4/4	0.83	0.15	48,48,50,52	0
6	EDO	A	714	4/4	0.87	0.26	46,50,54,59	0
6	EDO	E	712	4/4	0.88	0.18	34,35,41,43	0
5	TRS	E	706	8/8	0.88	0.12	33,37,42,49	0
3	SO4	A	706	5/5	0.90	0.10	42,43,47,48	5
4	MG	E	705	1/1	0.91	0.09	36,36,36,36	0
4	MG	A	709	1/1	0.94	0.06	37,37,37,37	0

Continued on next page...

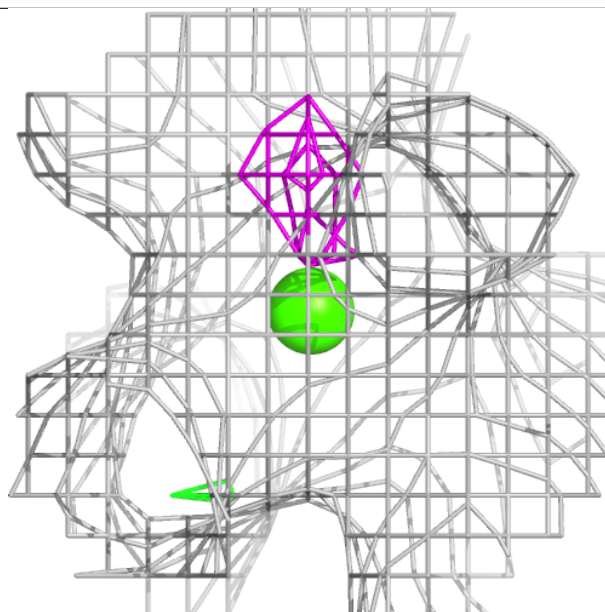
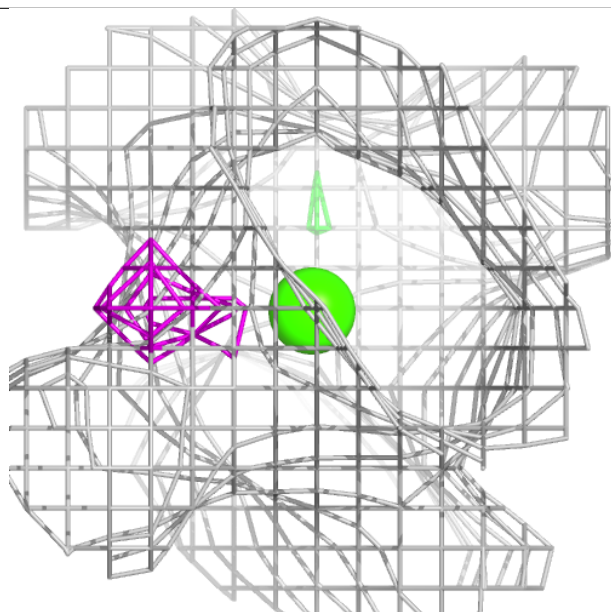
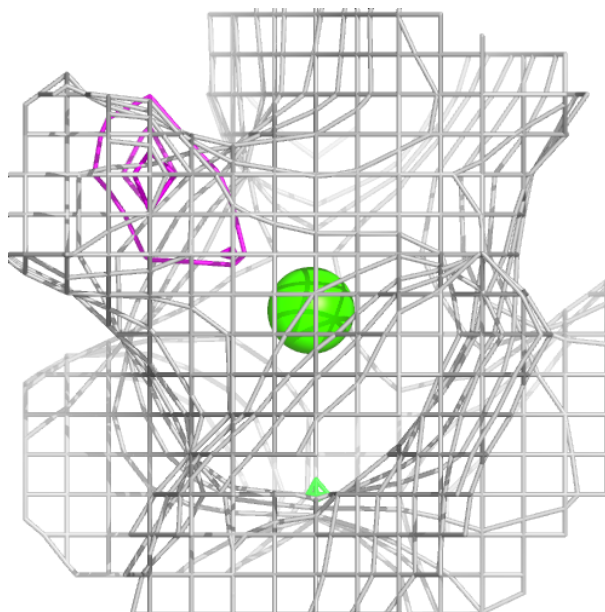
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	705	5/5	0.95	0.13	52,52,52,52	5
3	SO4	A	707	5/5	0.96	0.08	29,32,35,36	5
2	CA	A	701	1/1	0.97	0.06	31,31,31,31	0
2	CA	E	701	1/1	0.97	0.06	31,31,31,31	0
3	SO4	A	708	5/5	0.98	0.05	30,30,32,32	5
2	CA	E	703	1/1	0.98	0.04	33,33,33,33	0
2	CA	E	704	1/1	0.99	0.03	30,30,30,30	0
2	CA	A	704	1/1	0.99	0.04	39,39,39,39	0
2	CA	A	702	1/1	0.99	0.03	22,22,22,22	0
2	CA	E	702	1/1	0.99	0.03	31,31,31,31	0
2	CA	A	703	1/1	0.99	0.05	29,29,29,29	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.

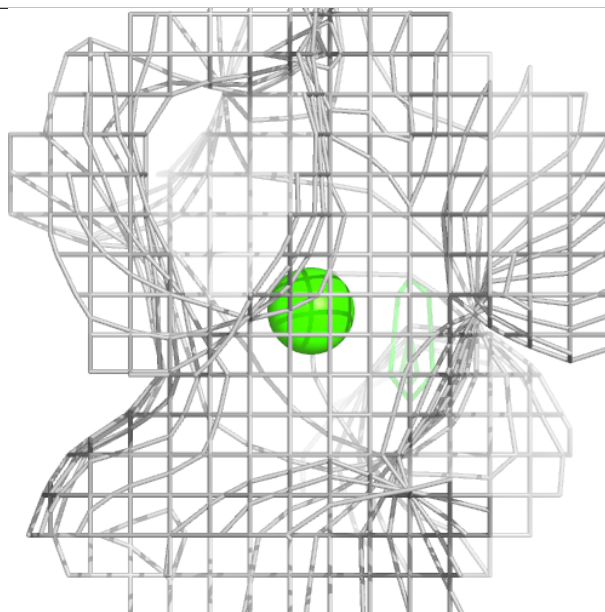
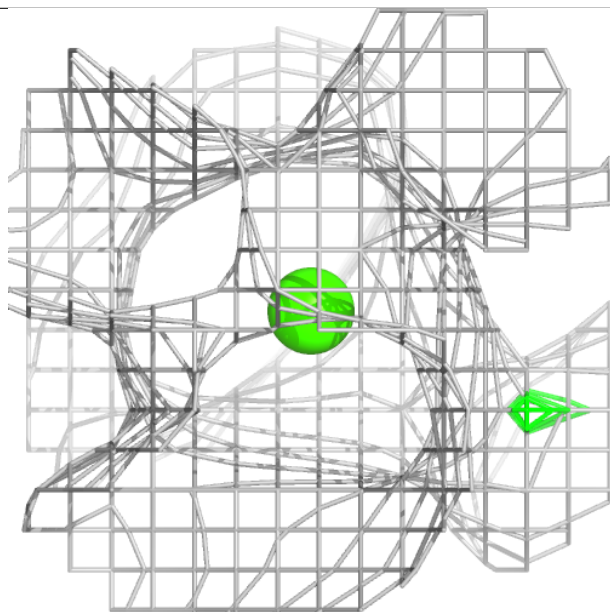
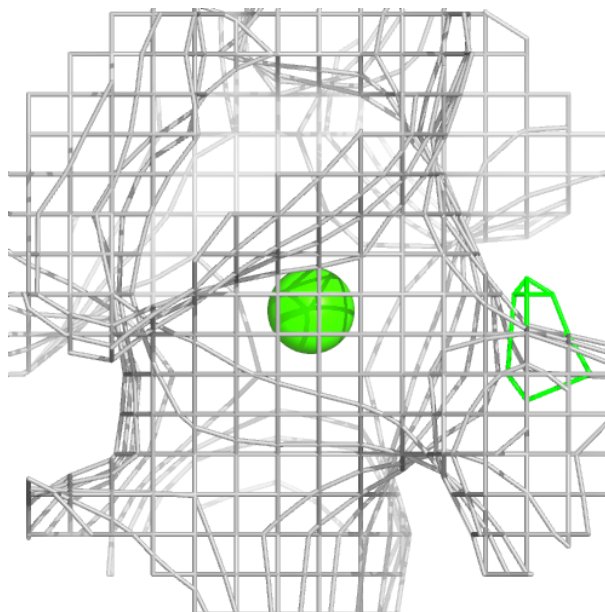
Electron density around CA A 701:

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



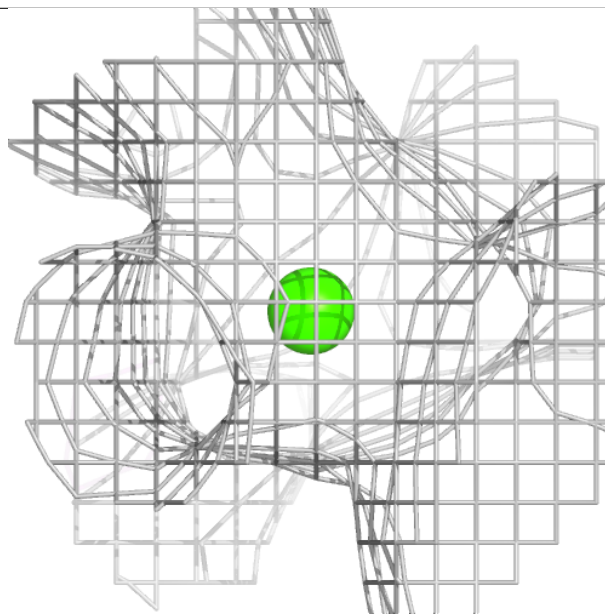
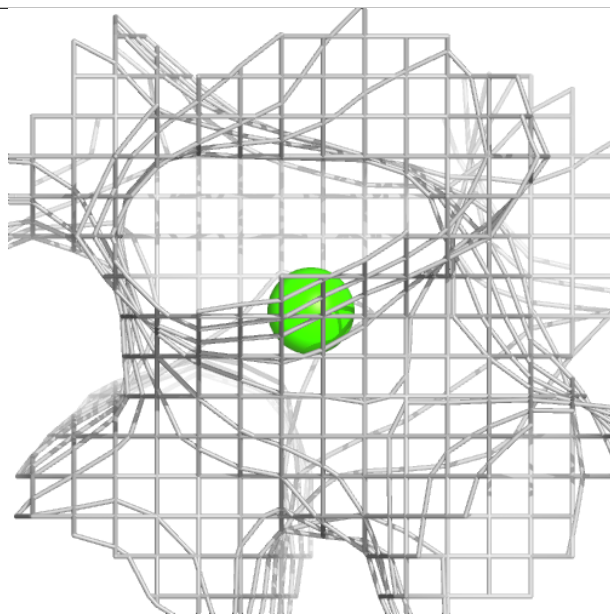
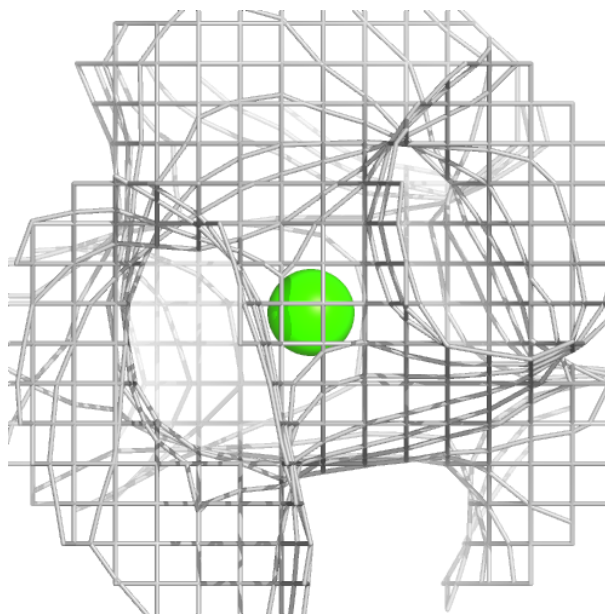
Electron density around CA E 701:

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



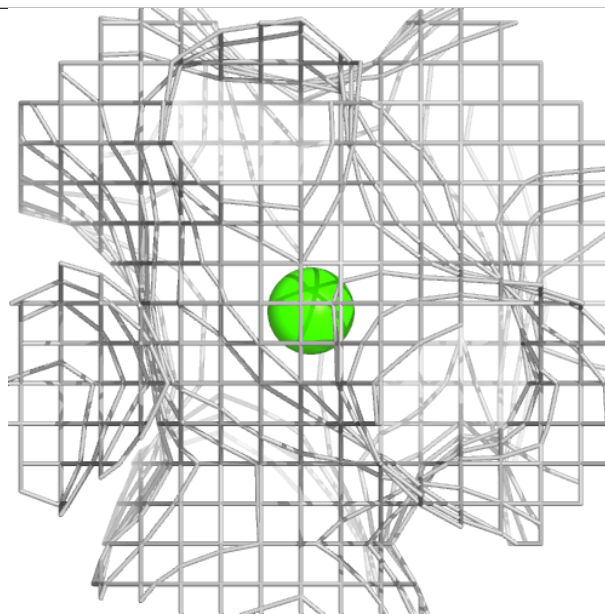
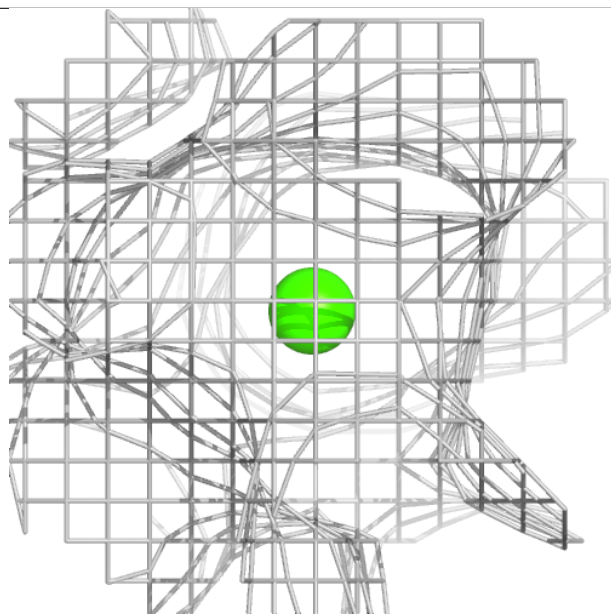
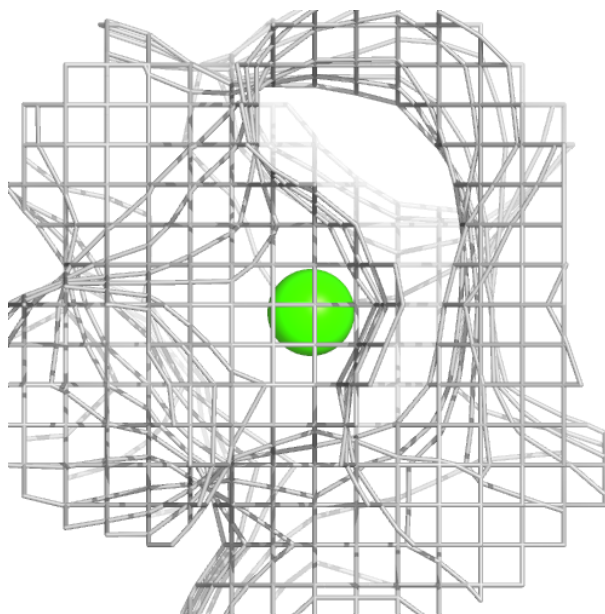
Electron density around CA E 703:

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



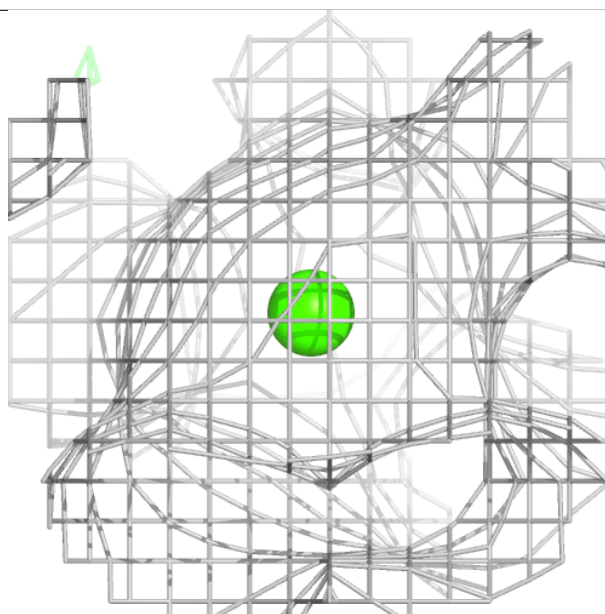
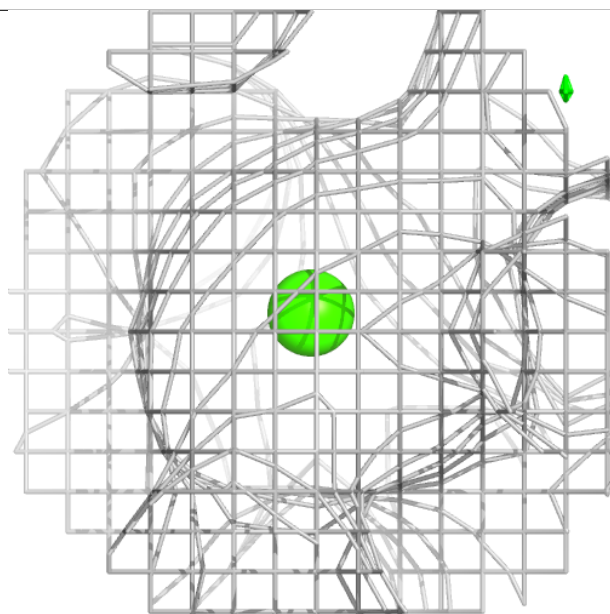
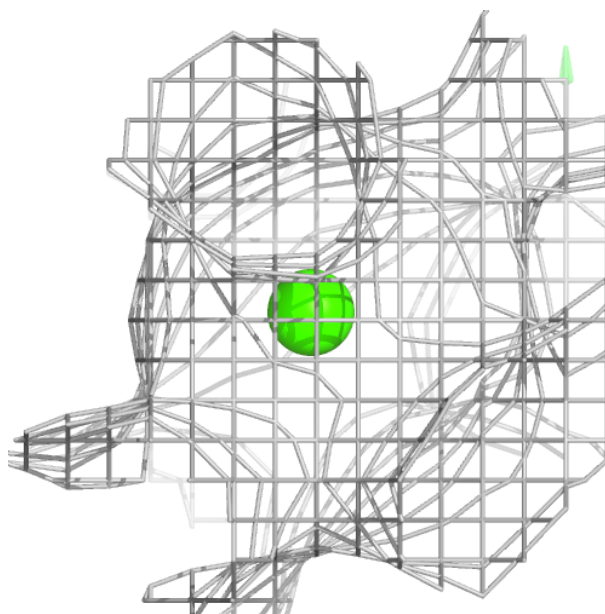
Electron density around CA E 704:

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



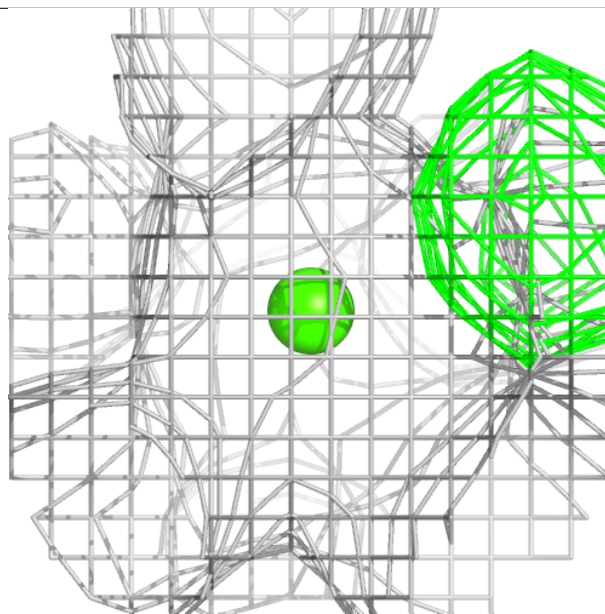
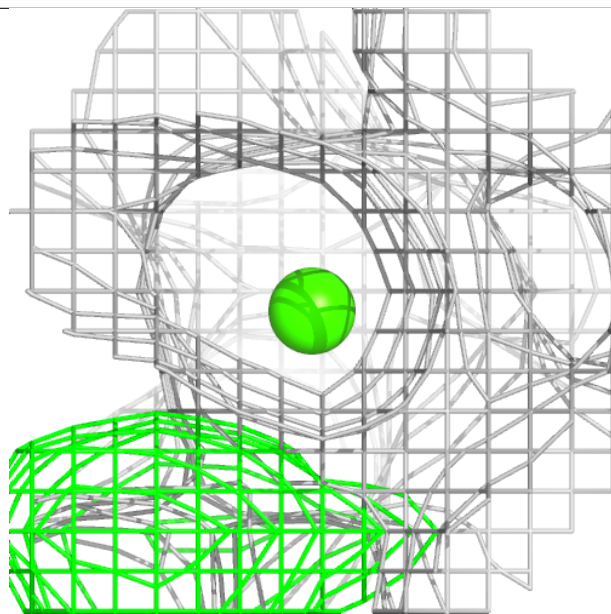
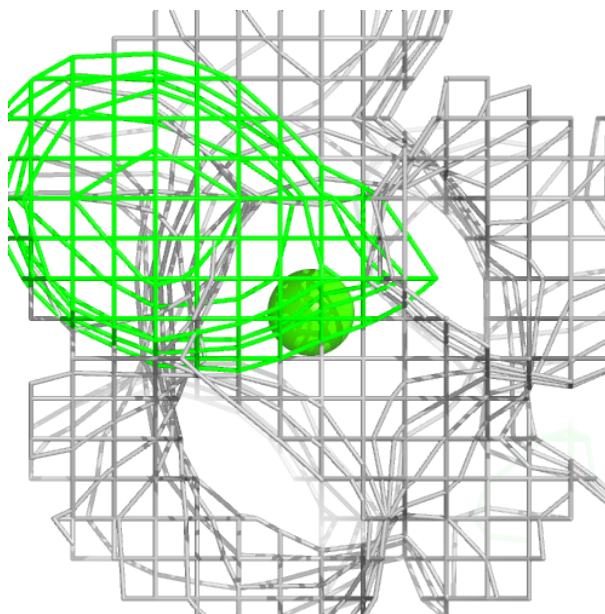
Electron density around CA A 704:

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



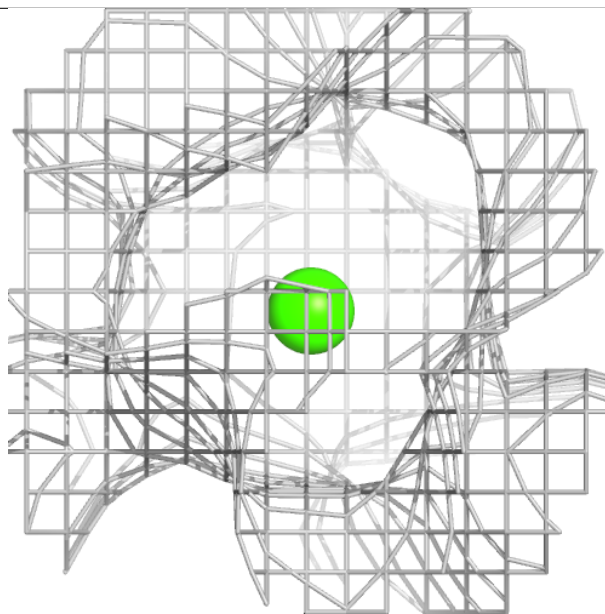
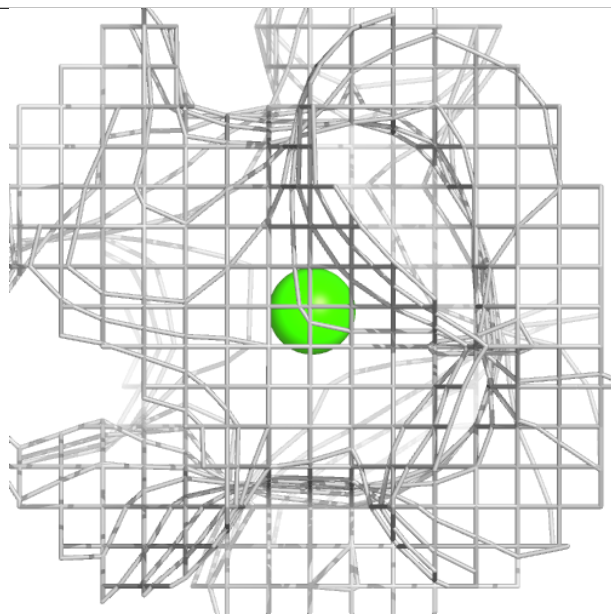
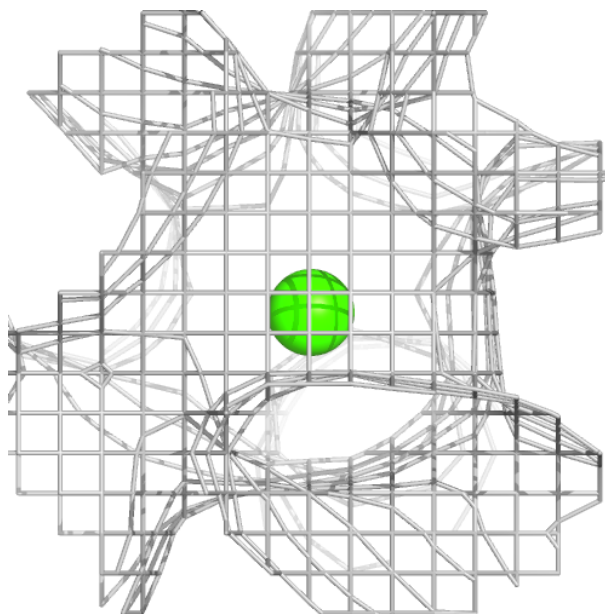
Electron density around CA A 702:

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



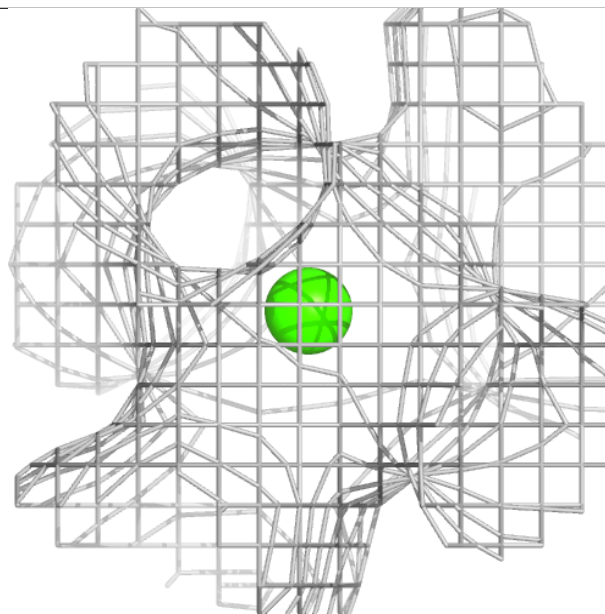
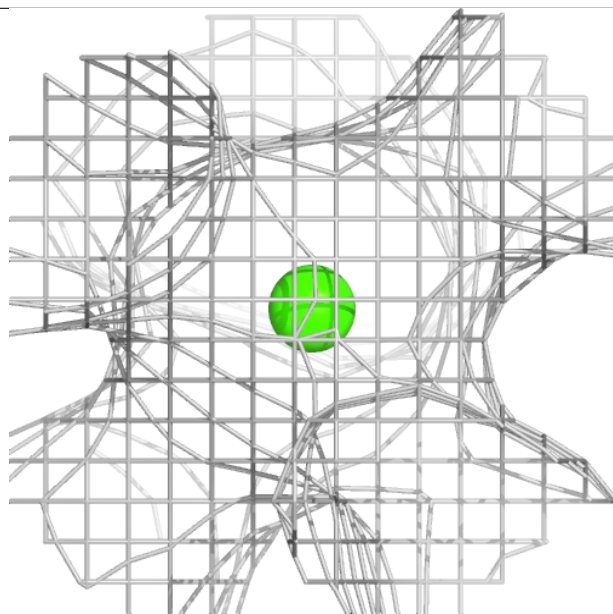
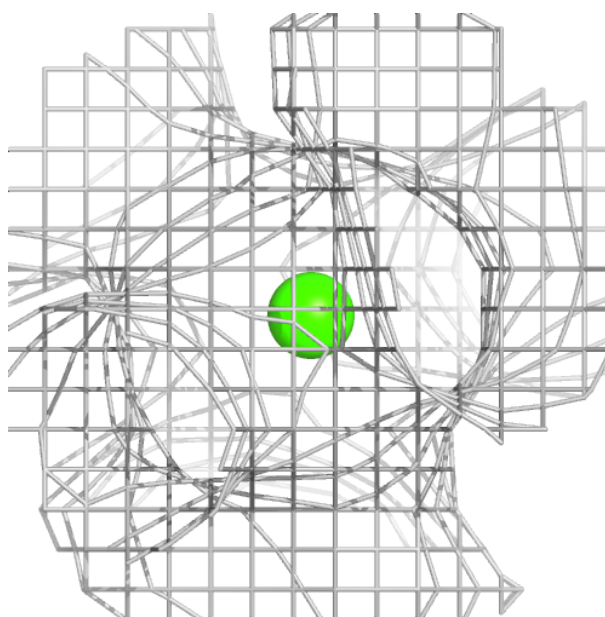
Electron density around CA E 702:

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



Electron density around CA A 703:

$2mF_o-DF_c$ (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.