



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:11 PM BST

PDB ID : 6VS7
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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13
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) : 2.13

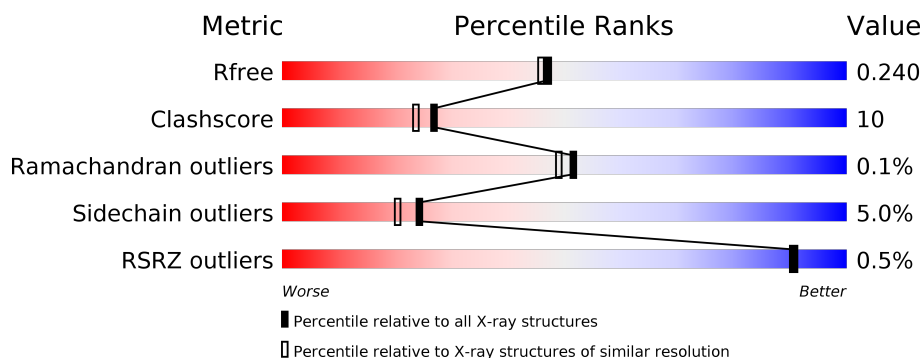
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	
1	E	409	

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	A	710	-	-	-	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.

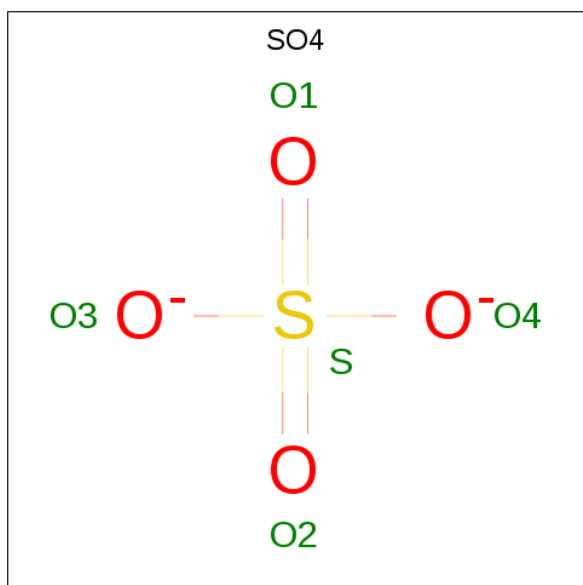
- Molecule 1 is a protein called Adhesin.

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 (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

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 (three-letter code: SO4) (formula: O₄S).

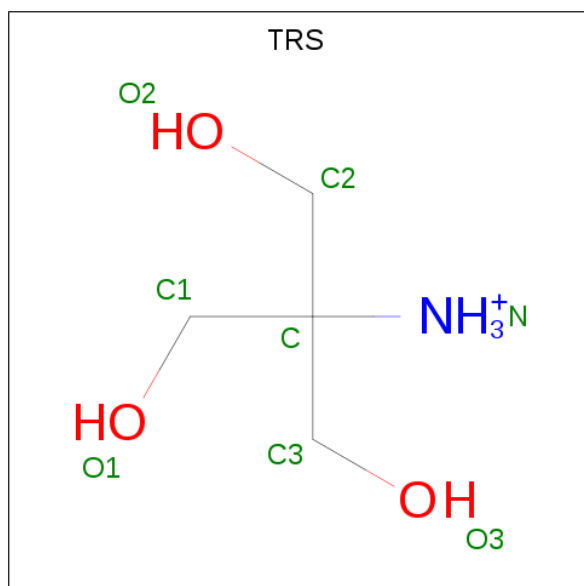


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: 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 (three-letter code: 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 (three-letter code: 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	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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

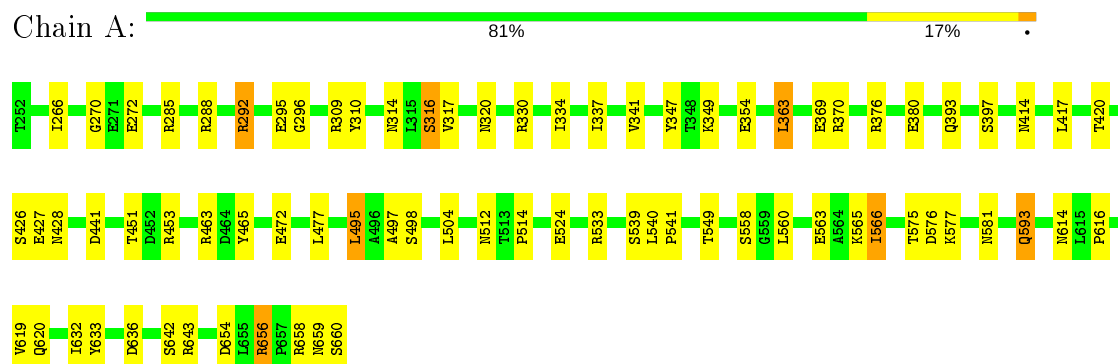
- Molecule 8 is water.

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

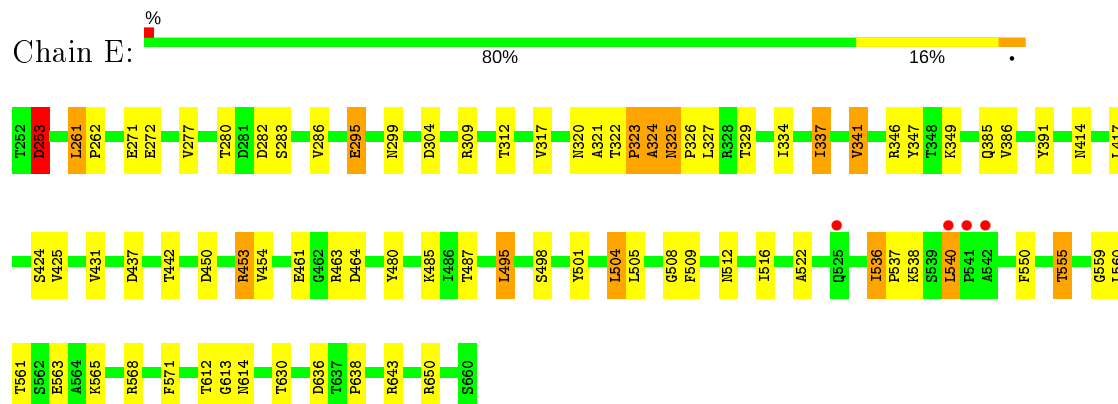
3 Residue-property plots

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	82.21 Å 269.86 Å 47.51 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 47.51 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.00) 82.2 (47.51-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.98 Å)	Xtriage
Refinement program	PHENIX v.1.17.1-3660	Depositor
R, R_{free}	0.211 , 0.240 0.211 , 0.240	Depositor DCC
R_{free} test set	3281 reflections (4.93%)	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)	0.33 , 41.6	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: GOL, MG, CA, EDO, SO4, TRS

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	0.75	2/3257 (0.1%)	0.73	6/4463 (0.1%)
1	E	0.75	2/3328 (0.1%)	0.70	3/4558 (0.1%)
All	All	0.75	4/6585 (0.1%)	0.72	9/9021 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	295	GLU	CD-OE1	-7.09	1.17	1.25
1	A	316	SER	CB-OG	-5.74	1.34	1.42
1	E	271	GLU	CD-OE2	-5.68	1.19	1.25
1	A	369	GLU	CD-OE1	-5.29	1.19	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	253	ASP	N-CA-CB	13.41	134.75	110.60
1	A	292	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	370	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	E	324	ALA	N-CA-C	7.73	131.88	111.00
1	A	292	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	E	325	ASN	N-CA-C	-7.10	91.82	111.00
1	A	370	ARG	NE-CZ-NH1	6.49	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	495	LEU	CA-CB-CG	-5.83	101.90	115.30

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 ⓘ

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	61	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	8	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	132	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 (132) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:THR:HG22	1:A:633:TYR:CD2	1.75	1.20
1:A:540:LEU:HA	8:A:801:HOH:O	1.40	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
6:A:714:EDO:H22	8:A:1160:HOH:O	1.52	1.10
1:E:613:GLY:C	8:E:802:HOH:O	1.95	1.03
1:E:613:GLY:HA2	8:E:802:HOH:O	1.56	1.01
1:A:658:ARG:C	8:A:803:HOH:O	1.97	1.00
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:427[A]:GLU:CD	1:A:427[A]:GLU:H	2.04	0.60
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:309:ARG:HD2	8:A:1034:HOH:O	2.04	0.58
1:A:285:ARG:HH21	1:A:316:SER:HB2	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:577:LYS:HE3	8:A:1190:HOH:O	2.14	0.47
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:E:349:LYS:HZ3	6:E:712:EDO:C2	2.28	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: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
5:E:706:TRS:N	8:E:817:HOH:O	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:HD3	1:A:465:TYR:CZ	2.54	0.41
1:E:324:ALA:C	1:E:326:PRO:HD3	2.40	0.41
1:E:495:LEU:HD22	1:E:495:LEU:HA	1.58	0.41
1:A:472:GLU:CD	1:A:533:ARG:HE	2.24	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:659:ASN:C	8:A:803:HOH:O	2.50	0.40
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 [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	414/409 (101%)	404 (98%)	10 (2%)	0	100	100
1	E	422/409 (103%)	408 (97%)	13 (3%)	1 (0%)	47	44
All	All	836/818 (102%)	812 (97%)	23 (3%)	1 (0%)	51	49

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%)	339 (95%)	17 (5%)	25	22
1	E	364/349 (104%)	340 (93%)	24 (7%)	16	12
All	All	720/698 (103%)	679 (94%)	41 (6%)	24	16

All (41) 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	656	ARG
1	A	660	SER
1	E	261	LEU
1	E	280	THR
1	E	282[A]	ASP
1	E	282[B]	ASP
1	E	295	GLU
1	E	299	ASN

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Mol	Chain	Res	Type
1	E	304	ASP
1	E	337	ILE
1	E	341	VAL
1	E	385[A]	GLN
1	E	385[B]	GLN
1	E	386	VAL
1	E	453[A]	ARG
1	E	453[B]	ARG
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
1	A	581	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 monosaccharides 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
3	SO4	A	705	-	4,4,4	0.18	0	6,6,6	0.17	0
5	TRS	E	706	-	7,7,7	1.10	0	9,9,9	1.52	2 (22%)
6	EDO	E	710	-	3,3,3	0.26	0	2,2,2	0.69	0
6	EDO	A	714	-	3,3,3	0.61	0	2,2,2	1.50	0
5	TRS	A	710	-	7,7,7	0.29	0	9,9,9	0.90	0
3	SO4	A	707	-	4,4,4	0.22	0	6,6,6	0.28	0
3	SO4	A	708	-	4,4,4	0.21	0	6,6,6	0.34	0
6	EDO	E	709	-	3,3,3	0.45	0	2,2,2	0.39	0
6	EDO	A	715	-	3,3,3	0.24	0	2,2,2	0.62	0
6	EDO	E	711	-	3,3,3	0.36	0	2,2,2	0.74	0
6	EDO	E	708	-	3,3,3	0.39	0	2,2,2	0.54	0
6	EDO	A	711	-	3,3,3	0.38	0	2,2,2	0.68	0
6	EDO	E	712	-	3,3,3	0.36	0	2,2,2	0.79	0
3	SO4	A	706	-	4,4,4	0.16	0	6,6,6	0.17	0
6	EDO	A	712	-	3,3,3	0.21	0	2,2,2	1.32	0
7	GOL	E	707	-	5,5,5	0.86	0	5,5,5	1.06	0
6	EDO	A	713	-	3,3,3	0.32	0	2,2,2	0.77	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
6	EDO	E	710	-	-	0/1/1/1	-
6	EDO	A	714	-	-	1/1/1/1	-
5	TRS	E	706	-	-	7/9/9/9	-
5	TRS	A	710	-	-	0/9/9/9	-
6	EDO	E	709	-	-	0/1/1/1	-
6	EDO	A	715	-	-	0/1/1/1	-
6	EDO	E	711	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	E	708	-	-	0/1/1/1	-
6	EDO	A	711	-	-	0/1/1/1	-
6	EDO	E	712	-	-	0/1/1/1	-
6	EDO	A	712	-	-	0/1/1/1	-
7	GOL	E	707	-	-	4/4/4/4	-
6	EDO	A	713	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	706	TRS	C2-C-C1	-2.62	102.70	110.81
5	E	706	TRS	O2-C2-C	2.07	117.57	111.00

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
6	A	714	EDO	O1-C1-C2-O2
7	E	707	GOL	C1-C2-C3-O3
7	E	707	GOL	O2-C2-C3-O3
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 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	706	TRS	5	0
6	A	714	EDO	1	0
5	A	710	TRS	0	1
6	E	711	EDO	6	0
6	E	712	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	706	SO4	1	0
6	A	712	EDO	1	0
6	A	713	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%)	-0.15	0 100 100	23, 32, 45, 63	0
1	E	409/409 (100%)	-0.03	4 (0%) 82 81	23, 35, 55, 115	0
All	All	818/818 (100%)	-0.09	4 (0%) 91 90	23, 33, 50, 115	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	525	GLN	2.9
1	E	542	ALA	2.4
1	E	540[A]	LEU	2.4
1	E	541	PRO	2.1

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 ⓘ

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
5	TRS	A	710	8/8	0.75	0.45	40,44,48,48	0

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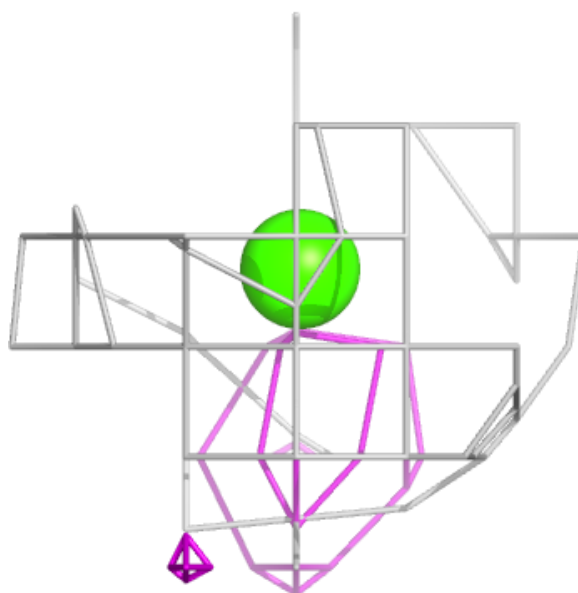
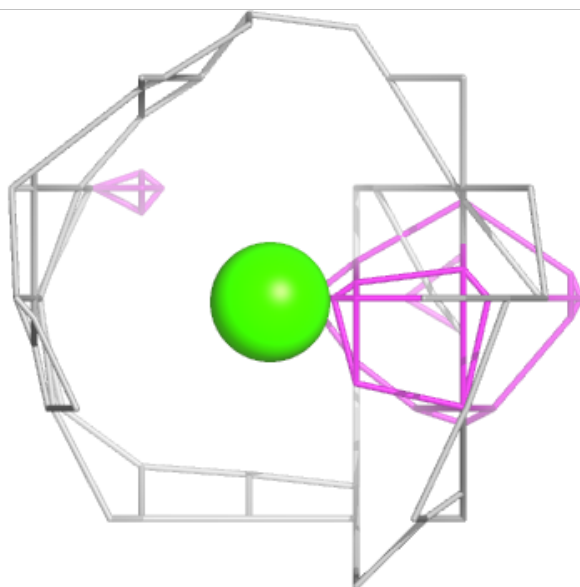
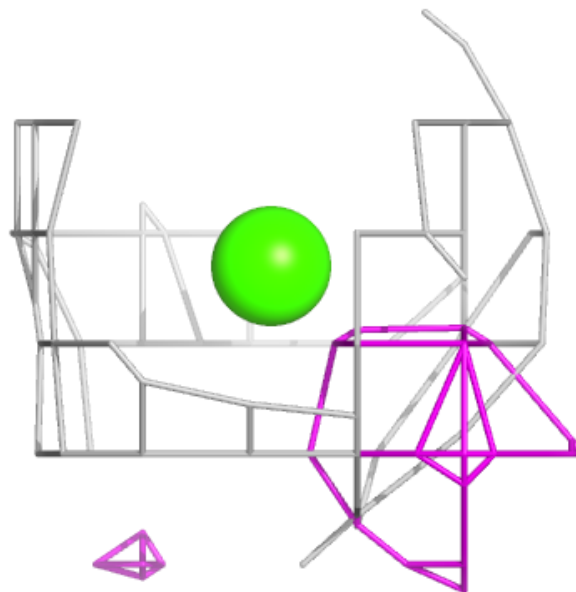
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	A	713	4/4	0.83	0.24	43,43,51,56	0
7	GOL	E	707	6/6	0.83	0.29	52,54,57,58	0
6	EDO	A	714	4/4	0.84	0.46	46,50,54,59	0
6	EDO	E	710	4/4	0.84	0.17	41,42,45,45	0
6	EDO	A	711	4/4	0.87	0.16	37,39,40,44	0
5	TRS	E	706	8/8	0.87	0.15	33,37,42,49	0
6	EDO	E	709	4/4	0.88	0.09	44,45,49,49	0
6	EDO	E	712	4/4	0.88	0.22	34,35,41,43	0
6	EDO	A	712	4/4	0.89	0.21	42,43,44,52	0
6	EDO	E	711	4/4	0.90	0.10	45,48,49,50	0
6	EDO	E	708	4/4	0.91	0.14	48,48,50,52	0
6	EDO	A	715	4/4	0.93	0.32	44,45,48,55	0
3	SO4	A	706	5/5	0.93	0.16	42,43,47,48	5
4	MG	E	705	1/1	0.95	0.13	36,36,36,36	0
4	MG	A	709	1/1	0.96	0.05	37,37,37,37	0
2	CA	A	701	1/1	0.96	0.08	31,31,31,31	0
3	SO4	A	705	5/5	0.97	0.17	52,52,52,52	5
2	CA	A	703	1/1	0.98	0.05	29,29,29,29	0
2	CA	E	703	1/1	0.98	0.04	33,33,33,33	0
3	SO4	A	707	5/5	0.98	0.15	29,32,35,36	5
2	CA	E	701	1/1	0.98	0.06	31,31,31,31	0
3	SO4	A	708	5/5	0.99	0.12	30,30,32,32	5
2	CA	E	704	1/1	0.99	0.08	30,30,30,30	0
2	CA	A	704	1/1	0.99	0.07	39,39,39,39	0
2	CA	E	702	1/1	0.99	0.09	31,31,31,31	0
2	CA	A	702	1/1	1.00	0.09	22,22,22,22	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.

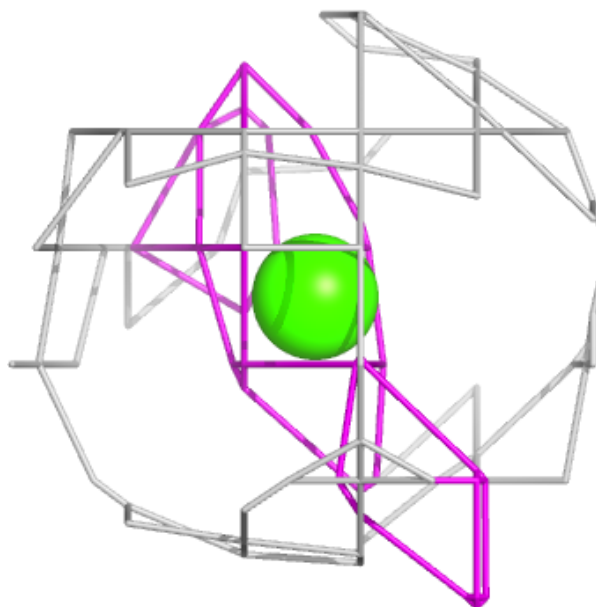
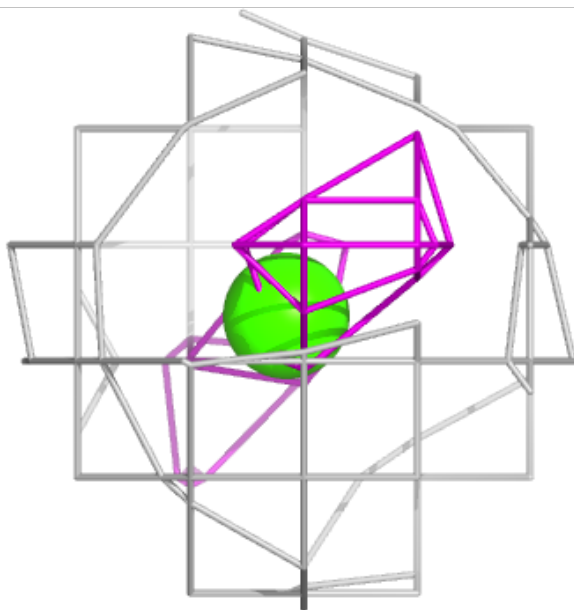
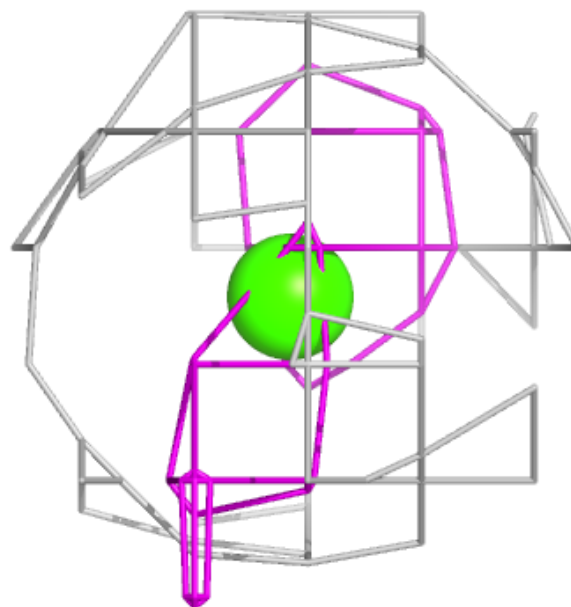
Electron density around CA A 701:

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



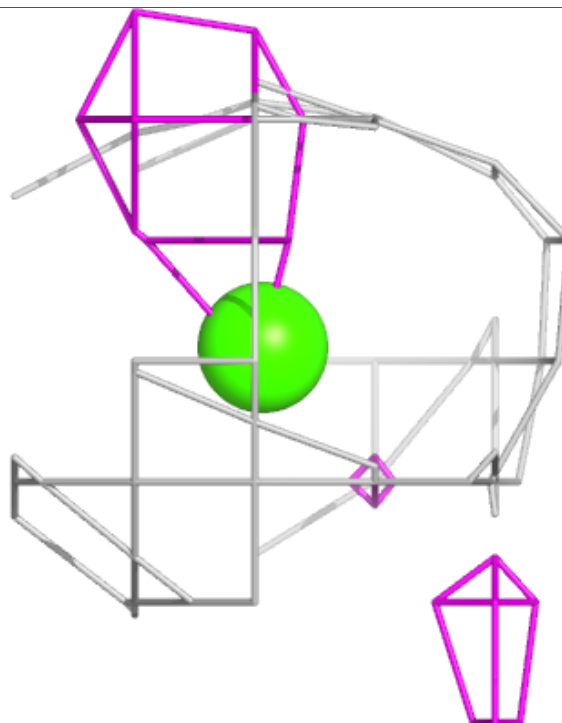
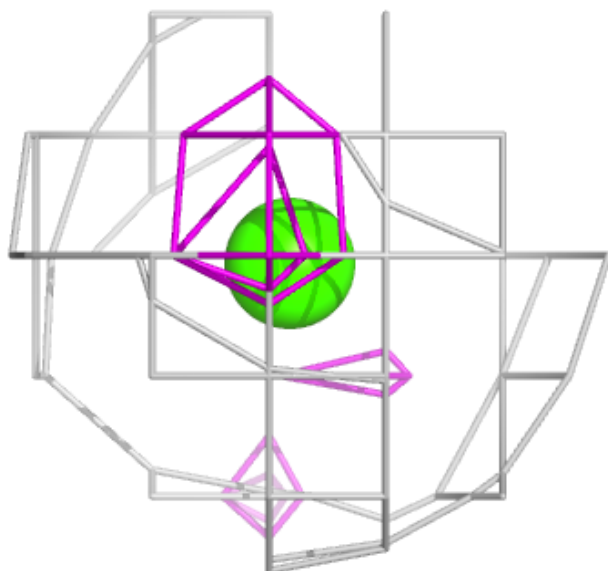
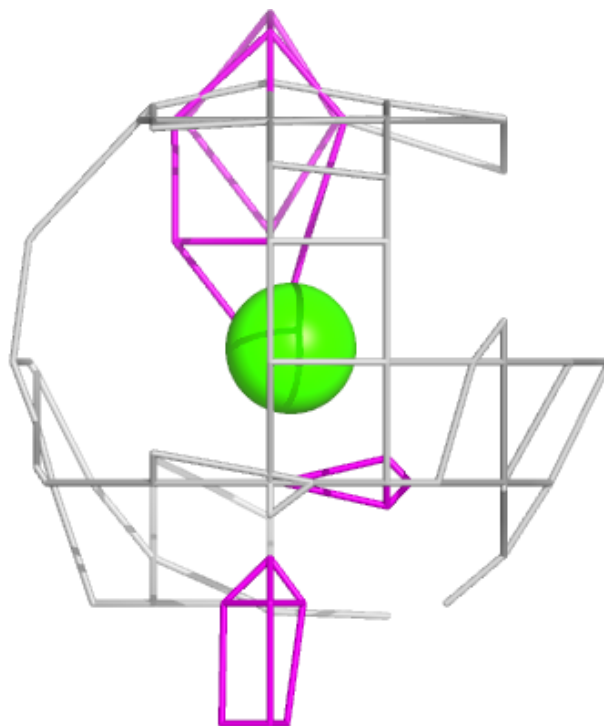
Electron density around CA A 703:

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and green (positive)



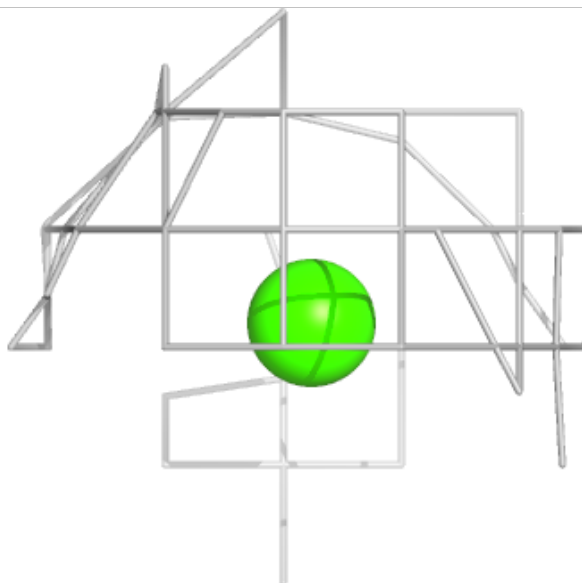
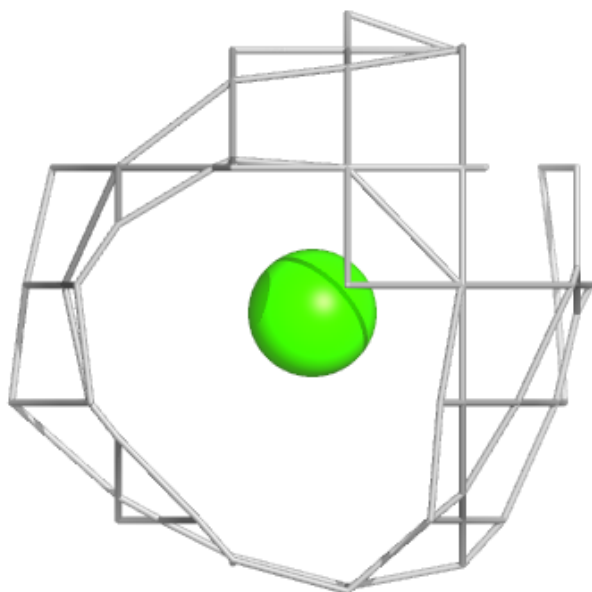
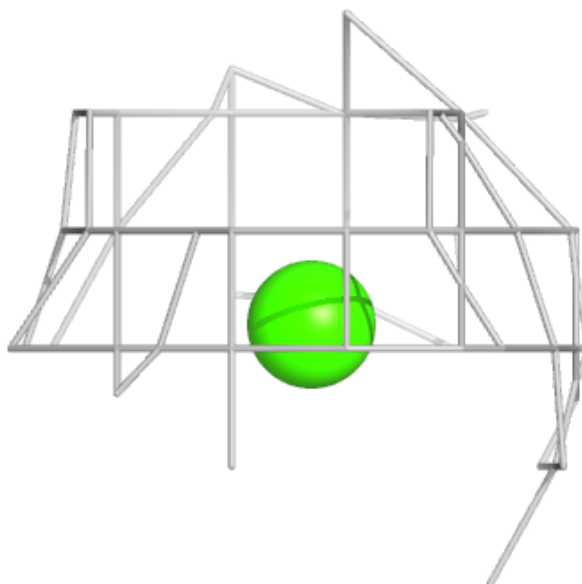
Electron density around CA E 703:

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and green (positive)



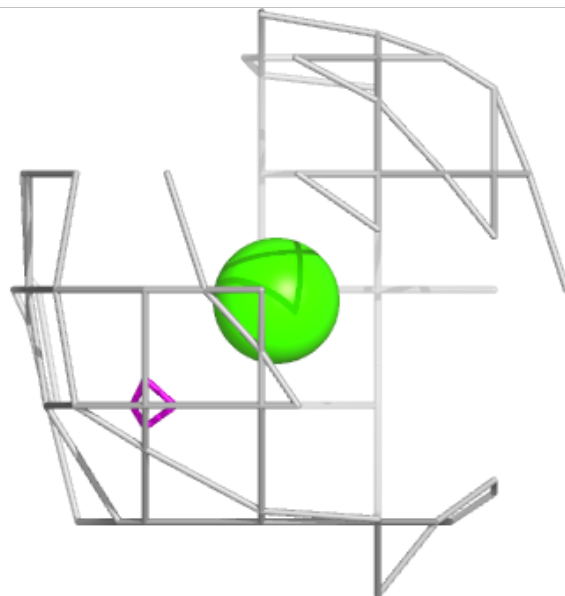
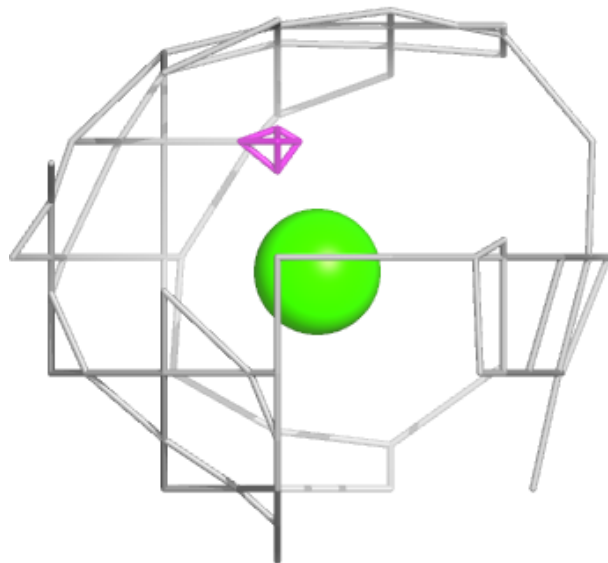
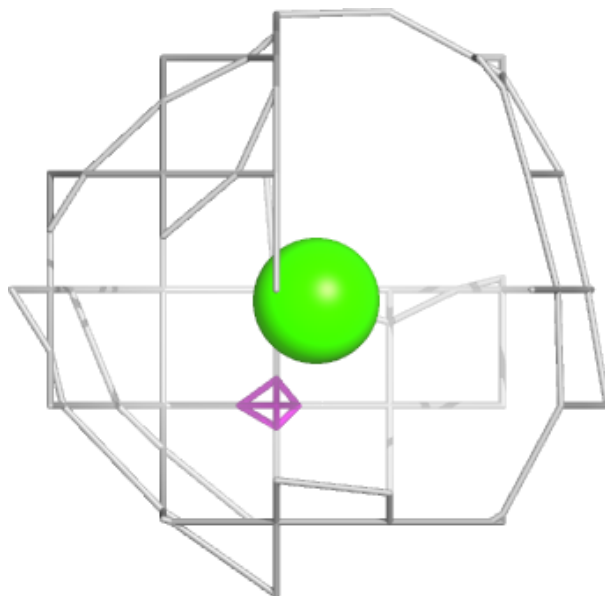
Electron density around CA E 701:

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and green (positive)



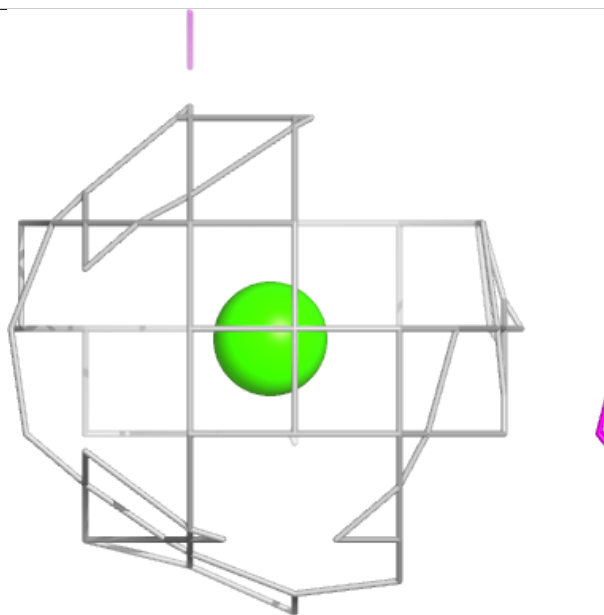
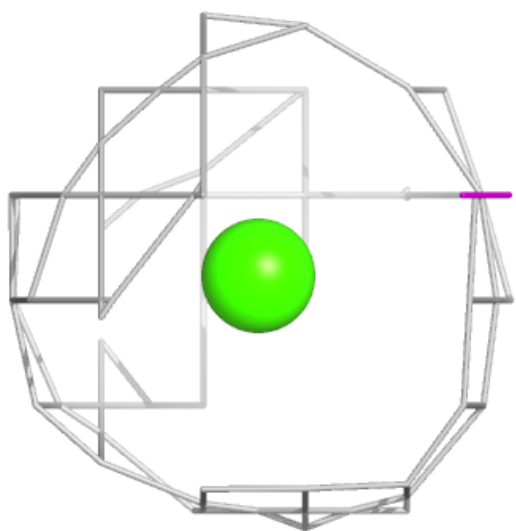
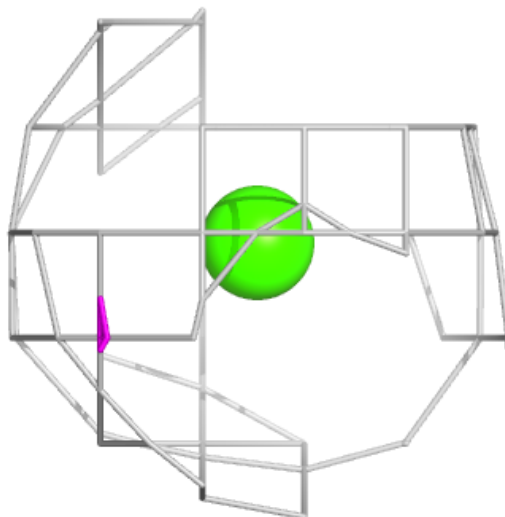
Electron density around CA E 704:

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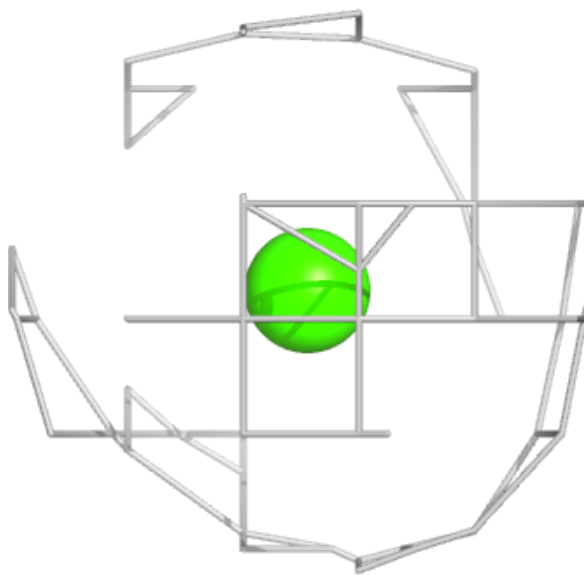
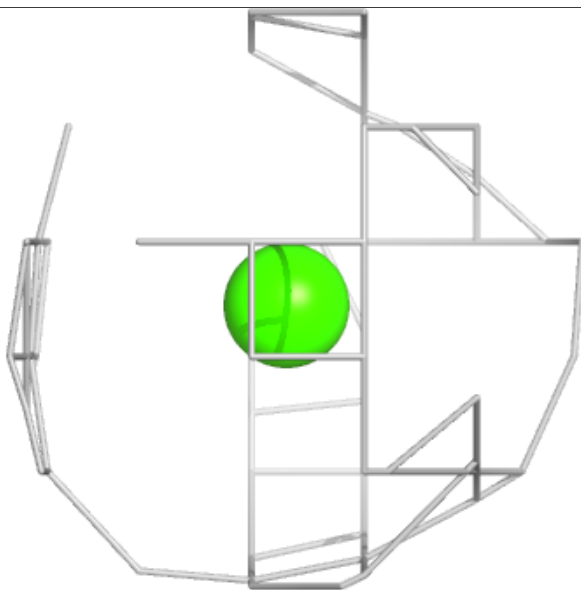
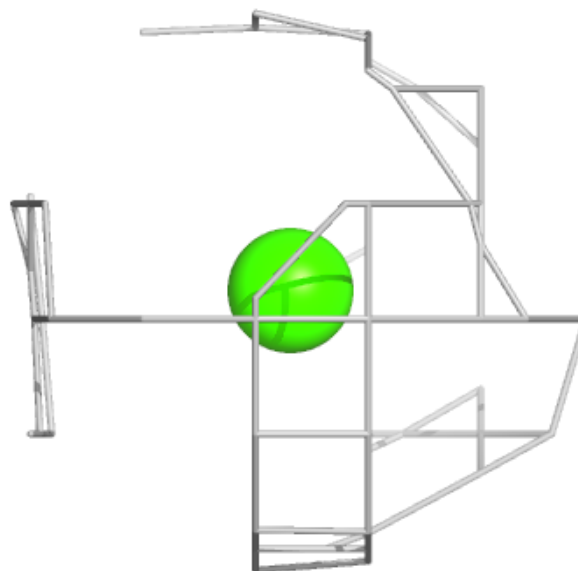
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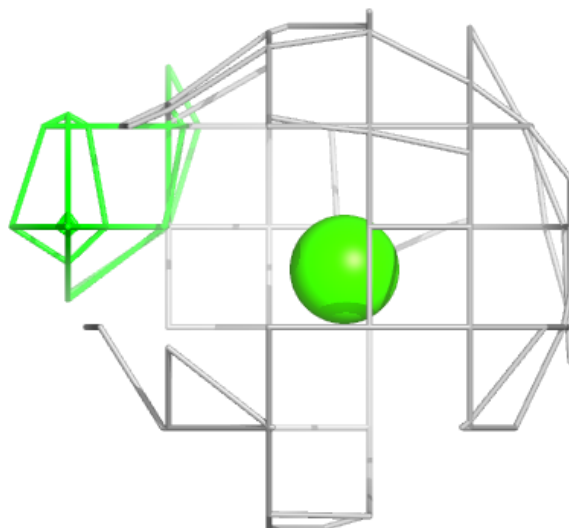
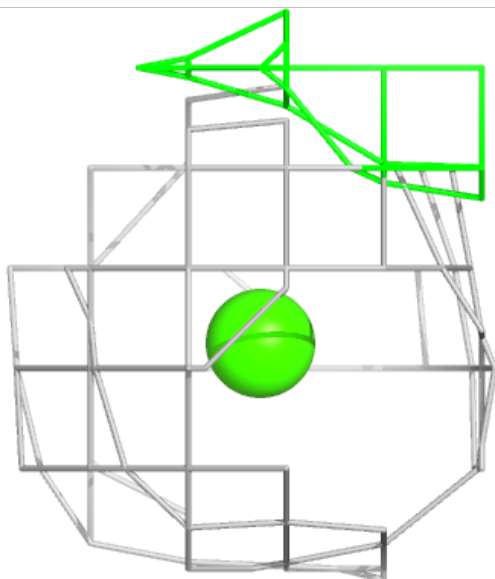
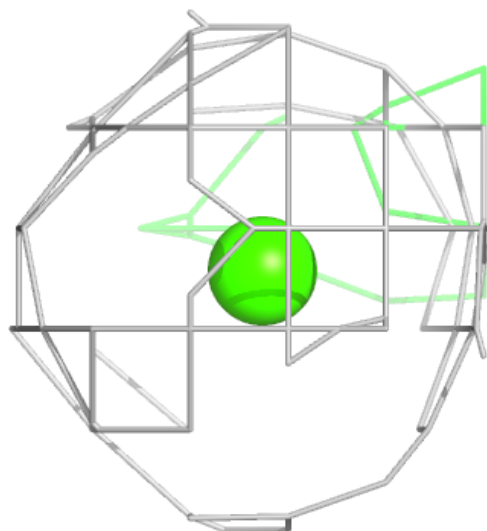
Electron density around CA E 702:

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



Electron density around CA A 702:

$2mF_o-DF_c$ (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.