



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:39 AM UTC

PDB ID : 9G66 / pdb_00009g66
Title : Crystal structure of WT Rhizobium etli L-asparaginase ReAV in complex with L-Asn
Authors : Pokrywka, K.; Grzechowiak, M.; Sliwiak, J.; Worsztynowicz, P.; Loch, J.I.; Ruszkowski, M.; Gilski, M.; Jaskolski, M.
Deposited on : 2024-07-18
Resolution : 1.79 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

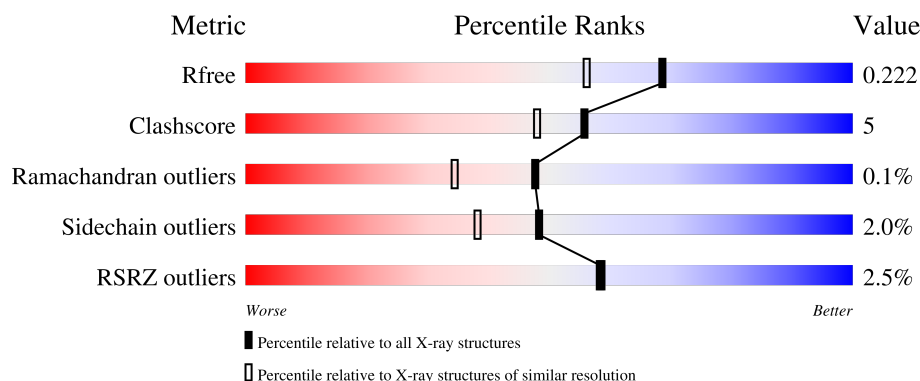
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	373	
1	B	373	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	404	-	-	X	-
3	PEG	B	407	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6206 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 L-asparaginase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	10	0
			2653	1642	486	502	23			
1	B	369	Total	C	N	O	S	0	10	0
			2790	1727	510	529	24			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q2K0Z2
A	-4	ILE	-	expression tag	UNP Q2K0Z2
A	-3	ASP	-	expression tag	UNP Q2K0Z2
A	-2	PRO	-	expression tag	UNP Q2K0Z2
A	-1	PHE	-	expression tag	UNP Q2K0Z2
A	0	THR	-	expression tag	UNP Q2K0Z2
B	-5	GLY	-	expression tag	UNP Q2K0Z2
B	-4	ILE	-	expression tag	UNP Q2K0Z2
B	-3	ASP	-	expression tag	UNP Q2K0Z2
B	-2	PRO	-	expression tag	UNP Q2K0Z2
B	-1	PHE	-	expression tag	UNP Q2K0Z2
B	0	THR	-	expression tag	UNP Q2K0Z2

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



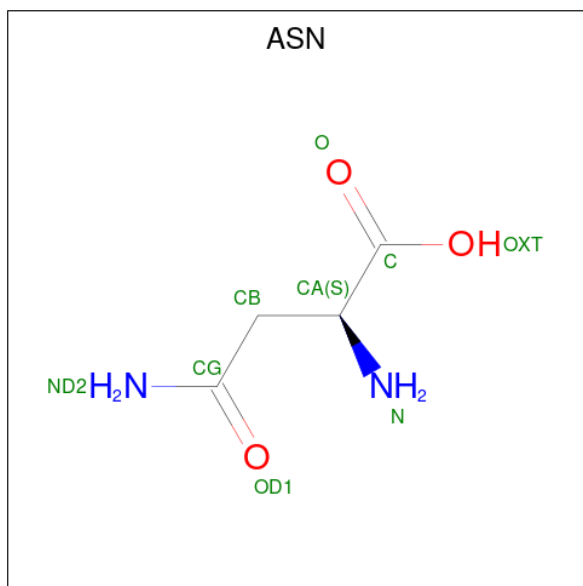
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ASPARAGINE (CCD ID: ASN) (formula: $C_4H_8N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			9	4	2	3		
5	B	1	Total	C	N	O	0	1
			9	4	2	3		

- Molecule 6 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Cd 1	0	0
6	B	1	Total 1	Cd 1	0	0

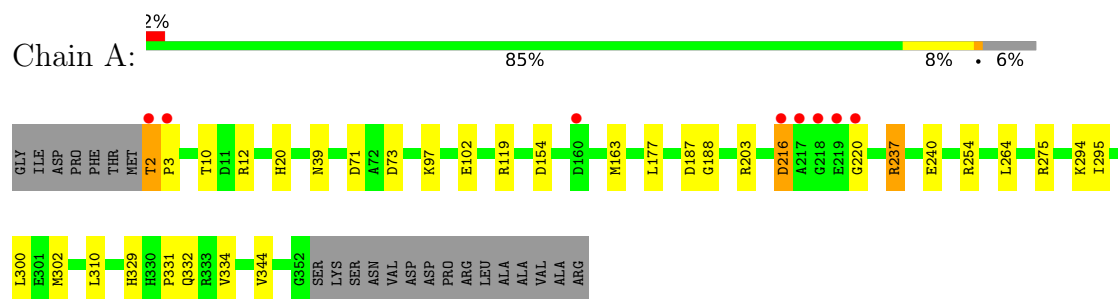
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	308	Total 308	O 308	0	1
7	B	327	Total 327	O 327	0	1

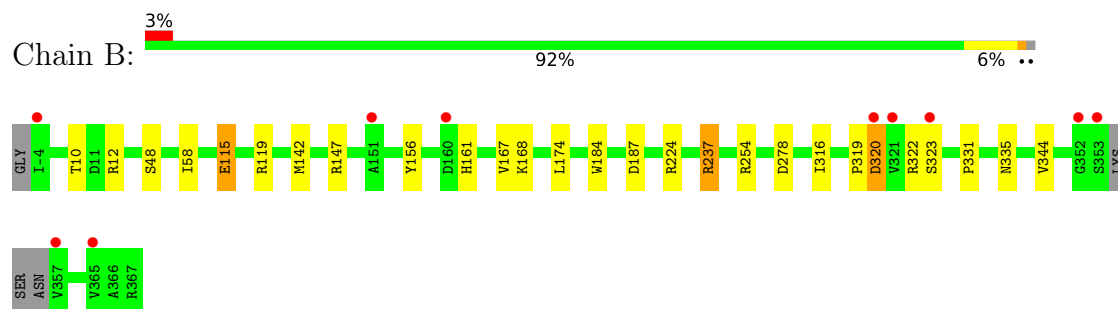
3 Residue-property plots [i](#)

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

- Molecule 1: L-asparaginase II protein



- Molecule 1: L-asparaginase II protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.96Å 91.33Å 106.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.66 – 1.79 45.66 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.66-1.79) 99.4 (45.66-1.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.174 , 0.221 0.174 , 0.222	Depositor DCC
R_{free} test set	1000 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtrriage
Anisotropy	0.561	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6206	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8160e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CSO, CD, PEG, GOL, EDO

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	0.43	0/2720	0.61	0/3671
1	B	0.49	0/2859	0.62	0/3859
All	All	0.46	0/5579	0.61	0/7530

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2653	0	2649	27	0
1	B	2790	0	2786	23	0
2	A	56	0	84	7	0
2	B	32	0	48	4	0
3	A	7	0	10	5	0
3	B	7	0	10	4	0
4	A	6	0	8	0	0
5	A	9	0	5	1	0
5	B	9	0	5	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	308	0	0	4	0
7	B	327	0	0	3	0
All	All	6206	0	5605	53	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 5.

All (53) 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:B:224:ARG:HH11	3:B:407:PEG:H22	1.46	0.81
1:B:10:THR:HG22	1:B:344[B]:VAL:HG22	1.66	0.76
1:A:119:ARG:HH12	3:A:404:PEG:H12	1.54	0.72
5:B:409[A]:ASN:ND2	7:B:501:HOH:O	2.29	0.66
5:A:413[A]:ASN:ND2	7:A:502:HOH:O	2.29	0.66
1:A:119:ARG:HH22	3:A:404:PEG:H12	1.60	0.66
1:A:12:ARG:HH12	2:A:406:EDO:H22	1.62	0.64
1:A:264:LEU:HD11	1:A:300:LEU:HD21	1.80	0.64
1:B:115:GLU:O	1:B:119:ARG:HG3	1.99	0.62
1:A:10:THR:HG22	1:A:344[A]:VAL:HG22	1.81	0.62
1:A:2:THR:HG23	1:A:3:PRO:HD3	1.84	0.60
1:B:12:ARG:HH12	2:B:401:EDO:H12	1.68	0.58
1:A:39:ASN:HD22	2:A:403:EDO:C1	2.18	0.56
1:A:177:LEU:HD23	2:A:416:EDO:H11	1.86	0.56
1:B:115:GLU:HG2	1:B:119:ARG:NH2	2.20	0.56
1:A:119:ARG:NH1	3:A:404:PEG:H12	2.23	0.53
1:A:203:ARG:HH12	2:A:415:EDO:H22	1.74	0.52
1:A:240:GLU:HB3	1:A:254:ARG:NH2	2.25	0.52
1:B:48:SER:OG	5:B:409[A]:ASN:CG	2.53	0.51
1:B:316:ILE:O	1:B:322:ARG:HD3	2.11	0.51
1:B:254:ARG:HE	2:B:411:EDO:C1	2.24	0.51
1:B:254:ARG:HG2	2:B:411:EDO:H11	1.93	0.51
1:B:224:ARG:NH1	3:B:407:PEG:H22	2.22	0.50
1:A:332:GLN:HG2	7:A:627:HOH:O	2.11	0.50
1:B:331:PRO:HD2	1:B:344[A]:VAL:HG11	1.93	0.49
1:A:10:THR:HG22	1:A:344[B]:VAL:HG12	1.95	0.49
1:B:174:LEU:HD23	3:B:407:PEG:H11	1.93	0.49
1:A:102[B]:GLU:HG2	7:A:755:HOH:O	2.13	0.48
1:B:142[B]:MET:HE2	1:B:167:VAL:HG21	1.93	0.48
1:B:147:ARG:HD2	7:B:690:HOH:O	2.13	0.48
1:A:20:HIS:CD2	1:A:302:MET:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:SER:HG	5:B:409[A]:ASN:N	2.12	0.47
1:A:119:ARG:NH2	3:A:404:PEG:H12	2.27	0.47
1:A:237[A]:ARG:NH2	7:A:506:HOH:O	2.42	0.47
1:A:331:PRO:HD2	1:A:344[B]:VAL:HG21	1.97	0.47
1:A:216:ASP:CG	1:A:275:ARG:HH22	2.22	0.46
1:B:237:ARG:NH1	7:B:509:HOH:O	2.41	0.46
1:A:73:ASP:OD2	1:A:97:LYS:NZ	2.40	0.46
1:A:163[A]:MET:HA	1:A:163[A]:MET:HE2	1.97	0.46
1:B:58:ILE:HD11	1:B:142[A]:MET:HE2	1.97	0.46
1:A:329:HIS:HB2	2:A:412:EDO:H11	1.98	0.45
3:A:404:PEG:H41	3:A:404:PEG:H22	1.63	0.45
1:B:319:PRO:O	1:B:323:SER:HB3	2.17	0.45
3:B:407:PEG:H31	3:B:407:PEG:H12	1.40	0.44
1:B:320:ASP:OD1	1:B:320:ASP:N	2.51	0.43
1:B:156:TYR:HA	1:B:161:HIS:CD2	2.53	0.43
1:A:154:ASP:OD1	2:A:402:EDO:H12	2.18	0.43
1:B:168:LYS:HG2	1:B:184:TRP:CZ2	2.54	0.43
1:A:294:LYS:HE3	1:A:295:ILE:O	2.19	0.42
1:B:335:ASN:HB3	2:B:401:EDO:H11	2.01	0.42
1:A:329:HIS:CB	2:A:412:EDO:H11	2.50	0.42
1:A:71:ASP:HB2	1:A:237[B]:ARG:HH21	1.84	0.41
1:A:188:GLY:HA2	1:B:335:ASN:HB2	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/373 (96%)	349 (98%)	8 (2%)	1 (0%)	36	25
1	B	374/373 (100%)	365 (98%)	9 (2%)	0	100	100
All	All	732/746 (98%)	714 (98%)	17 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	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	274/282 (97%)	267 (97%)	7 (3%)	40	28
1	B	289/282 (102%)	283 (98%)	6 (2%)	47	36
All	All	563/564 (100%)	550 (98%)	13 (2%)	48	33

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	187	ASP
1	A	216	ASP
1	A	237[A]	ARG
1	A	237[B]	ARG
1	A	310	LEU
1	A	334	VAL
1	B	115	GLU
1	B	187	ASP
1	B	237	ARG
1	B	278[A]	ASP
1	B	278[B]	ASP
1	B	320	ASP

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

Mol	Chain	Res	Type
1	A	39	ASN
1	B	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CSO	B	225	1	3,6,7	0.62	0	1,6,8	0.58	0
1	CSO	A	225	1	3,6,7	0.48	0	1,6,8	0.31	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
1	CSO	B	225	1	-	0/1/5/7	-
1	CSO	A	225	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	PEG	A	404	-	6,6,6	0.19	0	5,5,5	0.46	0
5	ASN	B	409[A]	6	7,8,8	1.23	1 (14%)	6,10,10	0.91	0
5	ASN	A	413[A]	6	7,8,8	1.41	2 (28%)	6,10,10	1.05	1 (16%)
2	EDO	A	403	-	3,3,3	0.37	0	2,2,2	0.76	0
2	EDO	A	402	-	3,3,3	0.44	0	2,2,2	0.18	0
2	EDO	A	411	-	3,3,3	0.54	0	2,2,2	0.35	0
2	EDO	B	411	-	3,3,3	0.54	0	2,2,2	0.33	0
3	PEG	B	407	-	6,6,6	0.34	0	5,5,5	0.37	0
2	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	A	401	-	3,3,3	0.45	0	2,2,2	0.56	0
2	EDO	B	406	-	3,3,3	0.50	0	2,2,2	0.39	0
4	GOL	A	409	-	5,5,5	0.79	0	5,5,5	1.33	1 (20%)
2	EDO	A	407	-	3,3,3	0.47	0	2,2,2	0.58	0
2	EDO	A	410	-	3,3,3	0.45	0	2,2,2	0.70	0
2	EDO	A	417	-	3,3,3	0.60	0	2,2,2	0.21	0
2	EDO	B	403	-	3,3,3	0.53	0	2,2,2	0.36	0
2	EDO	B	402	-	3,3,3	0.42	0	2,2,2	0.60	0
2	EDO	A	416	-	3,3,3	0.59	0	2,2,2	0.25	0
2	EDO	A	405	-	3,3,3	0.18	0	2,2,2	0.27	0
2	EDO	B	405	-	3,3,3	0.52	0	2,2,2	0.44	0
2	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.65	0
2	EDO	A	408	-	3,3,3	0.41	0	2,2,2	0.54	0
2	EDO	A	415	-	3,3,3	0.48	0	2,2,2	0.48	0
2	EDO	A	406	-	3,3,3	0.56	0	2,2,2	0.46	0
2	EDO	A	414	-	3,3,3	0.43	0	2,2,2	0.33	0
2	EDO	A	412	-	3,3,3	0.34	0	2,2,2	0.46	0
2	EDO	B	408	-	3,3,3	0.47	0	2,2,2	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	404	-	-	4/4/4/4	-
5	ASN	B	409[A]	6	-	4/8/8/8	-
5	ASN	A	413[A]	6	-	2/8/8/8	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-
2	EDO	B	411	-	-	1/1/1/1	-
3	PEG	B	407	-	-	2/4/4/4	-
2	EDO	B	404	-	-	1/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	B	406	-	-	0/1/1/1	-
4	GOL	A	409	-	-	2/4/4/4	-
2	EDO	A	407	-	-	1/1/1/1	-
2	EDO	A	410	-	-	1/1/1/1	-
2	EDO	A	417	-	-	0/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	B	402	-	-	1/1/1/1	-
2	EDO	A	416	-	-	1/1/1/1	-
2	EDO	A	405	-	-	1/1/1/1	-
2	EDO	B	405	-	-	1/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	A	415	-	-	1/1/1/1	-
2	EDO	A	406	-	-	1/1/1/1	-
2	EDO	A	414	-	-	0/1/1/1	-
2	EDO	A	412	-	-	1/1/1/1	-
2	EDO	B	408	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	413[A]	ASN	OXT-C	-3.05	1.20	1.30
5	B	409[A]	ASN	OXT-C	-3.00	1.21	1.30
5	A	413[A]	ASN	CB-CG	-2.05	1.46	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	409	GOL	C3-C2-C1	-2.30	103.36	111.80
5	A	413[A]	ASN	OXT-C-O	-2.21	119.07	124.08

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	407	PEG	C1-C2-O2-C3
4	A	409	GOL	O1-C1-C2-C3
5	A	413[A]	ASN	N-CA-CB-CG
3	A	404	PEG	C4-C3-O2-C2
3	A	404	PEG	O2-C3-C4-O4
2	B	411	EDO	O1-C1-C2-O2
4	A	409	GOL	O1-C1-C2-O2
5	B	409[A]	ASN	OXT-C-CA-CB
5	B	409[A]	ASN	N-CA-CB-CG
5	B	409[A]	ASN	O-C-CA-CB
3	B	407	PEG	C4-C3-O2-C2
3	A	404	PEG	O1-C1-C2-O2
2	A	412	EDO	O1-C1-C2-O2
2	B	404	EDO	O1-C1-C2-O2
2	A	405	EDO	O1-C1-C2-O2
2	A	410	EDO	O1-C1-C2-O2
2	A	415	EDO	O1-C1-C2-O2
2	A	416	EDO	O1-C1-C2-O2
2	B	401	EDO	O1-C1-C2-O2
2	B	402	EDO	O1-C1-C2-O2
2	B	405	EDO	O1-C1-C2-O2
5	A	413[A]	ASN	C-CA-CB-CG
5	B	409[A]	ASN	OXT-C-CA-N
2	A	407	EDO	O1-C1-C2-O2
2	A	411	EDO	O1-C1-C2-O2
3	A	404	PEG	C1-C2-O2-C3
2	A	406	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 24 short contacts:

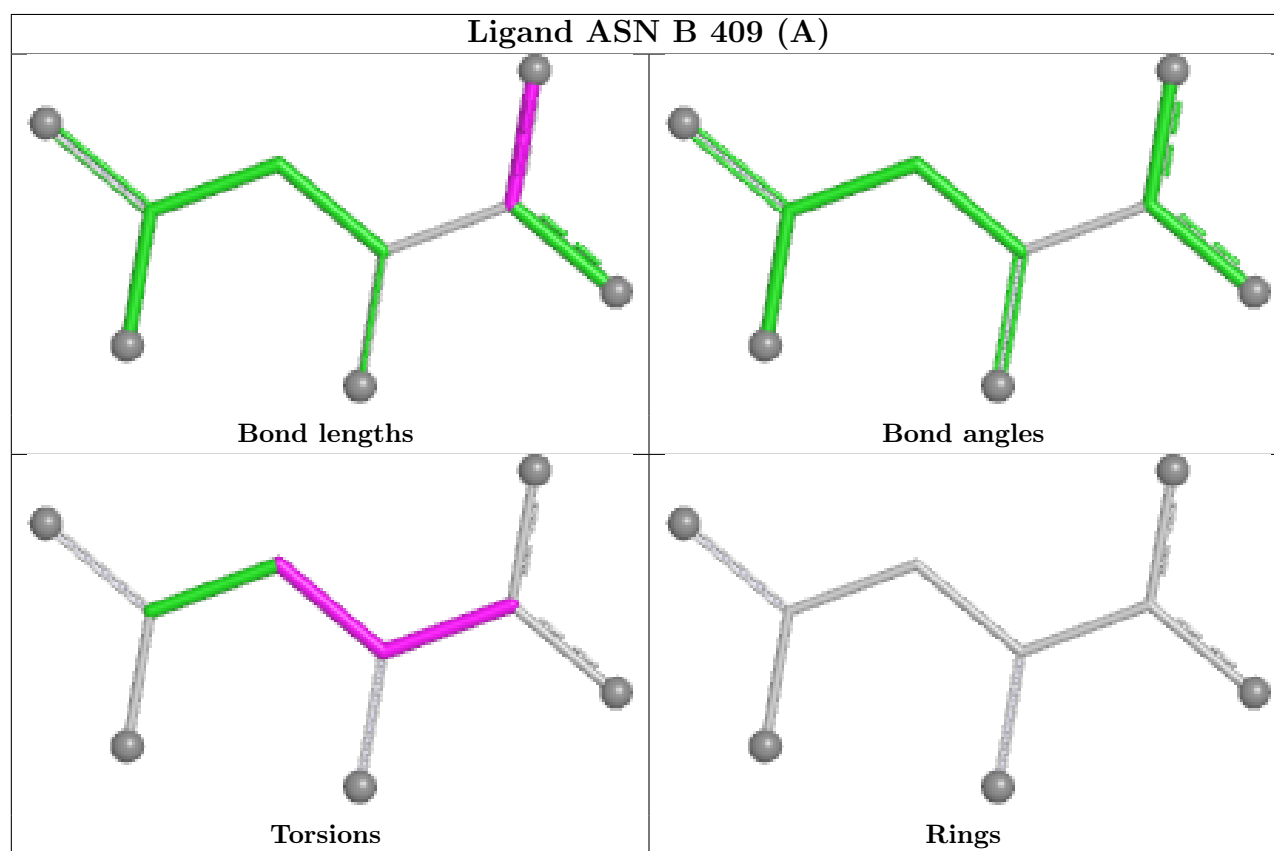
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	PEG	5	0
5	B	409[A]	ASN	3	0
5	A	413[A]	ASN	1	0
2	A	403	EDO	1	0
2	A	402	EDO	1	0
2	B	411	EDO	2	0
3	B	407	PEG	4	0
2	A	416	EDO	1	0

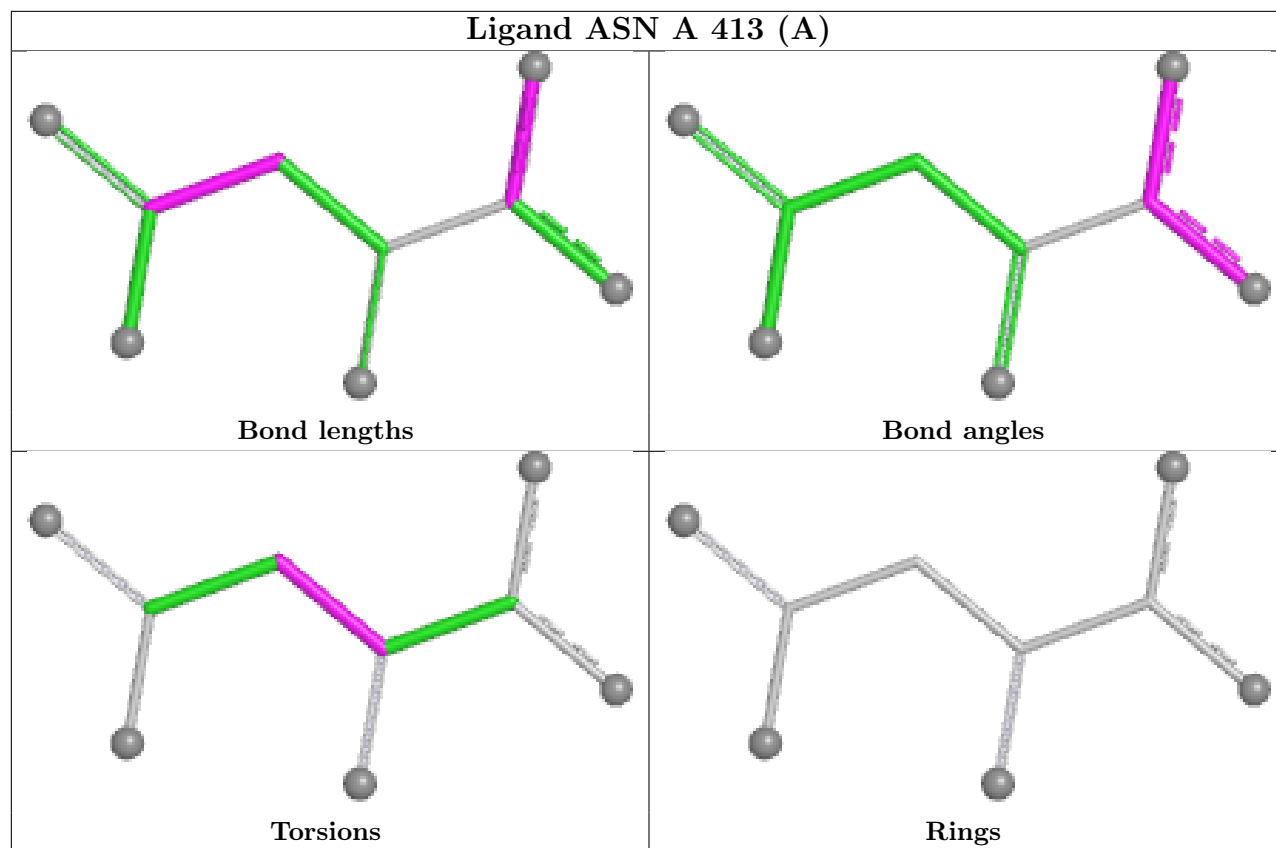
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	EDO	2	0
2	A	415	EDO	1	0
2	A	406	EDO	1	0
2	A	412	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	350/373 (93%)	0.38	8 (2%) 61 61	11, 23, 39, 97	10 (2%)
1	B	368/373 (98%)	0.32	10 (2%) 56 56	11, 21, 38, 63	10 (2%)
All	All	718/746 (96%)	0.35	18 (2%) 58 58	11, 22, 39, 97	20 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	GLY	5.5
1	B	-4	ILE	5.2
1	B	357	VAL	5.1
1	A	217	ALA	4.0
1	B	352	GLY	4.0
1	B	160	ASP	3.7
1	B	353	SER	3.3
1	A	219	GLU	3.1
1	B	320	ASP	2.8
1	B	151	ALA	2.6
1	A	2	THR	2.5
1	A	160	ASP	2.4
1	B	321	VAL	2.4
1	A	218	GLY	2.4
1	A	3	PRO	2.4
1	A	216	ASP	2.3
1	B	365	VAL	2.2
1	B	323	SER	2.1

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

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
1	CSO	A	225	7/8	0.91	0.12	35,37,49,58	0
1	CSO	B	225	7/8	0.91	0.09	20,21,29,33	0

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
5	ASN	B	409[A]	9/9	0.64	0.21	24,24,26,27	9
2	EDO	A	416	4/4	0.71	0.16	34,40,41,47	0
2	EDO	B	411	4/4	0.72	0.17	37,40,41,41	0
2	EDO	B	406	4/4	0.73	0.16	39,41,41,41	0
2	EDO	A	402	4/4	0.74	0.17	41,42,43,47	0
2	EDO	A	415	4/4	0.74	0.14	43,44,46,47	0
3	PEG	B	407	7/7	0.75	0.15	22,30,37,37	0
3	PEG	A	404	7/7	0.75	0.13	28,28,35,41	0
5	ASN	A	413[A]	9/9	0.76	0.18	20,22,26,27	9
2	EDO	B	405	4/4	0.76	0.21	36,37,41,41	0
2	EDO	A	403	4/4	0.77	0.20	29,33,33,34	0
4	GOL	A	409	6/6	0.78	0.14	38,40,41,43	0
2	EDO	A	410	4/4	0.80	0.15	35,41,42,42	0
2	EDO	B	403	4/4	0.81	0.18	24,37,43,44	0
2	EDO	B	404	4/4	0.81	0.14	40,46,49,50	0
2	EDO	A	406	4/4	0.81	0.13	26,35,37,37	0
2	EDO	A	414	4/4	0.81	0.17	35,36,39,45	0
2	EDO	B	401	4/4	0.81	0.14	25,28,34,40	0
2	EDO	A	401	4/4	0.82	0.19	36,38,38,41	0
2	EDO	A	417	4/4	0.83	0.16	27,34,34,35	0
2	EDO	A	411	4/4	0.87	0.12	31,31,34,40	0
2	EDO	A	407	4/4	0.88	0.13	34,38,38,39	0
2	EDO	B	402	4/4	0.88	0.12	30,30,33,39	0
2	EDO	B	408	4/4	0.88	0.13	20,23,27,36	4
2	EDO	A	412	4/4	0.89	0.20	29,33,34,38	0

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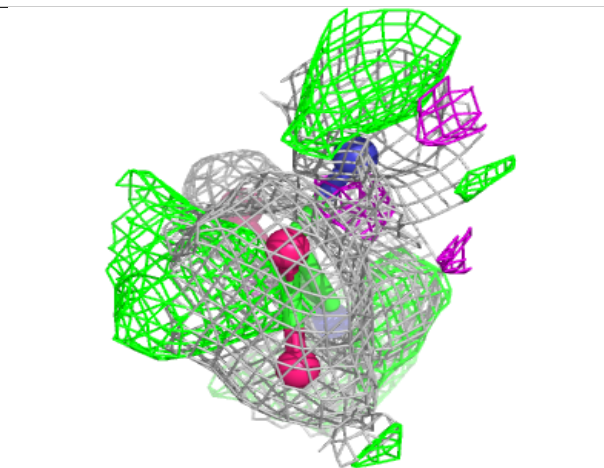
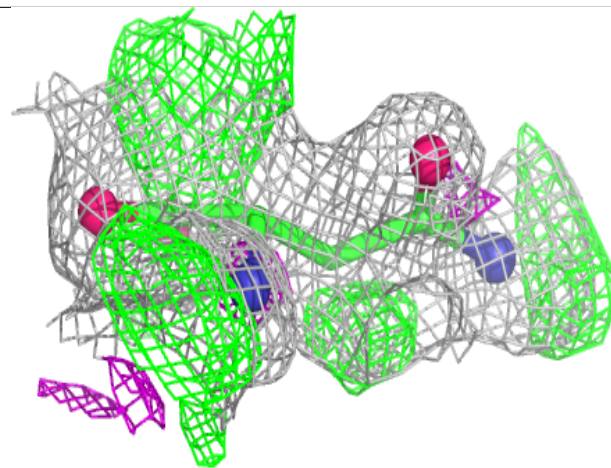
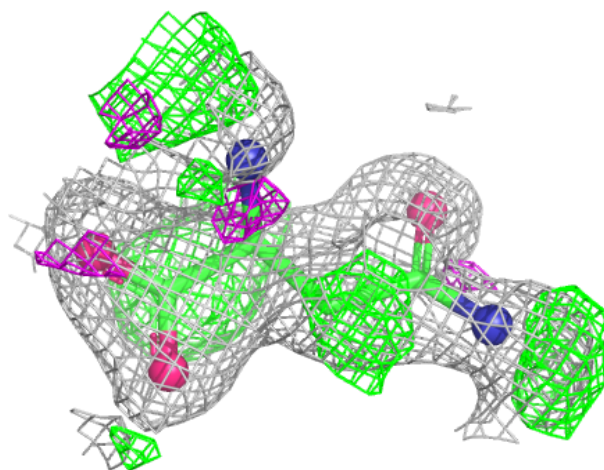
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	408	4/4	0.89	0.14	28,28,34,35	0
2	EDO	A	405	4/4	0.91	0.09	37,37,37,38	0
6	CD	A	418	1/1	0.98	0.05	25,25,25,25	0
6	CD	B	410	1/1	0.98	0.04	25,25,25,25	0

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.

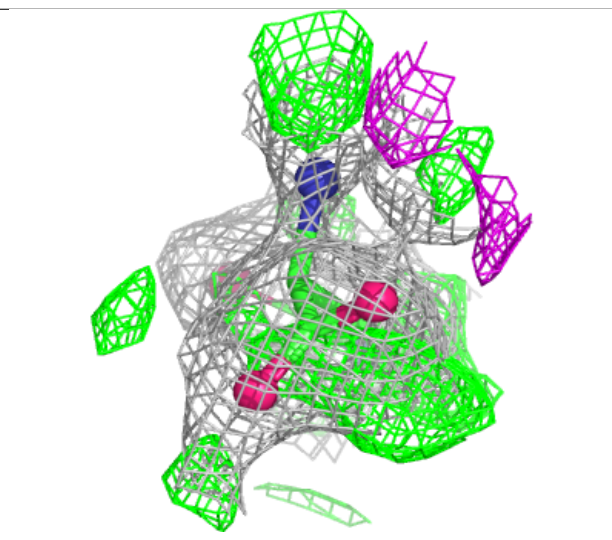
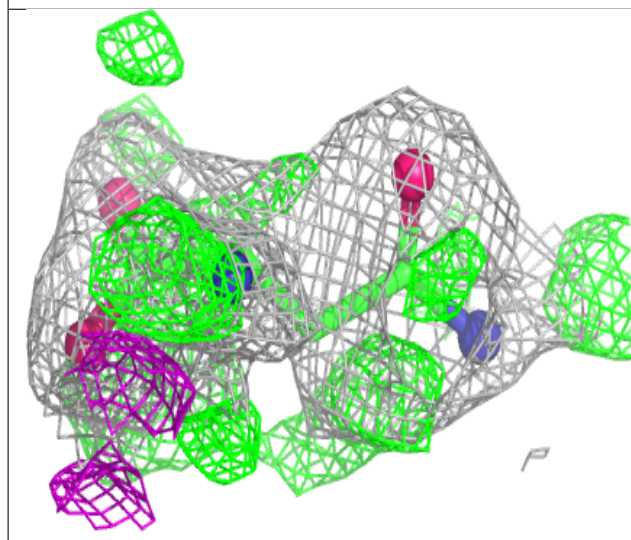
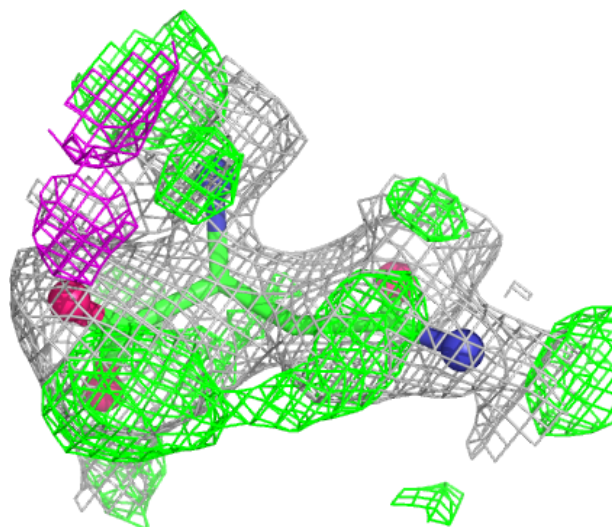
Electron density around ASN B 409 (A):

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 ASN A 413 (A):

$2mF_o-DF_c$ (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.