



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 06:19 PM JST

PDB ID : 9V83 / pdb_00009v83
Title : Crystal Structure of Asparagine Synthetase from Entamoeba histolytica
Authors : Mishra, S.; Yadav, L.; Gautam, A.K.; Gourinath, S.
Deposited on : 2025-05-29
Resolution : 2.38 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>.

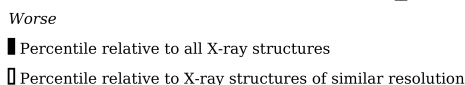
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

i

X-RAY DIFFRACTION

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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	345	<div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	B	345	<div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	C	345	<div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	D	345	<div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	604	-	-	X	-
3	PEG	B	403	-	-	X	-

2 Entry composition [i](#)

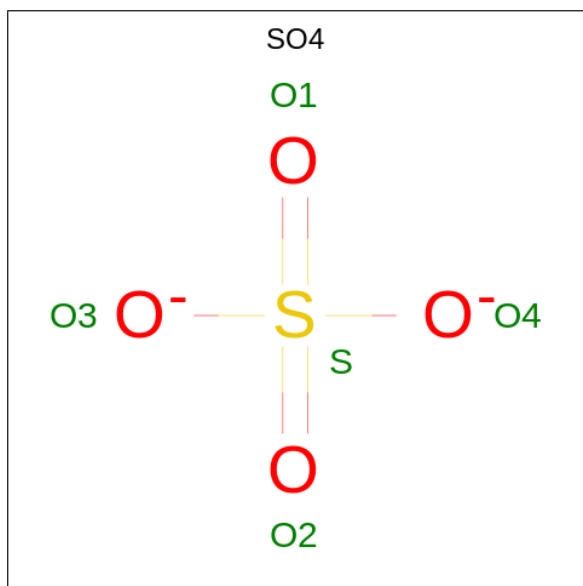
There are 5 unique types of molecules in this entry. The entry contains 11804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aspergine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	1
			2706	1731	452	510	13			
1	B	337	Total	C	N	O	S	0	0	0
			2671	1711	448	499	13			
1	C	339	Total	C	N	O	S	0	0	0
			2734	1746	463	512	13			
1	D	341	Total	C	N	O	S	0	0	0
			2723	1739	456	515	13			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



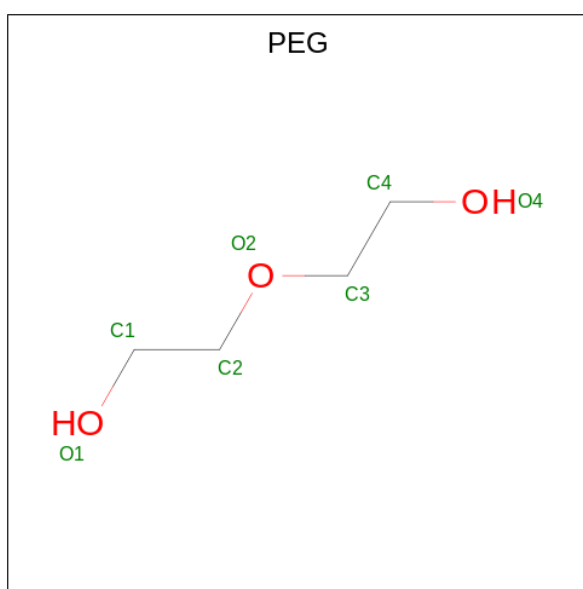
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



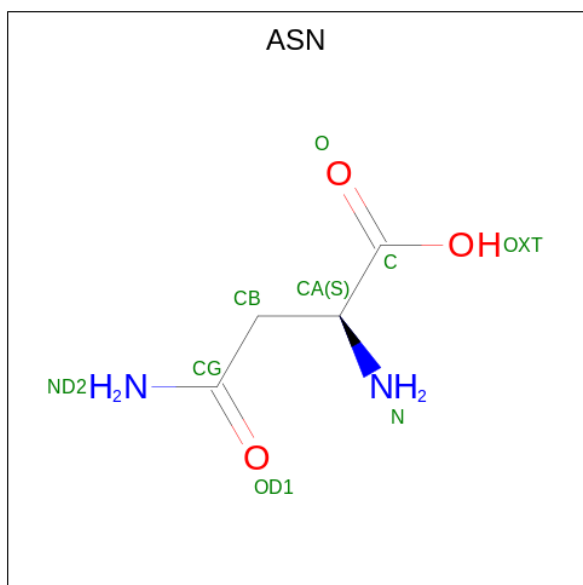
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 4 is ASPARAGINE (CCD ID: ASN) (formula: $C_4H_8N_2O_3$) (labeled as "Ligand of Interest" by depositor).



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

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

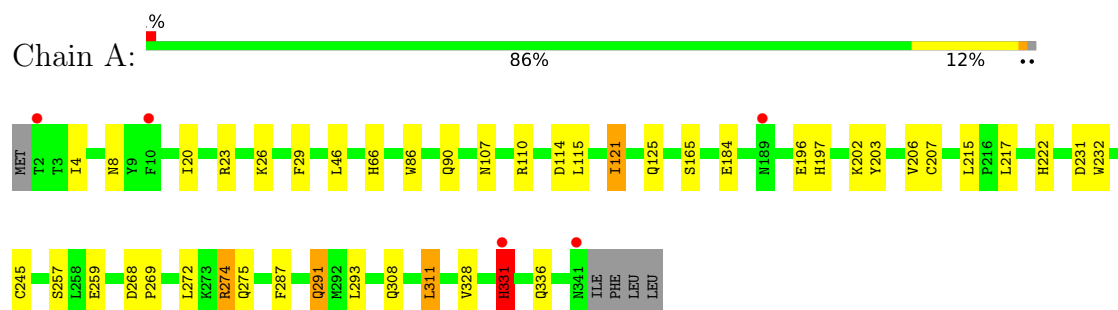
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	157	Total	O	0	0
			157	157		
5	B	166	Total	O	0	0
			166	166		
5	C	221	Total	O	0	0
			221	221		
5	D	212	Total	O	0	0
			212	212		

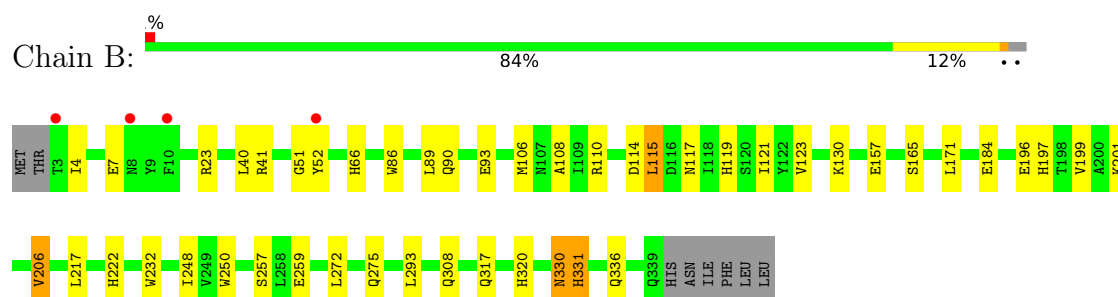
3 Residue-property plots [i](#)

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.

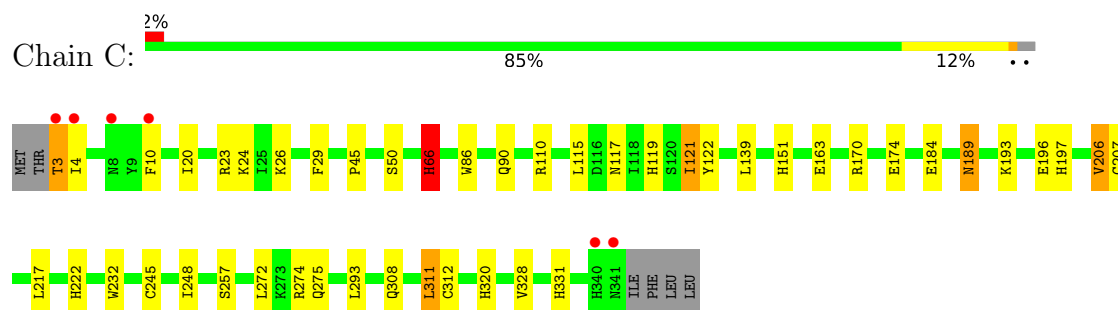
- Molecule 1: Aspergine synthetase



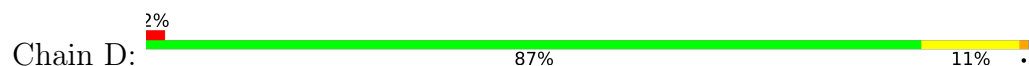
- Molecule 1: Aspergine synthetase

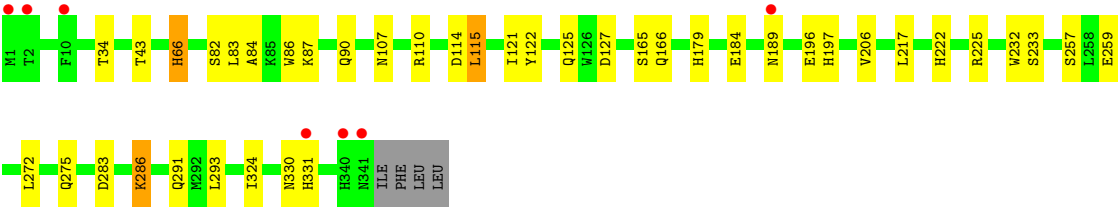


- Molecule 1: Aspergine synthetase



- Molecule 1: Aspergine synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.25Å 149.85Å 170.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.25 – 2.38 85.25 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.2 (85.25-2.38) 97.2 (85.25-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.178 , 0.225 0.186 , 0.186	Depositor DCC
R_{free} test set	4445 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11804	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: PEG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/2770	0.99	6/3763 (0.2%)
1	B	0.56	0/2734	1.00	5/3714 (0.1%)
1	C	0.60	0/2798	1.03	3/3793 (0.1%)
1	D	0.57	0/2787	1.01	5/3785 (0.1%)
All	All	0.57	0/11089	1.01	19/15055 (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	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	HIS	CB-CG-CD2	-10.01	118.19	131.20
1	D	66	HIS	CB-CG-CD2	-9.28	119.14	131.20
1	C	66	HIS	CB-CG-ND1	7.77	134.35	122.70
1	C	10	PHE	CA-CB-CG	-7.67	106.13	113.80
1	B	66	HIS	CB-CA-C	-7.48	95.16	109.66
1	D	66	HIS	CB-CG-ND1	7.22	133.53	122.70
1	A	66	HIS	CB-CG-CD2	7.21	140.57	131.20
1	A	66	HIS	CB-CG-ND1	-7.05	112.13	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	ASN	N-CA-CB	6.56	119.37	110.38
1	A	331	HIS	CA-CB-CG	-6.19	107.61	113.80
1	D	114	ASP	CB-CA-C	-6.04	101.49	110.67
1	A	66	HIS	CB-CA-C	-5.91	99.07	109.71
1	D	166	GLN	CB-CA-C	-5.55	98.61	110.32
1	D	66	HIS	CA-CB-CG	5.36	119.16	113.80
1	B	330	ASN	CA-CB-CG	5.20	117.80	112.60
1	B	308	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	114	ASP	CB-CA-C	-5.03	103.03	110.67
1	A	274	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	B	331	HIS	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	A	274	ARG	Sidechain
1	B	23	ARG	Sidechain
1	C	23	ARG	Sidechain
1	D	225	ARG	Sidechain

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	2706	0	2606	30	1
1	B	2671	0	2577	26	1
1	C	2734	0	2674	36	0
1	D	2723	0	2620	20	0
2	A	10	0	0	0	0
2	B	5	0	0	1	0
2	C	15	0	0	1	0
3	A	35	0	50	7	0
3	B	21	0	30	5	0
3	C	21	0	29	2	0
3	D	35	0	50	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	10	3	0
4	B	18	0	10	1	0
4	C	18	0	10	2	0
4	D	18	0	10	2	0
5	A	157	0	0	3	0
5	B	166	0	0	4	0
5	C	221	0	0	7	0
5	D	212	0	0	3	0
All	All	11804	0	10676	118	1

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 (118) 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)
3:C:602:PEG:O1	3:C:602:PEG:H32	1.64	0.94
1:B:123:VAL:HG22	2:B:404:SO4:O3	1.83	0.79
1:A:272:LEU:HD22	1:A:293:LEU:HD23	1.64	0.77
1:C:206:VAL:HG23	1:C:248:ILE:HG12	1.69	0.74
1:B:272:LEU:HD22	1:B:293:LEU:HD22	1.71	0.71
1:C:206:VAL:HG23	1:C:248:ILE:CG1	2.21	0.69
1:C:121:ILE:HD11	1:C:328:VAL:CG2	2.24	0.67
3:A:607:PEG:H22	5:A:807:HOH:O	1.95	0.65
1:A:328:VAL:HG12	3:A:605:PEG:H42	1.80	0.64
1:C:26:LYS:HE3	1:C:308:GLN:HE22	1.63	0.63
1:A:20:ILE:HA	3:B:403:PEG:H11	1.81	0.63
1:C:189:ASN:ND2	1:C:189:ASN:H	1.98	0.61
1:C:110:ARG:O	1:C:121:ILE:HG22	2.01	0.61
1:B:206:VAL:HG23	1:B:248:ILE:CG1	2.30	0.60
1:A:46:LEU:HD13	3:A:604:PEG:H12	1.83	0.60
1:D:232:TRP:H	1:D:275:GLN:HE22	1.50	0.60
1:B:196:GLU:OE2	1:B:222:HIS:HE1	1.85	0.59
1:A:196:GLU:OE2	1:A:222:HIS:HE1	1.86	0.59
1:C:196:GLU:OE2	1:C:222:HIS:HE1	1.85	0.58
1:C:331:HIS:HD2	5:C:804:HOH:O	1.86	0.58
1:D:196:GLU:OE2	1:D:222:HIS:HE1	1.86	0.58
1:B:86:TRP:CH2	1:B:90:GLN:HG3	2.40	0.56
1:B:41:ARG:H	3:B:403:PEG:H32	1.70	0.56
1:C:20:ILE:HA	3:D:405:PEG:H41	1.87	0.55
1:D:125:GLN:HE22	4:D:406:ASN:ND2	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ARG:HH22	4:C:607:ASN:HD21	1.54	0.55
1:C:197:HIS:CD2	1:C:257:SER:H	2.23	0.55
1:B:40:LEU:HD12	3:B:403:PEG:H12	1.89	0.55
1:A:29:PHE:CE1	1:A:311:LEU:HD21	2.42	0.55
1:A:26:LYS:HE3	1:A:308:GLN:HE22	1.72	0.54
1:B:206:VAL:HG23	1:B:248:ILE:HG12	1.90	0.54
1:A:232:TRP:H	1:A:275:GLN:HE22	1.55	0.54
1:D:283:ASP:O	1:D:286:LYS:HD2	2.08	0.54
1:A:4:ILE:H	1:A:336:GLN:HE22	1.57	0.53
1:D:86:TRP:CH2	1:D:90:GLN:HG3	2.45	0.52
1:C:119:HIS:NE2	2:C:604:SO4:O1	2.41	0.52
1:D:272:LEU:HD22	1:D:293:LEU:HD23	1.92	0.51
1:B:110:ARG:HH22	4:B:405:ASN:HD21	1.58	0.51
1:C:86:TRP:CH2	1:C:90:GLN:HG3	2.45	0.51
1:B:232:TRP:H	1:B:275:GLN:HE22	1.57	0.51
1:D:34:THR:HG21	3:D:405:PEG:H12	1.93	0.51
1:D:197:HIS:CD2	1:D:257:SER:H	2.29	0.51
1:A:110:ARG:HH22	4:A:608:ASN:HD21	1.58	0.51
5:B:506:HOH:O	1:C:151:HIS:HE1	1.94	0.50
3:A:607:PEG:H32	5:A:807:HOH:O	2.10	0.50
1:A:215:LEU:HD11	1:A:222:HIS:HB2	1.94	0.49
1:A:125:GLN:HE22	4:A:608:ASN:ND2	2.10	0.49
1:C:197:HIS:HD2	1:C:257:SER:OG	1.94	0.49
1:B:40:LEU:HD12	3:B:403:PEG:H31	1.95	0.49
1:B:115:LEU:HD21	1:B:121:ILE:HD11	1.94	0.48
1:A:202:LYS:HE2	1:A:203:TYR:OH	2.13	0.48
1:A:8:ASN:CB	5:A:710:HOH:O	2.62	0.48
1:A:115:LEU:HD21	1:A:121:ILE:HD13	1.96	0.48
1:A:86:TRP:CH2	1:A:90:GLN:HG3	2.47	0.48
1:A:107:ASN:HB2	3:A:604:PEG:C1	2.43	0.47
1:B:197:HIS:CD2	1:B:257:SER:H	2.31	0.47
1:A:46:LEU:CD1	3:A:604:PEG:H12	2.45	0.47
1:B:199:VAL:HG23	1:B:206:VAL:HG21	1.97	0.47
1:C:66:HIS:HD2	5:C:750:HOH:O	1.96	0.47
1:A:110:ARG:HH22	4:A:608:ASN:ND2	2.12	0.47
1:B:184:GLU:CD	1:B:217:LEU:HB2	2.40	0.47
1:C:121:ILE:HD11	1:C:328:VAL:HG23	1.97	0.47
1:C:3:THR:HG22	5:C:706:HOH:O	2.14	0.46
1:C:272:LEU:HD22	1:C:293:LEU:HD22	1.97	0.46
1:B:197:HIS:HD2	1:B:257:SER:OG	1.98	0.46
3:B:403:PEG:H12	3:B:403:PEG:H31	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:HIS:HD2	1:D:257:SER:OG	1.98	0.46
1:B:51:GLY:C	1:B:52:TYR:HD1	2.23	0.46
1:C:331:HIS:CD2	5:C:804:HOH:O	2.66	0.46
1:D:184:GLU:CD	1:D:217:LEU:HB2	2.40	0.46
1:C:274:ARG:HD2	5:C:753:HOH:O	2.16	0.45
1:D:330:ASN:ND2	5:D:504:HOH:O	2.39	0.45
1:D:43:THR:HG23	3:D:402:PEG:H11	1.99	0.45
1:D:110:ARG:HH22	4:D:406:ASN:HD21	1.65	0.45
1:C:222:HIS:HD2	5:C:796:HOH:O	1.99	0.45
1:D:107:ASN:ND2	1:D:122:TYR:OH	2.50	0.45
1:C:121:ILE:HD11	1:C:328:VAL:HG22	1.99	0.45
1:C:184:GLU:CD	1:C:217:LEU:HB2	2.41	0.44
1:C:24:LYS:NZ	1:C:163:GLU:OE1	2.46	0.44
1:C:232:TRP:H	1:C:275:GLN:HE22	1.66	0.44
1:C:189:ASN:ND2	1:C:189:ASN:N	2.65	0.44
1:B:130:LYS:NZ	5:B:503:HOH:O	2.44	0.44
1:A:110:ARG:O	1:A:121:ILE:HG22	2.18	0.43
1:A:184:GLU:CD	1:A:217:LEU:HB2	2.43	0.43
1:C:29:PHE:CE2	1:C:311:LEU:HD21	2.54	0.43
1:C:117:ASN:HA	1:C:320:HIS:CD2	2.54	0.43
1:D:233:SER:CB	1:D:275:GLN:HE21	2.32	0.43
1:A:207:CYS:SG	1:A:245:CYS:SG	3.17	0.43
1:D:115:LEU:HD21	1:D:121:ILE:HD11	2.00	0.43
1:C:197:HIS:HB3	5:C:879:HOH:O	2.17	0.42
1:D:83:LEU:O	1:D:84:ALA:C	2.62	0.42
1:A:197:HIS:HD2	1:A:257:SER:OG	2.02	0.42
1:C:193:LYS:HA	1:C:193:LYS:HD2	1.91	0.42
1:D:179:HIS:HD2	5:D:544:HOH:O	2.02	0.42
1:A:231:ASP:HA	1:A:275:GLN:HE22	1.85	0.42
3:A:604:PEG:H31	5:B:574:HOH:O	2.19	0.42
1:A:268:ASP:HB2	1:A:269:PRO:HD2	2.02	0.42
1:C:115:LEU:HD21	1:C:121:ILE:HG23	2.02	0.42
1:B:317:GLN:CG	5:B:634:HOH:O	2.68	0.42
1:C:45:PRO:HD3	1:C:86:TRP:CZ2	2.55	0.42
1:C:207:CYS:SG	1:C:245:CYS:SG	3.18	0.42
1:D:324:ILE:C	1:D:324:ILE:HD12	2.45	0.42
1:B:106:MET:SD	1:B:108:ALA:HB2	2.60	0.41
1:B:201:LYS:HB2	1:B:250:TRP:CZ3	2.55	0.41
1:A:268:ASP:HB2	1:A:269:PRO:CD	2.51	0.41
1:A:197:HIS:CD2	1:A:257:SER:H	2.38	0.41
1:B:114:ASP:O	1:B:119:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:O	1:B:93:GLU:HG2	2.19	0.41
1:D:87:LYS:NZ	1:D:127:ASP:OD1	2.48	0.41
1:C:312:CYS:SG	4:C:608:ASN:ND2	2.94	0.41
1:A:121:ILE:H	1:A:121:ILE:HG12	1.67	0.41
1:A:287:PHE:O	1:A:291:GLN:HB2	2.20	0.41
3:D:402:PEG:H21	5:D:669:HOH:O	2.20	0.41
1:A:232:TRP:H	1:A:275:GLN:NE2	2.18	0.40
1:B:4:ILE:H	1:B:336:GLN:HE22	1.70	0.40
1:B:117:ASN:HA	1:B:320:HIS:CD2	2.57	0.40
1:B:157:GLU:OE1	1:B:171:LEU:HB2	2.21	0.40
1:C:122:TYR:O	3:C:601:PEG:O4	2.27	0.40

All (1) 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:331:HIS:ND1	1:B:7:GLU:O[1_655]	2.10	0.10

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	338/345 (98%)	330 (98%)	8 (2%)	0	100	100
1	B	335/345 (97%)	326 (97%)	9 (3%)	0	100	100
1	C	337/345 (98%)	329 (98%)	8 (2%)	0	100	100
1	D	339/345 (98%)	330 (97%)	9 (3%)	0	100	100
All	All	1349/1380 (98%)	1315 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	290/315 (92%)	283 (98%)	7 (2%)	43	63
1	B	285/315 (90%)	279 (98%)	6 (2%)	47	67
1	C	299/315 (95%)	288 (96%)	11 (4%)	30	47
1	D	293/315 (93%)	283 (97%)	10 (3%)	32	51
All	All	1167/1260 (93%)	1133 (97%)	34 (3%)	36	57

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ILE
1	A	165	SER
1	A	206	VAL
1	A	259	GLU
1	A	291	GLN
1	A	311	LEU
1	A	331	HIS
1	B	115	LEU
1	B	165	SER
1	B	206	VAL
1	B	259	GLU
1	B	330	ASN
1	B	331	HIS
1	C	3	THR
1	C	4	ILE
1	C	50	SER
1	C	66	HIS
1	C	121	ILE
1	C	139	LEU
1	C	170	ARG
1	C	174	GLU
1	C	189	ASN
1	C	206	VAL
1	C	311	LEU

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Mol	Chain	Res	Type
1	D	66	HIS
1	D	82	SER
1	D	115	LEU
1	D	165	SER
1	D	189	ASN
1	D	206	VAL
1	D	259	GLU
1	D	286	LYS
1	D	291	GLN
1	D	331	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	92	HIS
1	A	119	HIS
1	A	151	HIS
1	A	197	HIS
1	A	222	HIS
1	A	241	HIS
1	A	255	GLN
1	A	275	GLN
1	A	308	GLN
1	A	317	GLN
1	A	325	GLN
1	A	330	ASN
1	A	336	GLN
1	B	90	GLN
1	B	92	HIS
1	B	119	HIS
1	B	144	ASN
1	B	151	HIS
1	B	197	HIS
1	B	222	HIS
1	B	275	GLN
1	B	291	GLN
1	B	336	GLN
1	C	27	GLN
1	C	107	ASN
1	C	117	ASN
1	C	151	HIS

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Mol	Chain	Res	Type
1	C	189	ASN
1	C	197	HIS
1	C	222	HIS
1	C	255	GLN
1	C	275	GLN
1	C	291	GLN
1	C	308	GLN
1	C	336	GLN
1	D	27	GLN
1	D	74	ASN
1	D	107	ASN
1	D	125	GLN
1	D	151	HIS
1	D	197	HIS
1	D	222	HIS
1	D	255	GLN
1	D	275	GLN
1	D	291	GLN
1	D	308	GLN
1	D	317	GLN
1	D	336	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 ligands 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	$\# Z > 2$
3	PEG	A	607	-	6,6,6	0.13	0	5,5,5	0.11	0
4	ASN	D	407	-	6,8,8	0.81	0	8,10,10	0.79	0
4	ASN	B	405	-	6,8,8	0.69	0	8,10,10	0.89	0
3	PEG	A	603	-	6,6,6	0.43	0	5,5,5	0.21	0
4	ASN	C	607	-	6,8,8	0.76	0	8,10,10	0.85	0
2	SO4	A	602	-	4,4,4	0.35	0	6,6,6	0.12	0
3	PEG	A	605	-	6,6,6	0.25	0	5,5,5	0.19	0
3	PEG	D	403	-	6,6,6	0.47	0	5,5,5	0.32	0
3	PEG	A	604	-	6,6,6	0.79	0	5,5,5	0.48	0
3	PEG	C	601	-	6,6,6	0.26	0	5,5,5	0.21	0
3	PEG	D	404	-	6,6,6	0.23	0	5,5,5	0.16	0
3	PEG	D	405	-	6,6,6	0.76	0	5,5,5	0.65	0
3	PEG	B	403	-	6,6,6	0.69	0	5,5,5	0.73	0
4	ASN	B	406	-	6,8,8	0.91	1 (16%)	8,10,10	0.60	0
4	ASN	A	608	-	6,8,8	0.88	0	8,10,10	0.79	0
4	ASN	D	406	-	6,8,8	0.82	0	8,10,10	0.91	0
3	PEG	C	602	-	6,6,6	0.53	0	5,5,5	0.37	0
3	PEG	C	603	-	6,6,6	0.30	0	5,5,5	0.12	0
2	SO4	C	604	-	4,4,4	0.41	0	6,6,6	0.11	0
2	SO4	C	605	-	4,4,4	0.37	0	6,6,6	0.12	0
3	PEG	D	401	-	6,6,6	0.37	0	5,5,5	0.22	0
2	SO4	B	404	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	A	601	-	4,4,4	0.32	0	6,6,6	0.08	0
3	PEG	B	401	-	6,6,6	0.59	0	5,5,5	0.48	0
2	SO4	C	606	-	4,4,4	0.34	0	6,6,6	0.10	0
4	ASN	A	609	-	6,8,8	0.83	0	8,10,10	0.77	0
4	ASN	C	608	-	6,8,8	0.68	0	8,10,10	1.53	1 (12%)
3	PEG	A	606	-	6,6,6	0.43	0	5,5,5	0.24	0
3	PEG	B	402	-	6,6,6	0.13	0	5,5,5	0.14	0
3	PEG	D	402	-	6,6,6	0.78	0	5,5,5	0.49	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	607	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ASN	D	407	-	-	0/8/8/8	-
4	ASN	B	405	-	-	2/8/8/8	-
3	PEG	A	603	-	-	3/4/4/4	-
4	ASN	C	607	-	-	2/8/8/8	-
3	PEG	A	605	-	-	4/4/4/4	-
3	PEG	D	403	-	-	3/4/4/4	-
3	PEG	A	604	-	-	3/4/4/4	-
3	PEG	C	601	-	-	1/4/4/4	-
3	PEG	D	404	-	-	3/4/4/4	-
3	PEG	D	405	-	-	3/4/4/4	-
3	PEG	B	403	-	-	3/4/4/4	-
4	ASN	B	406	-	-	0/8/8/8	-
4	ASN	A	608	-	-	2/8/8/8	-
4	ASN	D	406	-	-	2/8/8/8	-
3	PEG	C	602	-	-	2/4/4/4	-
3	PEG	C	603	-	-	4/4/4/4	-
3	PEG	D	401	-	-	3/4/4/4	-
3	PEG	B	401	-	-	1/4/4/4	-
4	ASN	C	608	-	-	2/8/8/8	-
4	ASN	A	609	-	-	0/8/8/8	-
3	PEG	A	606	-	-	2/4/4/4	-
3	PEG	B	402	-	-	2/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	406	ASN	OXT-C	-2.08	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	608	ASN	CA-CB-CG	-2.99	106.29	112.24

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	608	ASN	C-CA-CB-CG
3	B	403	PEG	C1-C2-O2-C3
3	D	403	PEG	C4-C3-O2-C2
3	A	604	PEG	O2-C3-C4-O4
3	C	602	PEG	C1-C2-O2-C3
3	B	402	PEG	O1-C1-C2-O2
3	D	402	PEG	O1-C1-C2-O2
3	D	403	PEG	O1-C1-C2-O2
4	D	406	ASN	CA-CB-CG-OD1
3	D	405	PEG	O1-C1-C2-O2
3	A	604	PEG	O1-C1-C2-O2
3	B	402	PEG	O2-C3-C4-O4
3	C	601	PEG	O1-C1-C2-O2
3	D	402	PEG	O2-C3-C4-O4
4	C	608	ASN	N-CA-CB-CG
4	A	608	ASN	CA-CB-CG-OD1
4	A	608	ASN	CA-CB-CG-ND2
4	B	405	ASN	CA-CB-CG-ND2
4	C	607	ASN	CA-CB-CG-OD1
4	C	607	ASN	CA-CB-CG-ND2
4	D	406	ASN	CA-CB-CG-ND2
3	A	603	PEG	O2-C3-C4-O4
3	D	401	PEG	O2-C3-C4-O4
3	A	606	PEG	O1-C1-C2-O2
3	B	403	PEG	O1-C1-C2-O2
4	B	405	ASN	CA-CB-CG-OD1
3	A	603	PEG	O1-C1-C2-O2
3	D	404	PEG	O2-C3-C4-O4
3	A	603	PEG	C4-C3-O2-C2
3	C	603	PEG	O2-C3-C4-O4
3	C	602	PEG	C4-C3-O2-C2
3	D	405	PEG	C4-C3-O2-C2
3	A	605	PEG	C4-C3-O2-C2
3	D	402	PEG	C1-C2-O2-C3
3	D	401	PEG	C1-C2-O2-C3
3	C	603	PEG	C4-C3-O2-C2
3	A	604	PEG	C4-C3-O2-C2
3	A	605	PEG	O2-C3-C4-O4
3	A	606	PEG	O2-C3-C4-O4
3	C	603	PEG	O1-C1-C2-O2
3	D	404	PEG	O1-C1-C2-O2
3	C	603	PEG	C1-C2-O2-C3
3	A	605	PEG	C1-C2-O2-C3

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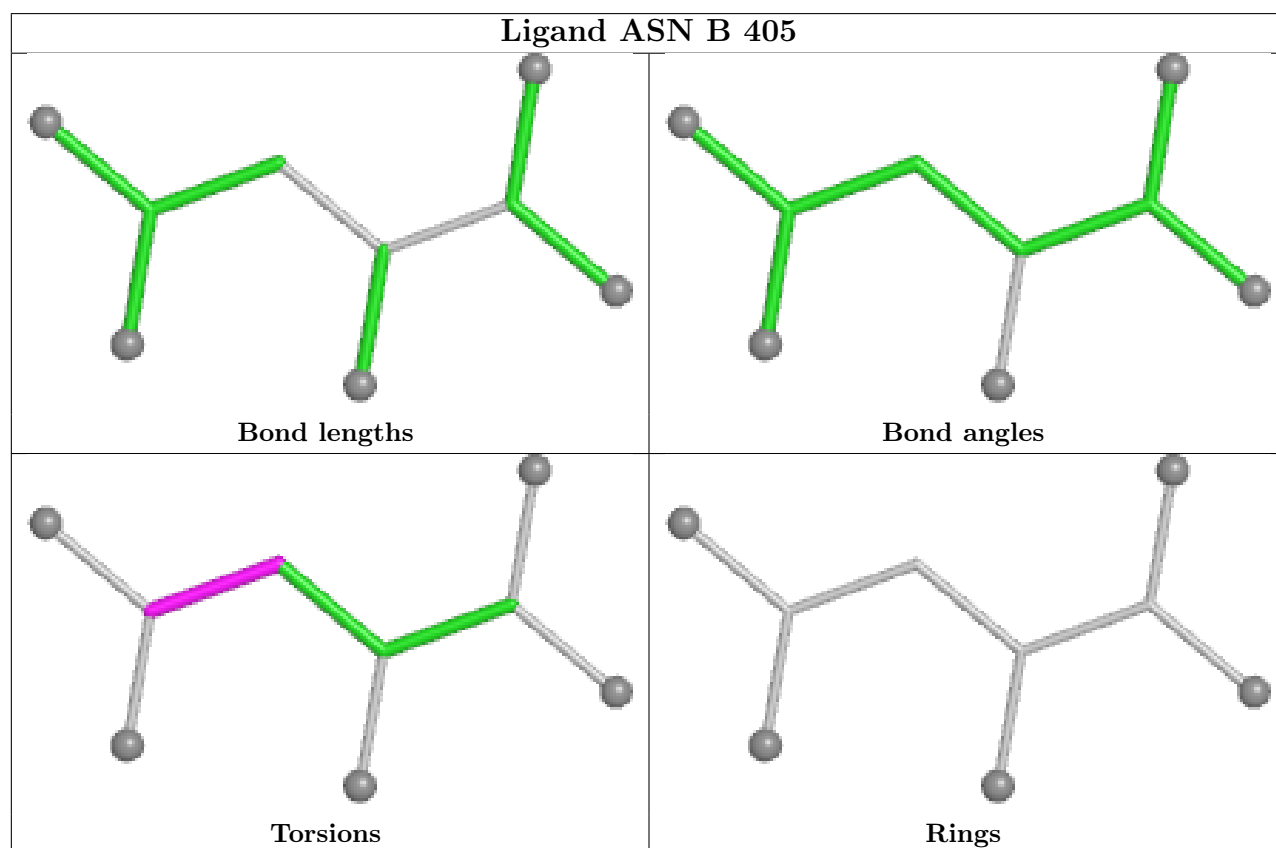
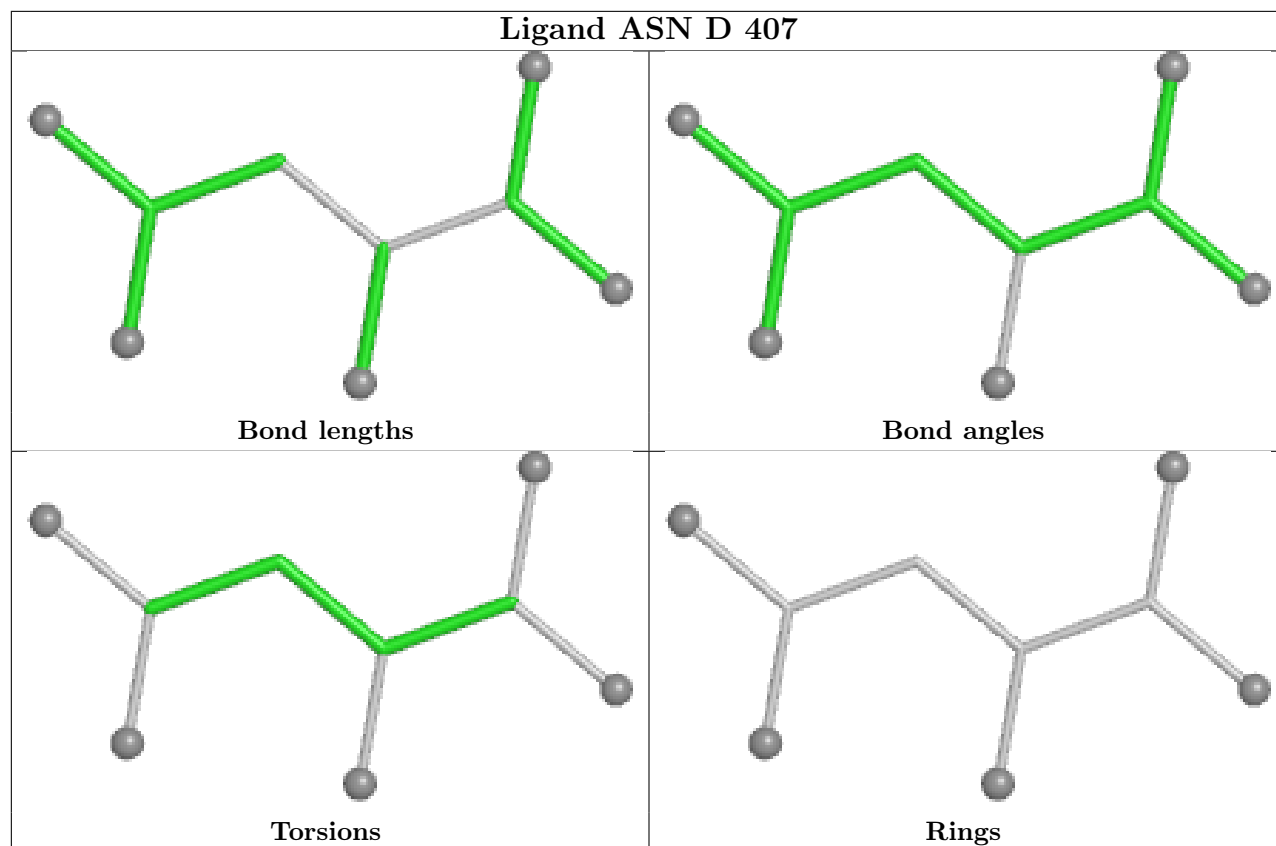
Mol	Chain	Res	Type	Atoms
3	B	401	PEG	C1-C2-O2-C3
3	A	605	PEG	O1-C1-C2-O2
3	D	403	PEG	O2-C3-C4-O4
3	D	401	PEG	O1-C1-C2-O2
3	D	404	PEG	C4-C3-O2-C2
3	A	607	PEG	O2-C3-C4-O4
3	B	403	PEG	O2-C3-C4-O4
3	D	405	PEG	C1-C2-O2-C3

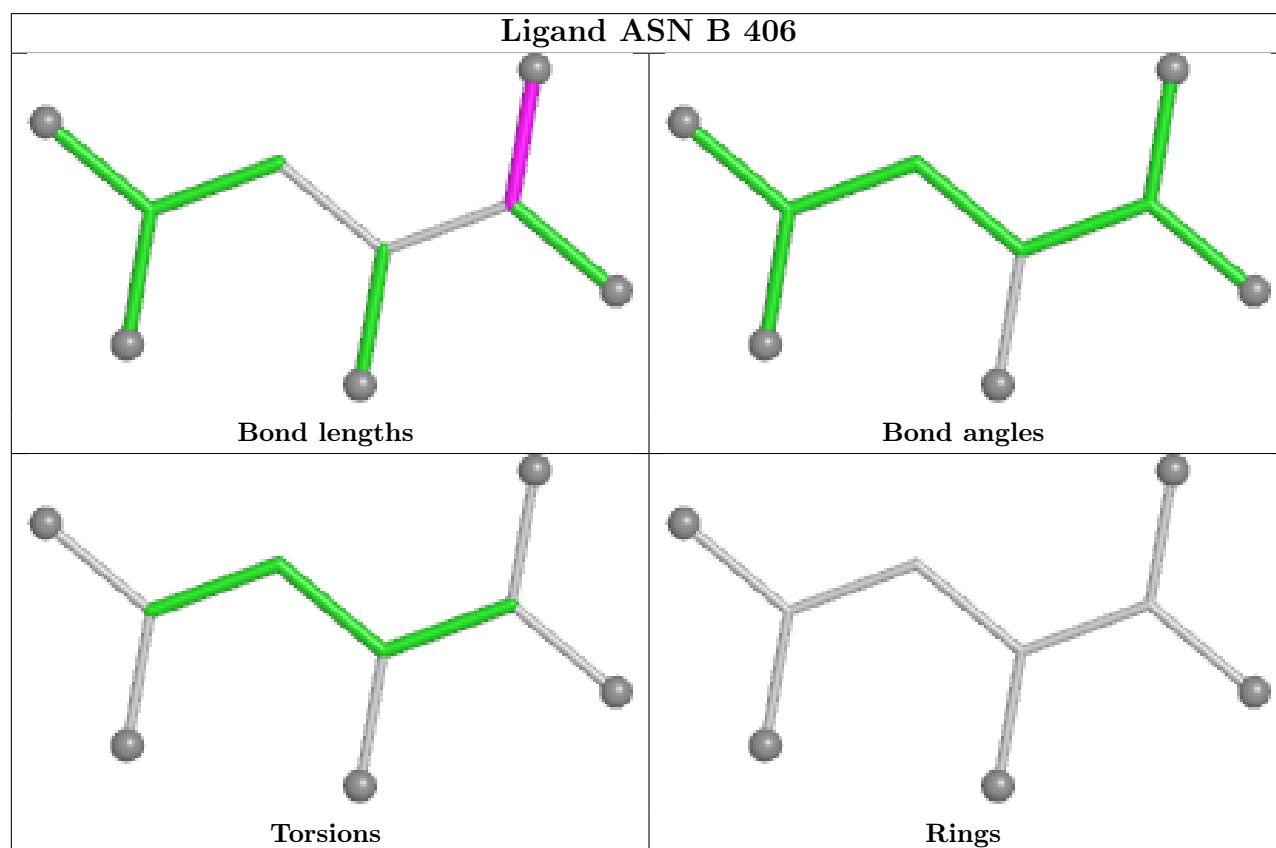
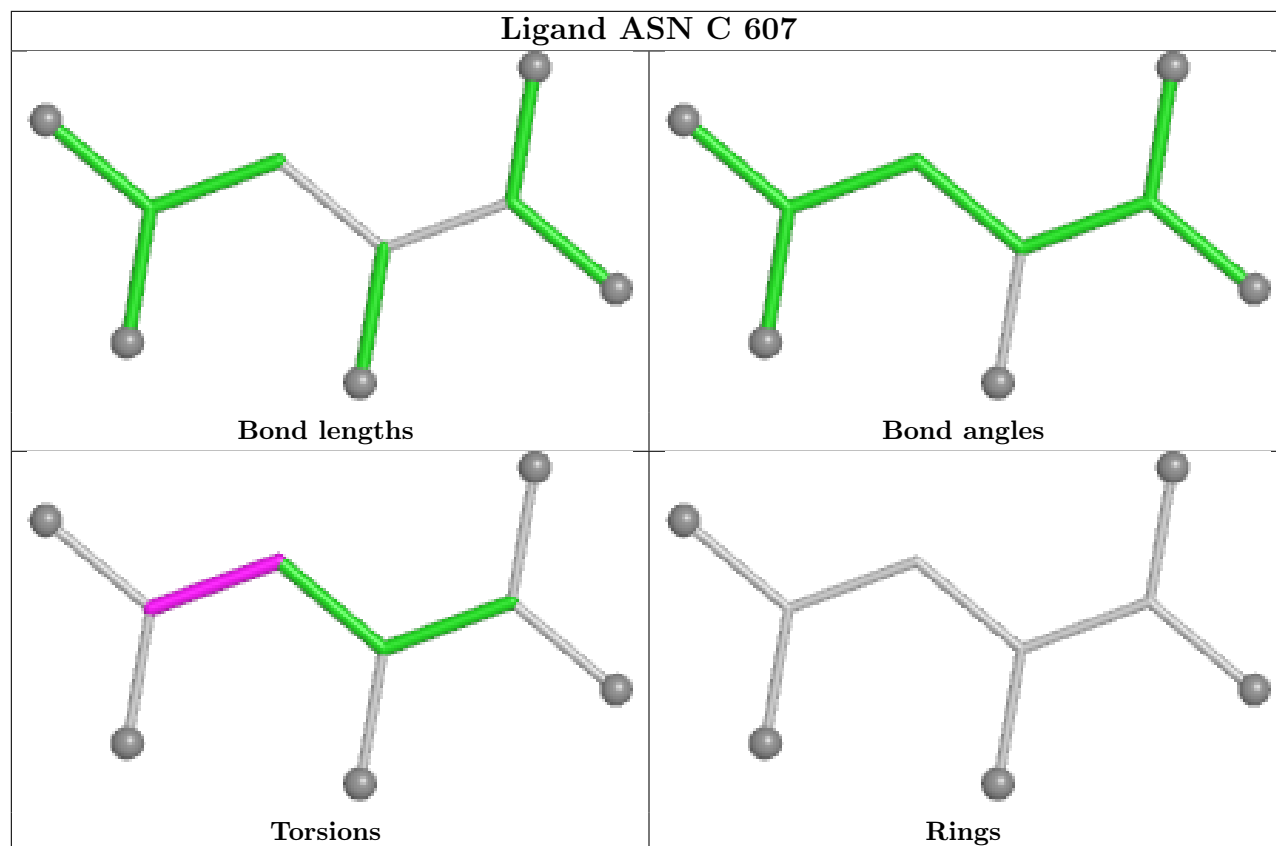
There are no ring outliers.

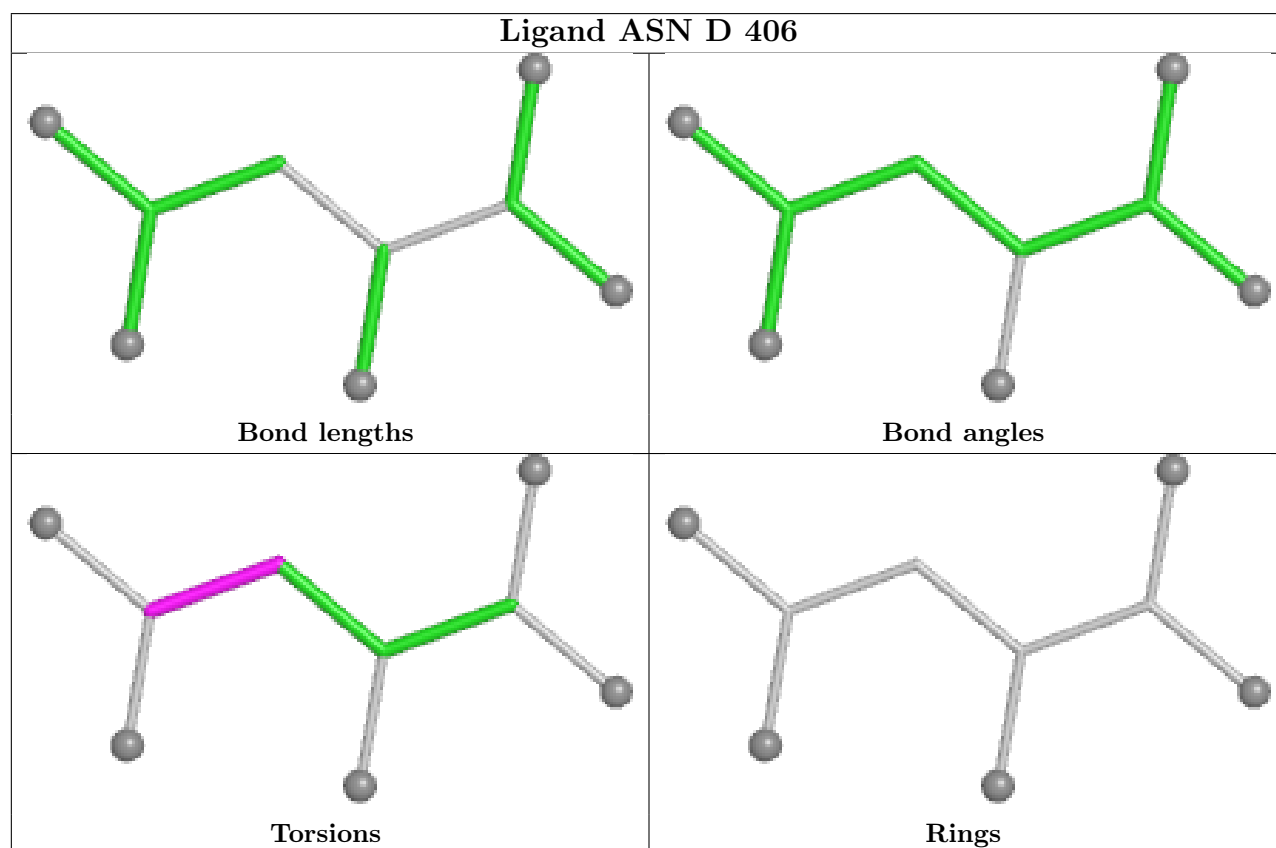
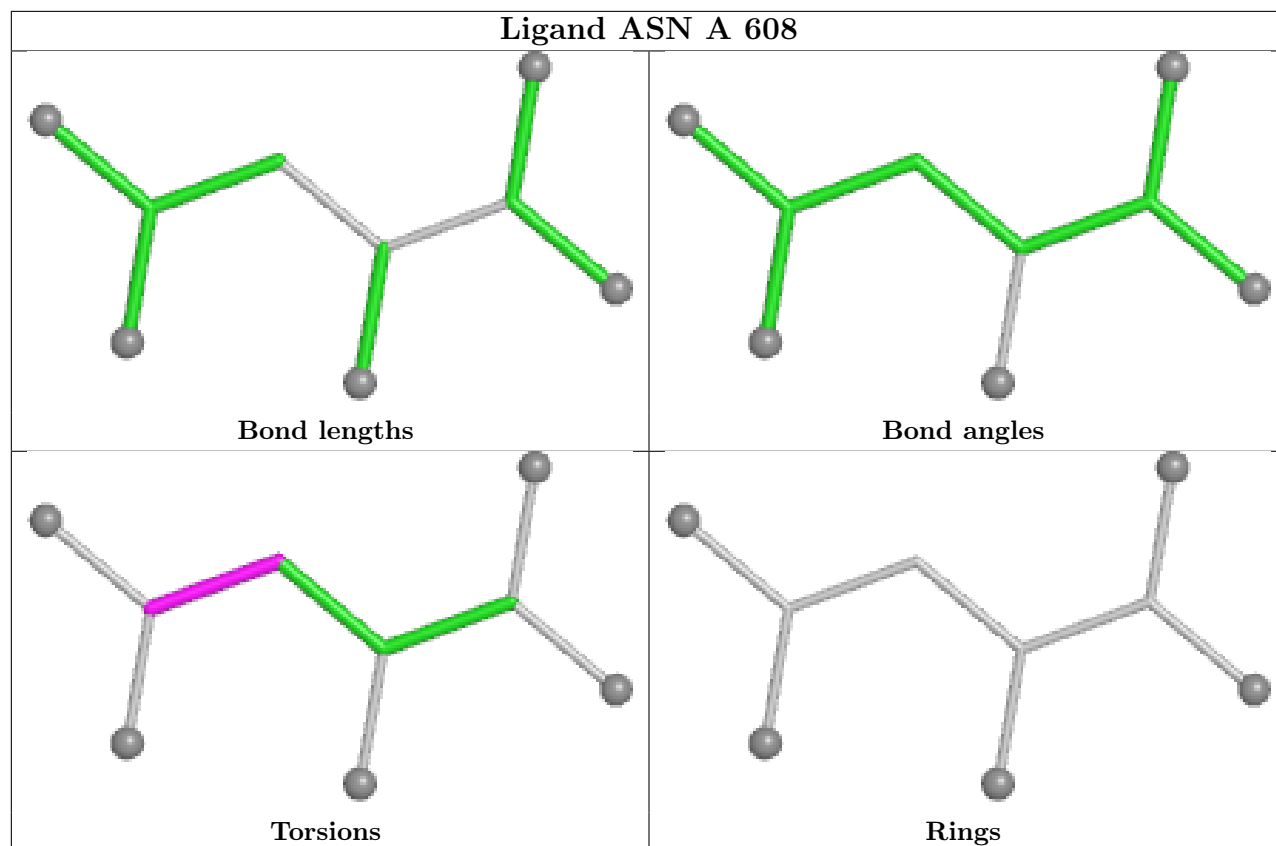
15 monomers are involved in 28 short contacts:

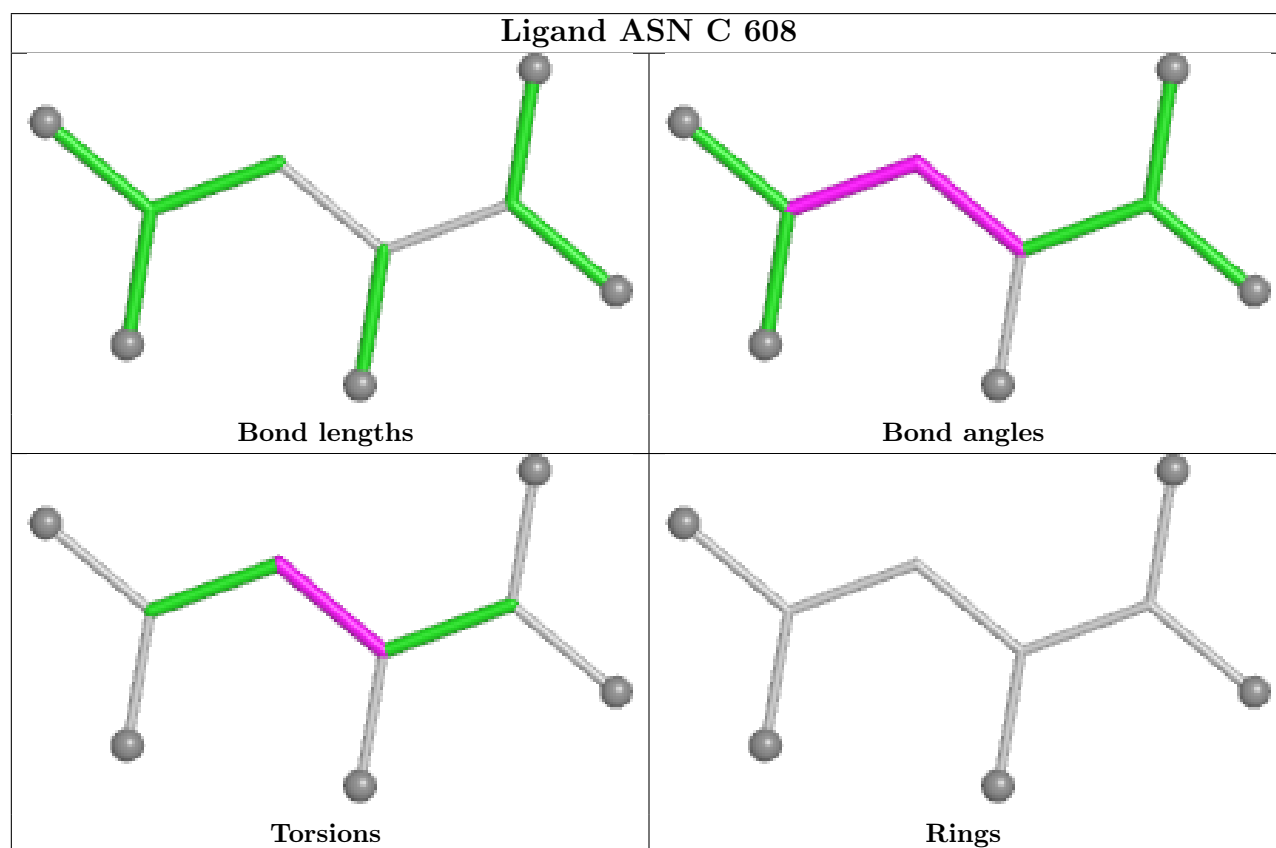
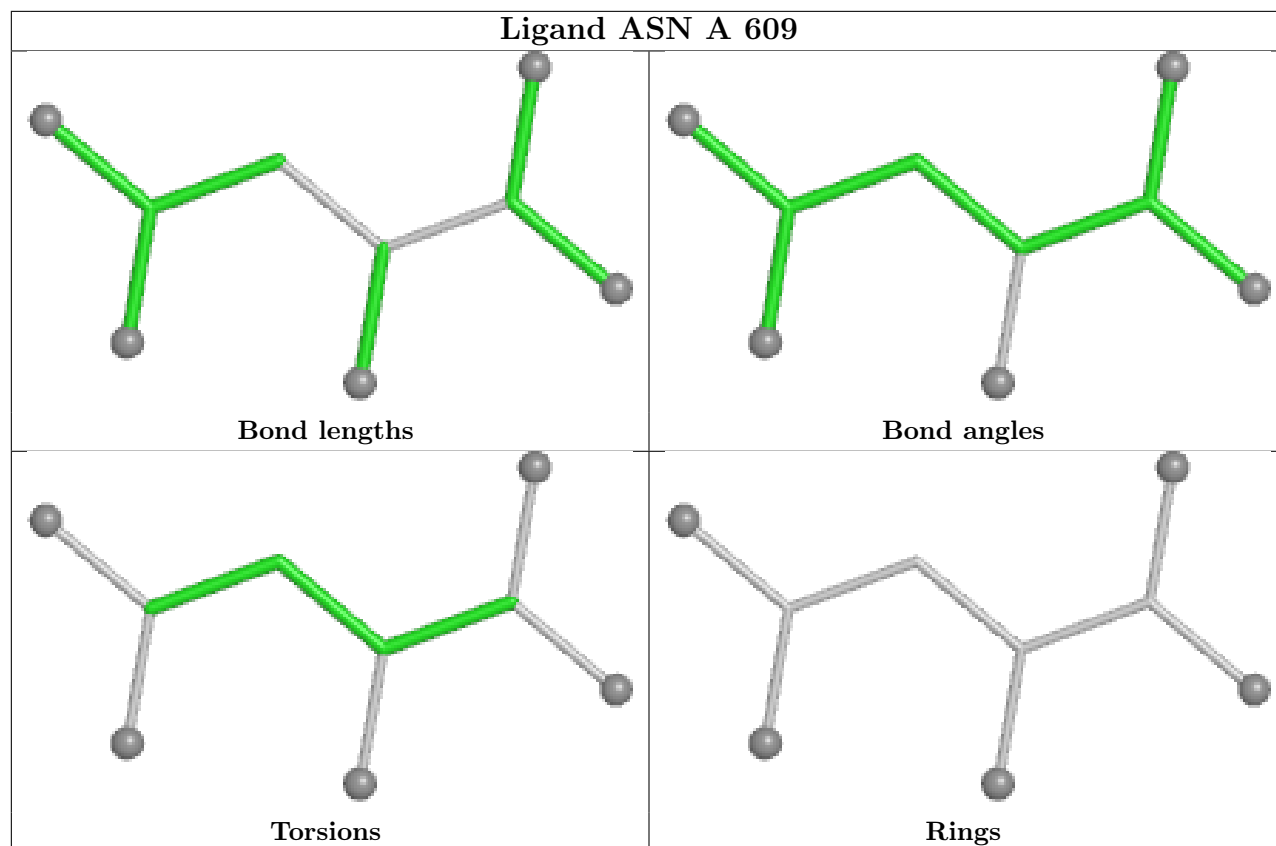
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	607	PEG	2	0
4	B	405	ASN	1	0
4	C	607	ASN	1	0
3	A	605	PEG	1	0
3	A	604	PEG	4	0
3	C	601	PEG	1	0
3	D	405	PEG	2	0
3	B	403	PEG	5	0
4	A	608	ASN	3	0
4	D	406	ASN	2	0
3	C	602	PEG	1	0
2	C	604	SO4	1	0
2	B	404	SO4	1	0
4	C	608	ASN	1	0
3	D	402	PEG	2	0

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	340/345 (98%)	-0.07	5 (1%) 72 71	22, 33, 54, 77	0
1	B	337/345 (97%)	-0.05	4 (1%) 76 76	22, 34, 55, 69	0
1	C	339/345 (98%)	-0.27	6 (1%) 67 66	20, 27, 44, 96	0
1	D	341/345 (98%)	-0.15	7 (2%) 63 62	20, 31, 51, 83	0
All	All	1357/1380 (98%)	-0.14	22 (1%) 70 69	20, 31, 52, 96	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	ASN	6.1
1	C	10	PHE	4.6
1	D	341	ASN	4.3
1	D	331	HIS	4.3
1	B	10	PHE	4.0
1	B	3	THR	3.5
1	C	4	ILE	3.2
1	D	1	MET	3.1
1	A	331	HIS	3.0
1	D	10	PHE	2.9
1	C	340	HIS	2.8
1	D	340	HIS	2.8
1	C	8	ASN	2.7
1	A	10	PHE	2.7
1	D	2	THR	2.7
1	C	341	ASN	2.6
1	A	2	THR	2.6
1	C	3	THR	2.5
1	A	189	ASN	2.4
1	B	8	ASN	2.3
1	B	52	TYR	2.0
1	D	189	ASN	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(\AA^2)	Q<0.9
2	SO4	A	602	5/5	0.62	0.20	110,112,121,122	0
2	SO4	C	606	5/5	0.70	0.13	70,77,86,88	0
3	PEG	D	402	7/7	0.76	0.20	32,46,50,51	0
3	PEG	A	603	7/7	0.78	0.19	56,60,64,65	0
3	PEG	A	606	7/7	0.80	0.21	56,62,69,70	0
3	PEG	C	603	7/7	0.82	0.17	45,56,65,65	0
3	PEG	A	607	7/7	0.82	0.18	50,56,62,62	0
2	SO4	A	601	5/5	0.83	0.21	87,99,106,112	0
3	PEG	A	604	7/7	0.83	0.13	31,32,34,37	0
2	SO4	C	605	5/5	0.84	0.20	93,93,105,107	0
3	PEG	B	402	7/7	0.85	0.16	57,61,63,64	0
3	PEG	B	403	7/7	0.85	0.21	35,39,44,45	0
3	PEG	D	403	7/7	0.85	0.16	39,43,50,51	0
3	PEG	D	405	7/7	0.85	0.22	33,39,40,41	0
3	PEG	D	401	7/7	0.86	0.17	54,61,67,68	0
3	PEG	B	401	7/7	0.86	0.13	35,39,40,45	0
4	ASN	C	608	9/9	0.87	0.14	25,29,40,47	0
2	SO4	B	404	5/5	0.88	0.15	74,76,92,97	0
3	PEG	A	605	7/7	0.89	0.14	54,59,61,62	0
3	PEG	C	602	7/7	0.89	0.15	38,43,44,46	0
3	PEG	C	601	7/7	0.90	0.15	45,47,49,50	0
3	PEG	D	404	7/7	0.92	0.11	61,63,66,67	0
4	ASN	B	405	9/9	0.93	0.08	28,29,30,31	0
4	ASN	A	608	9/9	0.93	0.09	29,31,34,34	0
4	ASN	A	609	9/9	0.94	0.07	25,26,27,28	0
4	ASN	B	406	9/9	0.95	0.07	27,29,33,35	0
4	ASN	C	607	9/9	0.95	0.07	24,26,27,32	0

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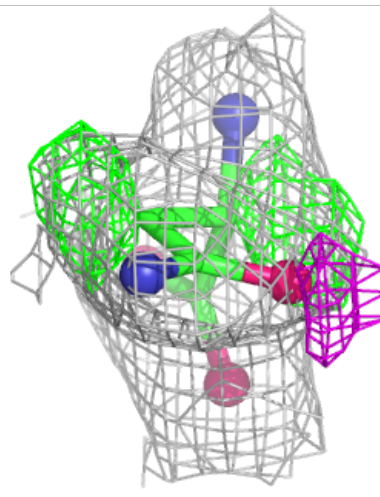
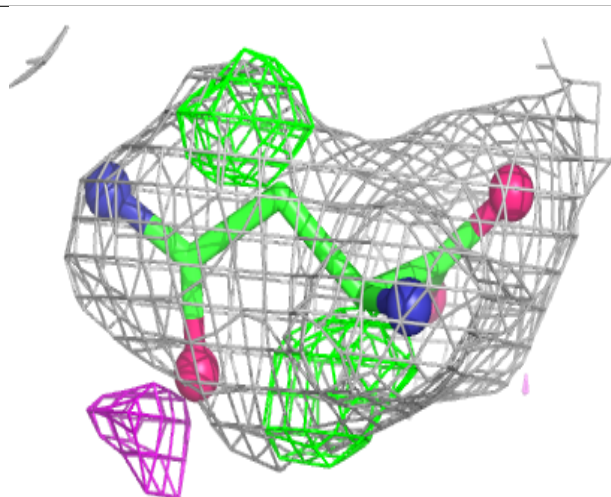
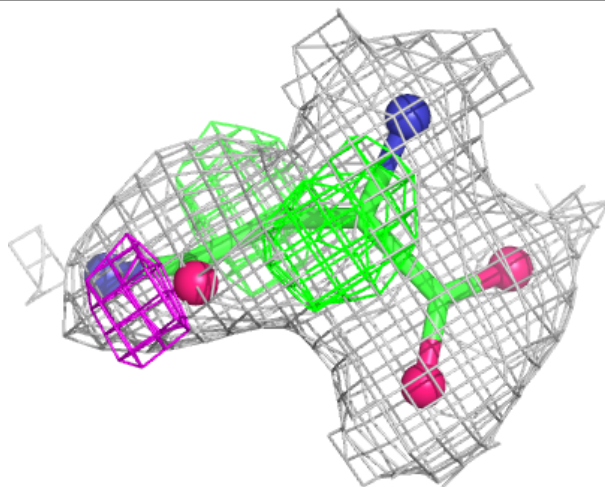
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	C	604	5/5	0.95	0.11	67,68,70,73	0
4	ASN	D	406	9/9	0.97	0.06	25,31,35,40	0
4	ASN	D	407	9/9	0.97	0.05	24,25,26,26	0

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.

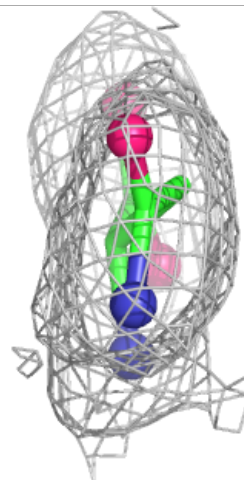
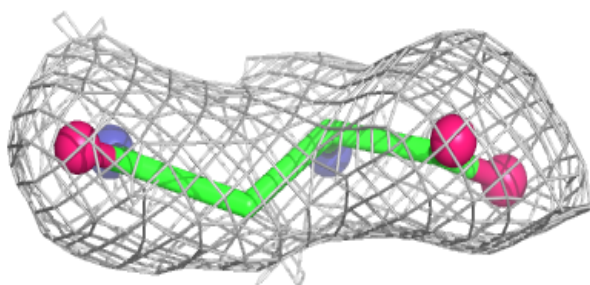
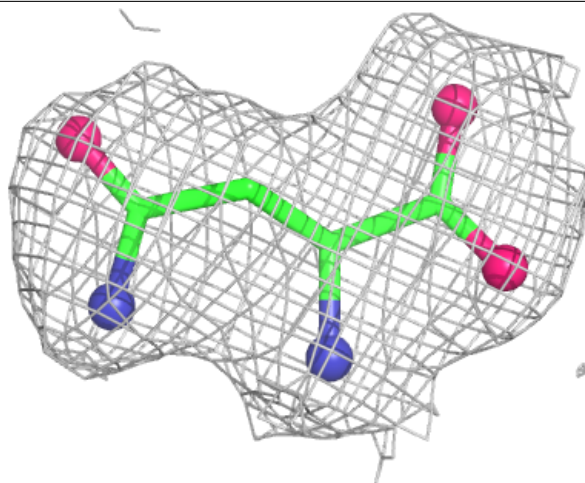
Electron density around ASN C 608:

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



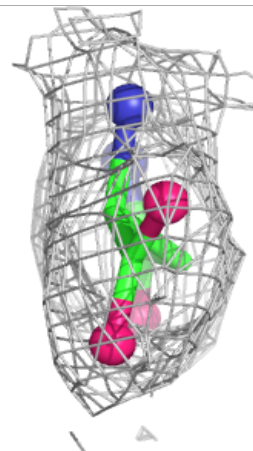
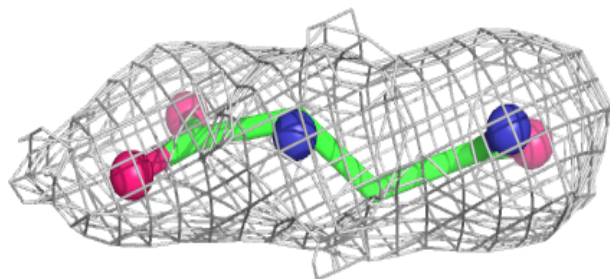
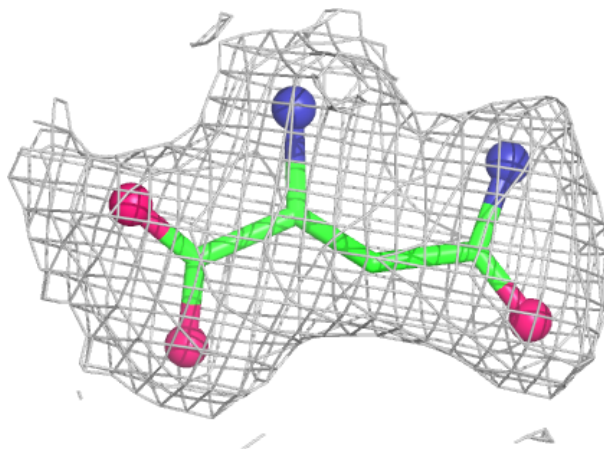
Electron density around ASN B 405:

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



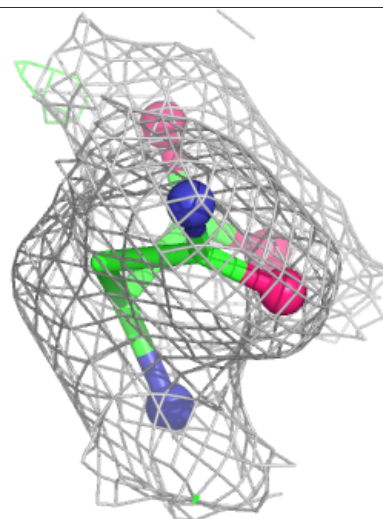
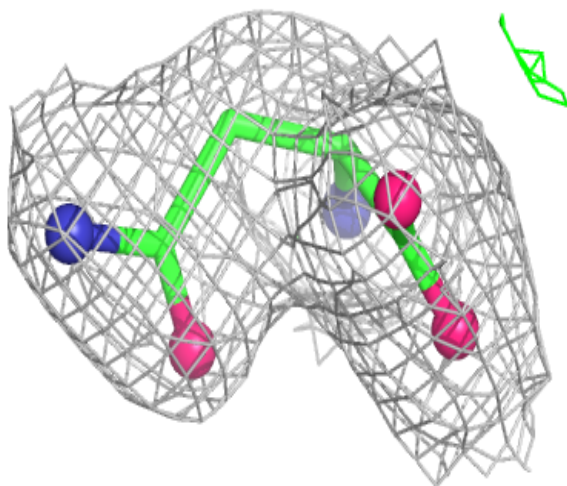
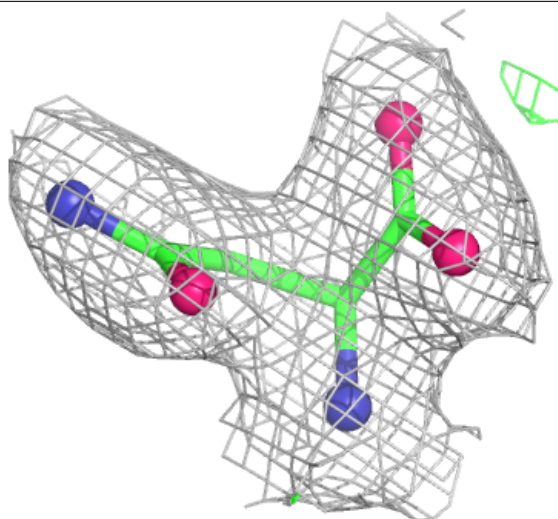
Electron density around ASN A 608:

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



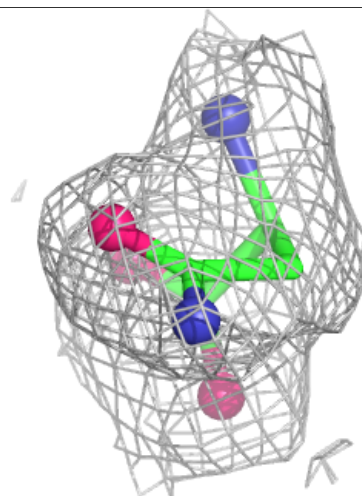
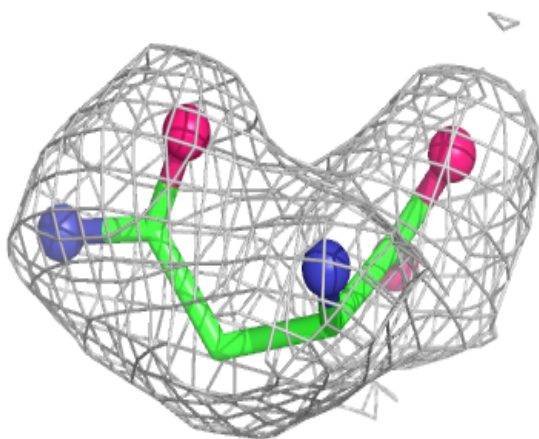
Electron density around ASN A 609:

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



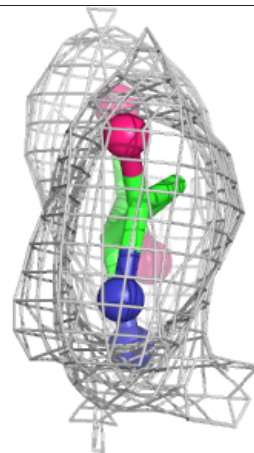
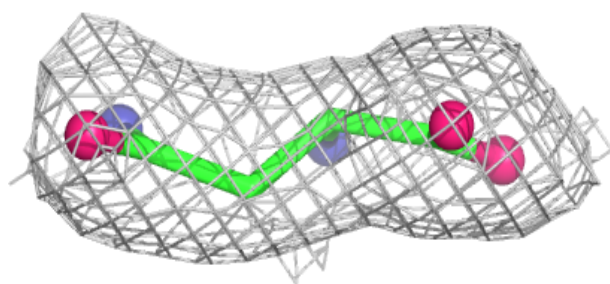
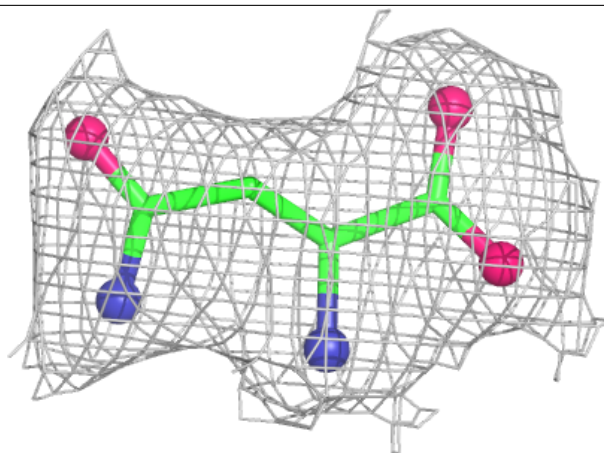
Electron density around ASN B 406:

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



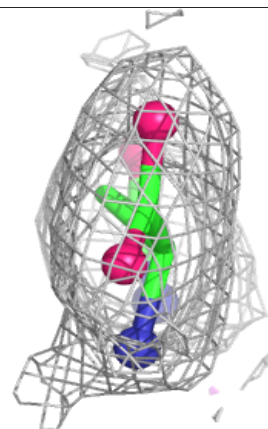
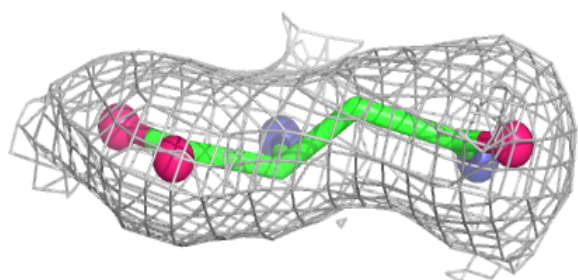
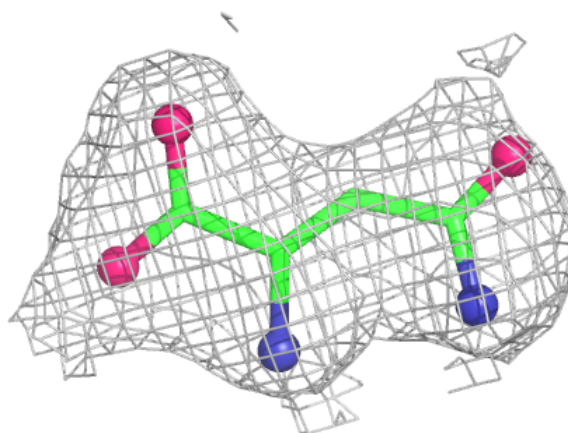
Electron density around ASN C 607:

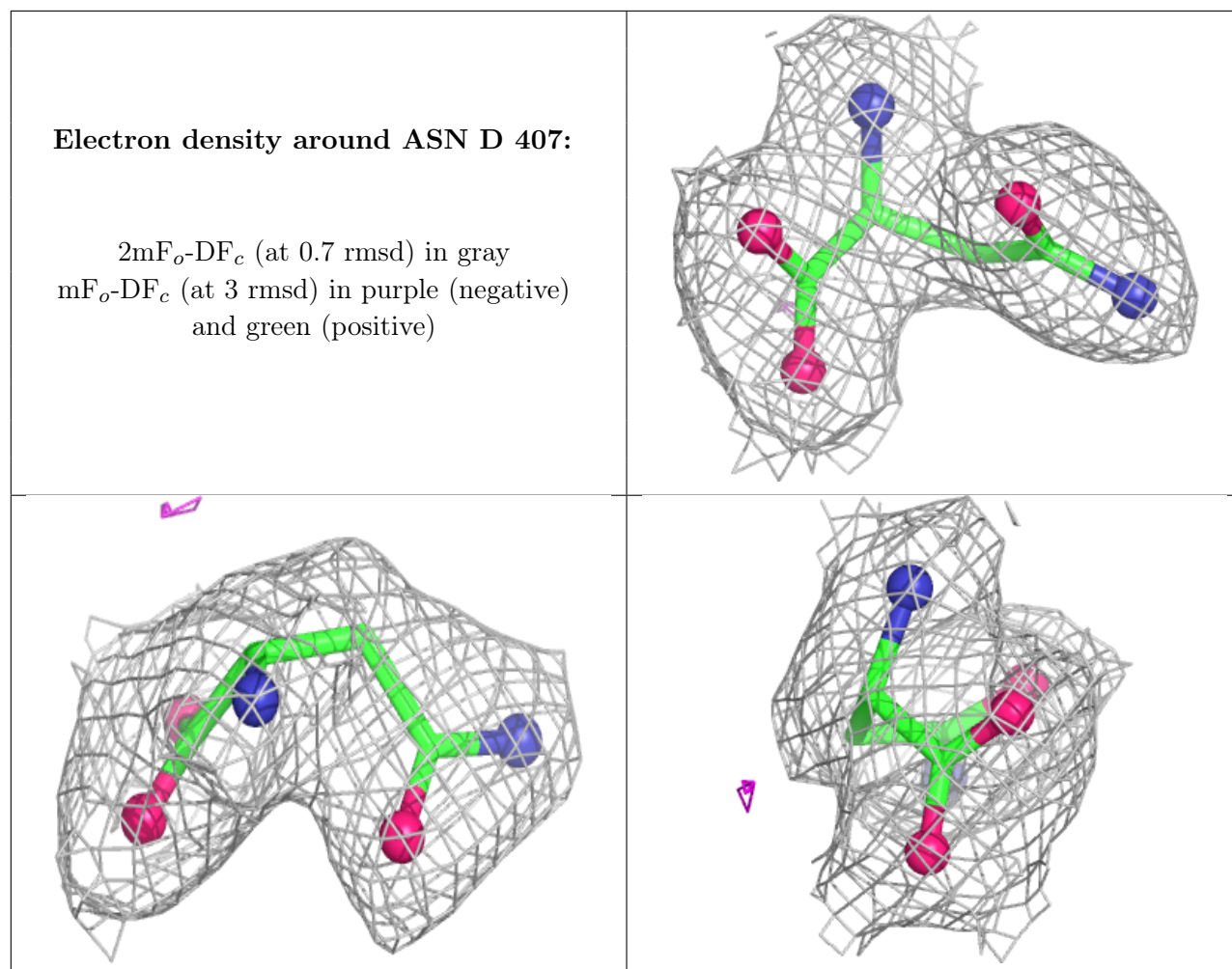
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ASN D 406:

$2mF_o-DF_c$ (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.