



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 01:50 PM EDT

PDB ID : 6UOG
Title : Asparaginase II from Escherichia coli
Authors : Araujo, T.S.; Almeida, M.S.; Lima, L.M.T.R.
Deposited on : 2019-10-14
Resolution : 2.29 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 : 2.23.2
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) : 2.23.2

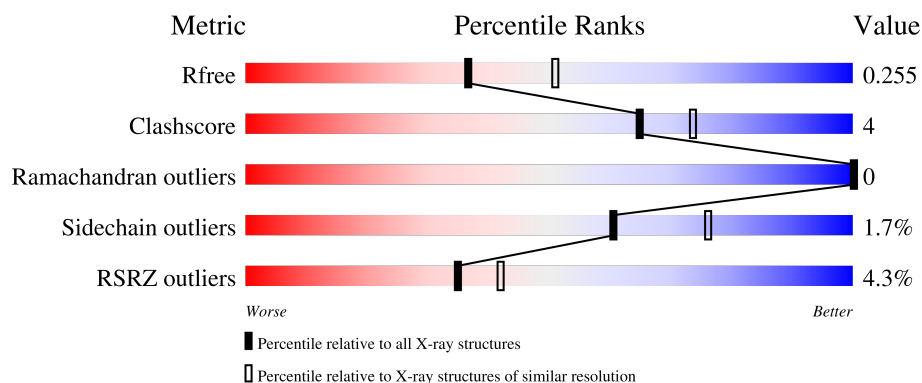
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	326	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	326	<div> <div></div> <div>93%</div> <div>7%</div> </div>
1	C	326	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	326	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	E	326	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	326	<div><div></div><div>16%</div><div></div><div>92%</div><div></div><div>8%</div></div>
1	G	326	<div><div></div><div>10%</div><div></div><div>84%</div><div></div><div>15%</div><div></div><div>•</div></div>
1	H	326	<div><div></div><div>3%</div><div></div><div>92%</div><div></div><div>8%</div></div>

2 Entry composition

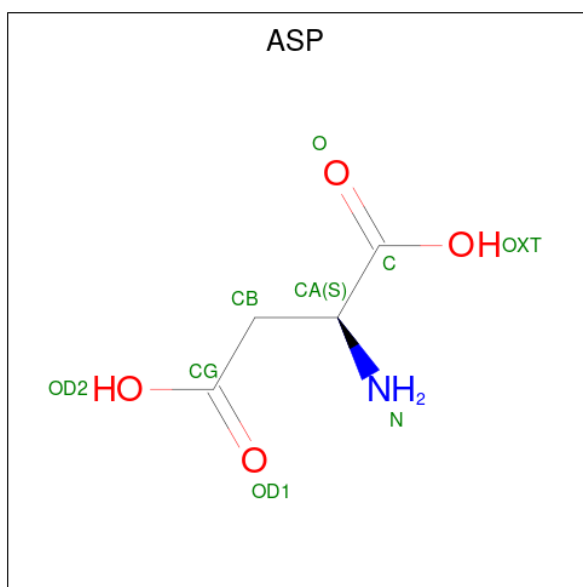
There are 3 unique types of molecules in this entry. The entry contains 20127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			
1	B	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			
1	C	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			
1	D	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			
1	E	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			
1	F	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			
1	G	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			
1	H	326	Total	C	N	O	S	0	0	0
			2430	1515	416	491	8			

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		
2	C	1	Total	C	N	O	0	0
			9	4	1	4		
2	D	1	Total	C	N	O	0	0
			9	4	1	4		
2	E	1	Total	C	N	O	0	0
			9	4	1	4		
2	F	1	Total	C	N	O	0	0
			9	4	1	4		
2	G	1	Total	C	N	O	0	0
			9	4	1	4		
2	H	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	99	Total	O	0	0
			99	99		
3	C	98	Total	O	0	0
			98	98		
3	D	95	Total	O	0	0
			95	95		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	79	Total 79	O 79	0	0
3	F	40	Total 40	O 40	0	0
3	G	53	Total 53	O 53	0	0
3	H	61	Total 61	O 61	0	0

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.

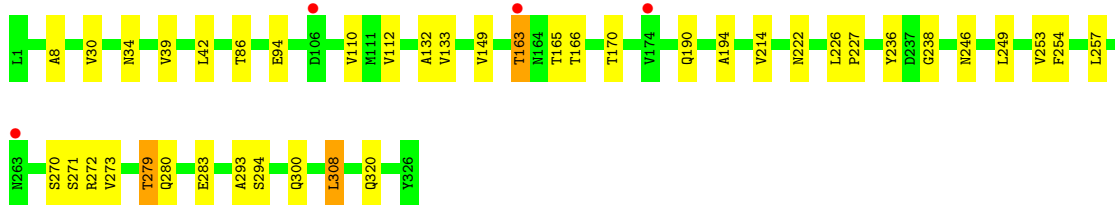
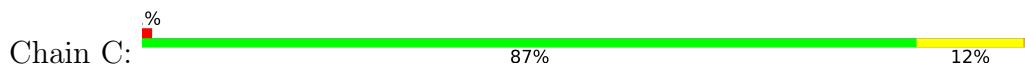
- Molecule 1: L-asparaginase 2



- Molecule 1: L-asparaginase 2



- Molecule 1: L-asparaginase 2

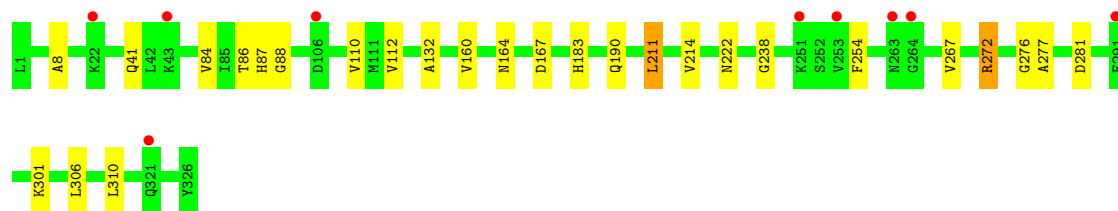


- Molecule 1: L-asparaginase 2

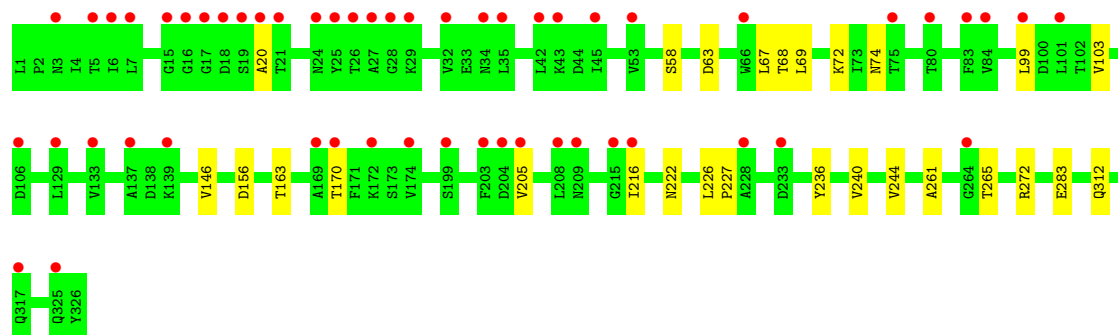
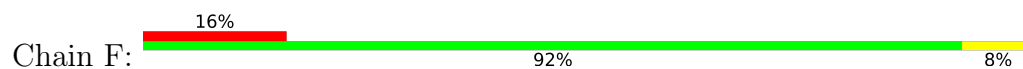


- Molecule 1: L-asparaginase 2

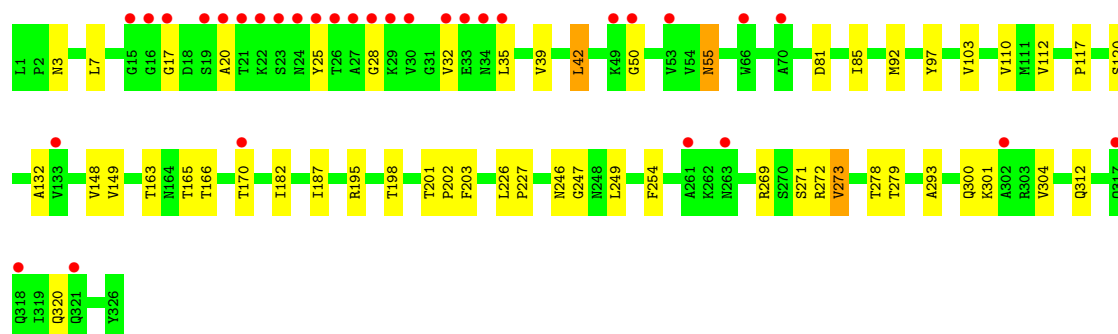
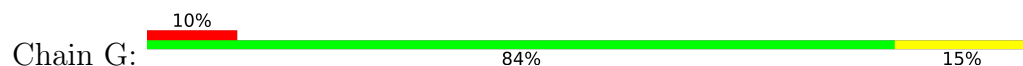




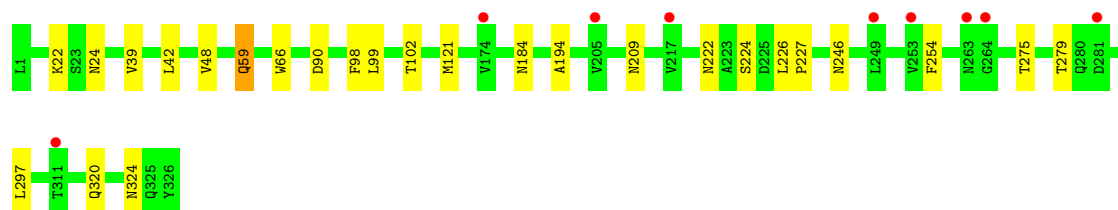
● Molecule 1: L-asparaginase 2



● Molecule 1: L-asparaginase 2



● Molecule 1: L-asparaginase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.99Å 60.16Å 151.11Å 90.00° 117.31° 90.00°	Depositor
Resolution (Å)	47.07 – 2.29 47.07 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.07-2.29) 98.5 (47.07-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.225 , 0.262 0.222 , 0.255	Depositor DCC
R_{free} test set	4868 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.863 for H, K, L 0.137 for -H, -K, H+L	Depositor
Outliers	5 of 100054 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20127	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.49 % 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 2.7163e-05. 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 [i](#)

5.1 Standard geometry [i](#)

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	0.66	0/2467	0.73	0/3359
1	B	0.65	0/2467	0.72	0/3359
1	C	0.65	0/2467	0.74	0/3359
1	D	0.66	0/2467	0.73	0/3359
1	E	0.66	0/2467	0.73	0/3359
1	F	0.67	0/2467	0.73	0/3359
1	G	0.66	0/2467	0.74	0/3359
1	H	0.66	0/2467	0.73	0/3359
All	All	0.66	0/19736	0.73	0/26872

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2430	0	2419	21	0
1	B	2430	0	2419	17	0
1	C	2430	0	2419	36	0
1	D	2430	0	2419	18	0
1	E	2430	0	2419	19	0
1	F	2430	0	2419	18	0
1	G	2430	0	2419	42	0
1	H	2430	0	2419	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	0	3	1	0
2	B	9	0	3	0	0
2	C	9	0	3	0	0
2	D	9	0	3	0	0
2	E	9	0	3	0	0
2	F	9	0	3	1	0
2	G	9	0	3	0	0
2	H	9	0	3	1	0
3	A	90	0	0	0	0
3	B	99	0	0	1	0
3	C	98	0	0	0	0
3	D	95	0	0	0	0
3	E	79	0	0	0	0
3	F	40	0	0	0	0
3	G	53	0	0	0	0
3	H	61	0	0	0	0
All	All	20127	0	19376	161	0

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

All (161) 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:112:VAL:HG11	1:A:132:ALA:HB2	1.44	1.00
1:C:112:VAL:HG21	1:C:132:ALA:HB2	1.45	0.97
1:G:246:ASN:HD21	1:G:279:THR:HG22	1.29	0.93
1:D:246:ASN:HD21	1:D:279:THR:HG22	1.37	0.90
1:C:112:VAL:HG21	1:C:132:ALA:CB	2.02	0.89
1:A:112:VAL:CG1	1:A:132:ALA:HB2	2.08	0.84
1:E:112:VAL:CG1	1:E:132:ALA:HB2	2.09	0.83
1:E:112:VAL:HG11	1:E:132:ALA:HB2	1.60	0.83
1:B:164:ASN:HD22	1:D:275:THR:HG22	1.44	0.82
1:C:112:VAL:CG2	1:C:132:ALA:HB2	2.09	0.82
1:H:59:GLN:H	1:H:59:GLN:HE21	1.28	0.81
1:A:277:ALA:O	1:C:165:THR:HG21	1.84	0.79
1:H:246:ASN:HD21	1:H:279:THR:HG22	1.46	0.78
1:E:164:ASN:HD22	1:E:167:ASP:H	1.34	0.74
1:E:112:VAL:HG11	1:E:132:ALA:CB	2.18	0.74
1:F:163:THR:O	1:H:275:THR:HG22	1.88	0.73
1:G:246:ASN:HD21	1:G:279:THR:CG2	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG11	1:A:132:ALA:CB	2.18	0.72
1:B:164:ASN:HD22	1:D:275:THR:CG2	2.01	0.72
1:G:32:VAL:HG11	1:G:50:GLY:HA3	1.73	0.71
1:F:163:THR:HB	1:F:170:THR:O	1.89	0.71
1:G:112:VAL:HG21	1:G:132:ALA:CB	2.19	0.71
1:C:163:THR:HG22	1:C:170:THR:O	1.92	0.68
1:D:246:ASN:ND2	1:D:279:THR:HG22	2.08	0.68
1:C:293:ALA:H	1:C:320:GLN:HE22	1.42	0.67
1:G:246:ASN:ND2	1:G:279:THR:HG22	2.06	0.66
1:C:112:VAL:CG2	1:C:132:ALA:CB	2.72	0.66
1:B:164:ASN:ND2	1:D:275:THR:HG22	2.11	0.66
1:D:246:ASN:HD21	1:D:279:THR:CG2	2.08	0.66
1:A:63:ASP:H	1:C:222:ASN:HD22	1.44	0.66
1:G:293:ALA:H	1:G:320:GLN:HE22	1.42	0.65
1:E:112:VAL:CG1	1:E:132:ALA:CB	2.75	0.64
1:G:165:THR:HG23	1:G:166:THR:HG23	1.80	0.64
1:G:112:VAL:CG2	1:G:132:ALA:CB	2.76	0.64
1:B:74:ASN:HD21	1:B:104:LYS:H	1.46	0.63
1:H:246:ASN:ND2	1:H:279:THR:HG22	2.13	0.62
1:G:39:VAL:HG13	1:G:42:LEU:HD22	1.82	0.61
1:G:20:ALA:HA	1:G:120:SER:HA	1.82	0.61
1:C:271:SER:OG	1:C:273:VAL:HG13	2.02	0.60
1:G:201:THR:CG2	1:G:203:PHE:CD2	2.86	0.59
1:C:165:THR:HG23	1:C:166:THR:HG23	1.83	0.59
1:G:271:SER:OG	1:G:273:VAL:HG13	2.02	0.59
1:H:246:ASN:HD21	1:H:279:THR:CG2	2.16	0.58
1:G:32:VAL:HA	1:G:35:LEU:HD12	1.86	0.58
1:F:63:ASP:CG	1:H:222:ASN:HD22	2.07	0.58
1:G:32:VAL:HG11	1:G:50:GLY:CA	2.34	0.57
1:A:183:HIS:CE1	1:D:279:THR:HG21	2.40	0.57
1:E:277:ALA:O	1:G:165:THR:HG21	2.06	0.56
1:F:58:SER:OG	2:F:401:ASP:O	2.21	0.55
1:G:28:GLY:C	1:G:55:ASN:HD21	2.09	0.55
1:G:249:LEU:HD22	1:G:249:LEU:N	2.21	0.55
1:C:246:ASN:HD21	1:C:279:THR:HG22	1.71	0.55
1:G:112:VAL:CG2	1:G:132:ALA:HB2	2.37	0.55
1:G:226:LEU:HB2	1:G:227:PRO:HD3	1.88	0.54
1:A:112:VAL:CG1	1:A:132:ALA:CB	2.83	0.54
1:G:202:PRO:HB2	1:G:312:GLN:HE22	1.71	0.54
1:A:163:THR:HB	1:A:170:THR:O	2.07	0.54
1:A:272:ARG:CZ	1:C:300:GLN:HG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:ASN:O	1:G:81:ASP:HB2	2.09	0.53
1:H:99:LEU:HA	1:H:102:THR:HG22	1.90	0.52
1:E:183:HIS:CE1	1:H:279:THR:HG21	2.44	0.52
1:B:74:ASN:ND2	1:B:104:LYS:H	2.07	0.52
1:B:30:VAL:HG13	1:B:34:ASN:HD22	1.75	0.52
1:D:195:ARG:NH1	1:D:323:PHE:O	2.43	0.52
1:E:281:ASP:OD1	1:H:184:ASN:ND2	2.42	0.52
1:B:163:THR:O	1:D:275:THR:HB	2.10	0.51
1:G:17:GLY:HA2	1:G:25:TYR:HB3	1.92	0.51
1:G:92:MET:HE2	1:G:148:VAL:HG13	1.90	0.51
1:H:22:LYS:HG2	1:H:24:ASN:HD22	1.76	0.51
1:C:30:VAL:CG1	1:C:34:ASN:HB3	2.39	0.51
1:H:39:VAL:HG23	1:H:42:LEU:HD13	1.92	0.51
2:A:401:ASP:N	1:C:283:GLU:OE2	2.44	0.50
1:D:219:ASN:HD22	1:D:250:TYR:H	1.59	0.50
1:G:103:VAL:O	1:G:198:THR:HA	2.11	0.50
1:C:226:LEU:HB2	1:C:227:PRO:HD3	1.94	0.50
1:F:67:LEU:HD23	1:F:205:VAL:CG1	2.42	0.50
1:G:182:ILE:HG12	1:G:187:ILE:HG12	1.94	0.50
1:C:94:GLU:HG2	1:C:300:GLN:HB3	1.94	0.49
1:C:246:ASN:HD21	1:C:279:THR:CG2	2.24	0.49
1:G:92:MET:CE	1:G:148:VAL:HG13	2.43	0.49
1:G:201:THR:HG21	1:G:203:PHE:CD2	2.48	0.49
1:B:183:HIS:CE1	1:C:279:THR:HG21	2.48	0.49
1:E:87:HIS:HD2	1:E:88:GLY:O	1.96	0.49
1:F:244:VAL:HG22	1:H:90:ASP:HB3	1.95	0.49
1:B:84:VAL:HA	1:B:110:VAL:O	2.13	0.48
1:E:190:GLN:HA	1:H:194:ALA:HB3	1.95	0.48
1:F:67:LEU:HD23	1:F:205:VAL:HG11	1.95	0.48
1:A:243:GLY:O	1:A:272:ARG:HG2	2.13	0.48
1:C:279:THR:HG23	1:C:280:GLN:O	2.13	0.48
1:H:39:VAL:CG2	1:H:42:LEU:HD13	2.43	0.48
1:B:103:VAL:O	1:B:198:THR:HA	2.14	0.47
1:E:306:LEU:O	1:E:310:LEU:HG	2.14	0.47
1:F:99:LEU:HB3	1:F:146:VAL:HG21	1.97	0.47
1:F:226:LEU:HB2	1:F:227:PRO:HD3	1.96	0.47
1:B:60:ASP:HB3	1:D:251:LYS:HE2	1.97	0.46
1:A:87:HIS:HD2	1:A:88:GLY:O	1.98	0.46
1:A:272:ARG:NH2	1:C:300:GLN:HG3	2.31	0.45
1:G:32:VAL:CG1	1:G:50:GLY:HA3	2.44	0.45
1:F:68:THR:O	1:F:72:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LEU:O	1:G:85:ILE:HA	2.17	0.45
1:D:306:LEU:O	1:D:310:LEU:HG	2.17	0.45
1:F:67:LEU:CD2	1:F:205:VAL:CG1	2.95	0.45
1:F:261:ALA:HA	1:F:265:THR:O	2.15	0.45
1:C:8:ALA:HA	1:C:86:THR:OG1	2.17	0.45
1:D:84:VAL:HA	1:D:110:VAL:O	2.17	0.45
1:H:226:LEU:HB2	1:H:227:PRO:HD3	1.98	0.45
1:B:190:GLN:HA	1:C:194:ALA:HB3	1.99	0.45
1:B:194:ALA:HB3	1:C:190:GLN:HA	1.99	0.45
1:B:35:LEU:N	1:B:35:LEU:HD12	2.31	0.45
1:H:42:LEU:HD23	1:H:48:VAL:HG21	1.98	0.45
1:E:276:GLY:HA3	1:G:165:THR:HG22	2.00	0.44
1:B:218:TYR:HA	1:B:242:ALA:HB3	2.00	0.44
1:G:112:VAL:HG21	1:G:132:ALA:HB2	1.96	0.44
1:A:272:ARG:NH2	1:C:300:GLN:CG	2.81	0.44
1:E:84:VAL:HA	1:E:110:VAL:O	2.18	0.44
1:A:272:ARG:CZ	1:C:300:GLN:CG	2.96	0.44
1:F:216:ILE:HA	1:F:240:VAL:O	2.18	0.43
1:G:117:PRO:HG2	1:G:120:SER:HB3	2.00	0.43
1:A:167:ASP:O	1:A:170:THR:HB	2.17	0.43
1:F:69:LEU:HD12	1:F:69:LEU:HA	1.87	0.43
1:F:74:ASN:HD21	1:F:103:VAL:HA	1.84	0.43
1:A:224:SER:HB2	1:C:236:TYR:OH	2.19	0.43
1:C:253:VAL:HG12	1:C:257:LEU:HD22	2.00	0.43
1:B:151:ASN:ND2	3:B:502:HOH:O	2.46	0.43
1:D:42:LEU:HD22	1:D:133:VAL:HG21	2.01	0.43
1:E:211:LEU:HD12	1:E:211:LEU:HA	1.91	0.42
1:H:320:GLN:NE2	1:H:324:ASN:HD21	2.17	0.42
1:C:308:LEU:HD12	1:C:308:LEU:HA	1.90	0.42
1:G:269:ARG:O	1:G:278:THR:HG21	2.19	0.42
1:H:66:TRP:HB3	1:H:98:PHE:CE2	2.53	0.42
1:A:183:HIS:NE2	1:D:279:THR:HG21	2.34	0.42
1:C:270:SER:HA	1:C:294:SER:OG	2.20	0.42
1:G:39:VAL:HG23	1:H:121:MET:HE1	2.01	0.42
1:E:41:GLN:HE21	1:F:20:ALA:HB3	1.85	0.42
1:G:301:LYS:O	1:G:304:VAL:HG22	2.19	0.42
1:A:164:ASN:HD22	1:A:167:ASP:H	1.67	0.42
1:E:160:VAL:O	1:E:301:LYS:CE	2.68	0.42
1:E:272:ARG:CZ	1:G:300:GLN:HG2	2.49	0.42
1:A:84:VAL:HA	1:A:110:VAL:O	2.20	0.41
1:G:112:VAL:HG22	1:G:132:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:THR:HB	1:G:170:THR:O	2.20	0.41
1:C:110:VAL:HG13	1:C:149:VAL:HG23	2.02	0.41
1:C:246:ASN:ND2	1:C:279:THR:HG22	2.35	0.41
1:D:226:LEU:HB2	1:D:227:PRO:HD3	2.02	0.41
1:A:277:ALA:O	1:C:165:THR:CG2	2.64	0.41
1:C:214:VAL:HA	1:C:238:GLY:O	2.21	0.41
1:C:249:LEU:N	1:C:249:LEU:HD22	2.35	0.41
1:D:110:VAL:HG13	1:D:149:VAL:HG23	2.03	0.41
1:G:110:VAL:HG13	1:G:149:VAL:HG23	2.02	0.41
1:E:8:ALA:HA	1:E:86:THR:OG1	2.20	0.41
1:G:28:GLY:O	1:G:55:ASN:ND2	2.54	0.41
1:A:218:TYR:HA	1:A:242:ALA:HB3	2.02	0.41
1:F:236:TYR:OH	1:H:224:SER:HB2	2.20	0.41
1:F:283:GLU:OE2	2:H:401:ASP:N	2.54	0.41
1:C:39:VAL:HG13	1:C:42:LEU:CD1	2.50	0.41
1:C:42:LEU:HD22	1:C:133:VAL:HG21	2.02	0.41
1:B:220:TYR:CE2	1:B:223:ALA:HA	2.56	0.40
1:D:103:VAL:O	1:D:198:THR:HA	2.21	0.40
1:E:214:VAL:HA	1:E:238:GLY:O	2.21	0.40
1:G:247:GLY:HA3	1:G:278:THR:HG23	2.03	0.40
1:G:97:TYR:CD2	1:G:304:VAL:CG2	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/326 (99%)	318 (98%)	6 (2%)	0	100	100
1	B	324/326 (99%)	317 (98%)	7 (2%)	0	100	100
1	C	324/326 (99%)	318 (98%)	6 (2%)	0	100	100
1	D	324/326 (99%)	314 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	324/326 (99%)	312 (96%)	12 (4%)	0	100	100
1	F	324/326 (99%)	311 (96%)	13 (4%)	0	100	100
1	G	324/326 (99%)	316 (98%)	8 (2%)	0	100	100
1	H	324/326 (99%)	318 (98%)	6 (2%)	0	100	100
All	All	2592/2608 (99%)	2524 (97%)	68 (3%)	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	265/265 (100%)	258 (97%)	7 (3%)	46	63
1	B	265/265 (100%)	263 (99%)	2 (1%)	81	91
1	C	265/265 (100%)	260 (98%)	5 (2%)	57	73
1	D	265/265 (100%)	261 (98%)	4 (2%)	65	79
1	E	265/265 (100%)	260 (98%)	5 (2%)	57	73
1	F	265/265 (100%)	261 (98%)	4 (2%)	65	79
1	G	265/265 (100%)	259 (98%)	6 (2%)	50	67
1	H	265/265 (100%)	261 (98%)	4 (2%)	65	79
All	All	2120/2120 (100%)	2083 (98%)	37 (2%)	60	76

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	THR
1	A	209	ASN
1	A	211	LEU
1	A	222	ASN
1	A	226	LEU
1	A	272	ARG

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Mol	Chain	Res	Type
1	A	310	LEU
1	B	222	ASN
1	B	272	ARG
1	C	163	THR
1	C	254	PHE
1	C	272	ARG
1	C	279	THR
1	C	308	LEU
1	D	222	ASN
1	D	254	PHE
1	D	272	ARG
1	D	275	THR
1	E	211	LEU
1	E	222	ASN
1	E	254	PHE
1	E	267	VAL
1	E	272	ARG
1	F	156	ASP
1	F	222	ASN
1	F	272	ARG
1	F	312	GLN
1	G	42	LEU
1	G	55	ASN
1	G	195	ARG
1	G	254	PHE
1	G	272	ARG
1	G	273	VAL
1	H	59	GLN
1	H	209	ASN
1	H	254	PHE
1	H	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	164	ASN
1	A	190	GLN
1	A	197	HIS
1	A	209	ASN
1	A	312	GLN
1	B	34	ASN

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Mol	Chain	Res	Type
1	B	37	ASN
1	B	74	ASN
1	B	131	ASN
1	B	151	ASN
1	B	197	HIS
1	B	209	ASN
1	B	248	ASN
1	B	321	GLN
1	B	325	GLN
1	C	131	ASN
1	C	222	ASN
1	C	320	GLN
1	C	324	ASN
1	D	24	ASN
1	D	131	ASN
1	D	143	ASN
1	D	151	ASN
1	D	184	ASN
1	D	190	GLN
1	D	197	HIS
1	D	219	ASN
1	D	280	GLN
1	D	318	GLN
1	D	324	ASN
1	E	24	ASN
1	E	87	HIS
1	E	164	ASN
1	E	190	GLN
1	E	197	HIS
1	E	307	GLN
1	F	37	ASN
1	F	52	GLN
1	F	64	ASN
1	F	74	ASN
1	F	131	ASN
1	F	151	ASN
1	F	248	ASN
1	G	52	GLN
1	G	55	ASN
1	G	64	ASN
1	G	131	ASN
1	G	183	HIS

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Mol	Chain	Res	Type
1	G	209	ASN
1	G	320	GLN
1	G	324	ASN
1	H	24	ASN
1	H	59	GLN
1	H	64	ASN
1	H	131	ASN
1	H	151	ASN
1	H	197	HIS
1	H	222	ASN
1	H	324	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	ASP	A	401	-	2,8,8	0.73	0	1,10,10	0.95	0
2	ASP	D	401	-	2,8,8	0.83	0	1,10,10	1.19	0
2	ASP	G	401	-	2,8,8	0.80	0	1,10,10	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ASP	E	401	-	2,8,8	0.90	0	1,10,10	1.06	0
2	ASP	B	401	-	2,8,8	0.79	0	1,10,10	0.97	0
2	ASP	H	401	-	2,8,8	0.80	0	1,10,10	0.85	0
2	ASP	C	401	-	2,8,8	0.67	0	1,10,10	1.08	0
2	ASP	F	401	-	2,8,8	0.96	0	1,10,10	0.87	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
2	ASP	A	401	-	-	0/2/8/8	-
2	ASP	D	401	-	-	0/2/8/8	-
2	ASP	G	401	-	-	0/2/8/8	-
2	ASP	E	401	-	-	0/2/8/8	-
2	ASP	B	401	-	-	0/2/8/8	-
2	ASP	H	401	-	-	0/2/8/8	-
2	ASP	C	401	-	-	0/2/8/8	-
2	ASP	F	401	-	-	0/2/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

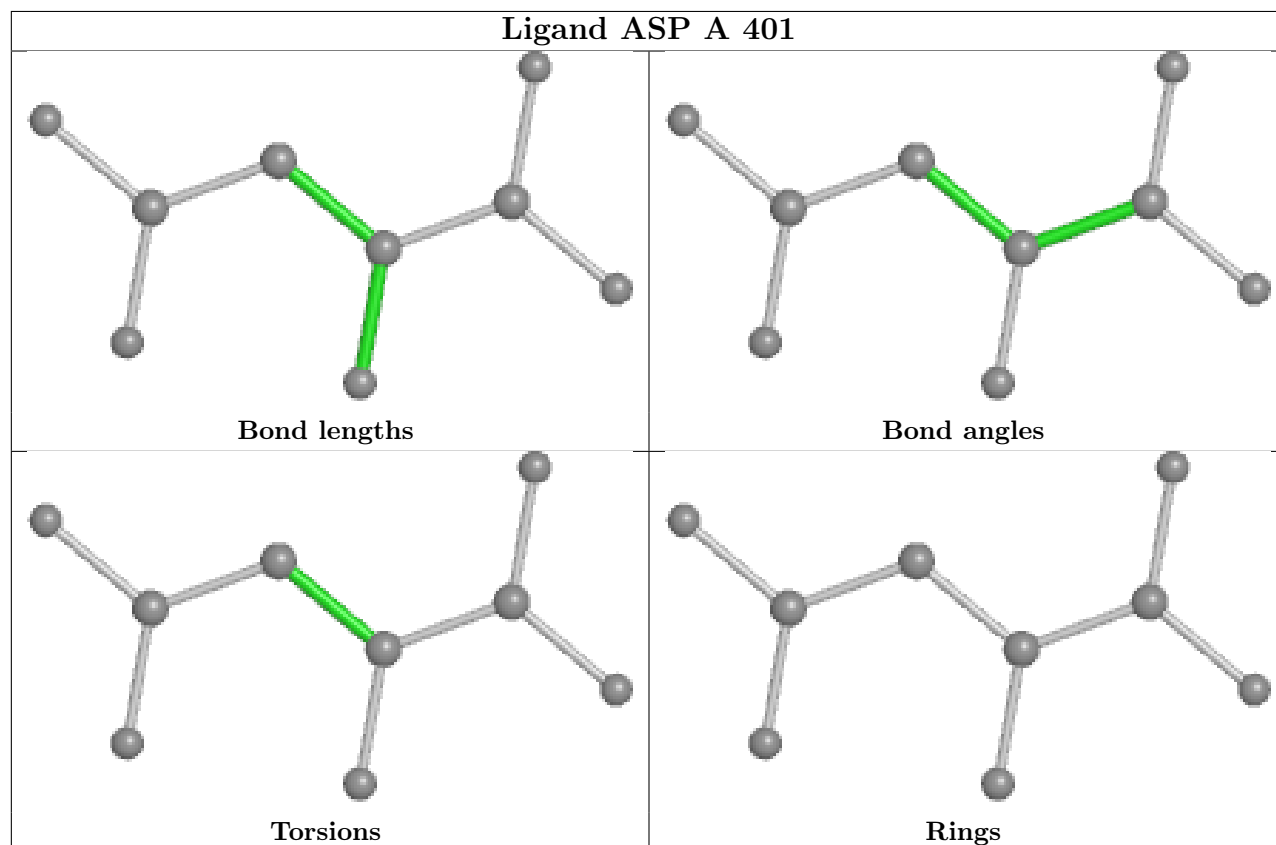
There are no ring outliers.

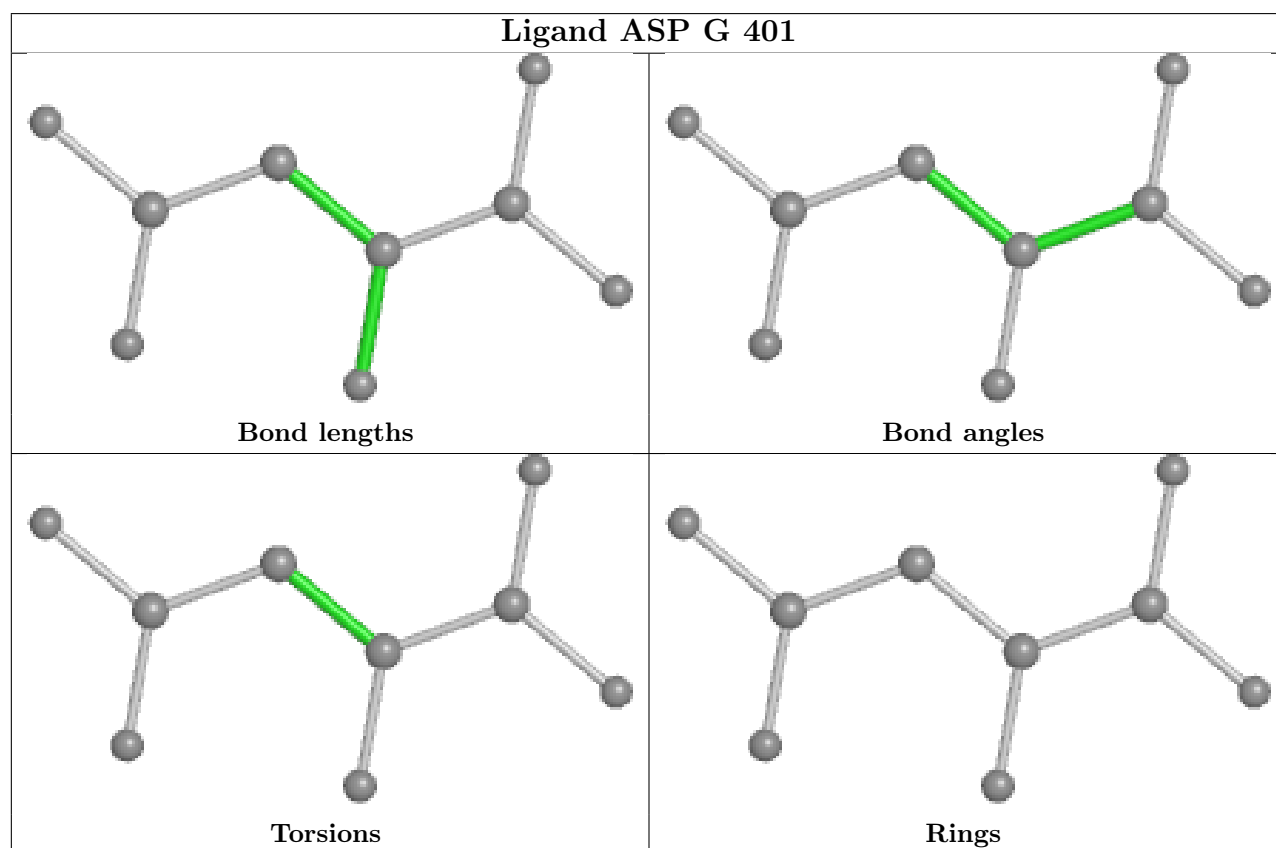
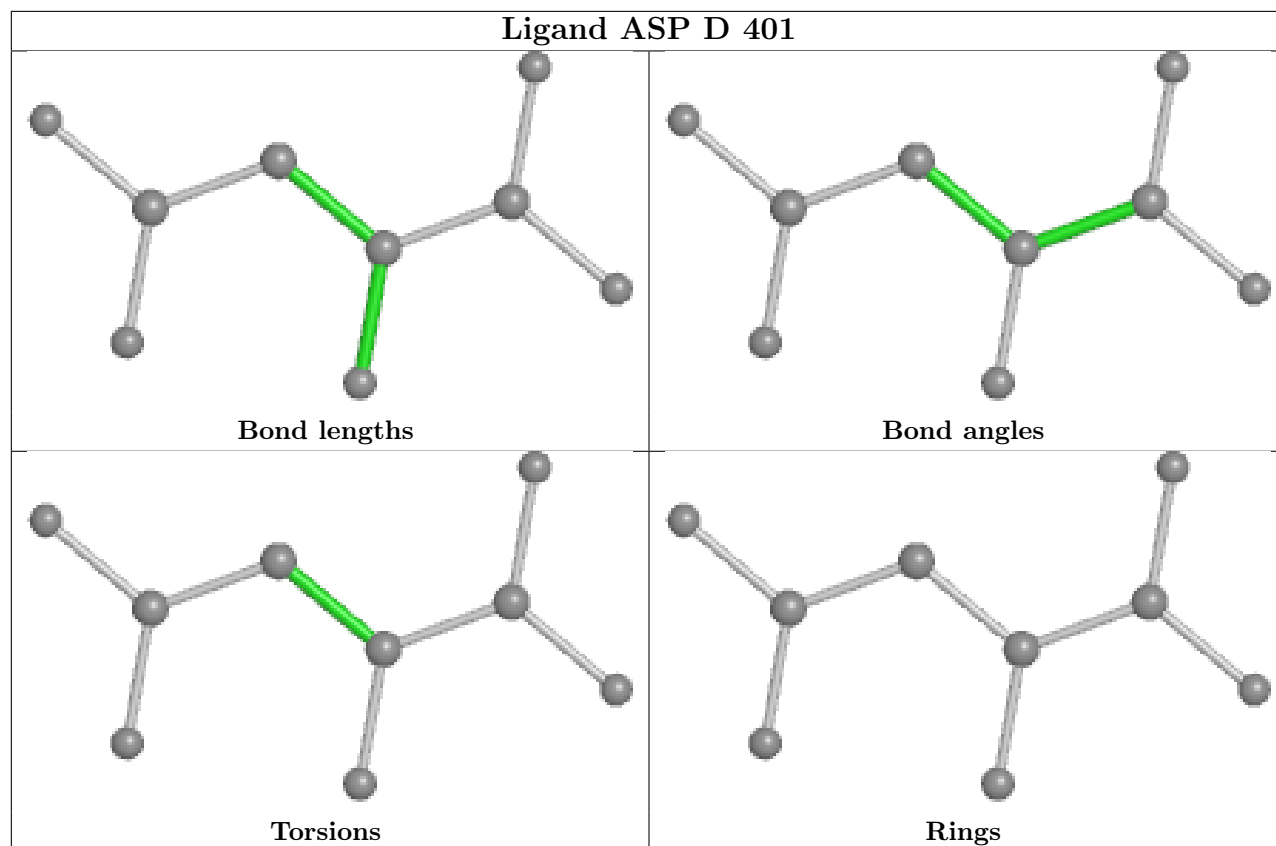
3 monomers are involved in 3 short contacts:

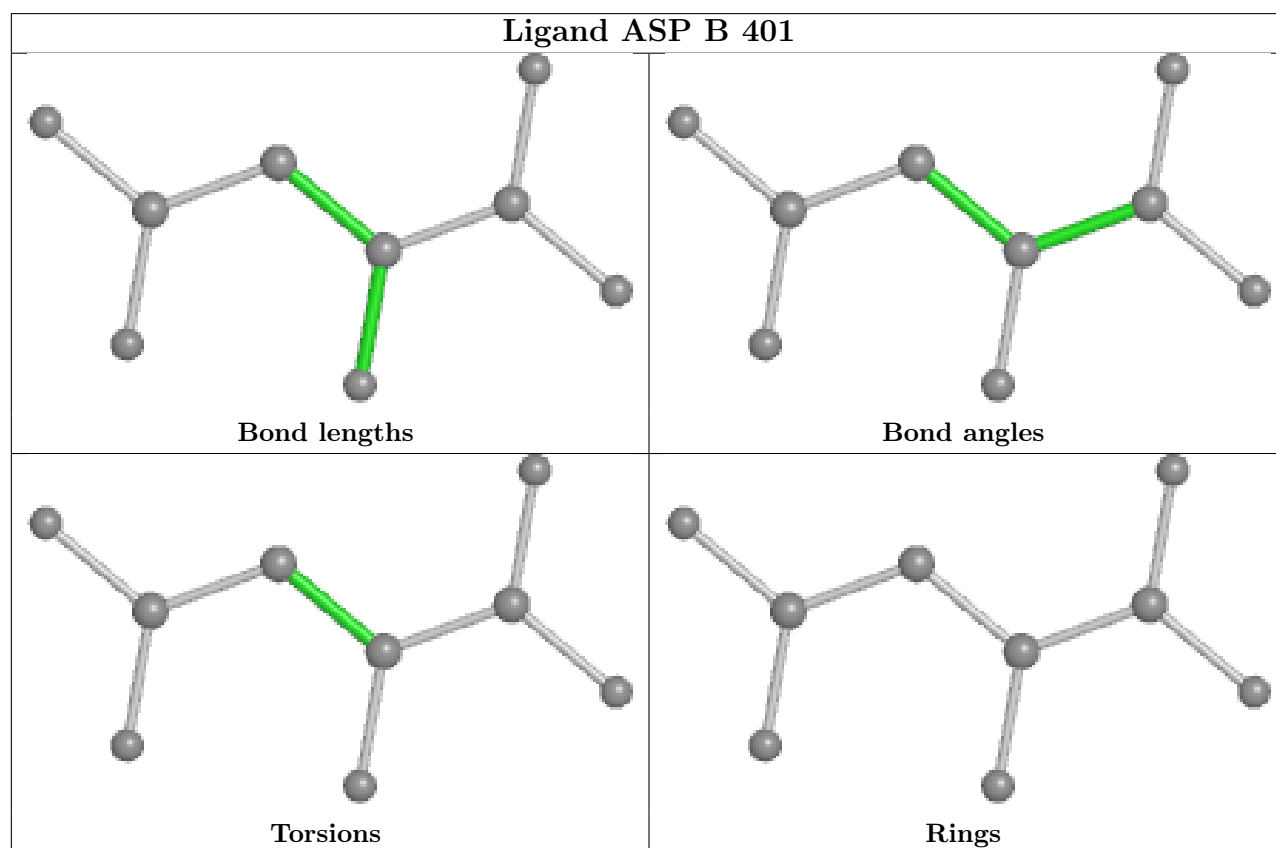
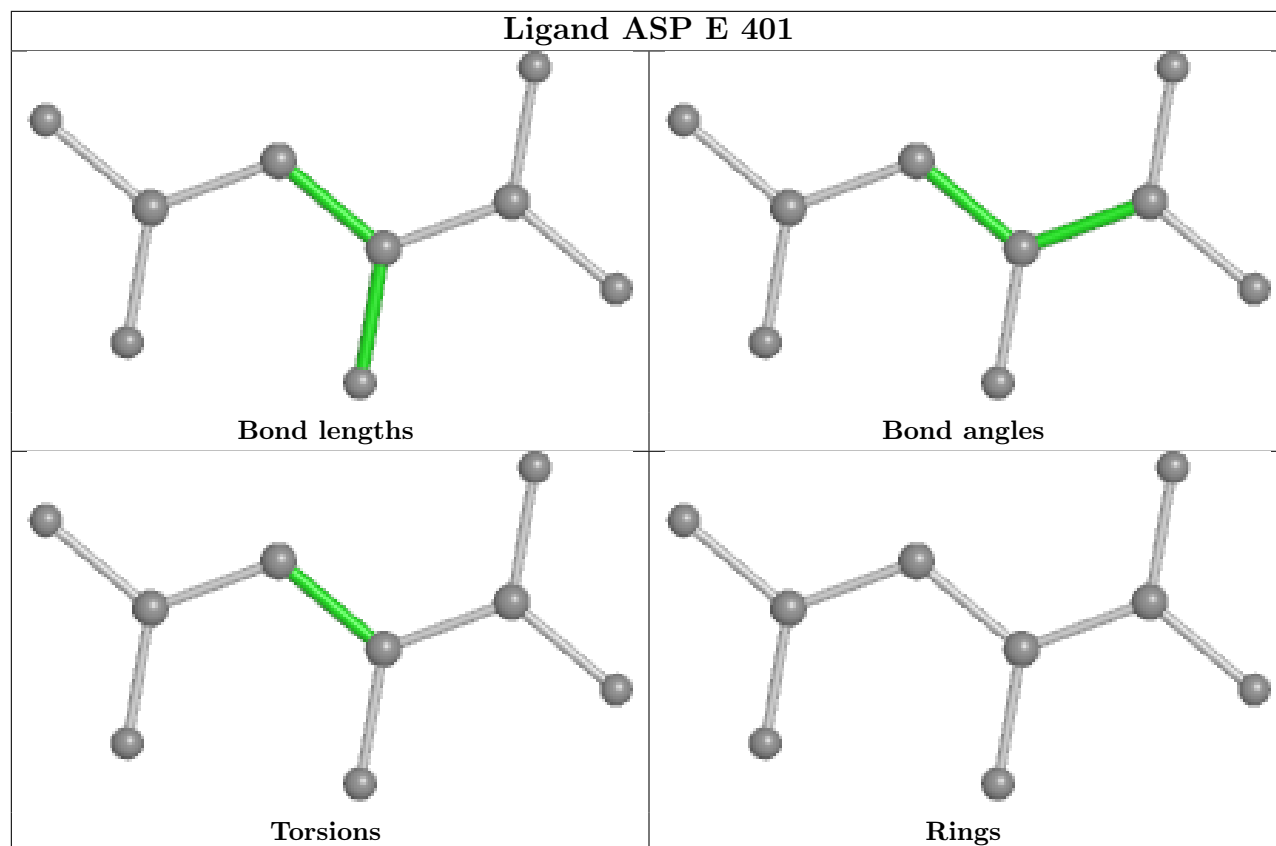
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ASP	1	0
2	H	401	ASP	1	0
2	F	401	ASP	1	0

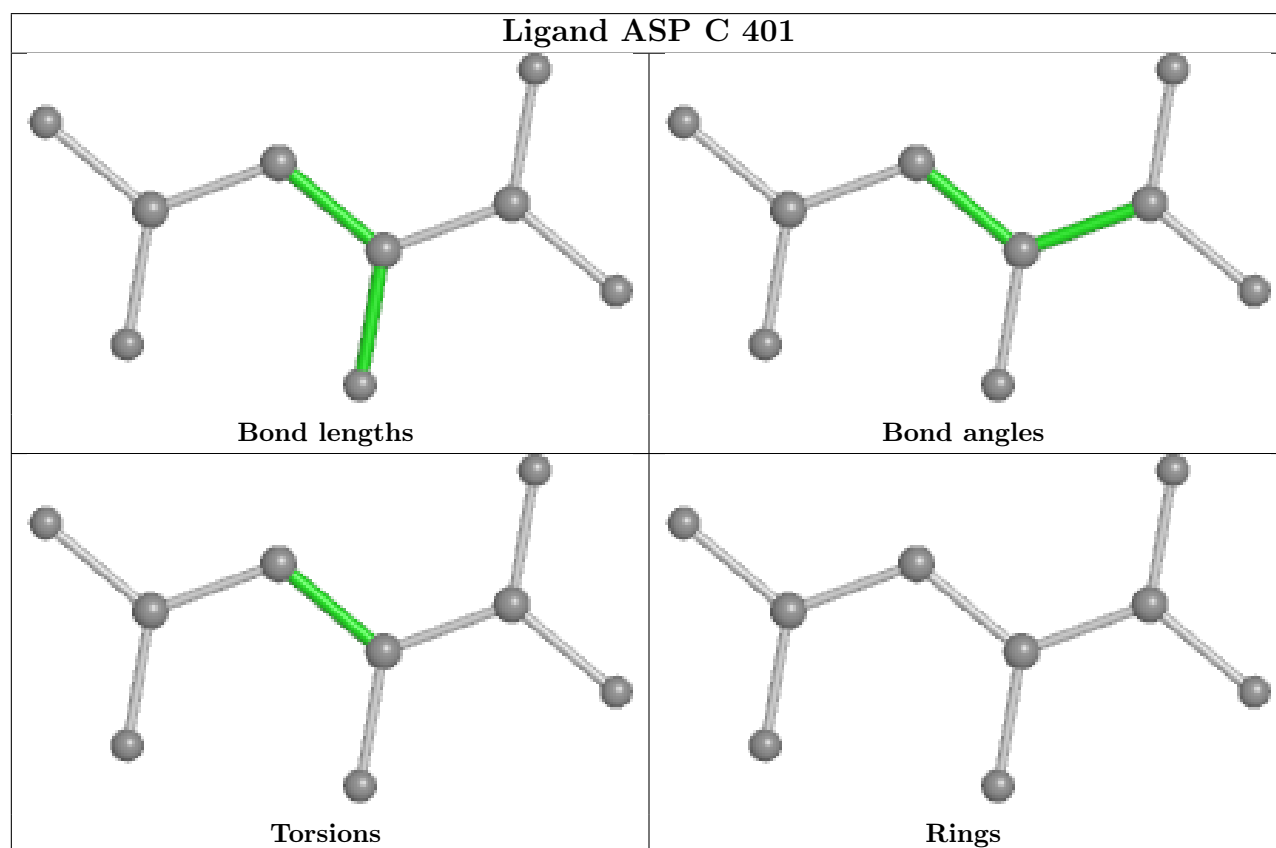
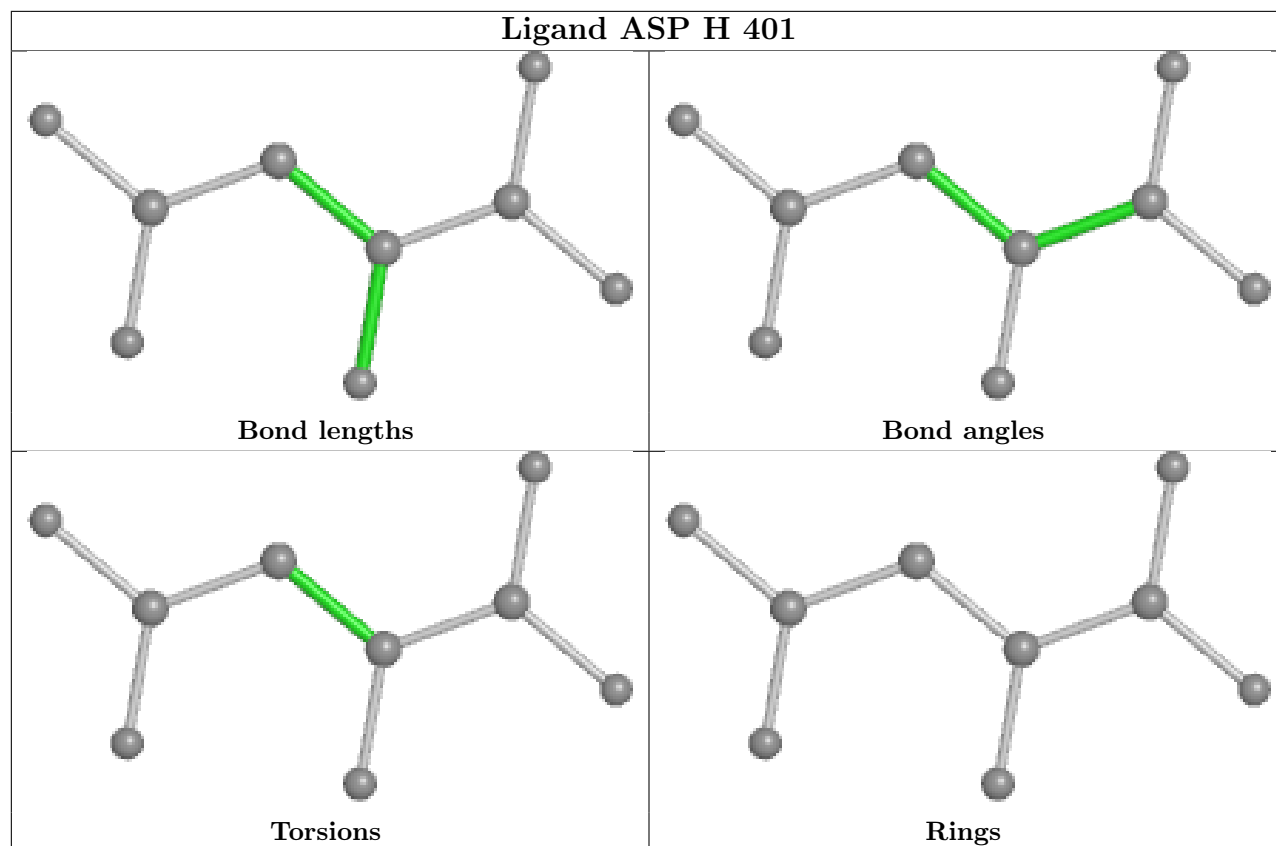
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

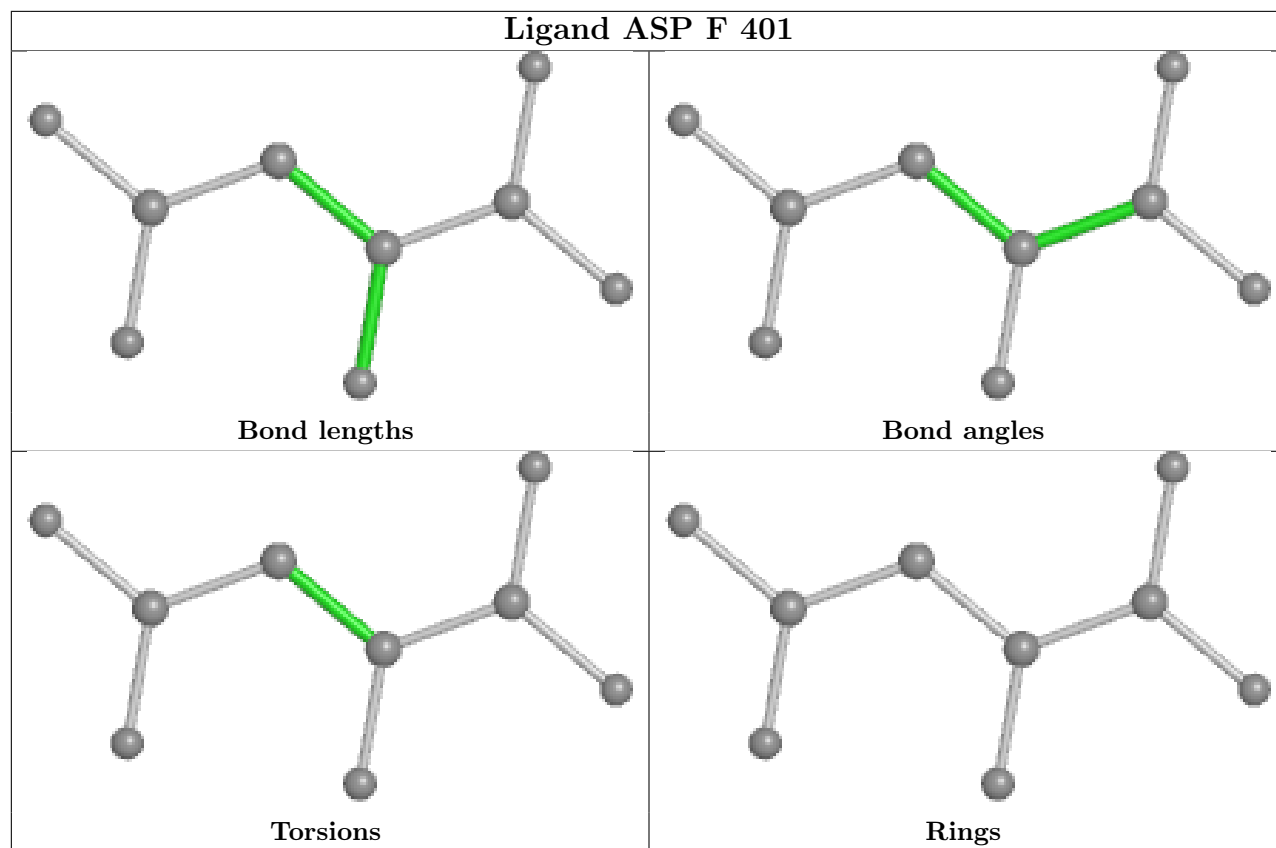
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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	326/326 (100%)	0.01	3 (0%) 84 88	22, 33, 50, 60	0
1	B	326/326 (100%)	-0.14	0 100 100	21, 30, 46, 55	0
1	C	326/326 (100%)	-0.06	4 (1%) 79 83	23, 32, 44, 55	0
1	D	326/326 (100%)	-0.09	3 (0%) 84 88	22, 33, 47, 55	0
1	E	326/326 (100%)	0.08	9 (2%) 53 60	28, 37, 54, 65	0
1	F	326/326 (100%)	0.90	53 (16%) 1 2	31, 53, 87, 114	0
1	G	326/326 (100%)	0.58	32 (9%) 7 10	30, 44, 88, 120	0
1	H	326/326 (100%)	0.14	9 (2%) 53 60	26, 39, 59, 67	0
All	All	2608/2608 (100%)	0.18	113 (4%) 35 42	21, 37, 63, 120	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	28	GLY	9.8
1	F	27	ALA	9.1
1	G	23	SER	8.7
1	G	27	ALA	7.6
1	G	20	ALA	6.2
1	F	139	LYS	5.7
1	G	32	VAL	5.5
1	G	25	TYR	5.5
1	F	18	ASP	5.5
1	F	264	GLY	5.2
1	G	35	LEU	5.2
1	F	29	LYS	5.2
1	F	43	LYS	5.2
1	F	205	VAL	5.1
1	G	15	GLY	5.1
1	G	26	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	26	THR	4.6
1	F	21	THR	4.4
1	F	35	LEU	4.4
1	F	25	TYR	4.4
1	F	106	ASP	4.3
1	H	264	GLY	4.3
1	F	83	PHE	4.2
1	F	20	ALA	4.1
1	F	15	GLY	4.0
1	G	321	GLN	3.8
1	F	16	GLY	3.6
1	C	106	ASP	3.6
1	E	106	ASP	3.6
1	G	24	ASN	3.5
1	F	6	ILE	3.5
1	G	33	GLU	3.4
1	G	16	GLY	3.3
1	F	133	VAL	3.2
1	G	19	SER	3.0
1	C	163	THR	3.0
1	G	17	GLY	2.9
1	E	263	ASN	2.9
1	G	66	TRP	2.9
1	F	17	GLY	2.8
1	F	24	ASN	2.8
1	H	263	ASN	2.8
1	F	203	PHE	2.7
1	A	1	LEU	2.7
1	G	21	THR	2.7
1	G	29	LYS	2.7
1	F	28	GLY	2.7
1	F	3	ASN	2.7
1	G	50	GLY	2.7
1	F	99	LEU	2.6
1	G	22	LYS	2.6
1	E	251	LYS	2.6
1	F	84	VAL	2.6
1	G	318	GLN	2.6
1	G	302	ALA	2.6
1	F	208	LEU	2.5
1	F	204	ASP	2.5
1	G	30	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	317	GLN	2.5
1	G	317	GLN	2.5
1	F	42	LEU	2.5
1	F	7	LEU	2.5
1	F	216	ILE	2.5
1	F	129	LEU	2.5
1	D	264	GLY	2.4
1	F	137	ALA	2.4
1	F	45	ILE	2.4
1	G	53	VAL	2.4
1	G	133	VAL	2.4
1	F	101	LEU	2.4
1	F	169	ALA	2.4
1	F	34	ASN	2.4
1	G	261	ALA	2.4
1	F	75	THR	2.4
1	F	199	SER	2.4
1	E	264	GLY	2.3
1	F	66	TRP	2.3
1	E	291	PHE	2.3
1	E	253	VAL	2.3
1	E	321	GLN	2.3
1	F	80	THR	2.3
1	F	53	VAL	2.3
1	F	174	VAL	2.3
1	G	263	ASN	2.3
1	E	43	LYS	2.3
1	A	27	ALA	2.3
1	G	170	THR	2.2
1	E	22	LYS	2.2
1	F	172	LYS	2.2
1	G	49	LYS	2.2
1	F	325	GLN	2.2
1	H	205	VAL	2.2
1	F	5	THR	2.2
1	C	263	ASN	2.1
1	F	228	ALA	2.1
1	H	311	THR	2.1
1	A	321	GLN	2.1
1	F	209	ASN	2.1
1	H	249	LEU	2.1
1	F	32	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	217	VAL	2.1
1	H	281	ASP	2.1
1	D	275	THR	2.1
1	H	253	VAL	2.1
1	F	215	GLY	2.1
1	G	70	ALA	2.1
1	D	45	ILE	2.0
1	G	34	ASN	2.0
1	F	19	SER	2.0
1	H	174	VAL	2.0
1	C	174	VAL	2.0
1	F	170	THR	2.0
1	F	233	ASP	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 monosaccharides 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.

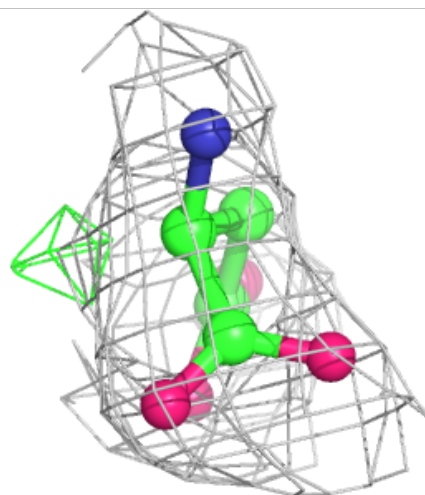
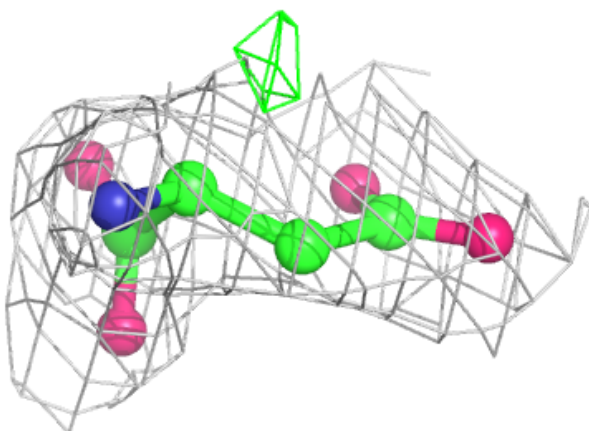
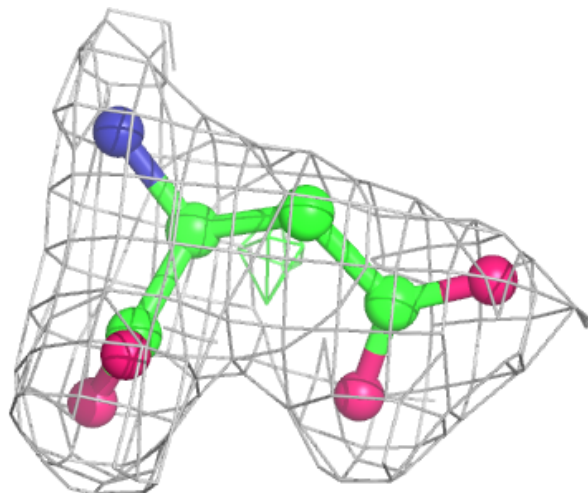
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ASP	F	401	9/9	0.89	0.12	45,47,50,50	0
2	ASP	G	401	9/9	0.91	0.10	36,37,38,38	0
2	ASP	D	401	9/9	0.92	0.13	27,27,27,28	0
2	ASP	E	401	9/9	0.92	0.12	30,30,31,31	0
2	ASP	H	401	9/9	0.93	0.12	29,31,34,35	0
2	ASP	C	401	9/9	0.94	0.11	23,24,25,25	0
2	ASP	A	401	9/9	0.95	0.09	28,29,30,30	0
2	ASP	B	401	9/9	0.97	0.09	23,23,24,24	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.

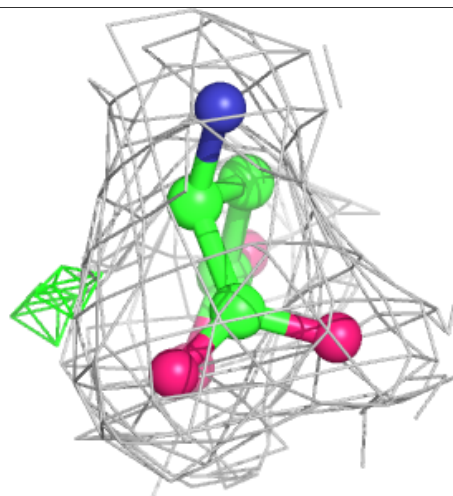
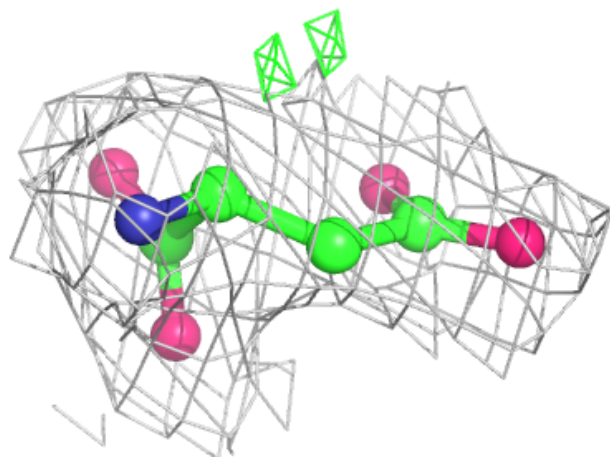
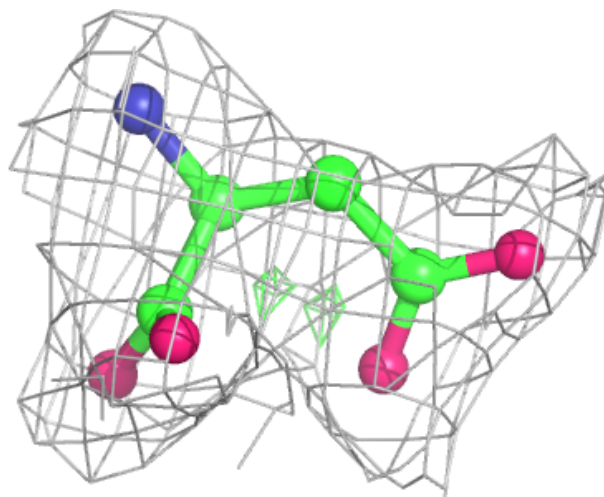
Electron density around ASP F 401:

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



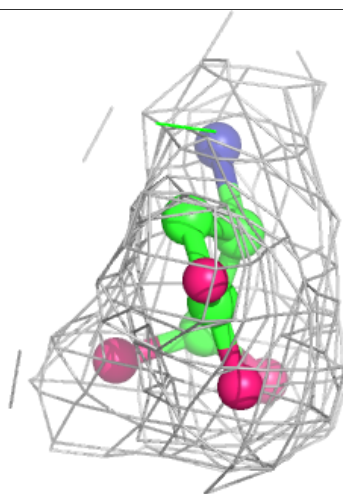
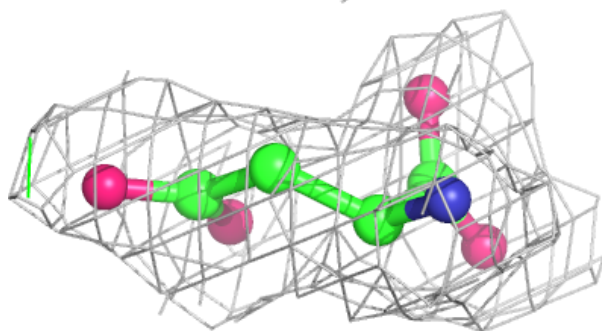
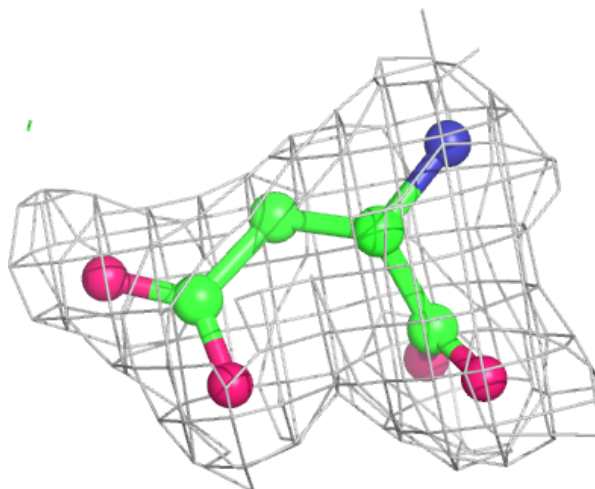
Electron density around ASP G 401:

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



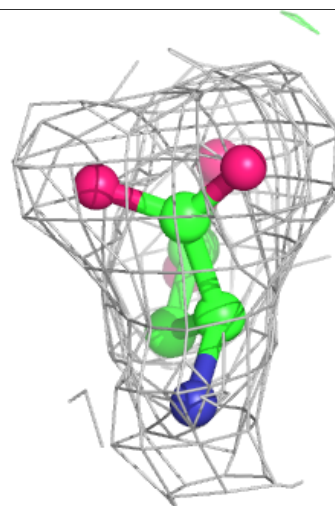
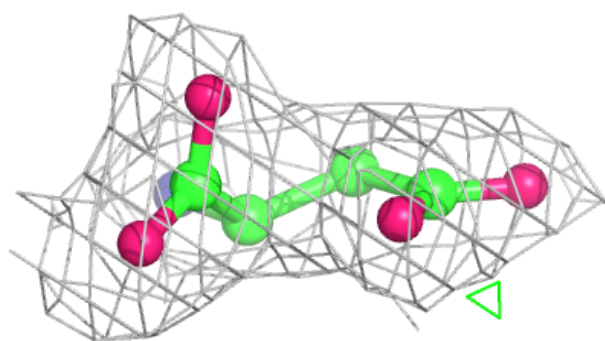
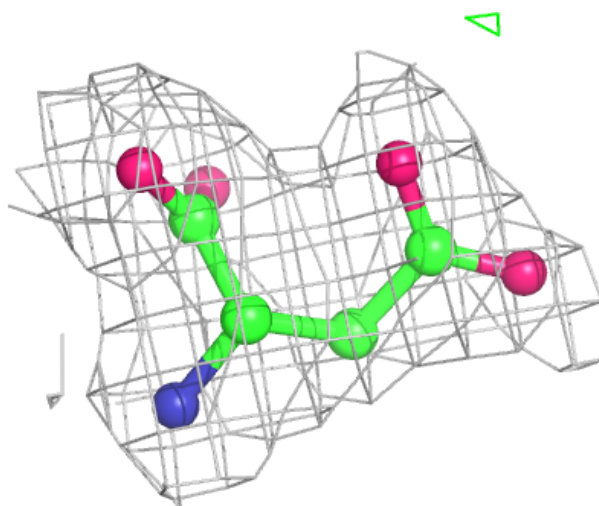
Electron density around ASP D 401:

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



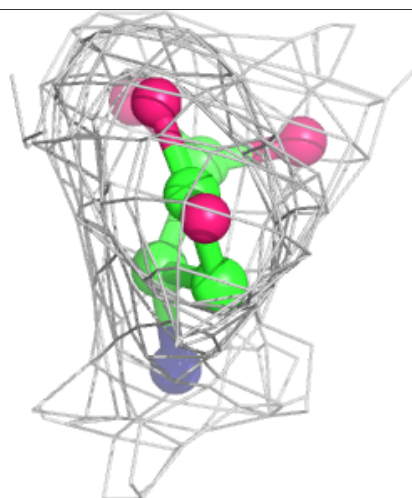
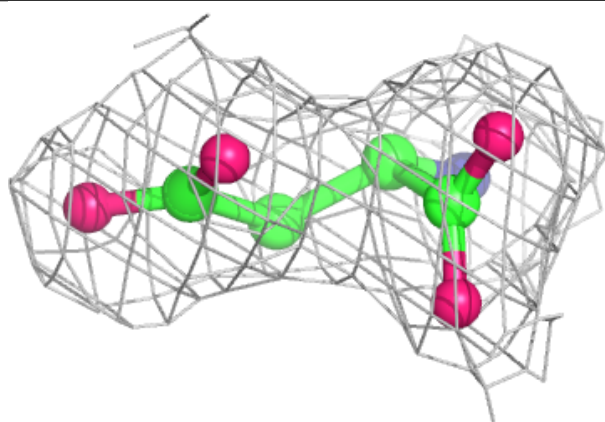
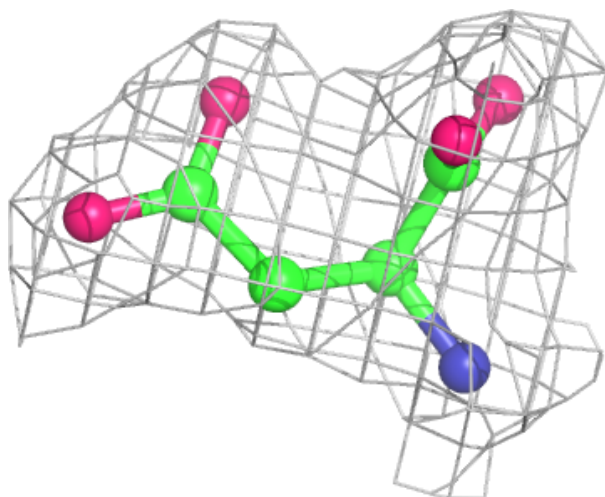
Electron density around ASP E 401:

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



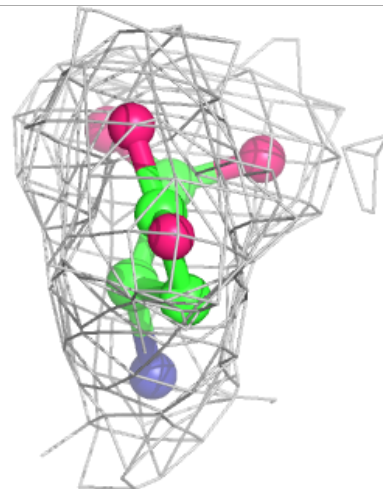
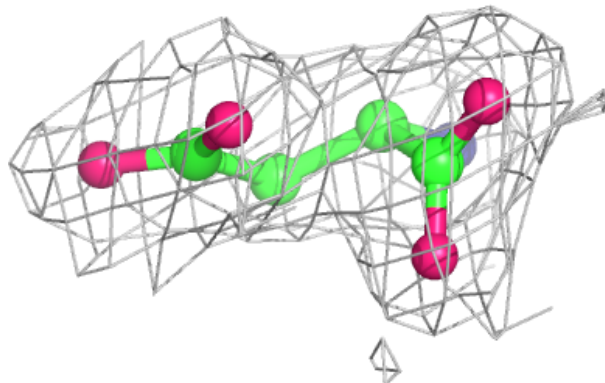
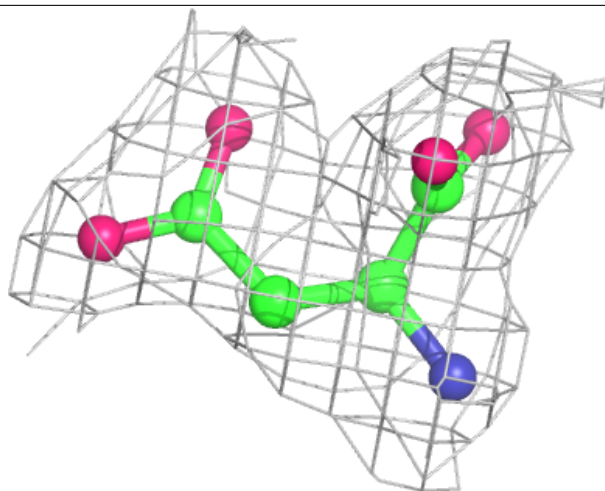
Electron density around ASP H 401:

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



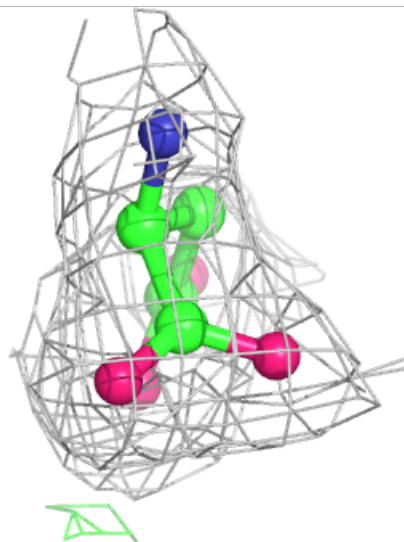
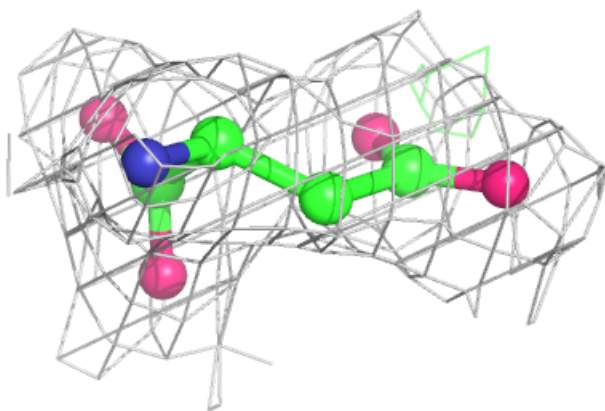
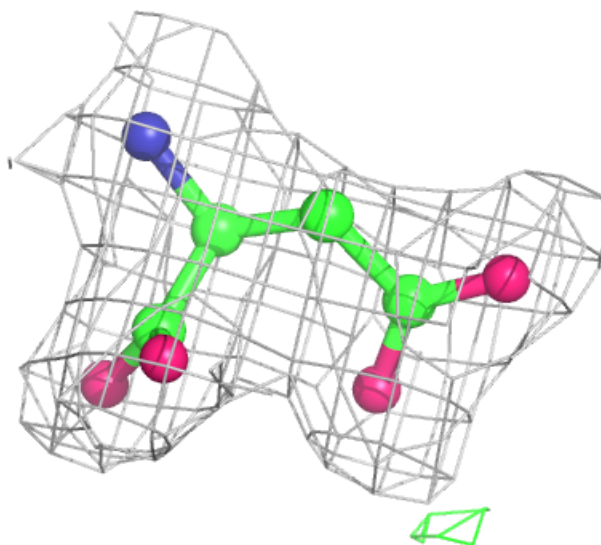
Electron density around ASP C 401:

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



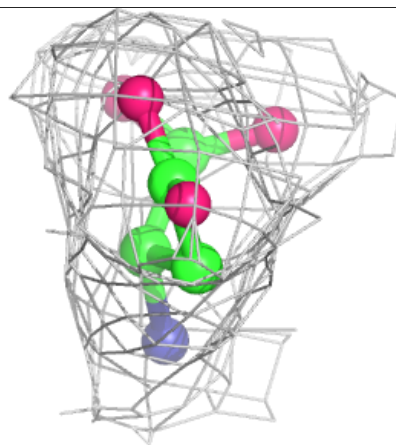
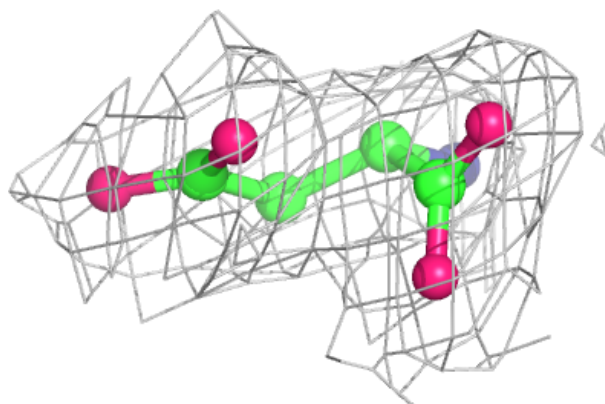
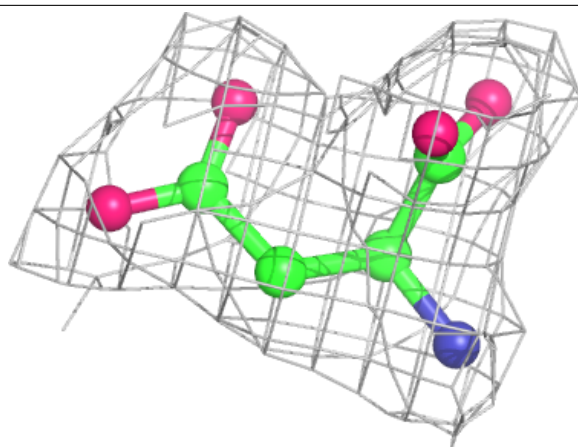
Electron density around ASP A 401:

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



Electron density around ASP B 401:

$2mF_o-DF_c$ (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.