



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:55 PM UTC

PDB ID : 6V25 / pdb_00006v25
Title : Complex of mutant (K162M) of E. coli L-asparaginase II with L-Asp
Authors : Lubkowski, J.; Wlodawer, A.
Deposited on : 2019-11-22
Resolution : 1.78 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

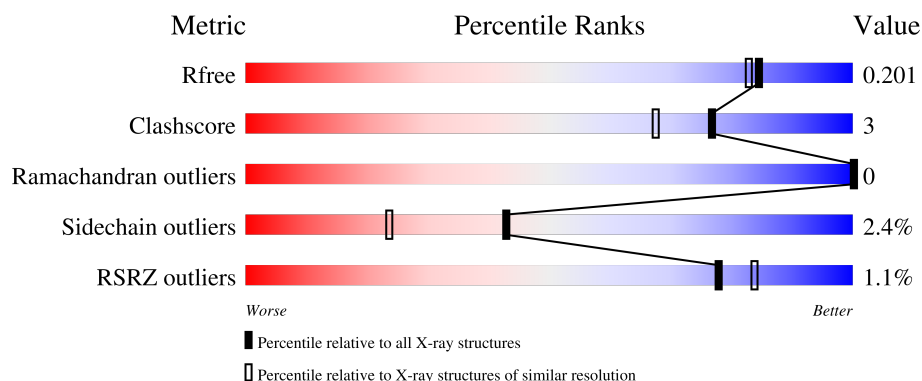
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	333	2% 82% 15% ..
1	B	333	77% 14% 8%
2	C	333	83% 14% ..
2	D	333	% 86% 12% .

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	ASP	A	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11175 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	2	0
			2440	1522	415	494	9			
1	B	305	Total	C	N	O	S	0	1	0
			2292	1433	389	461	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P00805
A	-5	HIS	-	expression tag	UNP P00805
A	-4	HIS	-	expression tag	UNP P00805
A	-3	HIS	-	expression tag	UNP P00805
A	-2	HIS	-	expression tag	UNP P00805
A	-1	HIS	-	expression tag	UNP P00805
A	0	HIS	-	expression tag	UNP P00805
A	162	MET	LYS	engineered mutation	UNP P00805
B	-6	MET	-	expression tag	UNP P00805
B	-5	HIS	-	expression tag	UNP P00805
B	-4	HIS	-	expression tag	UNP P00805
B	-3	HIS	-	expression tag	UNP P00805
B	-2	HIS	-	expression tag	UNP P00805
B	-1	HIS	-	expression tag	UNP P00805
B	0	HIS	-	expression tag	UNP P00805
B	162	MET	LYS	engineered mutation	UNP P00805

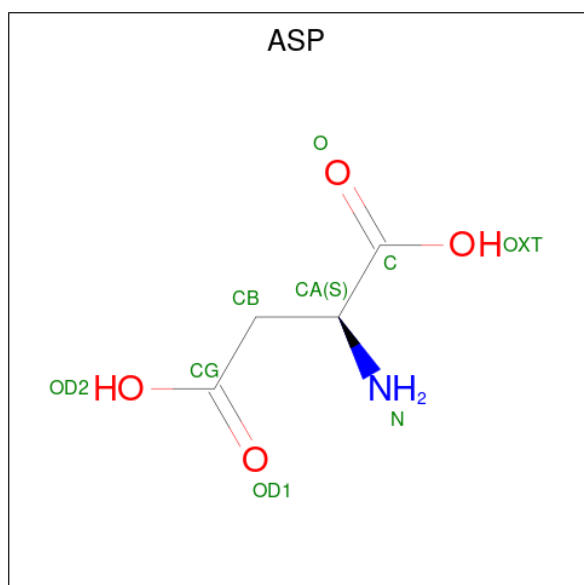
- Molecule 2 is a protein called L-asparaginase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	326	Total	C	N	O	S	0	0	0
			2438	1520	415	494	9			
2	D	332	Total	C	N	O	S	0	1	0
			2503	1561	433	500	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	expression tag	UNP P00805
C	-5	HIS	-	expression tag	UNP P00805
C	-4	HIS	-	expression tag	UNP P00805
C	-3	HIS	-	expression tag	UNP P00805
C	-2	HIS	-	expression tag	UNP P00805
C	-1	HIS	-	expression tag	UNP P00805
C	0	HIS	-	expression tag	UNP P00805
C	12	AEI	THR	modified residue	UNP P00805
C	162	MET	LYS	engineered mutation	UNP P00805
D	-6	MET	-	expression tag	UNP P00805
D	-5	HIS	-	expression tag	UNP P00805
D	-4	HIS	-	expression tag	UNP P00805
D	-3	HIS	-	expression tag	UNP P00805
D	-2	HIS	-	expression tag	UNP P00805
D	-1	HIS	-	expression tag	UNP P00805
D	0	HIS	-	expression tag	UNP P00805
D	12	AEI	THR	modified residue	UNP P00805
D	162	MET	LYS	engineered mutation	UNP P00805

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$) (labeled as "Ligand of Interest" by depositor).



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

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

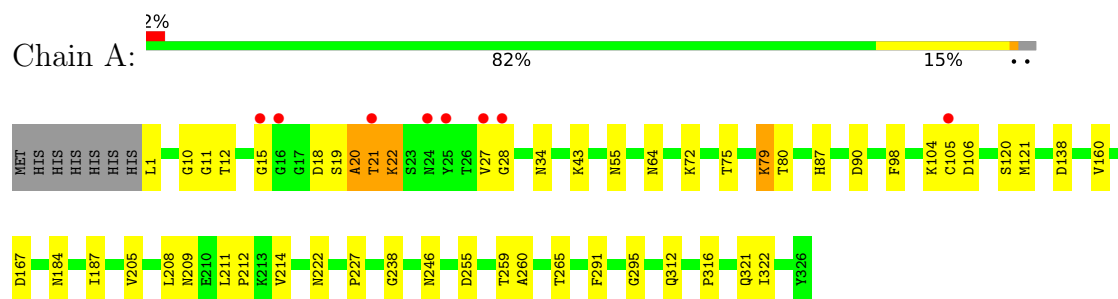
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	379	Total	O	0	4
			383	383		
4	C	378	Total	O	0	6
			384	384		
4	B	306	Total	O	0	7
			313	313		
4	D	393	Total	O	0	10
			404	404		

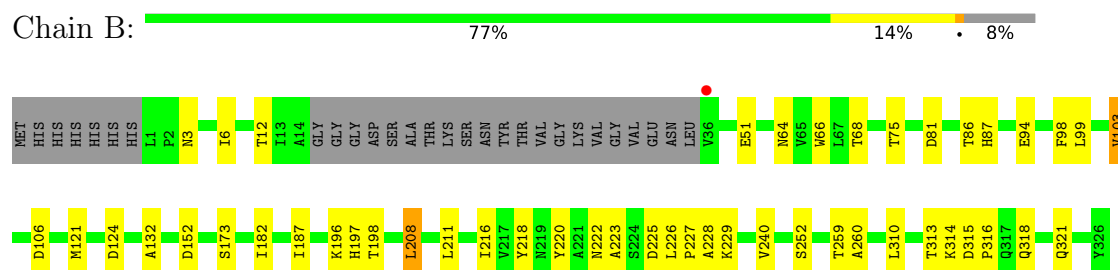
3 Residue-property plots

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

• Molecule 1: L-asparaginase 2



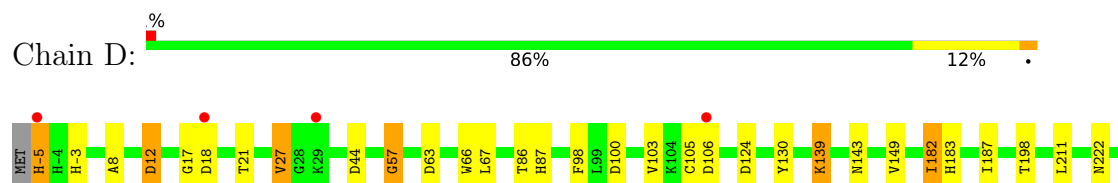
• Molecule 1: L-asparaginase 2



• Molecule 2: L-asparaginase 2



• Molecule 2: 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	61.53Å 123.97Å 76.30Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	24.61 – 1.78 24.61 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.0 (24.61-1.78) 93.0 (24.61-1.78)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.136 , 0.193 0.148 , 0.201	Depositor DCC
R_{free} test set	2442 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11175	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: AEI

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	1.48	18/2483 (0.7%)	1.51	18/3382 (0.5%)
1	B	1.43	16/2330 (0.7%)	1.45	7/3174 (0.2%)
2	C	1.50	23/2459 (0.9%)	1.46	12/3347 (0.4%)
2	D	1.45	15/2533 (0.6%)	1.45	16/3448 (0.5%)
All	All	1.46	72/9805 (0.7%)	1.47	53/13351 (0.4%)

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
2	D	0	1

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	ALA	C-O	9.11	1.34	1.24
1	A	105	CYS	N-CA	8.89	1.56	1.46
1	A	20	ALA	C-O	8.81	1.35	1.24
2	C	193	PRO	C-O	-8.69	1.14	1.23
1	B	173	SER	CA-CB	-8.55	1.41	1.52
1	A	212	PRO	C-O	-8.32	1.13	1.23
1	B	6	ILE	C-O	8.23	1.33	1.24
1	B	106	ASP	C-O	7.95	1.34	1.24
1	A	246	ASN	C-O	7.88	1.33	1.23
1	B	121	MET	C-O	7.46	1.32	1.23
2	C	281	ASP	CG-OD2	7.25	1.39	1.25
2	D	106	ASP	C-O	7.20	1.33	1.24
1	A	138	ASP	C-O	7.15	1.32	1.24
2	D	250	TYR	C-O	7.13	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	236	TYR	C-O	7.10	1.32	1.23
1	A	1	LEU	N-CA	7.10	1.59	1.46
1	B	51	GLU	C-O	6.96	1.31	1.23
2	C	151	ASN	C-O	6.73	1.32	1.23
2	D	281	ASP	CG-OD2	6.68	1.38	1.25
2	D	-3	HIS	CE1-NE2	6.60	1.39	1.32
2	D	182	ILE	C-O	6.55	1.31	1.24
2	C	204	ASP	C-O	6.44	1.31	1.24
2	C	223	ALA	C-O	-6.29	1.16	1.23
1	A	15	GLY	C-O	6.24	1.32	1.23
1	B	64	ASN	C-O	6.24	1.31	1.24
1	B	132	ALA	C-O	-6.22	1.16	1.24
1	A	80	THR	C-O	6.22	1.31	1.24
2	D	302	ALA	C-O	6.05	1.31	1.24
1	B	124	ASP	C-O	-6.04	1.16	1.24
2	C	183	HIS	CG-ND1	6.04	1.44	1.38
1	A	160	VAL	C-O	-5.94	1.17	1.24
1	B	229	LYS	N-CA	5.88	1.53	1.46
1	A	316	PRO	C-O	-5.87	1.17	1.24
2	C	301	LYS	C-O	5.87	1.31	1.24
1	A	187	ILE	C-O	-5.85	1.17	1.24
2	C	55	ASN	C-O	5.84	1.32	1.23
1	B	218	TYR	C-O	-5.74	1.17	1.23
1	A	72	LYS	C-O	5.74	1.30	1.24
2	D	-5	HIS	N-CA	5.68	1.57	1.46
1	A	98	PHE	C-O	5.68	1.30	1.24
2	D	67	LEU	C-O	5.65	1.30	1.24
2	C	67	LEU	C-O	5.56	1.30	1.24
1	B	197	HIS	CE1-NE2	5.54	1.38	1.32
2	C	118	SER	C-O	-5.47	1.17	1.24
2	C	293	ALA	C-O	5.47	1.30	1.24
2	C	65	VAL	C-O	-5.46	1.17	1.24
1	B	208	LEU	C-O	5.38	1.30	1.23
2	D	283	GLU	C-O	-5.37	1.17	1.24
2	C	280	GLN	C-O	5.36	1.31	1.23
1	B	196	LYS	C-O	5.32	1.30	1.23
1	A	184	ASN	C-O	5.31	1.30	1.23
2	C	96	ALA	C-O	5.30	1.30	1.24
1	B	260	ALA	C-O	5.27	1.30	1.24
2	D	245	GLY	C-O	5.27	1.30	1.24
2	D	57	GLY	C-O	5.25	1.29	1.23
2	D	18	ASP	C-O	5.24	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	268	VAL	C-O	5.22	1.29	1.24
1	A	87	HIS	CG-ND1	5.22	1.44	1.38
2	C	159	ASP	C-O	5.21	1.30	1.24
2	D	100	ASP	C-O	5.20	1.30	1.24
2	C	106	ASP	CG-OD1	5.15	1.35	1.25
2	C	87	HIS	C-O	5.11	1.29	1.23
2	C	170	THR	C-O	5.11	1.30	1.24
2	C	10	GLY	C-O	-5.08	1.17	1.23
1	B	86	THR	C-O	5.06	1.30	1.24
2	D	106	ASP	N-CA	5.05	1.51	1.46
1	A	322	ILE	C-O	5.04	1.30	1.24
2	C	128	ASN	C-O	-5.04	1.18	1.24
1	A	295	GLY	C-O	5.02	1.30	1.24
2	D	44	ASP	C-O	5.02	1.30	1.24
1	A	265	THR	N-CA	5.01	1.52	1.46
2	C	285	ASP	CG-OD1	5.01	1.34	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LYS	CA-C-N	10.12	135.09	120.71
1	A	104	LYS	C-N-CA	10.12	135.09	120.71
2	C	87	HIS	CA-CB-CG	9.27	123.07	113.80
1	A	104	LYS	CA-C-O	-9.06	108.82	119.15
1	A	167	ASP	CA-CB-CG	8.16	120.76	112.60
2	D	281	ASP	CB-CA-C	-7.96	99.06	111.39
2	C	63	ASP	CA-CB-CG	7.77	120.37	112.60
2	C	75	THR	CA-CB-OG1	-7.57	98.24	109.60
2	C	139	LYS	CB-CA-C	-7.39	98.12	110.68
1	B	75	THR	CA-CB-OG1	-7.21	98.79	109.60
2	D	63	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	105	CYS	N-CA-C	-7.16	99.85	110.23
1	A	312	GLN	N-CA-C	-6.86	105.53	114.04
2	C	106	ASP	CA-CB-CG	-6.67	105.93	112.60
1	A	259	THR	CA-CB-OG1	-6.61	99.68	109.60
2	C	192	THR	O-C-N	-6.47	117.32	121.85
2	D	17	GLY	CA-C-N	6.40	130.04	120.31
2	D	17	GLY	C-N-CA	6.40	130.04	120.31
1	A	321	GLN	N-CA-CB	6.39	119.51	110.12
1	A	105	CYS	CA-CB-SG	6.37	129.06	114.40
2	C	281	ASP	CB-CA-C	-6.30	102.78	111.73
1	B	87	HIS	CA-CB-CG	6.20	120.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	27	VAL	CA-C-O	-5.94	116.99	121.68
2	C	231	LEU	CA-C-O	-5.72	114.35	120.42
2	D	87	HIS	CA-CB-CG	5.65	119.45	113.80
1	A	255	ASP	CA-CB-CG	5.54	118.14	112.60
2	D	18	ASP	CB-CA-C	-5.52	100.07	110.67
2	D	124	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	306	LEU	N-CA-C	-5.50	105.36	111.36
2	D	229	LYS	CA-C-O	-5.49	114.74	120.55
2	C	259	THR	CA-CB-OG1	-5.39	101.52	109.60
1	A	260	ALA	N-CA-C	-5.35	105.45	111.28
1	B	259	THR	CA-CB-OG1	-5.34	101.59	109.60
2	D	-5	HIS	CA-CB-CG	5.33	119.13	113.80
1	A	75	THR	CA-CB-OG1	-5.27	101.70	109.60
1	A	106	ASP	N-CA-C	-5.25	106.46	112.92
2	D	143	ASN	CA-C-O	-5.24	114.10	120.12
2	C	73	ILE	CA-C-O	-5.23	115.51	120.95
2	C	73	ILE	O-C-N	5.21	126.92	121.87
1	A	104	LYS	CB-CA-C	5.17	118.65	109.65
2	C	26	THR	CA-CB-OG1	-5.14	101.89	109.60
2	D	254	PHE	N-CA-C	-5.14	104.94	111.11
1	B	321	GLN	CA-C-O	-5.12	115.12	120.55
1	A	90	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	205	VAL	CA-C-O	-5.11	114.32	119.89
1	B	152	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	209	ASN	CA-CB-CG	-5.09	107.51	112.60
1	B	94	GLU	N-CA-C	-5.07	105.21	111.40
1	B	68	THR	CA-CB-OG1	-5.06	102.01	109.60
2	D	21	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	291	PHE	CA-CB-CG	5.01	118.81	113.80
2	D	105	CYS	CA-C-N	-5.01	114.67	122.73
2	D	105	CYS	C-N-CA	-5.01	114.67	122.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	277	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2440	0	2430	18	0
1	B	2292	0	2284	14	0
2	C	2438	0	2423	13	0
2	D	2503	0	2476	14	0
3	A	9	0	3	4	0
3	B	9	0	3	1	0
4	A	383	0	0	2	0
4	B	313	0	0	0	0
4	C	384	0	0	4	0
4	D	404	0	0	7	0
All	All	11175	0	9619	56	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 3.

All (56) 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)
2:D:183:HIS:HB2	4:D:698:HOH:O	1.58	1.03
1:A:21:THR:HG21	4:D:425:HOH:O	1.72	0.89
2:C:12:AEI:CD	4:C:428:HOH:O	2.29	0.80
1:A:12:THR:OG1	3:A:401:ASP:CG	2.25	0.78
1:A:227:PRO:HB3	2:C:227:PRO:HB3	1.70	0.73
2:D:12:AEI:CD	4:D:533:HOH:O	2.43	0.65
2:D:149:VAL:HG12	4:D:479:HOH:O	1.97	0.63
1:B:12:THR:OG1	3:B:401:ASP:CG	2.41	0.63
1:A:21:THR:CG2	4:D:425:HOH:O	2.40	0.59
1:A:19:SER:HB3	1:A:22:LYS:HG3	1.88	0.54
1:A:121:MET:HE1	2:D:130:TYR:CD1	2.43	0.54
1:B:103:VAL:O	1:B:198:THR:HA	2.08	0.53
1:B:66:TRP:HB3	1:B:98:PHE:CE2	2.44	0.53
1:A:121:MET:HE1	2:D:130:TYR:CG	2.43	0.53
1:B:225:ASP:HB3	1:B:252:SER:HB3	1.90	0.53
1:B:313:THR:OG1	1:B:318:GLN:NE2	2.42	0.52
2:D:66:TRP:HB3	2:D:98:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:TYR:CZ	1:B:223:ALA:HA	2.44	0.51
2:C:73:ILE:HD11	2:C:85:ILE:HD11	1.92	0.51
1:A:64:ASN:ND2	4:A:503:HOH:O	2.40	0.48
2:D:103:VAL:O	2:D:198:THR:HA	2.14	0.47
1:A:214:VAL:HA	1:A:238:GLY:O	2.14	0.47
1:B:226:LEU:HB2	1:B:227:PRO:HD3	1.95	0.47
1:A:27:VAL:HG11	3:A:401:ASP:HA	1.95	0.47
2:C:35:LEU:HD23	2:C:35:LEU:HA	1.77	0.46
1:A:12:THR:CB	3:A:401:ASP:CG	2.90	0.45
1:B:315:ASP:OD1	1:B:316:PRO:HD2	2.17	0.45
2:D:182:ILE:HG12	2:D:187:ILE:HG12	1.98	0.45
2:C:121:MET:HB3	2:C:121:MET:HE2	1.52	0.45
2:D:27:VAL:HG21	2:D:57:GLY:CA	2.47	0.45
2:C:182:ILE:HG12	2:C:187:ILE:HG12	1.99	0.44
1:A:20:ALA:HA	1:A:120:SER:HA	1.99	0.44
2:C:317:GLN:HG3	4:C:458:HOH:O	2.17	0.44
1:B:99:LEU:O	1:B:103:VAL:HG13	2.18	0.44
1:A:10:GLY:HA2	1:A:55:ASN:ND2	2.31	0.44
2:D:260:ALA:HB1	2:D:265:THR:HB	1.98	0.44
2:C:84:VAL:HA	2:C:110:VAL:O	2.18	0.44
1:B:3:ASN:O	1:B:81:ASP:HB2	2.19	0.43
1:A:79:LYS:HD2	4:A:658:HOH:O	2.19	0.42
2:C:51:GLU:OE1	4:C:401:HOH:O	2.22	0.42
2:C:208:LEU:HD12	2:C:208:LEU:HA	1.90	0.42
2:C:268:VAL:HG22	2:C:292:VAL:HB	2.02	0.42
2:D:139:LYS:HG3	4:D:623:HOH:O	2.19	0.42
1:B:216:ILE:HA	1:B:240:VAL:O	2.20	0.42
1:B:66:TRP:HB3	1:B:98:PHE:CD2	2.54	0.41
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.95	0.41
2:C:139:LYS:HE3	2:C:139:LYS:HB2	1.95	0.41
2:D:8:ALA:HA	2:D:86:THR:OG1	2.21	0.41
2:C:162:MET:HE1	4:C:403:HOH:O	2.19	0.41
2:D:-5:HIS:N	4:D:423:HOH:O	2.53	0.41
1:A:28:GLY:HA2	1:A:55:ASN:ND2	2.36	0.41
1:B:182:ILE:HG12	1:B:187:ILE:HG12	2.02	0.40
2:D:261:ALA:HA	2:D:265:THR:O	2.22	0.40
1:A:11:GLY:HA2	3:A:401:ASP:OXT	2.21	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	326/333 (98%)	317 (97%)	9 (3%)	0	100	100
1	B	302/333 (91%)	297 (98%)	5 (2%)	0	100	100
2	C	323/333 (97%)	316 (98%)	7 (2%)	0	100	100
2	D	330/333 (99%)	323 (98%)	7 (2%)	0	100	100
All	All	1281/1332 (96%)	1253 (98%)	28 (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	268/273 (98%)	260 (97%)	8 (3%)	36	15
1	B	252/273 (92%)	247 (98%)	5 (2%)	48	29
2	C	265/272 (97%)	258 (97%)	7 (3%)	40	20
2	D	272/272 (100%)	267 (98%)	5 (2%)	51	33
All	All	1057/1090 (97%)	1032 (98%)	25 (2%)	43	24

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	21	THR

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Mol	Chain	Res	Type
1	A	22	LYS
1	A	43	LYS
1	A	79	LYS
1	A	208	LEU
1	A	211	LEU
1	A	222	ASN
2	C	33	GLU
2	C	43	LYS
2	C	139	LYS
2	C	208	LEU
2	C	211	LEU
2	C	222	ASN
2	C	229	LYS
1	B	103	VAL
1	B	208	LEU
1	B	211	LEU
1	B	222	ASN
1	B	314	LYS
2	D	139	LYS
2	D	211	LEU
2	D	222	ASN
2	D	251	LYS
2	D	314	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	64	ASN
1	A	143	ASN
2	C	183	HIS
2	C	248	ASN
2	C	318	GLN
1	B	64	ASN
1	B	280	GLN
1	B	318	GLN
1	B	321	GLN
2	D	64	ASN
2	D	318	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	$\# Z > 2$
2	AEI	C	12	2	12,14,15	2.05	2 (16%)	12,18,20	1.90	3 (25%)
2	AEI	D	12	2	12,14,15	1.93	4 (33%)	12,18,20	1.87	2 (16%)

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	AEI	C	12	2	-	5/16/18/20	-
2	AEI	D	12	2	-	5/16/18/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	12	AEI	OG1-CD	5.80	1.50	1.34
2	D	12	AEI	OG1-CD	4.17	1.46	1.34
2	C	12	AEI	OG1-CB	-3.02	1.42	1.46
2	D	12	AEI	OT1-CH2	2.88	1.30	1.22
2	D	12	AEI	OT2-CH2	-2.73	1.21	1.30
2	D	12	AEI	CE2-CD	2.16	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	AEI	CZ-CE2-CD	-5.23	101.39	112.77
2	C	12	AEI	CZ-CE2-CD	-4.08	103.87	112.77
2	C	12	AEI	OE1-CD-CE2	-3.02	117.63	124.65
2	C	12	AEI	OG1-CD-CE2	2.45	115.83	111.43
2	D	12	AEI	O-C-CA	-2.14	119.26	124.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	12	AEI	O-C-CA-CB
2	C	12	AEI	OT1-CH2-CZ-NH1
2	D	12	AEI	O-C-CA-CB
2	C	12	AEI	OT2-CH2-CZ-NH1
2	D	12	AEI	OT2-CH2-CZ-NH1
2	D	12	AEI	OT1-CH2-CZ-NH1
2	C	12	AEI	OE1-CD-CE2-CZ
2	D	12	AEI	OE1-CD-CE2-CZ
2	C	12	AEI	OG1-CD-CE2-CZ
2	D	12	AEI	OG1-CD-CE2-CZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	12	AEI	1	0
2	D	12	AEI	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	ASP	A	401	-	7,8,8	2.57	1 (14%)	6,10,10	1.02	1 (16%)
3	ASP	B	401	-	7,8,8	1.24	1 (14%)	6,10,10	1.58	1 (16%)

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	ASP	A	401	-	-	3/8/8/8	-
3	ASP	B	401	-	-	2/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ASP	OD1-CG	6.52	1.43	1.22
3	B	401	ASP	OD2-CG	2.60	1.39	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ASP	OD1-CG-CB	-2.90	113.95	122.84
3	A	401	ASP	OD1-CG-CB	-2.02	116.62	122.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

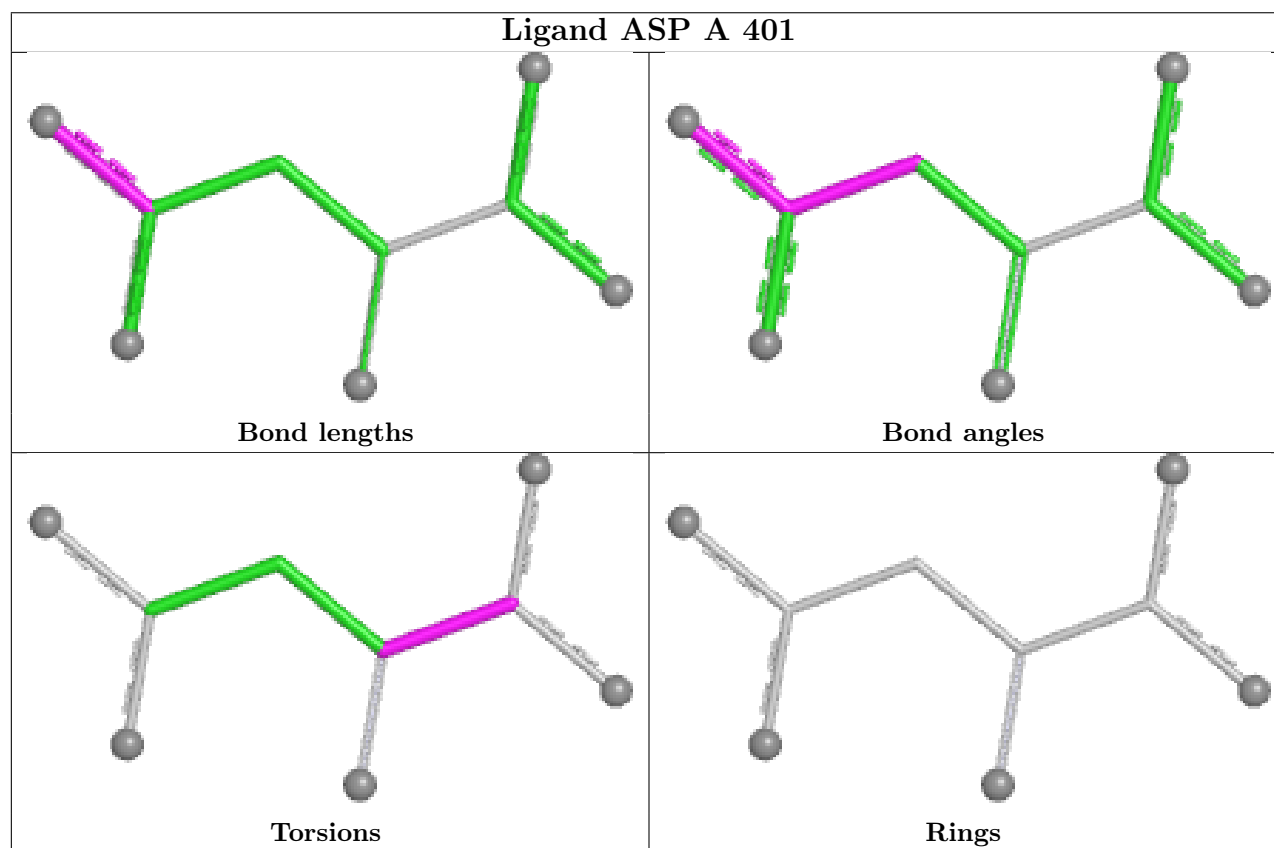
Mol	Chain	Res	Type	Atoms
3	B	401	ASP	O-C-CA-N
3	A	401	ASP	OXT-C-CA-N
3	B	401	ASP	OXT-C-CA-N
3	A	401	ASP	O-C-CA-N
3	A	401	ASP	OXT-C-CA-CB

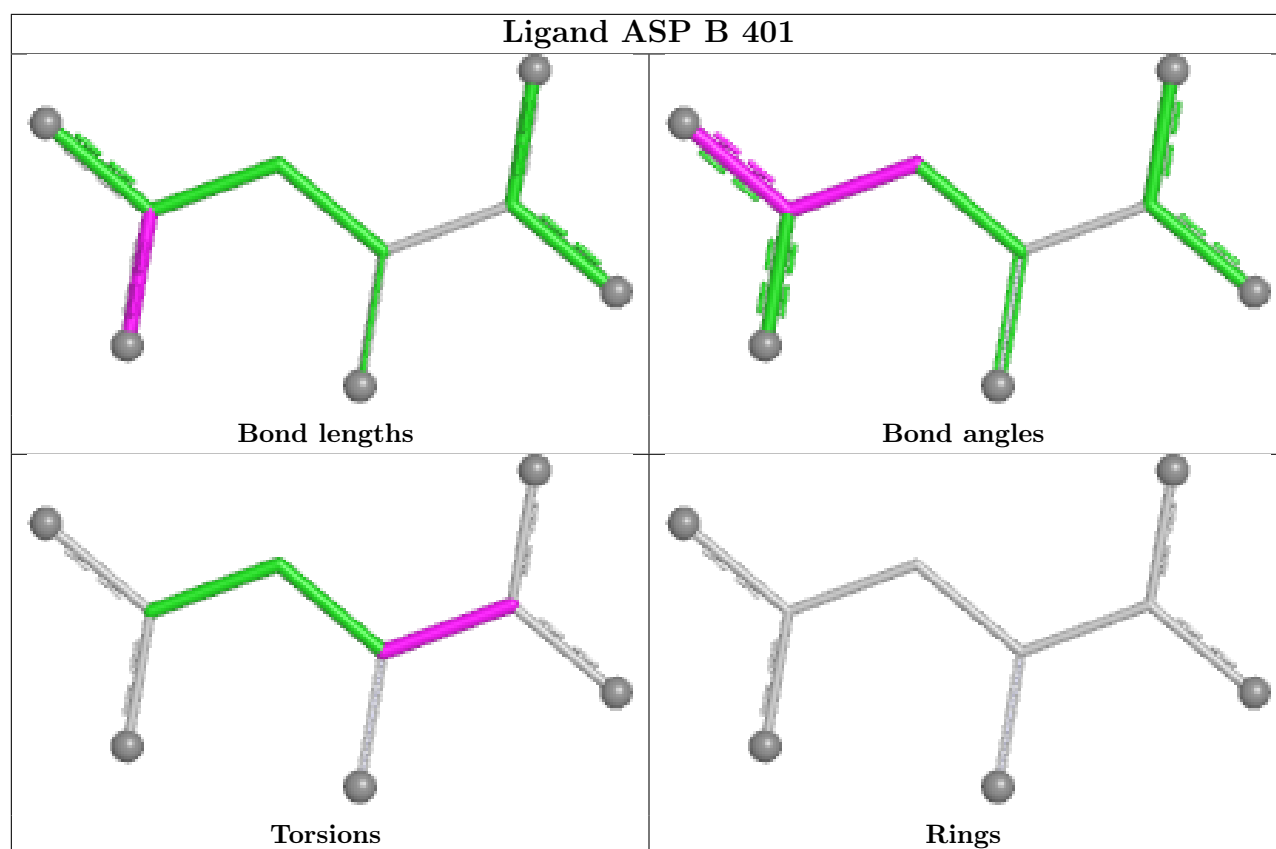
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ASP	4	0
3	B	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	326/333 (97%)	-0.15	8 (2%) 58 66	22, 28, 51, 78	2 (0%)
1	B	305/333 (91%)	-0.09	1 (0%) 90 93	23, 31, 49, 70	1 (0%)
2	C	325/333 (97%)	-0.22	1 (0%) 90 93	22, 28, 44, 56	0
2	D	331/333 (99%)	-0.18	4 (1%) 76 82	21, 29, 47, 69	1 (0%)
All	All	1287/1332 (96%)	-0.16	14 (1%) 78 84	21, 29, 47, 78	4 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	VAL	3.8
2	D	-5	HIS	3.0
1	A	25	TYR	3.0
2	C	26	THR	2.9
1	A	15	GLY	2.5
2	D	29	LYS	2.5
1	A	21	THR	2.4
1	A	24	ASN	2.3
1	A	27	VAL	2.2
2	D	18	ASP	2.2
2	D	106	ASP	2.2
1	A	105	CYS	2.1
1	A	16	GLY	2.0
1	A	28	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	AEI	D	12	15/16	0.97	0.05	23,26,29,31	0
2	AEI	C	12	15/16	0.98	0.05	23,26,36,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

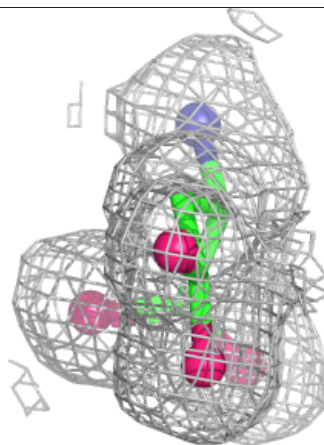
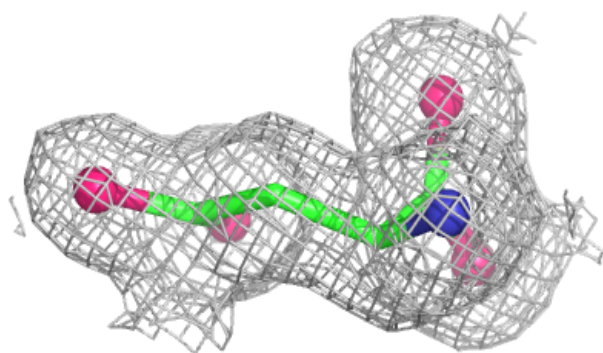
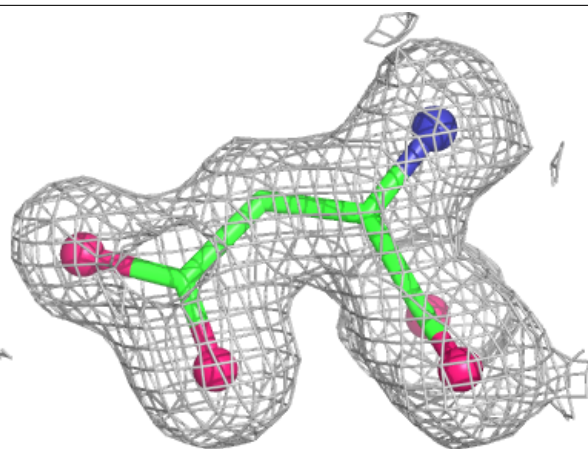
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ASP	A	401	9/9	0.96	0.07	24,25,32,32	0
3	ASP	B	401	9/9	0.97	0.06	26,29,33,35	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.

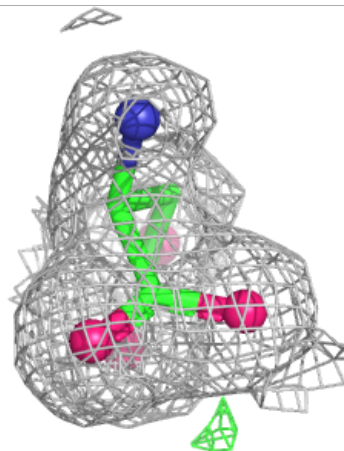
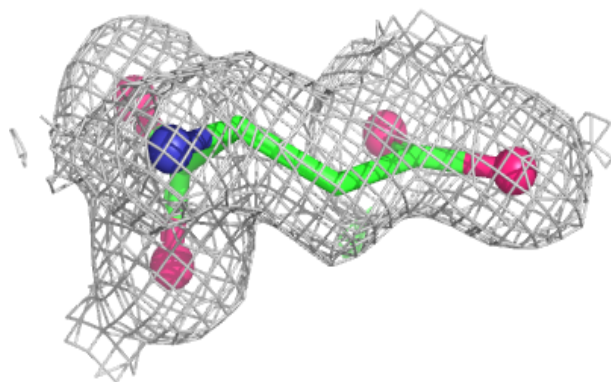
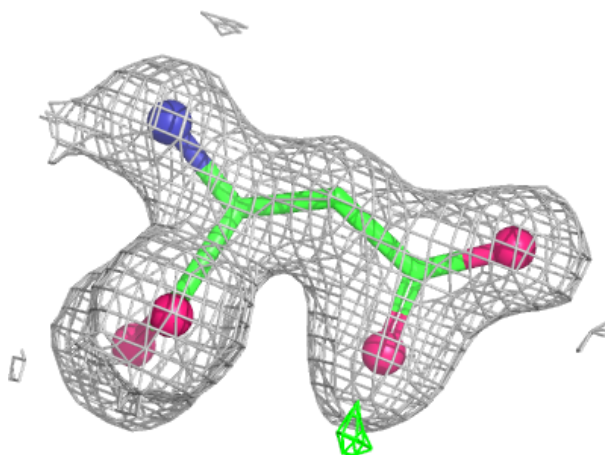
Electron density around ASP A 401:

$2mF_o-DF_c$ (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.