



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:02 AM UTC

PDB ID : 1NNS / pdb_00001nns
Title : L-asparaginase of E. coli in C2 space group and 1.95 Å resolution
Authors : Sanches, M.; Barbosa, J.A.R.G.; de Oliveira, R.T.; Neto, J.A.A.; Polikarpov, I.
Deposited on : 2003-01-14
Resolution : 1.95 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
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

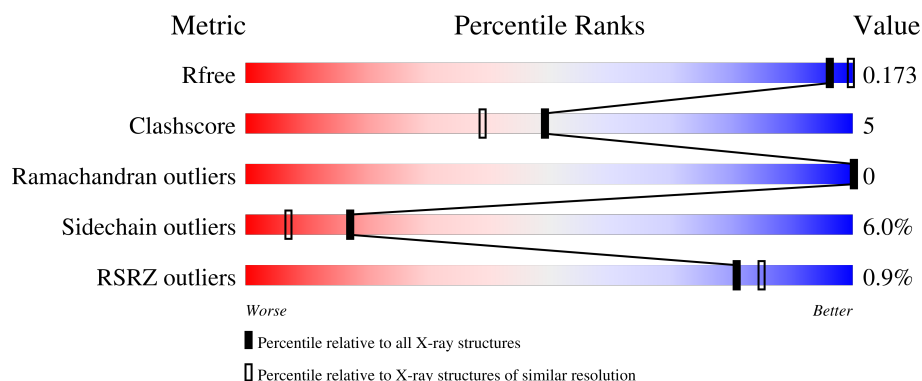
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	 86% 11% ..
1	B	326	 87% 11% .

2 Entry composition [i](#)

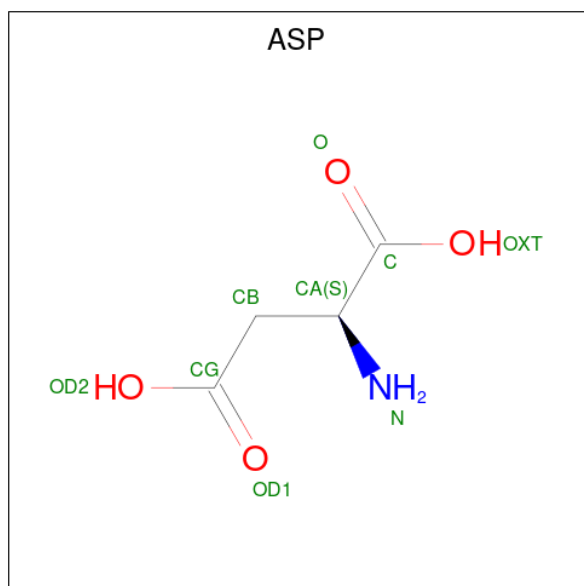
There are 3 unique types of molecules in this entry. The entry contains 5209 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-asparaginase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2431	1517	415	491	8			
1	B	326	Total	C	N	O	S	0	0	0
			2431	1517	415	491	8			

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



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		

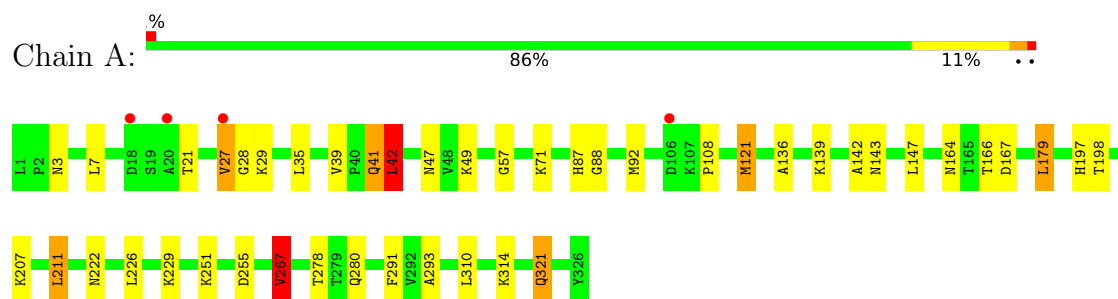
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	184	Total 184	O 184	0	0

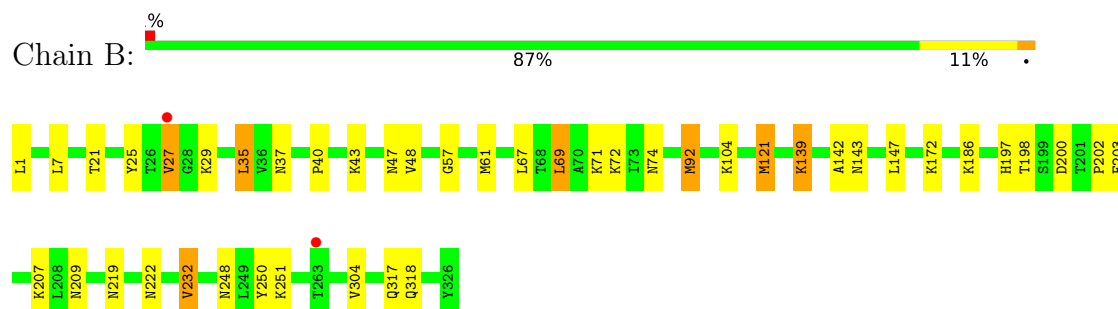
3 Residue-property plots

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 II



• Molecule 1: L-asparaginase II



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.30Å 134.62Å 64.87Å 90.00° 110.51° 90.00°	Depositor
Resolution (Å)	12.97 – 1.95 12.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.8 (12.97-1.95) 91.5 (12.97-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.09	Depositor
R, R_{free}	0.130 , 0.171 0.132 , 0.173	Depositor DCC
R_{free} test set	2045 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5209	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% 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

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	1.31	8/2468 (0.3%)	1.19	5/3361 (0.1%)
1	B	1.41	8/2468 (0.3%)	1.21	7/3361 (0.2%)
All	All	1.36	16/4936 (0.3%)	1.20	12/6722 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	MET	SD-CE	-8.89	1.57	1.79
1	B	142	ALA	CA-CB	7.44	1.65	1.53
1	B	92	MET	SD-CE	-7.24	1.61	1.79
1	B	304	VAL	CA-CB	6.39	1.61	1.54
1	B	121	MET	SD-CE	-6.01	1.64	1.79
1	A	211	LEU	CG-CD1	-5.84	1.33	1.52
1	A	267	VAL	CB-CG2	-5.52	1.34	1.52
1	A	293	ALA	CA-CB	5.44	1.61	1.53
1	A	278	THR	CA-CB	5.36	1.60	1.53
1	A	42	LEU	CG-CD2	-5.34	1.34	1.52
1	B	61	MET	SD-CE	-5.24	1.66	1.79
1	B	69	LEU	CG-CD1	-5.22	1.35	1.52
1	B	248	ASN	CG-ND2	-5.12	1.22	1.33
1	A	121	MET	SD-CE	-5.05	1.67	1.79
1	B	47	ASN	CB-CG	-5.01	1.39	1.52
1	A	92	MET	CG-SD	-5.00	1.68	1.80

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	LYS	CD-CE-NZ	-7.67	87.36	111.90
1	B	232	VAL	N-CA-CB	6.15	117.74	110.55
1	A	267	VAL	N-CA-C	6.05	116.57	108.11
1	A	35	LEU	CD1-CG-CD2	-5.51	98.69	110.80
1	B	48	VAL	N-CA-C	5.42	116.79	108.71
1	B	251	LYS	N-CA-C	5.42	117.61	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	LEU	CB-CG-CD1	5.33	126.70	110.70
1	B	35	LEU	CD1-CG-CD2	-5.33	99.07	110.80
1	B	47	ASN	CB-CA-C	-5.24	102.20	111.05
1	A	267	VAL	CA-CB-CG2	5.22	119.27	110.40
1	A	226	LEU	CD1-CG-CD2	-5.18	99.41	110.80
1	B	139	LYS	CA-CB-CG	-5.12	103.87	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2431	0	2424	23	2
1	B	2431	0	2424	30	0
2	A	9	0	3	0	0
2	B	9	0	3	2	0
3	A	145	0	0	7	2
3	B	184	0	0	11	4
All	All	5209	0	4854	53	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASN:HB2	3:B:605:HOH:O	1.25	1.30
1:B:202:PRO:HG2	3:B:608:HOH:O	1.31	1.27
1:B:318:GLN:HG2	3:B:607:HOH:O	1.30	1.25
1:B:37:ASN:HB2	3:B:598:HOH:O	1.69	0.92
1:B:74:ASN:HD21	1:B:104:LYS:H	1.19	0.90
1:B:27:VAL:HG21	1:B:57:GLY:HA2	1.59	0.83
1:B:200:ASP:HB3	3:B:595:HOH:O	1.85	0.76
1:A:136:ALA:O	3:A:507:HOH:O	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:HG21	1:B:57:GLY:CA	2.15	0.75
1:B:74:ASN:ND2	1:B:104:LYS:H	1.85	0.73
1:A:3:ASN:ND2	1:A:47:ASN:ND2	2.36	0.73
1:B:27:VAL:HG11	2:B:428:ASP:HA	1.74	0.70
1:A:3:ASN:ND2	1:A:47:ASN:HD22	1.92	0.67
1:B:27:VAL:CG2	1:B:57:GLY:HA2	2.25	0.66
1:B:27:VAL:CG2	1:B:57:GLY:CA	2.73	0.66
1:A:87:HIS:HD2	1:A:88:GLY:O	1.79	0.66
1:A:197:HIS:HE1	3:A:543:HOH:O	1.78	0.66
1:A:27:VAL:HG21	1:A:57:GLY:HA2	1.78	0.64
1:B:203:PHE:CD1	3:B:608:HOH:O	2.49	0.64
1:A:164:ASN:HD22	1:A:167:ASP:H	1.46	0.63
3:A:539:HOH:O	1:B:172:LYS:HE3	1.98	0.63
1:B:203:PHE:CE1	3:B:608:HOH:O	2.52	0.63
1:B:25:TYR:HE1	1:B:27:VAL:HG12	1.63	0.62
1:A:27:VAL:CG2	1:A:57:GLY:HA2	2.31	0.61
1:B:40:PRO:O	1:B:43:LYS:HG2	2.05	0.57
1:A:21:THR:HG22	1:A:121:MET:HE3	1.86	0.56
1:A:39:VAL:HB	1:A:42:LEU:HD22	1.90	0.53
1:A:3:ASN:HD21	1:A:47:ASN:HD22	1.54	0.53
1:B:202:PRO:CG	3:B:608:HOH:O	2.14	0.51
1:A:164:ASN:ND2	1:A:166:THR:H	2.09	0.49
1:B:219:ASN:HD22	1:B:250:TYR:H	1.61	0.49
1:A:197:HIS:HD2	1:A:198:THR:OG1	1.96	0.49
1:B:74:ASN:HD21	1:B:104:LYS:N	1.99	0.48
1:B:197:HIS:HD2	1:B:198:THR:OG1	1.95	0.48
1:B:21:THR:HG22	1:B:121:MET:HE3	1.95	0.47
1:A:164:ASN:HD22	1:A:166:THR:H	1.63	0.47
1:A:27:VAL:HG23	1:A:28:GLY:N	2.28	0.47
1:A:321:GLN:NE2	1:A:321:GLN:HA	2.29	0.47
1:A:41:GLN:H	1:A:41:GLN:NE2	2.14	0.46
1:B:318:GLN:CG	3:B:607:HOH:O	2.16	0.46
1:B:186:LYS:HB2	1:B:186:LYS:HE2	1.85	0.43
1:B:27:VAL:HG21	1:B:57:GLY:HA3	1.96	0.43
1:A:108:PRO:HG2	3:A:507:HOH:O	2.18	0.43
1:B:143:ASN:HB3	3:B:603:HOH:O	2.19	0.43
1:A:142:ALA:O	1:A:143:ASN:HB2	2.19	0.43
1:B:67:LEU:O	1:B:71:LYS:HG3	2.19	0.42
1:A:314:LYS:NZ	3:A:563:HOH:O	1.95	0.42
1:A:267:VAL:HG22	1:A:291:PHE:CD1	2.55	0.42
1:B:202:PRO:CD	3:B:608:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:HE2	3:A:534:HOH:O	2.20	0.41
1:B:27:VAL:HG11	2:B:428:ASP:CA	2.48	0.41
1:A:21:THR:HG22	1:A:121:MET:CE	2.51	0.40
3:A:539:HOH:O	1:B:172:LYS:CE	2.65	0.40

All (6) 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)
3:B:590:HOH:O	3:B:590:HOH:O[2_656]	1.43	0.77
1:A:47:ASN:OD1	1:A:47:ASN:OD1[2_555]	1.58	0.62
3:B:481:HOH:O	3:B:591:HOH:O[2_656]	1.61	0.59
3:A:505:HOH:O	3:A:505:HOH:O[2_656]	1.98	0.22
1:A:255:ASP:CB	3:B:593:HOH:O[4_646]	2.14	0.06
3:A:531:HOH:O	3:B:602:HOH:O[2_656]	2.14	0.06

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%)	320 (99%)	4 (1%)	0	100	100
1	B	324/326 (99%)	319 (98%)	5 (2%)	0	100	100
All	All	648/652 (99%)	639 (99%)	9 (1%)	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	266/266 (100%)	248 (93%)	18 (7%)	14	5
1	B	266/266 (100%)	252 (95%)	14 (5%)	20	9
All	All	532/532 (100%)	500 (94%)	32 (6%)	17	7

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	27	VAL
1	A	29	LYS
1	A	41	GLN
1	A	42	LEU
1	A	49	LYS
1	A	71	LYS
1	A	139	LYS
1	A	147	LEU
1	A	179	LEU
1	A	207	LYS
1	A	211	LEU
1	A	222	ASN
1	A	229	LYS
1	A	267	VAL
1	A	280	GLN
1	A	310	LEU
1	A	321	GLN
1	B	1	LEU
1	B	7	LEU
1	B	27	VAL
1	B	29	LYS
1	B	35	LEU
1	B	69	LEU
1	B	72	LYS
1	B	92	MET
1	B	139	LYS
1	B	147	LEU
1	B	207	LYS
1	B	222	ASN
1	B	232	VAL
1	B	317	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	34	ASN
1	A	41	GLN
1	A	64	ASN
1	A	87	HIS
1	A	164	ASN
1	A	190	GLN
1	A	197	HIS
1	A	209	ASN
1	A	248	ASN
1	A	307	GLN
1	A	321	GLN
1	B	34	ASN
1	B	37	ASN
1	B	64	ASN
1	B	74	ASN
1	B	131	ASN
1	B	151	ASN
1	B	183	HIS
1	B	197	HIS
1	B	219	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 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
2	ASP	B	428	-	7,8,8	1.14	1 (14%)	6,10,10	2.99	2 (33%)
2	ASP	A	427	-	7,8,8	1.30	1 (14%)	6,10,10	1.38	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
2	ASP	B	428	-	-	2/8/8/8	-
2	ASP	A	427	-	-	2/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	427	ASP	OXT-C	-2.08	1.24	1.30
2	B	428	ASP	OD2-CG	-2.03	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	428	ASP	OXT-C-O	-6.40	109.56	124.08
2	B	428	ASP	OD2-CG-OD1	-2.88	115.93	123.33
2	A	427	ASP	OXT-C-O	-2.69	117.98	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	427	ASP	O-C-CA-N
2	B	428	ASP	O-C-CA-N
2	B	428	ASP	OXT-C-CA-N
2	A	427	ASP	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	428	ASP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	326/326 (100%)	-0.08	4 (1%) 76 82	10, 15, 29, 40	0
1	B	326/326 (100%)	-0.64	2 (0%) 85 89	10, 15, 29, 40	0
All	All	652/652 (100%)	-0.36	6 (0%) 81 85	10, 15, 30, 40	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	3.3
1	A	106	ASP	3.1
1	A	18	ASP	2.4
1	A	27	VAL	2.2
1	B	27	VAL	2.2
1	B	263	THR	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($\text{\AA}^2$)	Q<0.9
2	ASP	A	427	9/9	0.97	0.05	24,25,28,30	0
2	ASP	B	428	9/9	0.98	0.05	18,20,22,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.