



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:48 AM UTC

PDB ID : 3ECA / pdb\_00003eca  
Title : CRYSTAL STRUCTURE OF ESCHERICHIA COLI L-ASPARAGINASE,  
AN ENZYME USED IN CANCER THERAPY (ELSPAR)  
Authors : Swain, A.L.; Jaskolski, M.; Housset, D.; Rao, J.K.M.; Wlodawer, A.  
Deposited on : 1993-07-02  
Resolution : 2.40 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](mailto: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>.

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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

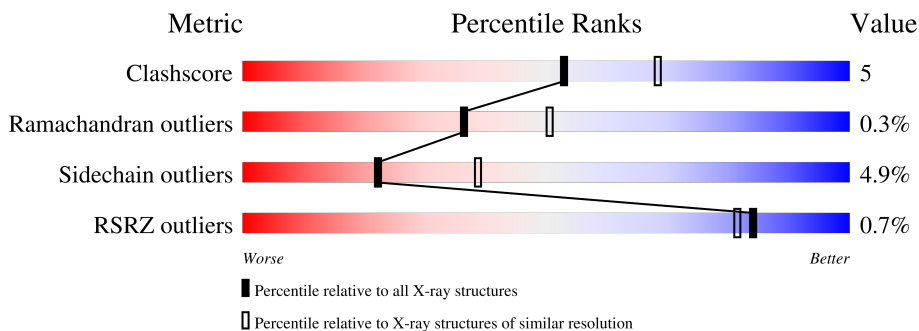
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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% 13% .
1	B	326	 80% 17% .
1	C	326	 79% 17% ..
1	D	326	 84% 14% .

## 2 Entry composition [i](#)

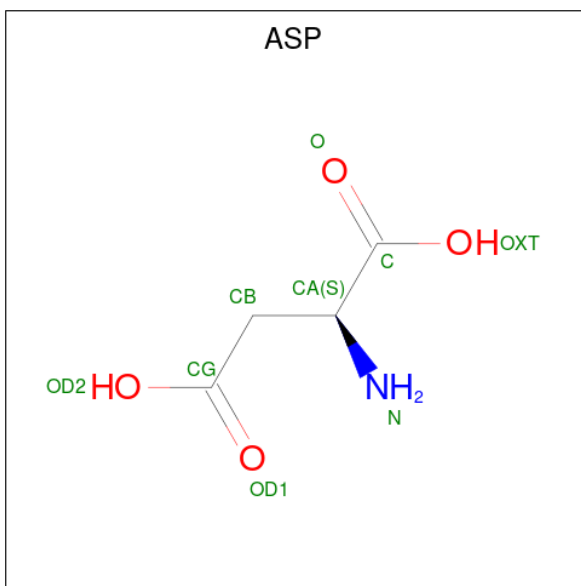
There are 3 unique types of molecules in this entry. The entry contains 10225 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	326	Total 2431	C 1516	N 415	O 492	S 8	0	0	0
1	B	326	Total 2431	C 1516	N 415	O 492	S 8	0	0	0
1	C	326	Total 2431	C 1516	N 415	O 492	S 8	0	0	0
1	D	326	Total 2431	C 1516	N 415	O 492	S 8	0	0	0

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

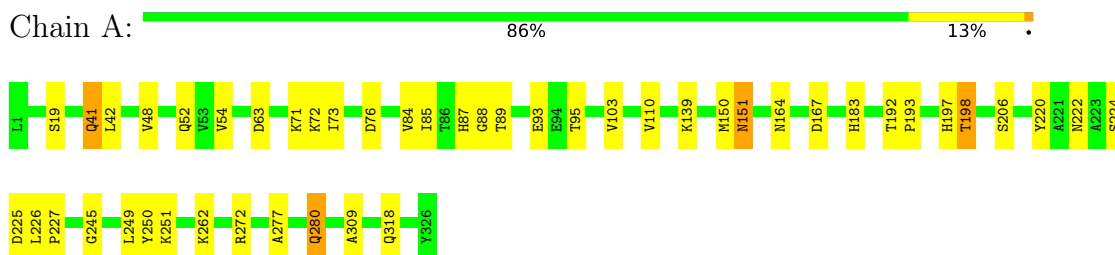
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	129	Total	O	0	0
			129	129		
3	C	109	Total	O	0	0
			109	109		
3	D	112	Total	O	0	0
			112	112		

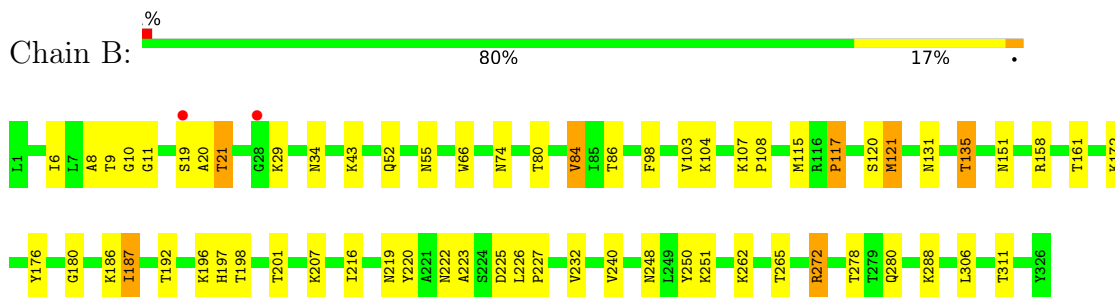
### 3 Residue-property plots [i](#)

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.

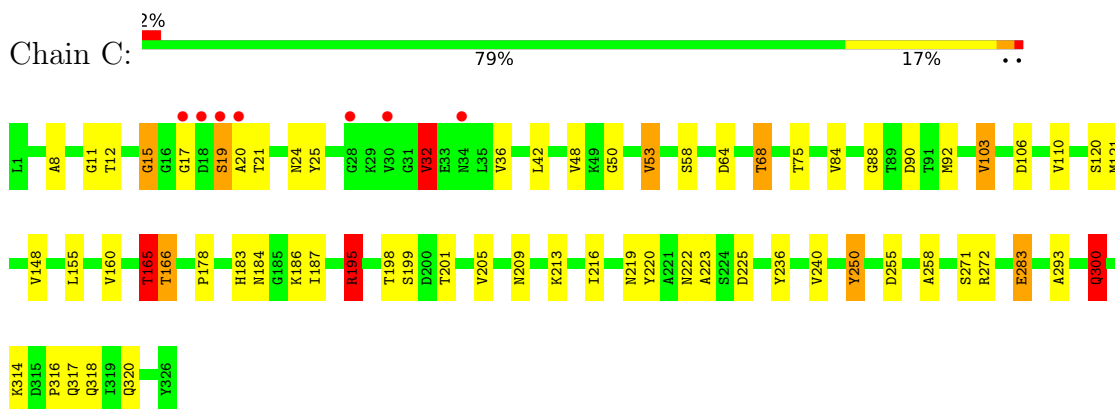
- Molecule 1: L-asparaginase 2



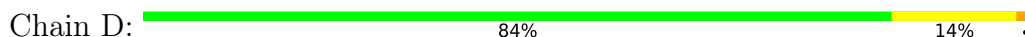
- Molecule 1: L-asparaginase 2

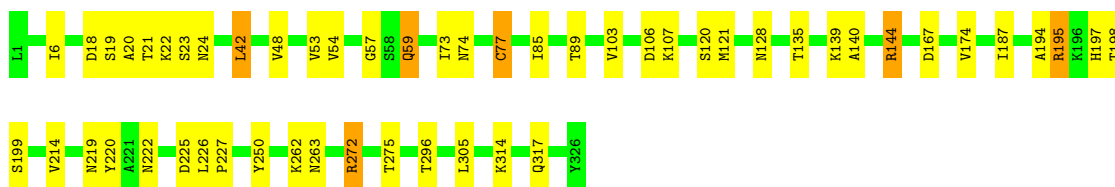


- Molecule 1: L-asparaginase 2



- Molecule 1: L-asparaginase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.70Å 96.10Å 111.30Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	9.99 – 2.40 9.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	85.3 (9.99-2.40) 85.3 (9.99-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.111 , (Not available) 0.121 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.1	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical 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	1.20	4/2468 (0.2%)	1.48	6/3361 (0.2%)
1	B	1.25	9/2468 (0.4%)	1.57	19/3361 (0.6%)
1	C	1.27	9/2468 (0.4%)	1.58	21/3361 (0.6%)
1	D	1.21	4/2468 (0.2%)	1.55	23/3361 (0.7%)
All	All	1.23	26/9872 (0.3%)	1.55	69/13444 (0.5%)

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	C	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	THR	C-O	-6.97	1.15	1.24
1	B	187	ILE	C-O	-6.53	1.17	1.24
1	D	53	VAL	C-O	-6.27	1.17	1.23
1	C	283	GLU	C-O	-6.21	1.16	1.24
1	B	115	MET	C-O	-6.17	1.16	1.24
1	B	248	ASN	C-O	6.00	1.31	1.23
1	B	52	GLN	C-O	-5.95	1.16	1.24
1	C	271	SER	C-O	-5.80	1.17	1.23
1	D	194	ALA	C-O	-5.76	1.16	1.24
1	B	180	GLY	C-O	-5.74	1.18	1.23
1	C	183	HIS	CE1-NE2	5.69	1.38	1.32
1	A	250	TYR	C-O	5.66	1.30	1.23
1	B	280	GLN	C-O	5.58	1.31	1.23
1	C	19	SER	C-O	5.49	1.30	1.24
1	C	48	VAL	C-O	-5.47	1.17	1.24
1	D	214	VAL	C-O	-5.47	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	TYR	C-O	-5.41	1.17	1.24
1	C	110	VAL	C-O	-5.29	1.18	1.24
1	B	135	THR	C-O	-5.28	1.18	1.24
1	C	84	VAL	C-O	-5.25	1.18	1.24
1	C	103	VAL	C-O	-5.23	1.18	1.24
1	D	48	VAL	C-O	-5.22	1.18	1.24
1	B	158	ARG	C-O	-5.07	1.18	1.24
1	A	193	PRO	C-O	-5.03	1.17	1.23
1	A	48	VAL	C-O	-5.03	1.18	1.24
1	A	183	HIS	CE1-NE2	5.01	1.37	1.32

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	GLN	CB-CA-C	-10.92	93.34	110.81
1	B	121	MET	CA-C-N	-8.04	111.30	122.87
1	B	121	MET	C-N-CA	-8.04	111.30	122.87
1	D	195	ARG	NE-CZ-NH1	-7.79	113.72	121.50
1	D	195	ARG	NE-CZ-NH2	7.57	126.02	119.20
1	D	53	VAL	N-CA-C	-7.54	104.44	111.45
1	C	314	LYS	N-CA-C	-7.45	102.43	113.61
1	A	225	ASP	CA-CB-CG	7.35	119.95	112.60
1	C	314	LYS	CB-CA-C	7.26	122.62	109.99
1	B	272	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	B	272	ARG	NE-CZ-NH1	-7.02	114.48	121.50
1	A	192	THR	CB-CA-C	6.73	119.20	109.45
1	D	272	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	C	50	GLY	CA-C-O	-6.53	114.61	120.75
1	D	272	ARG	NE-CZ-NH1	-6.51	114.99	121.50
1	D	54	VAL	CA-C-O	-6.51	115.26	121.64
1	D	272	ARG	CB-CG-CD	6.47	126.17	111.30
1	C	165	THR	N-CA-CB	-6.34	100.53	110.30
1	D	167	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	117	PRO	CA-C-N	6.12	129.31	120.38
1	B	117	PRO	C-N-CA	6.12	129.31	120.38
1	C	195	ARG	CG-CD-NE	6.05	125.31	112.00
1	D	77	CYS	CA-C-N	5.97	130.16	120.60
1	D	77	CYS	C-N-CA	5.97	130.16	120.60
1	C	258	ALA	CA-C-N	5.97	128.21	120.44
1	C	258	ALA	C-N-CA	5.97	128.21	120.44
1	B	192	THR	CB-CA-C	5.93	118.05	109.45
1	C	195	ARG	CD-NE-CZ	5.84	132.57	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ASN	CA-CB-CG	5.83	118.43	112.60
1	B	278	THR	CA-CB-OG1	-5.81	100.89	109.60
1	D	74	ASN	CA-C-N	5.78	127.95	120.44
1	D	74	ASN	C-N-CA	5.78	127.95	120.44
1	C	213	LYS	CB-CA-C	5.76	119.84	110.22
1	C	250	TYR	CA-C-O	-5.74	114.88	121.19
1	D	128	ASN	N-CA-C	-5.73	104.94	111.07
1	D	296	THR	CA-CB-OG1	-5.71	101.04	109.60
1	C	88	GLY	N-CA-C	-5.67	106.09	112.33
1	B	84	VAL	CA-C-O	-5.62	114.54	120.39
1	B	80	THR	CA-C-O	-5.62	115.44	121.45
1	C	53	VAL	N-CA-C	-5.62	107.34	112.96
1	B	265	THR	CA-CB-OG1	-5.60	101.19	109.60
1	C	75	THR	CA-CB-OG1	-5.58	101.23	109.60
1	B	9	THR	CA-CB-OG1	-5.58	101.23	109.60
1	C	209	ASN	N-CA-C	-5.50	105.36	113.61
1	D	305	LEU	N-CA-C	-5.50	105.30	112.23
1	C	300	GLN	CB-CG-CD	5.48	121.92	112.60
1	C	205	VAL	N-CA-C	-5.45	107.43	112.83
1	C	225	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	309	ALA	N-CA-C	-5.43	105.44	111.36
1	D	220	TYR	CA-C-O	-5.43	115.18	121.26
1	D	263	ASN	CA-CB-CG	-5.40	107.20	112.60
1	B	21	THR	CA-C-N	5.38	129.20	121.50
1	B	21	THR	C-N-CA	5.38	129.20	121.50
1	C	11	GLY	CA-C-O	-5.36	117.04	122.56
1	B	311	THR	N-CA-C	-5.34	106.76	113.28
1	B	225	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	151	ASN	CA-C-O	-5.26	115.74	121.84
1	D	144	ARG	CG-CD-NE	-5.25	100.44	112.00
1	D	6	ILE	CA-C-O	-5.25	114.65	120.74
1	D	195	ARG	CG-CD-NE	-5.24	100.47	112.00
1	D	225	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	53	VAL	CB-CA-C	5.17	115.61	111.06
1	A	54	VAL	CA-C-O	-5.12	116.32	121.49
1	B	34	ASN	CA-C-O	-5.11	115.00	120.42
1	D	57	GLY	CA-C-O	-5.11	116.98	121.58
1	B	196	LYS	CB-CA-C	5.10	118.38	109.65
1	A	52	GLN	CA-C-O	-5.05	115.17	120.58
1	D	195	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	161	THR	CA-CB-OG1	-5.00	102.09	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	300	GLN	Sidechain

## 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	2431	0	2419	24	0
1	B	2431	0	2419	25	0
1	C	2431	0	2419	30	0
1	D	2431	0	2419	25	0
2	A	9	0	3	2	0
2	B	9	0	3	1	0
2	C	9	0	3	1	0
2	D	9	0	3	2	0
3	A	115	0	0	5	0
3	B	129	0	0	4	0
3	C	109	0	0	0	0
3	D	112	0	0	2	0
All	All	10225	0	9688	98	0

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

All (98) 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:D:59:GLN:H	1:D:59:GLN:HE21	1.07	0.97
1:B:74:ASN:HD21	1:B:104:LYS:H	1.12	0.95
1:B:172:LYS:HE3	3:B:617:HOH:O	1.66	0.94
1:C:293:ALA:H	1:C:320:GLN:HE22	1.16	0.88
1:C:106:ASP:OD2	1:C:199:SER:OG	1.95	0.84
1:A:41:GLN:HE21	1:A:41:GLN:H	1.26	0.81
1:A:277:ALA:O	1:C:165:THR:HG21	1.80	0.80
1:B:74:ASN:ND2	1:B:104:LYS:H	1.80	0.78
1:A:164:ASN:HD22	1:A:167:ASP:H	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:HIS:HD2	1:D:198:THR:OG1	1.69	0.76
1:A:41:GLN:H	1:A:41:GLN:NE2	1.90	0.69
1:C:165:THR:HG23	1:C:166:THR:HG23	1.76	0.66
1:D:103:VAL:O	1:D:198:THR:HA	1.95	0.65
1:C:219:ASN:HD22	1:C:250:TYR:H	1.47	0.62
1:C:64:ASP:O	1:C:68:THR:HG23	1.99	0.62
1:C:293:ALA:H	1:C:320:GLN:NE2	1.94	0.61
1:B:74:ASN:HD21	1:B:104:LYS:N	1.92	0.61
1:A:87:HIS:HD2	1:A:88:GLY:O	1.84	0.60
1:C:17:GLY:HA2	1:C:25:TYR:HB3	1.84	0.59
1:C:293:ALA:N	1:C:320:GLN:HE22	1.96	0.58
1:B:219:ASN:ND2	1:B:250:TYR:H	2.03	0.55
1:C:21:THR:O	1:C:21:THR:HG22	2.05	0.55
1:B:117:PRO:O	1:B:120:SER:HB3	2.06	0.55
1:C:219:ASN:ND2	1:C:250:TYR:H	2.04	0.55
1:B:219:ASN:HD22	1:B:250:TYR:H	1.54	0.53
1:C:8:ALA:HB2	1:C:32:VAL:HG13	1.91	0.52
1:C:17:GLY:HA2	1:C:25:TYR:CB	2.40	0.52
1:C:20:ALA:HA	1:C:120:SER:HA	1.92	0.51
1:A:103:VAL:O	1:A:198:THR:HA	2.10	0.51
1:B:197:HIS:HD2	1:B:198:THR:OG1	1.94	0.51
1:B:172:LYS:CE	3:B:617:HOH:O	2.40	0.51
1:C:165:THR:CG2	1:C:166:THR:HG23	2.42	0.50
1:A:197:HIS:HE1	3:A:598:HOH:O	1.93	0.50
1:A:224:SER:HB2	1:C:236:TYR:OH	2.11	0.50
1:B:11:GLY:HA2	2:B:401:ASP:OXT	2.12	0.50
1:B:220:TYR:CZ	1:B:223:ALA:HA	2.47	0.50
1:C:58:SER:OG	2:C:401:ASP:OXT	2.25	0.49
1:A:73:ILE:HD11	1:A:85:ILE:HD11	1.94	0.49
3:A:595:HOH:O	1:D:195:ARG:HD3	2.11	0.49
1:D:107:LYS:HE2	3:D:509:HOH:O	2.12	0.49
1:D:59:GLN:HE21	1:D:59:GLN:N	1.91	0.49
1:D:197:HIS:HE1	3:D:590:HOH:O	1.94	0.49
1:A:280:GLN:HB3	3:A:576:HOH:O	2.12	0.48
1:B:19:SER:OG	1:B:20:ALA:N	2.46	0.48
1:C:184:ASN:HB2	1:D:23:SER:OG	2.14	0.47
1:B:21:THR:HG22	1:B:121:MET:HE1	1.96	0.47
1:D:140:ALA:O	1:D:144:ARG:HD2	2.14	0.47
1:B:10:GLY:HA2	1:B:55:ASN:OD1	2.14	0.47
1:A:197:HIS:HD2	1:A:198:THR:OG1	1.98	0.47
1:D:226:LEU:HB2	1:D:227:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:TRP:HB3	1:B:98:PHE:CE2	2.50	0.46
1:A:87:HIS:CE1	1:A:95:THR:OG1	2.68	0.46
1:D:59:GLN:H	1:D:59:GLN:NE2	1.92	0.46
1:D:77:CYS:O	1:D:107:LYS:NZ	2.41	0.46
1:A:226:LEU:HB2	1:A:227:PRO:HD3	1.98	0.46
1:A:84:VAL:HA	1:A:110:VAL:O	2.15	0.46
1:B:135:THR:HA	1:B:187:ILE:HD11	1.98	0.46
1:C:21:THR:O	1:C:21:THR:CG2	2.64	0.46
1:C:220:TYR:CZ	1:C:223:ALA:HA	2.51	0.46
1:B:103:VAL:O	1:B:198:THR:HA	2.17	0.45
3:B:584:HOH:O	1:C:195:ARG:HB2	2.17	0.45
1:B:216:ILE:HA	1:B:240:VAL:O	2.15	0.45
1:D:219:ASN:HD22	1:D:250:TYR:H	1.64	0.45
1:D:21:THR:CG2	1:D:121:MET:SD	3.05	0.45
1:D:106:ASP:OD2	1:D:199:SER:OG	2.32	0.45
1:A:72:LYS:NZ	1:A:76:ASP:OD2	2.48	0.44
1:A:277:ALA:O	1:C:165:THR:CG2	2.60	0.44
1:C:64:ASP:O	1:C:68:THR:CG2	2.65	0.44
1:D:174:VAL:HB	1:D:275:THR:HG22	1.99	0.44
1:D:19:SER:OG	1:D:22:LYS:HB3	2.17	0.44
1:B:216:ILE:HG12	1:B:240:VAL:HB	2.00	0.44
1:A:220:TYR:CD1	1:A:220:TYR:N	2.86	0.44
1:A:93:GLU:HG2	3:A:540:HOH:O	2.18	0.43
1:C:12:THR:HA	1:C:15:GLY:HA3	2.00	0.43
1:D:20:ALA:HA	1:D:120:SER:HA	2.00	0.43
1:A:150:MET:O	1:A:151:ASN:C	2.61	0.43
1:D:73:ILE:HD11	1:D:85:ILE:HD11	2.01	0.43
1:D:59:GLN:HE22	2:D:401:ASP:N	2.17	0.43
1:C:103:VAL:O	1:C:198:THR:HA	2.18	0.43
1:B:8:ALA:HA	1:B:86:THR:OG1	2.18	0.42
1:B:6:ILE:HA	1:B:84:VAL:O	2.19	0.42
1:A:89:THR:OG1	2:A:401:ASP:OD1	2.32	0.42
1:D:89:THR:OG1	2:D:401:ASP:OD2	2.32	0.42
1:D:22:LYS:HG2	1:D:24:ASN:HD22	1.85	0.42
1:A:245:GLY:HA3	1:C:90:ASP:OD1	2.20	0.42
1:A:87:HIS:HE1	1:A:95:THR:OG1	2.02	0.42
1:A:63:ASP:OD2	3:A:501:HOH:O	2.22	0.41
1:C:148:VAL:HG21	1:C:160:VAL:HG11	2.02	0.41
1:A:71:LYS:HE2	1:A:206:SER:O	2.20	0.41
2:A:401:ASP:N	1:C:283:GLU:OE2	2.53	0.41
1:C:155:LEU:HD23	1:C:178:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:THR:HA	1:D:187:ILE:HD11	2.03	0.41
1:B:107:LYS:HA	1:B:108:PRO:HD3	1.93	0.41
1:D:42:LEU:HD12	1:D:42:LEU:HA	1.85	0.40
1:B:226:LEU:HB2	1:B:227:PRO:HD3	2.03	0.40
1:B:151:ASN:ND2	3:B:512:HOH:O	2.55	0.40
1:B:227:PRO:HB3	1:D:227:PRO:HB3	2.03	0.40
1:C:216:ILE:HA	1:C:240:VAL:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/326 (99%)	319 (98%)	4 (1%)	1 (0%)	36	50
1	B	324/326 (99%)	314 (97%)	10 (3%)	0	100	100
1	C	324/326 (99%)	311 (96%)	10 (3%)	3 (1%)	14	22
1	D	324/326 (99%)	318 (98%)	6 (2%)	0	100	100
All	All	1296/1304 (99%)	1262 (97%)	30 (2%)	4 (0%)	36	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	19	SER
1	C	32	VAL
1	A	198	THR
1	C	15	GLY

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/265 (100%)	254 (96%)	11 (4%)	26	45
1	B	265/265 (100%)	252 (95%)	13 (5%)	22	39
1	C	265/265 (100%)	246 (93%)	19 (7%)	13	23
1	D	265/265 (100%)	256 (97%)	9 (3%)	32	54
All	All	1060/1060 (100%)	1008 (95%)	52 (5%)	22	39

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	41	GLN
1	A	42	LEU
1	A	139	LYS
1	A	222	ASN
1	A	249	LEU
1	A	251	LYS
1	A	262	LYS
1	A	272	ARG
1	A	280	GLN
1	A	318	GLN
1	B	29	LYS
1	B	43	LYS
1	B	131	ASN
1	B	186	LYS
1	B	201	THR
1	B	207	LYS
1	B	222	ASN
1	B	232	VAL
1	B	251	LYS
1	B	262	LYS
1	B	272	ARG
1	B	288	LYS
1	B	306	LEU

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Mol	Chain	Res	Type
1	C	32	VAL
1	C	36	VAL
1	C	42	LEU
1	C	53	VAL
1	C	68	THR
1	C	92	MET
1	C	121	MET
1	C	165	THR
1	C	186	LYS
1	C	187	ILE
1	C	195	ARG
1	C	201	THR
1	C	222	ASN
1	C	255	ASP
1	C	272	ARG
1	C	300	GLN
1	C	316	PRO
1	C	317	GLN
1	C	318	GLN
1	D	18	ASP
1	D	42	LEU
1	D	59	GLN
1	D	139	LYS
1	D	222	ASN
1	D	262	LYS
1	D	272	ARG
1	D	314	LYS
1	D	317	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	34	ASN
1	A	41	GLN
1	A	87	HIS
1	A	164	ASN
1	A	197	HIS
1	A	209	ASN
1	A	219	ASN
1	A	248	ASN
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	183	HIS
1	B	197	HIS
1	B	219	ASN
1	B	248	ASN
1	B	312	GLN
1	B	318	GLN
1	C	131	ASN
1	C	183	HIS
1	C	219	ASN
1	C	248	ASN
1	C	320	GLN
1	C	324	ASN
1	D	24	ASN
1	D	59	GLN
1	D	131	ASN
1	D	151	ASN
1	D	190	GLN
1	D	197	HIS
1	D	219	ASN
1	D	324	ASN
1	D	325	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

4 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	D	401	-	7,8,8	1.28	1 (14%)	6,10,10	0.91	0
2	ASP	B	401	-	7,8,8	1.27	2 (28%)	6,10,10	0.91	0
2	ASP	C	401	-	7,8,8	1.26	1 (14%)	6,10,10	1.59	1 (16%)
2	ASP	A	401	-	7,8,8	1.00	0	6,10,10	1.04	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	D	401	-	-	2/8/8/8	-
2	ASP	B	401	-	-	5/8/8/8	-
2	ASP	C	401	-	-	3/8/8/8	-
2	ASP	A	401	-	-	4/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ASP	OD1-CG	2.45	1.30	1.22
2	C	401	ASP	OXT-C	-2.30	1.23	1.30
2	B	401	ASP	OD2-CG	-2.16	1.23	1.30
2	D	401	ASP	OXT-C	-2.06	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ASP	OXT-C-O	-2.95	117.39	124.08

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ASP	O-C-CA-N
2	B	401	ASP	O-C-CA-N
2	C	401	ASP	O-C-CA-N
2	D	401	ASP	O-C-CA-N
2	A	401	ASP	OXT-C-CA-N
2	B	401	ASP	OXT-C-CA-N
2	D	401	ASP	OXT-C-CA-N
2	C	401	ASP	OXT-C-CA-N
2	A	401	ASP	O-C-CA-CB
2	A	401	ASP	OXT-C-CA-CB
2	B	401	ASP	O-C-CA-CB
2	B	401	ASP	OXT-C-CA-CB
2	C	401	ASP	C-CA-CB-CG
2	B	401	ASP	CA-CB-CG-OD1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	ASP	2	0
2	B	401	ASP	1	0
2	C	401	ASP	1	0
2	A	401	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	326/326 (100%)	-1.03	0 <b>100</b> <b>100</b>	10, 24, 50, 77	0
1	B	326/326 (100%)	-1.00	2 (0%) <b>85</b> <b>83</b>	10, 20, 64, 125	0
1	C	326/326 (100%)	-0.86	7 (2%) <b>63</b> <b>59</b>	11, 23, 99, 149	0
1	D	326/326 (100%)	-1.00	0 <b>100</b> <b>100</b>	9, 22, 58, 94	0
All	All	1304/1304 (100%)	-0.97	9 (0%) <b>84</b> <b>81</b>	9, 22, 60, 149	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	SER	4.3
1	C	20	ALA	4.1
1	B	19	SER	3.4
1	C	30	VAL	3.3
1	C	17	GLY	3.1
1	B	28	GLY	2.7
1	C	28	GLY	2.4
1	C	34	ASN	2.2
1	C	18	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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	ASP	C	401	9/9	0.93	0.10	39,51,56,58	0
2	ASP	B	401	9/9	0.97	0.06	22,30,35,36	0
2	ASP	A	401	9/9	0.98	0.04	18,23,26,27	0
2	ASP	D	401	9/9	0.98	0.04	16,21,26,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.