Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:35 PM BST

PDB ID	:	3ECA
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*
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 ①) were used in the production of this report:

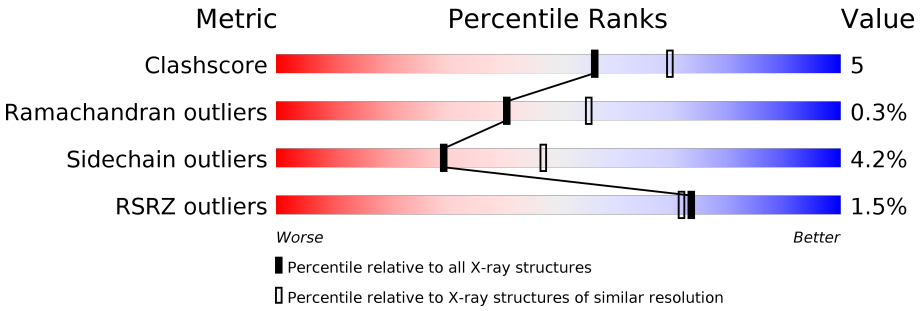
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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 <=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	88% 11% •
1	B	326	% 86% 14%
1	C	326	4% 87% 11% • •
1	D	326	% 88% 10% •

2 Entry composition

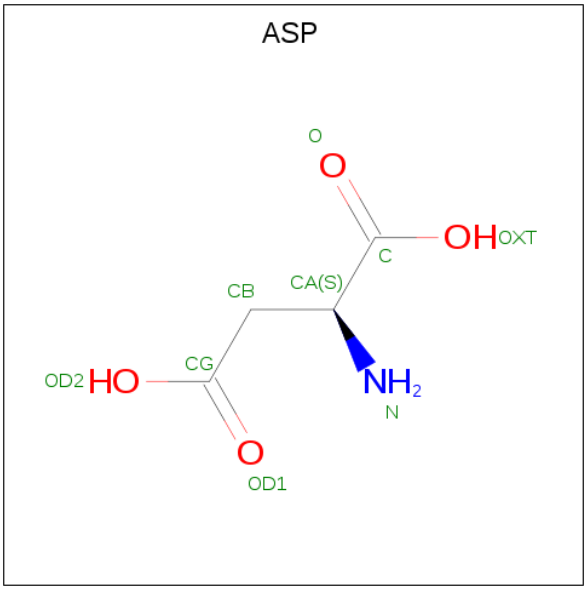
There are 3 unique types of molecules in this entry. The entry contains 10225 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is ASPARTIC ACID (three-letter code: 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		

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

- Molecule 3 is water.

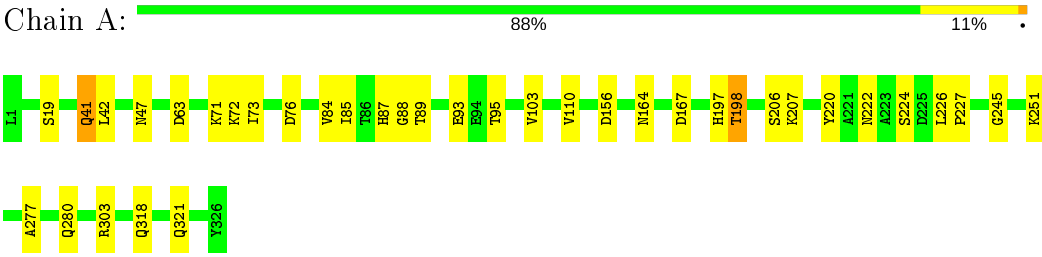
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	115	Total O 115 115	0	0
3	B	129	Total O 129 129	0	0
3	C	109	Total O 109 109	0	0
3	D	112	Total O 112 112	0	0

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.

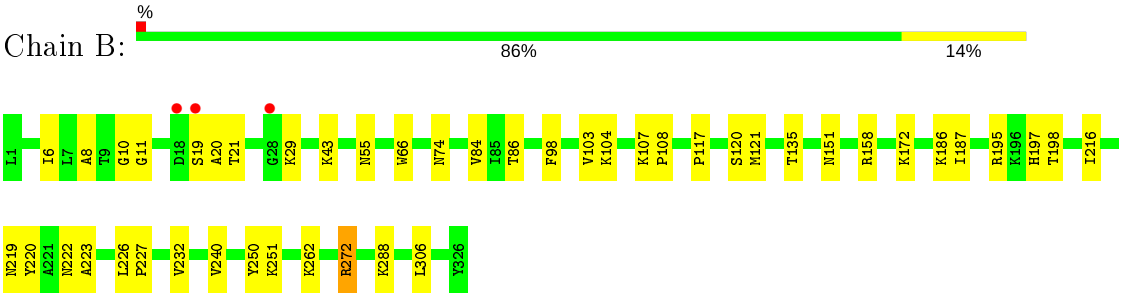
- Molecule 1: L-asparaginase 2

Chain A:



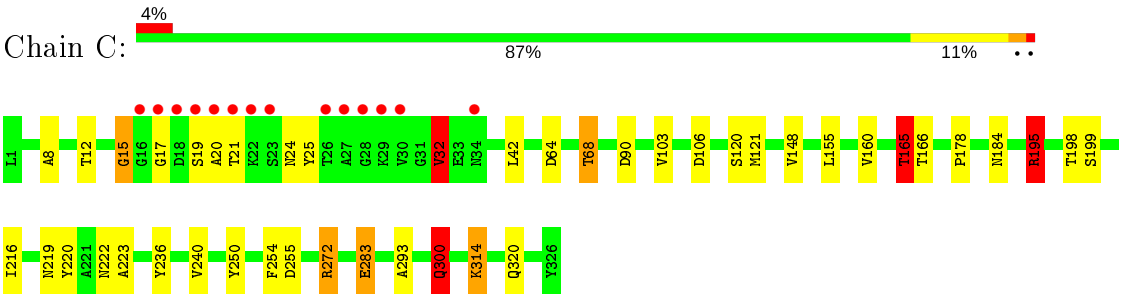
- Molecule 1: L-asparaginase 2

Chain B:



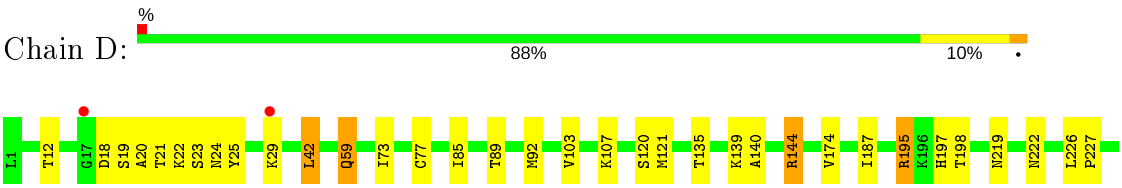
- Molecule 1: L-asparaginase 2

Chain C:



- Molecule 1: L-asparaginase 2

Chain D:




Y250
K262
R272
T275
Q317
Y326

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.70Å 96.10Å 111.30Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	9.99 – 2.40 9.99 – 2.31	Depositor EDS
% Data completeness (in resolution range)	85.3 (9.99-2.40) 81.3 (9.99-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
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^2)	20.1	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.6	EDS
L-test for twinning[1]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10225	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage'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.*

[1] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.81	0/2468	1.03	3/3361 (0.1%)
1	B	0.85	0/2468	1.11	6/3361 (0.2%)
1	C	0.86	1/2468 (0.0%)	1.10	9/3361 (0.3%)
1	D	0.82	0/2468	1.11	10/3361 (0.3%)
All	All	0.84	1/9872 (0.0%)	1.09	28/13444 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	283	GLU	CD-OE2	-6.97	1.18	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	195	ARG	NE-CZ-NH1	-13.17	113.72	120.30
1	B	272	ARG	NE-CZ-NH1	-11.64	114.48	120.30
1	D	195	ARG	NE-CZ-NH2	11.43	126.02	120.30
1	D	272	ARG	NE-CZ-NH1	-10.63	114.99	120.30
1	B	272	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	C	272	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	A	272	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	272	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	D	272	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	C	272	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	C	300	GLN	CB-CA-C	-8.53	93.34	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	144	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	C	195	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	D	144	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	C	195	ARG	CG-CD-NE	6.43	125.31	111.80
1	C	195	ARG	CD-NE-CZ	6.41	132.57	123.60
1	C	195	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	C	314	LYS	CB-CA-C	6.11	122.62	110.40
1	B	195	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	B	195	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	272	ARG	CB-CG-CD	5.60	126.17	111.60
1	D	195	ARG	CD-NE-CZ	5.60	131.44	123.60
1	D	144	ARG	CG-CD-NE	-5.41	100.44	111.80
1	B	158	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	195	ARG	CG-CD-NE	-5.39	100.47	111.80
1	C	165	THR	N-CA-CB	-5.14	100.53	110.30
1	A	303	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	272	ARG	CD-NE-CZ	5.02	130.62	123.60

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	23	0
1	B	2431	0	2419	26	0
1	C	2431	0	2419	29	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	0	0
2	D	9	0	3	2	0
3	A	115	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	97	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 (97) 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:H	1:A:41:GLN:HE21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:73:ILE:HD11	1:A:85:ILE:HD11	1.94	0.49
1:D:107:LYS:HE2	3:D:509:HOH:O	2.12	0.49
3:A:595:HOH:O	1:D:195:ARG:HD3	2.11	0.49
1:D:197:HIS:HE1	3:D:590:HOH:O	1.94	0.49
1:D:59:GLN:N	1:D:59:GLN:HE21	1.91	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: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:D:12:THR:HG1	1:D:25:TYR:HE2	1.61	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
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:NE2	1:D:59:GLN:H	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:CG2	1:C:21:THR:O	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: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:B:21:THR:HG22	1:B:121:MET:HE1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:21:THR:CG2	1:B:121:MET:HE1	2.51	0.41
1:C:155:LEU:HD23	1:C:178:PRO:HB3	2.03	0.41
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:HA	1:D:42:LEU:HD12	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:C:216:ILE:HA	1:C:240:VAL:O	2.21	0.40
1:B:227:PRO:HB3	1:D:227:PRO:HB3	2.03	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%)	41 55
1	B	324/326 (99%)	314 (97%)	10 (3%)	0	100 100
1	C	324/326 (99%)	311 (96%)	10 (3%)	3 (1%)	17 25
1	D	324/326 (99%)	318 (98%)	6 (2%)	0	100 100
All	All	1296/1304 (99%)	1262 (97%)	30 (2%)	4 (0%)	41 55

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 (i)

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%)	253 (96%)	12 (4%)	27 44
1	B	265/265 (100%)	255 (96%)	10 (4%)	33 51
1	C	265/265 (100%)	252 (95%)	13 (5%)	25 40
1	D	265/265 (100%)	255 (96%)	10 (4%)	33 51
All	All	1060/1060 (100%)	1015 (96%)	45 (4%)	30 47

All (45) 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	47	ASN
1	A	156	ASP
1	A	207	LYS
1	A	222	ASN

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Mol	Chain	Res	Type
1	A	251	LYS
1	A	254	PHE
1	A	272	ARG
1	A	318	GLN
1	A	321	GLN
1	B	29	LYS
1	B	43	LYS
1	B	186	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
1	C	24	ASN
1	C	32	VAL
1	C	42	LEU
1	C	68	THR
1	C	121	MET
1	C	165	THR
1	C	195	ARG
1	C	222	ASN
1	C	254	PHE
1	C	255	ASP
1	C	272	ARG
1	C	300	GLN
1	C	314	LYS
1	D	18	ASP
1	D	29	LYS
1	D	42	LEU
1	D	59	GLN
1	D	92	MET
1	D	139	LYS
1	D	222	ASN
1	D	262	LYS
1	D	272	ARG
1	D	317	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	47	ASN
1	A	87	HIS
1	A	164	ASN
1	A	190	GLN
1	A	197	HIS
1	A	209	ASN
1	A	219	ASN
1	B	37	ASN
1	B	74	ASN
1	B	131	ASN
1	B	151	ASN
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	318	GLN
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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.95	0 100 100	10, 24, 50, 77	0
1	B	326/326 (100%)	-0.96	3 (0%) 84 82	10, 20, 64, 125	0
1	C	326/326 (100%)	-0.75	14 (4%) 35 33	11, 23, 99, 149	0
1	D	326/326 (100%)	-0.94	2 (0%) 89 88	9, 22, 58, 94	0
All	All	1304/1304 (100%)	-0.90	19 (1%) 73 72	9, 22, 60, 149	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	SER	6.0
1	C	22	LYS	5.7
1	C	23	SER	5.3
1	C	26	THR	5.0
1	C	18	ASP	5.0
1	C	28	GLY	4.6
1	B	18	ASP	4.5
1	C	30	VAL	4.0
1	C	29	LYS	3.9
1	B	28	GLY	3.5
1	B	19	SER	3.4
1	C	34	ASN	3.1
1	C	16	GLY	2.8
1	C	21	THR	2.8
1	C	27	ALA	2.6
1	C	20	ALA	2.5
1	C	17	GLY	2.4
1	D	17	GLY	2.4
1	D	29	LYS	2.3

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, 95^{th} 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^2)	Q<0.9
2	ASP	C	401	9/9	0.94	0.19	39,51,56,58	0
2	ASP	A	401	9/9	0.98	0.08	18,23,26,27	0
2	ASP	B	401	9/9	0.98	0.10	22,30,35,36	0
2	ASP	D	401	9/9	0.98	0.09	16,21,26,27	0

6.5 Other polymers (i)

There are no such residues in this entry.