



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 1BRM / pdb_00001brm
Title : ASPARTATE BETA-SEMIALDEHYDE DEHYDROGENASE FROM ES-
CHERICHIA COLI
Authors : Hadfield, A.T.; Kryger, G.; Ouyang, J.; Ringe, D.; Petsko, G.A.; Viola, R.E.
Deposited on : 1998-08-24
Resolution : 2.50 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
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

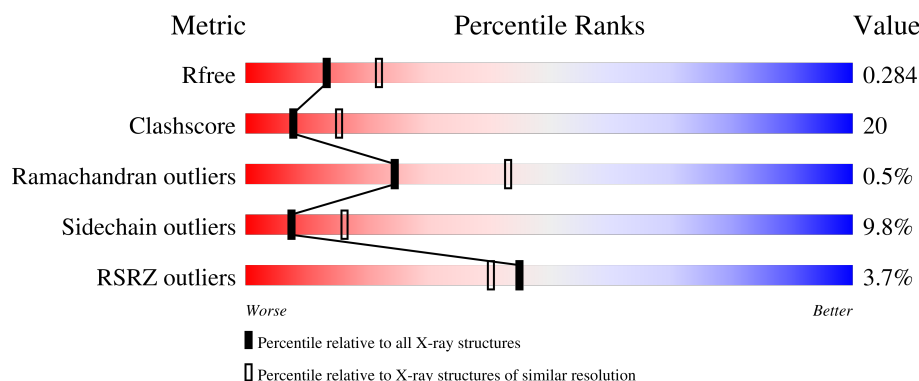
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	367	4% 57% 34% 6%
1	B	367	2% 59% 33% 6%
1	C	367	5% 60% 31% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8499 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 ASPARTATE-SEMIALDEHYDE DEHYDROGENASE.

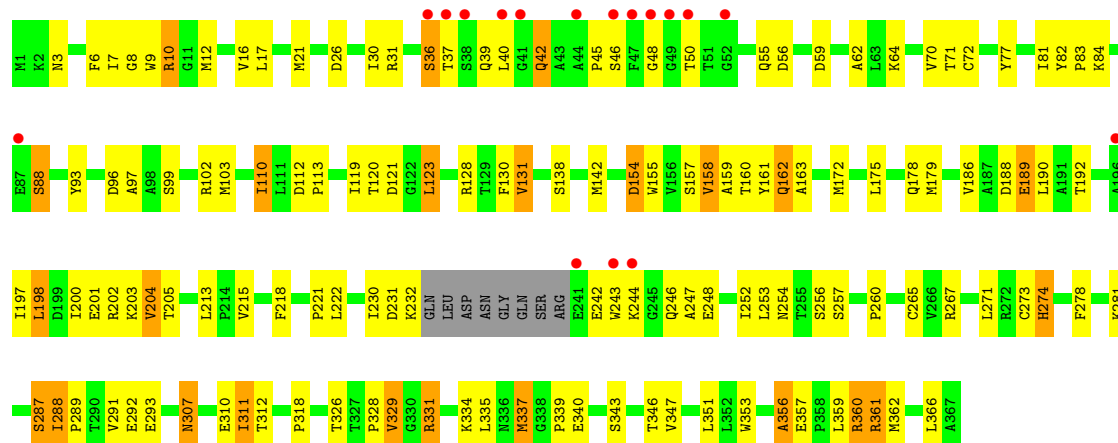
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2720	1722	472	510	16			
1	B	357	Total	C	N	O	S	0	0	0
			2729	1727	473	513	16			
1	C	359	Total	C	N	O	S	0	0	0
			2747	1738	476	517	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	113	Total	O	0	0
			113	113		
2	C	117	Total	O	0	0
			117	117		

● Molecule 1: ASPARTATE-SEMIALDEHYDE DEHYDROGENASE

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.89Å 117.05Å 58.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 2.50 28.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	82.6 (28.00-2.50) 82.5 (28.00-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 2.50Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.225 , 0.294 0.216 , 0.284	Depositor DCC
R_{free} test set	3466 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8499	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.39	0/2772	0.92	10/3764 (0.3%)
1	B	0.39	0/2781	0.93	12/3776 (0.3%)
1	C	0.38	0/2799	0.90	6/3799 (0.2%)
All	All	0.39	0/8352	0.91	28/11339 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	ILE	N-CA-C	7.92	119.99	108.58
1	B	110	ILE	N-CA-C	7.82	119.84	108.58
1	A	110	ILE	N-CA-C	7.82	119.83	108.58
1	C	356	ALA	N-CA-C	7.03	119.97	111.40
1	A	72	CYS	N-CA-C	-7.01	101.96	112.54
1	B	356	ALA	N-CA-C	6.94	119.87	111.40
1	A	356	ALA	N-CA-C	6.92	119.85	111.40
1	B	72	CYS	N-CA-C	-6.79	102.28	112.54
1	C	72	CYS	N-CA-C	-6.76	102.33	112.54
1	C	158	VAL	N-CA-C	5.87	118.43	108.86
1	B	44	ALA	CA-C-N	5.72	127.00	119.84
1	B	44	ALA	C-N-CA	5.72	127.00	119.84
1	B	158	VAL	N-CA-C	5.67	118.11	108.86
1	C	162	GLN	N-CA-C	5.61	119.06	110.20
1	A	327	THR	CA-C-N	5.60	125.55	119.78
1	A	327	THR	C-N-CA	5.60	125.55	119.78
1	A	162	GLN	N-CA-C	5.59	119.03	110.20
1	A	158	VAL	N-CA-C	5.55	117.80	108.81
1	B	162	GLN	N-CA-C	5.53	118.93	110.20
1	B	39	GLN	N-CA-C	5.48	117.56	110.65
1	C	81	ILE	N-CA-C	5.44	115.64	110.53
1	A	299	ASN	N-CA-C	5.40	113.08	108.22
1	B	340	GLU	N-CA-C	-5.36	106.52	113.16
1	B	81	ILE	N-CA-C	5.33	115.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	327	THR	CA-C-N	5.21	125.15	119.78
1	B	327	THR	C-N-CA	5.21	125.15	119.78
1	A	28	ASP	N-CA-C	5.14	116.89	111.28
1	A	81	ILE	N-CA-C	5.06	115.29	110.53

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	2720	0	2737	111	0
1	B	2729	0	2743	112	0
1	C	2747	0	2762	111	0
2	A	73	0	0	4	0
2	B	113	0	0	6	0
2	C	117	0	0	4	0
All	All	8499	0	8242	325	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 20.

All (325) 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:39:GLN:HB3	1:B:42:GLN:HG3	1.32	1.10
1:C:40:LEU:HD22	1:C:56:ASP:HA	1.44	0.99
1:A:1:MET:HE3	1:A:31:ARG:HG2	1.44	0.98
1:C:56:ASP:HB3	1:C:59:ASP:HB2	1.44	0.97
1:C:12:MET:HE3	1:C:351:LEU:HD11	1.45	0.96
1:C:289:PRO:O	1:C:293:GLU:HG3	1.70	0.92
1:C:39:GLN:HB3	1:C:42:GLN:HG3	1.50	0.90
1:B:186:VAL:HG12	1:B:190:LEU:HG	1.54	0.90
1:A:169:ALA:HB1	1:B:197:ILE:HG21	1.52	0.90
1:C:40:LEU:CD2	1:C:56:ASP:HA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:HB3	1:A:131:VAL:HG13	1.63	0.78
1:B:208:THR:HA	1:B:213:LEU:HD22	1.66	0.77
1:B:17:LEU:HG	1:B:21:MET:HE3	1.66	0.76
1:B:7:ILE:HB	1:B:71:THR:HG22	1.68	0.75
1:C:218:PHE:HE1	1:C:267:ARG:HD3	1.52	0.75
1:B:218:PHE:HE1	1:B:267:ARG:HD3	1.51	0.74
1:A:218:PHE:HE1	1:A:267:ARG:HD3	1.50	0.74
1:B:218:PHE:CE1	1:B:267:ARG:HD3	2.22	0.74
1:A:218:PHE:CE1	1:A:267:ARG:HD3	2.23	0.74
1:A:306:PRO:HD2	1:A:311:ILE:HD13	1.70	0.73
1:B:186:VAL:HG11	1:B:200:ILE:HG23	1.71	0.73
1:C:218:PHE:CE1	1:C:267:ARG:HD3	2.24	0.73
1:C:232:LYS:HB2	1:C:243:TRP:HZ3	1.52	0.72
1:A:289:PRO:O	1:A:293:GLU:HG3	1.90	0.72
1:A:335:LEU:HD21	1:A:343:SER:HB3	1.73	0.71
1:C:232:LYS:HB2	1:C:243:TRP:CZ3	2.26	0.71
1:C:335:LEU:HD21	1:C:343:SER:HB3	1.73	0.70
1:C:175:LEU:HD13	1:C:222:LEU:HD23	1.74	0.70
1:C:7:ILE:HB	1:C:71:THR:HG22	1.74	0.69
1:B:335:LEU:HD21	1:B:343:SER:HB3	1.74	0.69
1:B:24:GLU:O	1:B:25:ARG:HG2	1.92	0.69
1:B:245:GLY:HA2	2:B:804:HOH:O	1.93	0.68
1:C:12:MET:HE2	1:C:351:LEU:HD21	1.76	0.68
1:A:134:ASN:OD1	2:A:875:HOH:O	2.11	0.68
1:C:40:LEU:HD22	1:C:56:ASP:CA	2.22	0.68
1:C:112:ASP:CG	1:C:113:PRO:HD3	2.18	0.67
1:A:7:ILE:HB	1:A:71:THR:HG22	1.76	0.67
1:C:288:ILE:O	1:C:292:GLU:HG3	1.94	0.67
1:B:158:VAL:HG22	1:B:278:PHE:CD1	2.30	0.67
1:A:158:VAL:HG22	1:A:278:PHE:CD1	2.30	0.66
1:C:188:ASP:HB2	1:C:189:GLU:OE1	1.94	0.66
1:C:186:VAL:HG12	1:C:186:VAL:O	1.93	0.66
1:B:186:VAL:HG12	1:B:186:VAL:O	1.95	0.66
1:C:158:VAL:HG22	1:C:278:PHE:CD1	2.31	0.65
1:A:44:ALA:HB1	1:A:45:PRO:HD2	1.78	0.65
1:A:56:ASP:HB3	1:A:59:ASP:HB2	1.77	0.65
1:A:202:ARG:O	1:A:206:THR:HG23	1.97	0.64
1:C:307:ASN:HD21	1:C:331:ARG:HD2	1.63	0.64
1:A:340:GLU:HB2	2:A:533:HOH:O	1.96	0.64
1:C:287:SER:OG	1:C:289:PRO:HD2	1.98	0.64
1:B:307:ASN:HD21	1:B:331:ARG:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ARG:NH1	1:C:36:SER:HB2	2.12	0.63
1:C:3:ASN:OD1	1:C:31:ARG:HD2	1.99	0.62
1:A:307:ASN:ND2	1:A:331:ARG:HA	2.14	0.62
1:B:39:GLN:HB3	1:B:42:GLN:CG	2.21	0.62
1:B:307:ASN:ND2	1:B:331:ARG:HA	2.14	0.62
1:B:112:ASP:CG	1:B:113:PRO:HD3	2.25	0.61
1:C:186:VAL:O	1:C:186:VAL:CG1	2.47	0.61
1:C:329:VAL:HG13	1:C:346:THR:HG22	1.80	0.61
1:A:169:ALA:O	1:A:173:ARG:HG3	2.01	0.61
1:C:307:ASN:ND2	1:C:331:ARG:HA	2.14	0.60
1:A:171:HIS:CE1	1:A:217:ASN:HB3	2.37	0.60
1:A:287:SER:OG	1:A:289:PRO:HD2	2.00	0.60
1:C:186:VAL:HG11	1:C:200:ILE:HB	1.84	0.59
1:A:303:LYS:NZ	1:A:315:GLU:HG2	2.17	0.59
1:A:83:PRO:O	1:A:87:GLU:HG2	2.03	0.59
1:C:186:VAL:HG13	1:C:189:GLU:HG2	1.83	0.59
1:A:307:ASN:HD21	1:A:331:ARG:HD2	1.66	0.59
1:B:267:ARG:HD2	2:B:776:HOH:O	2.01	0.59
1:B:329:VAL:HG13	1:B:346:THR:HG22	1.84	0.59
1:B:45:PRO:HB2	1:B:47:PHE:CD2	2.38	0.59
1:B:7:ILE:HG22	1:B:73:GLN:HB2	1.85	0.58
1:B:18:MET:HE1	1:B:34:PHE:HE1	1.67	0.58
1:C:7:ILE:HD13	1:C:77:TYR:OH	2.04	0.58
1:A:21:MET:HG2	1:A:26:ASP:HB2	1.86	0.58
1:A:160:THR:OG1	1:A:265:CYS:HA	2.04	0.58
1:A:303:LYS:HZ1	1:A:315:GLU:HG2	1.68	0.58
1:B:123:LEU:HD13	1:B:130:PHE:CZ	2.38	0.58
1:A:112:ASP:CG	1:A:113:PRO:HD3	2.29	0.57
1:A:99:SER:HA	1:A:102:ARG:HG3	1.86	0.57
1:B:186:VAL:O	1:B:186:VAL:CG1	2.52	0.57
1:A:12:MET:SD	1:B:197:ILE:HD13	2.44	0.57
1:C:99:SER:HA	1:C:102:ARG:HG3	1.87	0.57
1:C:103:MET:HB2	2:C:851:HOH:O	2.04	0.57
1:B:99:SER:HA	1:B:102:ARG:HG3	1.87	0.56
1:B:283:LYS:O	1:B:284:LYS:HG3	2.05	0.56
1:B:309:ARG:HG2	1:B:313:MET:HE3	1.86	0.56
1:B:132:GLY:HA3	2:B:601:HOH:O	2.05	0.56
1:C:112:ASP:OD1	1:C:113:PRO:HD3	2.05	0.56
1:C:244:LYS:HD3	1:C:265:CYS:SG	2.46	0.56
1:C:160:THR:OG1	1:C:265:CYS:HA	2.05	0.56
1:B:112:ASP:OD1	1:B:113:PRO:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:HG13	1:C:189:GLU:CG	2.36	0.55
1:B:18:MET:HE1	1:B:34:PHE:CE1	2.40	0.55
1:A:96:ASP:HB3	1:A:131:VAL:CG1	2.35	0.55
1:B:197:ILE:HD12	1:B:198:LEU:HD23	1.88	0.55
1:A:309:ARG:HG3	1:B:229:TRP:NE1	2.22	0.55
1:C:288:ILE:HD11	1:C:334:LYS:HG2	1.88	0.55
1:A:248:GLU:HG3	2:A:814:HOH:O	2.07	0.54
1:C:172:MET:HB3	1:C:271:LEU:HD22	1.90	0.54
1:A:35:PHE:CZ	1:A:66:LEU:HD11	2.42	0.54
1:C:310:GLU:CD	1:C:310:GLU:H	2.16	0.54
1:C:158:VAL:HG22	1:C:278:PHE:HD1	1.70	0.54
1:A:158:VAL:HG22	1:A:278:PHE:HD1	1.71	0.54
1:B:160:THR:OG1	1:B:265:CYS:HA	2.08	0.54
1:B:360:ARG:HH12	1:B:361:ARG:HD2	1.74	0.53
1:C:7:ILE:HD12	1:C:71:THR:CG2	2.37	0.53
1:A:310:GLU:H	1:A:310:GLU:CD	2.17	0.53
1:C:178:GLN:NE2	1:C:215:VAL:HG12	2.23	0.53
1:A:360:ARG:HH12	1:A:361:ARG:HD2	1.73	0.53
1:A:37:THR:HG21	1:A:58:PHE:HE2	1.73	0.53
1:B:39:GLN:CB	1:B:42:GLN:HG3	2.23	0.52
1:B:189:GLU:CD	1:B:189:GLU:H	2.16	0.52
1:C:307:ASN:ND2	1:C:331:ARG:HD2	2.24	0.52
1:B:267:ARG:NH2	2:B:607:HOH:O	2.42	0.52
1:B:310:GLU:CD	1:B:310:GLU:H	2.16	0.52
1:C:7:ILE:HD13	1:C:77:TYR:CZ	2.44	0.52
1:C:97:ALA:HB2	1:C:359:LEU:HD11	1.91	0.52
1:C:175:LEU:HG	1:C:179:MET:HE3	1.90	0.52
1:A:36:SER:O	1:A:36:SER:OG	2.26	0.52
1:C:360:ARG:HH12	1:C:361:ARG:HD2	1.74	0.52
1:A:17:LEU:HG	1:A:21:MET:HE3	1.92	0.52
1:B:97:ALA:HB2	1:B:359:LEU:HD11	1.90	0.52
1:B:123:LEU:HD13	1:B:130:PHE:HZ	1.74	0.52
1:B:162:GLN:HE22	1:B:265:CYS:HB3	1.72	0.52
1:A:229:TRP:NE1	1:B:309:ARG:HG3	2.24	0.51
1:C:232:LYS:CB	1:C:243:TRP:HZ3	2.19	0.51
1:C:288:ILE:CD1	1:C:334:LYS:HG2	2.40	0.51
1:B:175:LEU:O	1:B:179:MET:HG3	2.10	0.51
1:C:39:GLN:CB	1:C:42:GLN:HG3	2.31	0.51
1:C:186:VAL:HG22	1:C:203:LYS:HD3	1.90	0.51
1:B:35:PHE:HB3	1:B:57:ALA:HB2	1.93	0.51
1:B:64:LYS:HE2	1:B:88:SER:OG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HE2	1:A:88:SER:OG	2.10	0.51
1:B:158:VAL:HG22	1:B:278:PHE:HD1	1.71	0.51
1:A:93:TYR:CE1	1:A:128:ARG:HD3	2.45	0.51
1:B:10:ARG:HH12	1:B:36:SER:HB2	1.74	0.51
1:C:162:GLN:HE22	1:C:265:CYS:HB3	1.75	0.51
1:B:186:VAL:HG13	1:B:189:GLU:CG	2.41	0.50
1:B:186:VAL:O	1:B:190:LEU:HG	2.11	0.50
1:A:306:PRO:CD	1:A:311:ILE:HD13	2.41	0.50
1:B:185:HIS:O	1:B:203:LYS:HE2	2.10	0.50
1:B:288:ILE:N	1:B:289:PRO:CD	2.75	0.50
1:A:97:ALA:HB2	1:A:359:LEU:HD11	1.92	0.50
1:B:307:ASN:ND2	1:B:331:ARG:HD2	2.26	0.50
1:B:309:ARG:O	1:B:313:MET:HG3	2.11	0.50
1:A:2:LYS:O	1:A:31:ARG:HG3	2.12	0.50
1:A:143:SER:HB3	1:A:329:VAL:HG22	1.93	0.50
1:C:200:ILE:O	1:C:204:VAL:HG13	2.12	0.50
1:C:6:PHE:CD1	1:C:70:VAL:HB	2.47	0.49
1:A:84:LYS:O	1:A:88:SER:HB3	2.12	0.49
1:A:167:GLY:HA3	1:A:171:HIS:CD2	2.47	0.49
1:A:267:ARG:NH2	2:A:751:HOH:O	2.44	0.49
1:B:17:LEU:CG	1:B:21:MET:HE3	2.40	0.49
1:B:142:MET:HE2	1:B:353:TRP:CE2	2.48	0.49
1:A:307:ASN:ND2	1:A:331:ARG:HD2	2.26	0.49
1:A:21:MET:HG2	1:A:26:ASP:CB	2.42	0.49
1:A:288:ILE:HD11	1:A:334:LYS:HG2	1.94	0.49
1:C:7:ILE:HD12	1:C:71:THR:HG22	1.95	0.49
1:B:130:PHE:CG	1:B:362:MET:HE2	2.48	0.49
1:C:288:ILE:N	1:C:289:PRO:CD	2.76	0.49
1:A:299:ASN:HB2	1:A:300:PRO:HD2	1.94	0.49
1:C:64:LYS:HE2	1:C:88:SER:OG	2.13	0.49
1:C:158:VAL:HG12	1:C:159:ALA:N	2.28	0.49
1:A:244:LYS:HE3	1:A:262:ASP:OD1	2.13	0.49
1:B:311:ILE:HG23	1:B:312:THR:N	2.28	0.49
1:C:84:LYS:O	1:C:88:SER:HB3	2.13	0.49
1:B:6:PHE:HE1	1:B:21:MET:HE1	1.78	0.48
1:C:9:TRP:CH2	1:C:45:PRO:HG3	2.48	0.48
1:A:162:GLN:HE22	1:A:265:CYS:HB3	1.77	0.48
1:A:12:MET:HE3	1:A:351:LEU:HD11	1.95	0.48
1:A:207:LEU:HD12	1:A:210:SER:OG	2.13	0.48
1:B:287:SER:O	1:B:291:VAL:HG23	2.13	0.48
1:C:36:SER:O	1:C:40:LEU:CD2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASP:HB3	1:C:62:ALA:HB3	1.96	0.48
1:A:34:PHE:CE2	1:A:45:PRO:HG2	2.48	0.48
1:B:244:LYS:HD3	1:B:265:CYS:SG	2.53	0.48
1:B:155:TRP:HZ3	1:B:157:SER:HB2	1.79	0.48
1:C:17:LEU:O	1:C:21:MET:HG3	2.14	0.48
1:C:155:TRP:HZ3	1:C:157:SER:HB2	1.79	0.48
1:B:175:LEU:HD13	1:B:222:LEU:HD23	1.95	0.47
1:A:158:VAL:HG12	1:A:159:ALA:N	2.29	0.47
1:A:163:ALA:HB2	1:A:273:CYS:O	2.14	0.47
1:B:309:ARG:CG	1:B:313:MET:HE3	2.44	0.47
1:A:155:TRP:HZ3	1:A:157:SER:HB2	1.79	0.47
1:C:6:PHE:HD1	1:C:70:VAL:HB	1.79	0.47
1:A:309:ARG:O	1:A:313:MET:HG3	2.14	0.47
1:B:162:GLN:NE2	1:B:265:CYS:HB3	2.30	0.47
1:C:163:ALA:HB2	1:C:273:CYS:O	2.15	0.47
1:A:36:SER:O	1:A:37:THR:C	2.56	0.47
1:A:155:TRP:NE1	1:A:281:LYS:HD3	2.30	0.47
1:B:158:VAL:HG12	1:B:159:ALA:N	2.29	0.47
1:A:35:PHE:HZ	1:A:66:LEU:HD11	1.78	0.47
1:B:84:LYS:O	1:B:88:SER:HB3	2.14	0.47
1:B:130:PHE:CD1	1:B:362:MET:HE2	2.50	0.47
1:C:162:GLN:NE2	1:C:265:CYS:HB3	2.30	0.47
1:A:246:GLN:OE1	1:A:260:PRO:HA	2.15	0.47
1:B:186:VAL:HG13	1:B:189:GLU:HG3	1.96	0.47
1:B:248:GLU:O	1:B:252:ILE:HG13	2.15	0.47
1:C:197:ILE:HG23	1:C:198:LEU:HD23	1.97	0.46
1:A:248:GLU:O	1:A:252:ILE:HG13	2.15	0.46
1:B:246:GLN:OE1	1:B:260:PRO:HA	2.15	0.46
1:B:284:LYS:O	1:B:286:VAL:HG23	2.15	0.46
1:C:328:PRO:HD2	1:C:347:VAL:O	2.15	0.46
1:A:34:PHE:CD2	1:A:45:PRO:HD2	2.50	0.46
1:B:48:GLY:C	1:B:50:THR:N	2.71	0.46
1:C:8:GLY:C	1:C:10:ARG:H	2.24	0.46
1:A:178:GLN:NE2	1:A:215:VAL:HG12	2.31	0.46
1:C:123:LEU:HD21	1:C:366:LEU:CD2	2.46	0.46
1:A:178:GLN:HE22	1:A:221:PRO:HA	1.81	0.46
1:B:300:PRO:HD2	1:B:301:TRP:CE3	2.50	0.46
1:A:186:VAL:HG23	1:A:190:LEU:HD12	1.98	0.46
1:C:96:ASP:HB3	1:C:131:VAL:HG13	1.97	0.46
1:B:297:ALA:O	1:B:298:HIS:C	2.58	0.45
1:A:58:PHE:HD1	1:A:81:ILE:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ILE:HG13	1:B:251:LYS:HE2	1.98	0.45
1:A:82:TYR:HB3	1:A:83:PRO:HD3	1.99	0.45
1:B:20:ARG:NH1	1:B:23:GLU:CD	2.74	0.45
1:C:130:PHE:CG	1:C:362:MET:HE2	2.52	0.45
1:C:246:GLN:OE1	1:C:260:PRO:HA	2.17	0.45
1:A:162:GLN:NE2	1:A:265:CYS:HB3	2.32	0.45
1:B:163:ALA:HB2	1:B:273:CYS:O	2.17	0.45
1:C:267:ARG:NH2	2:C:508:HOH:O	2.50	0.45
1:A:262:ASP:OD2	1:B:333:ARG:NH2	2.50	0.45
1:A:161:TYR:N	1:A:161:TYR:CD1	2.85	0.45
1:C:334:LYS:HD2	1:C:339:PRO:O	2.17	0.45
1:A:12:MET:HE3	1:A:351:LEU:HD21	1.98	0.45
1:B:103:MET:HE2	1:B:247:ALA:HB1	1.97	0.45
1:B:334:LYS:HD2	1:B:339:PRO:O	2.17	0.44
1:A:7:ILE:CD1	1:A:69:ILE:HG23	2.47	0.44
1:A:87:GLU:OE1	1:A:87:GLU:HA	2.18	0.44
1:B:71:THR:HB	2:B:679:HOH:O	2.18	0.44
1:B:82:TYR:HB3	1:B:83:PRO:HD3	2.00	0.44
1:C:21:MET:HE3	1:C:26:ASP:HB3	1.98	0.44
1:C:40:LEU:HD13	1:C:56:ASP:CB	2.48	0.44
1:A:18:MET:HE3	1:A:27:PHE:HZ	1.82	0.44
1:C:12:MET:O	1:C:16:VAL:HG23	2.17	0.44
1:A:285:ASP:OD1	1:A:285:ASP:C	2.61	0.44
1:C:123:LEU:HD21	1:C:366:LEU:HD21	1.99	0.44
1:C:198:LEU:O	1:C:202:ARG:HB2	2.17	0.44
1:C:230:ILE:HG22	1:C:232:LYS:HG2	2.00	0.44
1:C:288:ILE:HD12	1:C:334:LYS:HE3	2.00	0.44
1:A:311:ILE:CG2	1:A:314:ARG:HH21	2.30	0.44
1:C:311:ILE:HG23	1:C:312:THR:N	2.33	0.44
1:C:161:TYR:CD1	1:C:161:TYR:N	2.86	0.43
1:B:161:TYR:N	1:B:161:TYR:CD1	2.85	0.43
1:C:267:ARG:NH1	2:C:541:HOH:O	2.51	0.43
1:C:46:SER:C	1:C:48:GLY:H	2.26	0.43
1:C:204:VAL:CG2	1:C:205:THR:N	2.81	0.43
1:A:35:PHE:CD2	1:A:55:GLN:HB2	2.53	0.43
1:B:142:MET:HE2	1:B:353:TRP:CD2	2.53	0.43
1:B:273:CYS:HB2	1:B:318:PRO:HB3	2.01	0.43
1:C:200:ILE:CG1	1:C:201:GLU:N	2.82	0.43
1:A:273:CYS:HB2	1:A:318:PRO:HB3	2.00	0.43
1:B:184:GLY:C	1:B:186:VAL:H	2.26	0.43
1:A:333:ARG:NH2	1:B:262:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:O	1:C:252:ILE:HG13	2.18	0.43
1:B:39:GLN:O	1:B:54:LEU:HD12	2.19	0.43
1:B:332:LEU:HB2	2:B:540:HOH:O	2.17	0.43
1:C:154:ASP:HB2	1:C:281:LYS:O	2.18	0.43
1:B:110:ILE:HG21	1:B:130:PHE:HB3	2.01	0.43
1:C:357:GLU:O	1:C:361:ARG:CG	2.67	0.43
1:A:175:LEU:HD13	1:A:222:LEU:HD23	2.00	0.42
1:A:271:LEU:CD1	1:B:204:VAL:HG21	2.49	0.42
1:B:50:THR:HG23	1:B:51:THR:N	2.34	0.42
1:B:357:GLU:O	1:B:361:ARG:CG	2.68	0.42
1:C:119:ILE:HG22	1:C:123:LEU:HD12	2.01	0.42
1:C:242:GLU:CD	1:C:247:ALA:HB2	2.44	0.42
1:A:37:THR:CG2	1:A:58:PHE:HE2	2.31	0.42
1:C:244:LYS:CD	1:C:265:CYS:SG	3.07	0.42
1:C:82:TYR:HB3	1:C:83:PRO:HD3	2.00	0.42
1:C:110:ILE:CG2	1:C:130:PHE:HB3	2.49	0.42
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.90	0.42
1:B:300:PRO:HD2	1:B:301:TRP:CZ3	2.55	0.42
1:C:340:GLU:HB2	2:C:795:HOH:O	2.19	0.42
1:A:183:TYR:CD1	1:A:183:TYR:C	2.96	0.42
1:A:288:ILE:N	1:A:289:PRO:CD	2.83	0.42
1:A:335:LEU:HB3	1:A:337:MET:HE2	2.01	0.42
1:A:356:ALA:O	1:A:357:GLU:C	2.63	0.42
1:C:12:MET:CE	1:C:351:LEU:HD21	2.45	0.42
1:A:110:ILE:HG22	1:A:119:ILE:HD11	2.01	0.42
1:A:142:MET:HE2	1:A:353:TRP:CE2	2.54	0.42
1:B:6:PHE:CE1	1:B:21:MET:HE1	2.53	0.42
1:C:335:LEU:HB3	1:C:337:MET:HE2	2.01	0.42
1:A:286:VAL:CG1	1:A:290:THR:HG21	2.50	0.42
1:B:18:MET:HE3	1:B:47:PHE:CD2	2.55	0.42
1:A:253:LEU:O	1:A:254:ASN:C	2.63	0.41
1:C:110:ILE:HG21	1:C:130:PHE:HB3	2.02	0.41
1:A:258:VAL:O	1:A:260:PRO:HD3	2.21	0.41
1:B:109:ILE:HA	1:B:131:VAL:O	2.20	0.41
1:C:253:LEU:O	1:C:254:ASN:C	2.63	0.41
1:A:12:MET:SD	1:B:197:ILE:CD1	3.09	0.41
1:A:163:ALA:H	1:A:274:HIS:CE1	2.39	0.41
1:B:122:GLY:HA2	1:B:125:ASN:HD22	1.85	0.41
1:B:357:GLU:O	1:B:361:ARG:HG3	2.21	0.41
1:B:20:ARG:O	1:B:23:GLU:HB3	2.20	0.41
1:B:188:ASP:O	1:B:191:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LEU:O	1:B:254:ASN:C	2.62	0.41
1:A:357:GLU:O	1:A:361:ARG:CG	2.68	0.41
1:C:273:CYS:HB2	1:C:318:PRO:HB3	2.02	0.41
1:B:289:PRO:O	1:B:293:GLU:HG3	2.21	0.41
1:A:37:THR:HG22	1:A:57:ALA:HB3	2.03	0.41
1:A:311:ILE:HG23	1:A:314:ARG:HH21	1.85	0.41
1:B:297:ALA:O	1:B:299:ASN:N	2.54	0.41
1:C:178:GLN:HE22	1:C:221:PRO:HA	1.86	0.41
1:A:37:THR:HG21	1:A:58:PHE:CE2	2.55	0.41
1:A:244:LYS:HE3	1:A:263:GLY:H	1.85	0.41
1:C:40:LEU:HD22	1:C:55:GLN:C	2.46	0.41
1:C:163:ALA:H	1:C:274:HIS:CE1	2.38	0.41
1:A:40:LEU:H	1:A:40:LEU:HG	1.66	0.41
1:A:115:ASN:ND2	1:A:252:ILE:HG23	2.35	0.41
1:A:321:VAL:O	1:A:322:THR:C	2.64	0.41
1:B:20:ARG:HD2	1:B:20:ARG:HA	1.78	0.41
1:C:93:TYR:CE1	1:C:128:ARG:HD3	2.56	0.41
1:C:178:GLN:HE22	1:C:215:VAL:HG12	1.85	0.41
1:A:130:PHE:CG	1:A:362:MET:HE2	2.55	0.40
1:B:110:ILE:CG2	1:B:130:PHE:HB3	2.50	0.40
1:B:163:ALA:H	1:B:274:HIS:CE1	2.39	0.40
1:C:356:ALA:O	1:C:357:GLU:C	2.64	0.40
1:C:186:VAL:HG12	1:C:190:LEU:HG	2.03	0.40
1:A:357:GLU:O	1:A:361:ARG:HG3	2.21	0.40
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.91	0.40
1:A:110:ILE:HG21	1:A:130:PHE:HB3	2.03	0.40
1:A:337:MET:HE2	1:B:262:ASP:HB3	2.03	0.40
1:C:142:MET:HE2	1:C:353:TRP:CE2	2.56	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	352/367 (96%)	324 (92%)	27 (8%)	1 (0%)	36	55
1	B	353/367 (96%)	320 (91%)	31 (9%)	2 (1%)	21	38
1	C	355/367 (97%)	319 (90%)	34 (10%)	2 (1%)	21	38
All	All	1060/1101 (96%)	963 (91%)	92 (9%)	5 (0%)	24	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	B	298	HIS
1	C	42	GLN
1	C	231	ASP
1	B	45	PRO

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	292/302 (97%)	264 (90%)	28 (10%)	8	17
1	B	293/302 (97%)	266 (91%)	27 (9%)	8	19
1	C	295/302 (98%)	264 (90%)	31 (10%)	6	14
All	All	880/906 (97%)	794 (90%)	86 (10%)	7	16

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	12	MET
1	A	18	MET
1	A	30	ILE
1	A	33	VAL
1	A	36	SER
1	A	40	LEU
1	A	50	THR

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Mol	Chain	Res	Type
1	A	88	SER
1	A	123	LEU
1	A	131	VAL
1	A	135	CYS
1	A	138	SER
1	A	154	ASP
1	A	192	THR
1	A	257	SER
1	A	274	HIS
1	A	284	LYS
1	A	287	SER
1	A	288	ILE
1	A	307	ASN
1	A	311	ILE
1	A	315	GLU
1	A	326	THR
1	A	331	ARG
1	A	337	MET
1	A	360	ARG
1	A	361	ARG
1	B	25	ARG
1	B	36	SER
1	B	40	LEU
1	B	50	THR
1	B	88	SER
1	B	120	THR
1	B	123	LEU
1	B	135	CYS
1	B	138	SER
1	B	154	ASP
1	B	177	THR
1	B	189	GLU
1	B	192	THR
1	B	195	SER
1	B	197	ILE
1	B	202	ARG
1	B	213	LEU
1	B	256	SER
1	B	274	HIS
1	B	288	ILE
1	B	307	ASN
1	B	326	THR

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Mol	Chain	Res	Type
1	B	329	VAL
1	B	331	ARG
1	B	337	MET
1	B	360	ARG
1	B	361	ARG
1	C	10	ARG
1	C	30	ILE
1	C	36	SER
1	C	37	THR
1	C	50	THR
1	C	88	SER
1	C	120	THR
1	C	121	ASP
1	C	123	LEU
1	C	131	VAL
1	C	138	SER
1	C	154	ASP
1	C	189	GLU
1	C	192	THR
1	C	198	LEU
1	C	204	VAL
1	C	213	LEU
1	C	256	SER
1	C	257	SER
1	C	274	HIS
1	C	287	SER
1	C	288	ILE
1	C	291	VAL
1	C	307	ASN
1	C	311	ILE
1	C	326	THR
1	C	329	VAL
1	C	331	ARG
1	C	337	MET
1	C	360	ARG
1	C	361	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	150	ASN

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Mol	Chain	Res	Type
1	A	162	GLN
1	A	171	HIS
1	A	276	GLN
1	A	307	ASN
1	B	3	ASN
1	B	125	ASN
1	B	162	GLN
1	B	181	HIS
1	B	276	GLN
1	B	307	ASN
1	C	116	GLN
1	C	150	ASN
1	C	162	GLN
1	C	171	HIS
1	C	307	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	356/367 (97%)	0.43	15 (4%) 40 36	17, 40, 72, 95	0
1	B	357/367 (97%)	0.13	8 (2%) 62 58	13, 34, 64, 90	0
1	C	359/367 (97%)	0.16	17 (4%) 36 32	13, 34, 69, 93	0
All	All	1072/1101 (97%)	0.24	40 (3%) 45 40	13, 36, 69, 95	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	LEU	5.2
1	B	38	SER	4.4
1	B	243	TRP	4.1
1	A	50	THR	3.5
1	B	36	SER	3.4
1	A	49	GLY	3.3
1	A	47	PHE	3.2
1	C	48	GLY	3.1
1	C	38	SER	3.0
1	A	243	TRP	2.9
1	C	87	GLU	2.9
1	C	44	ALA	2.8
1	C	243	TRP	2.7
1	C	37	THR	2.7
1	B	151	ASP	2.6
1	C	52	GLY	2.6
1	A	38	SER	2.6
1	A	51	THR	2.6
1	C	36	SER	2.6
1	B	338	GLY	2.5
1	C	46	SER	2.5
1	A	1	MET	2.5
1	B	40	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	117	ASP	2.4
1	A	40	LEU	2.4
1	A	54	LEU	2.4
1	B	231	ASP	2.3
1	C	47	PHE	2.3
1	A	149	ALA	2.2
1	C	50	THR	2.2
1	C	244	LYS	2.2
1	B	37	THR	2.2
1	C	196	ALA	2.2
1	A	43	ALA	2.1
1	A	125	ASN	2.1
1	C	41	GLY	2.1
1	C	241	GLU	2.1
1	A	36	SER	2.1
1	C	49	GLY	2.1
1	A	71	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.