



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 10:07 PM EST

PDB ID : 1NDB
Title : Crystal structure of Carnitine Acetyltransferase
Authors : Jogl, G.; Tong, L.
Deposited on : 2002-12-09
Resolution : 1.80 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

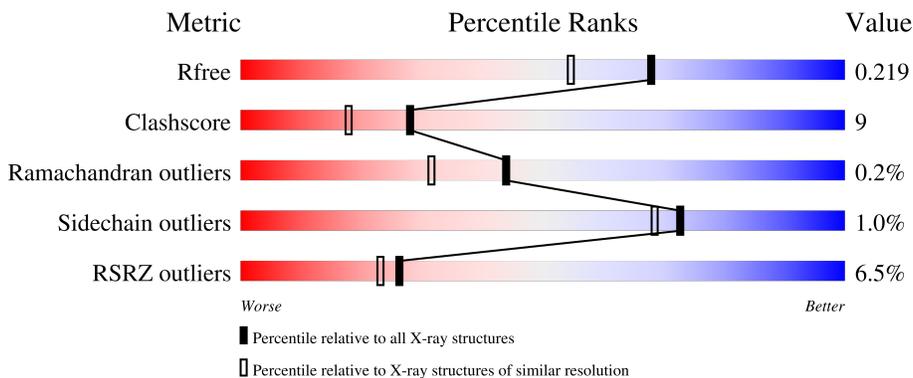
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	596	 5% 83% 17%
1	B	596	 8% 80% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10560 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 Carnitine Acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	596	4757	3034	820	875	8	20	0	0	0
1	B	596	4757	3034	820	875	8	20	0	0	0

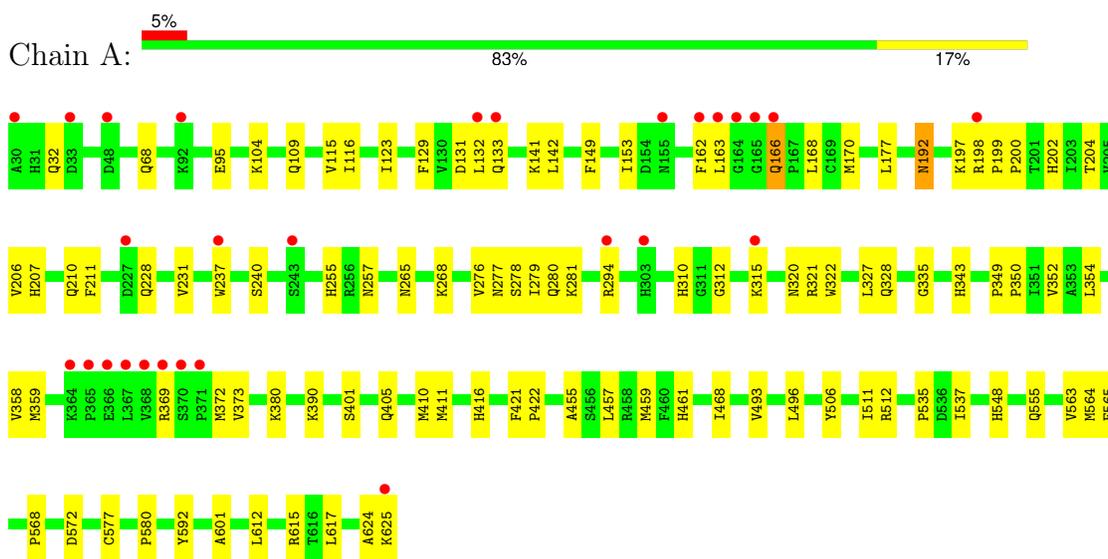
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	584	Total	O	0	0
			584	584		
2	B	462	Total	O	0	0
			462	462		

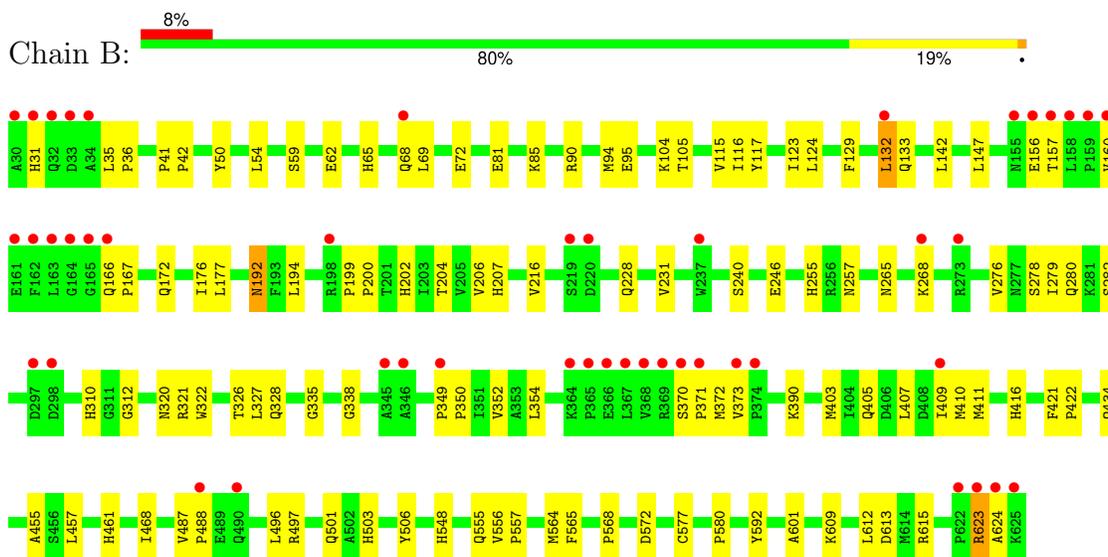
3 Residue-property plots [i](#)

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: Carnitine Acetyltransferase



- Molecule 1: Carnitine Acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.88Å 89.65Å 119.44Å 90.00° 127.46° 90.00°	Depositor
Resolution (Å)	29.69 – 1.80 29.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.69-1.80) 97.5 (29.69-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 1.79Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.219 0.192 , 0.219	Depositor DCC
R_{free} test set	8796 reflections (7.28%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10560	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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 [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	0.31	0/4852	0.57	0/6540
1	B	0.29	0/4852	0.56	0/6540
All	All	0.30	0/9704	0.56	0/13080

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4757	0	4733	86	0
1	B	4757	0	4733	80	0
2	A	584	0	0	12	0
2	B	462	0	0	6	0
All	All	10560	0	9466	166	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 9.

All (166) 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:A:372:MSE:HG2	1:A:373:VAL:H	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD22	1:A:132:LEU:H	1.39	0.87
1:A:624:ALA:O	1:A:625:LYS:HB2	1.76	0.86
1:B:623:ARG:HB3	1:B:623:ARG:NH1	1.90	0.85
1:A:32:GLN:HE22	1:A:170:MSE:H	1.28	0.81
1:B:265:ASN:HA	1:B:268:LYS:HE3	1.64	0.80
1:B:310:HIS:HD2	1:B:312:GLY:H	1.30	0.79
1:A:277:ASN:HD21	1:A:281:LYS:HE3	1.48	0.77
1:A:310:HIS:HD2	1:A:312:GLY:H	1.30	0.77
1:A:163:LEU:HB2	1:A:166:GLN:HG3	1.68	0.76
1:A:372:MSE:HG2	1:A:373:VAL:N	2.01	0.76
1:A:535:PRO:HB2	2:A:990:HOH:O	1.86	0.76
1:B:623:ARG:HB3	1:B:623:ARG:HH11	1.51	0.74
1:A:315:LYS:HG2	2:A:824:HOH:O	1.89	0.72
1:B:370:SER:HB2	1:B:371:PRO:HD2	1.73	0.69
1:A:310:HIS:CD2	1:A:312:GLY:H	2.12	0.68
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.76	0.67
1:A:459:MSE:HE3	1:A:511:ILE:HG22	1.75	0.67
1:A:255:HIS:HD2	1:A:257:ASN:H	1.41	0.67
1:A:537:ILE:HG22	2:A:990:HOH:O	1.94	0.66
1:B:117:TYR:CE1	1:B:403:MSE:HE3	2.30	0.66
1:B:132:LEU:HD12	1:B:133:GLN:H	1.60	0.66
1:B:310:HIS:CD2	1:B:312:GLY:H	2.12	0.66
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.78	0.66
1:A:123:ILE:HG13	1:A:565:PHE:CE2	2.32	0.65
1:A:322:TRP:H	1:A:328:GLN:NE2	1.96	0.64
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.33	0.64
1:A:277:ASN:ND2	1:A:281:LYS:HE3	2.12	0.64
1:A:255:HIS:CD2	1:A:257:ASN:H	2.15	0.63
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.64	0.63
1:A:132:LEU:H	1:A:132:LEU:CD2	2.12	0.61
1:A:358:VAL:HG12	1:A:359:MSE:HE2	1.82	0.61
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.82	0.61
1:A:132:LEU:HD22	1:A:132:LEU:N	2.16	0.59
1:B:497:ARG:O	1:B:501:GLN:HG2	2.03	0.59
1:B:95:GLU:OE1	1:B:461:HIS:HE1	1.86	0.59
1:A:322:TRP:H	1:A:328:GLN:HE22	1.51	0.58
1:B:104:LYS:HG3	1:B:105:THR:N	2.19	0.58
1:B:246:GLU:OE2	1:B:390:LYS:HE2	2.03	0.58
1:B:555:GLN:HE21	1:B:580:PRO:HG2	1.69	0.57
1:A:163:LEU:CB	1:A:166:GLN:HG3	2.34	0.57
1:A:555:GLN:HE21	1:A:580:PRO:HG2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:VAL:O	1:B:280:GLN:HG3	2.04	0.56
1:A:493:VAL:HG22	1:A:617:LEU:HG	1.87	0.55
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.88	0.55
1:A:162:PHE:O	1:A:163:LEU:HD22	2.06	0.55
1:A:410:MSE:HG2	1:A:601:ALA:HA	1.88	0.55
1:B:457:LEU:HG	2:B:767:HOH:O	2.07	0.55
1:A:354:LEU:C	1:A:354:LEU:HD23	2.27	0.55
1:A:32:GLN:NE2	1:A:170:MSE:H	2.01	0.54
1:B:322:TRP:H	1:B:328:GLN:NE2	2.05	0.54
1:B:81:GLU:HG3	2:B:688:HOH:O	2.07	0.54
1:A:537:ILE:CG2	2:A:990:HOH:O	2.54	0.54
1:A:197:LYS:HG2	2:A:935:HOH:O	2.07	0.53
1:B:268:LYS:HG2	2:B:914:HOH:O	2.08	0.53
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.43	0.53
1:B:407:LEU:HD21	1:B:409:ILE:HD11	1.88	0.53
1:A:410:MSE:HE3	1:A:411:MSE:O	2.09	0.53
1:B:59:SER:OG	1:B:62:GLU:HG3	2.09	0.52
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.91	0.52
1:A:123:ILE:HD12	1:A:411:MSE:HE2	1.92	0.52
1:B:354:LEU:C	1:B:354:LEU:HD23	2.30	0.52
1:B:410:MSE:HE3	1:B:411:MSE:O	2.09	0.52
1:B:132:LEU:CD1	1:B:133:GLN:H	2.23	0.52
1:A:207:HIS:HD2	1:A:240:SER:OG	1.93	0.51
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.46	0.51
1:B:623:ARG:HH11	1:B:623:ARG:CB	2.22	0.51
1:A:129:PHE:CZ	1:A:335:GLY:HA2	2.45	0.51
1:A:163:LEU:CD2	1:A:168:LEU:HD11	2.40	0.51
1:B:129:PHE:CZ	1:B:335:GLY:HA2	2.45	0.51
1:B:555:GLN:HG2	1:B:557:PRO:HD3	1.92	0.51
1:A:276:VAL:O	1:A:280:GLN:HG3	2.10	0.50
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.46	0.50
1:B:496:LEU:C	1:B:496:LEU:HD23	2.33	0.50
1:A:132:LEU:HD12	1:A:237:TRP:CZ2	2.47	0.49
1:B:81:GLU:O	1:B:85:LYS:HG2	2.12	0.49
1:B:116:ILE:HD12	1:B:403:MSE:HE2	1.93	0.49
1:A:163:LEU:HD23	1:A:168:LEU:HD11	1.95	0.49
1:A:231:VAL:HG21	1:A:372:MSE:HE1	1.93	0.49
1:B:202:HIS:HD2	2:B:666:HOH:O	1.95	0.49
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.48	0.48
1:A:123:ILE:HG13	1:A:565:PHE:CZ	2.48	0.48
1:A:204:THR:HG21	1:A:279:ILE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:HG	2:A:720:HOH:O	2.13	0.48
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.95	0.48
1:B:123:ILE:HD12	1:B:411:MSE:HE2	1.96	0.48
1:B:231:VAL:HG21	1:B:372:MSE:SE	2.62	0.48
1:B:255:HIS:HD2	1:B:257:ASN:HB2	1.78	0.48
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.78	0.48
1:B:322:TRP:H	1:B:328:GLN:HE22	1.60	0.48
1:A:123:ILE:HG13	1:A:565:PHE:HE2	1.77	0.48
1:B:349:PRO:HA	1:B:352:VAL:HG22	1.95	0.48
1:A:131:ASP:OD1	1:A:133:GLN:HG3	2.14	0.48
1:B:410:MSE:HG2	1:B:601:ALA:HA	1.96	0.47
1:B:204:THR:HG21	1:B:279:ILE:HA	1.96	0.47
1:A:265:ASN:HA	1:A:268:LYS:HE3	1.96	0.47
1:A:228:GLN:HG2	1:A:372:MSE:HG3	1.96	0.47
1:B:352:VAL:HG11	1:B:556:VAL:HG12	1.96	0.47
1:A:104:LYS:HG2	1:A:109:GLN:CD	2.35	0.47
1:A:198:ARG:O	1:A:198:ARG:HG3	2.15	0.47
1:A:210:GLN:HE21	1:A:380:LYS:NZ	2.13	0.47
1:A:401:SER:O	1:A:405:GLN:HG3	2.15	0.47
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.96	0.47
1:B:177:LEU:HD23	1:B:327:LEU:HD12	1.97	0.47
1:A:411:MSE:CE	1:A:563:VAL:HG11	2.45	0.46
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.98	0.46
1:A:141:LYS:HZ1	1:A:369:ARG:NH2	2.13	0.46
1:A:390:LYS:HB3	1:A:390:LYS:NZ	2.31	0.46
1:B:31:HIS:CE1	1:B:167:PRO:HB3	2.51	0.46
1:A:68:GLN:NE2	2:A:1063:HOH:O	2.49	0.46
1:B:255:HIS:HE1	2:B:842:HOH:O	1.99	0.46
1:B:609:LYS:HE2	1:B:613:ASP:OD1	2.15	0.46
1:A:548:HIS:HE1	1:A:572:ASP:OD1	1.99	0.45
1:A:405:GLN:HG3	2:A:953:HOH:O	2.15	0.45
1:B:202:HIS:HE1	1:B:278:SER:O	1.98	0.45
1:B:207:HIS:HD2	1:B:240:SER:OG	1.99	0.45
1:A:142:LEU:C	1:A:142:LEU:HD23	2.37	0.45
1:A:177:LEU:HD23	1:A:327:LEU:HD12	1.98	0.45
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.28	0.45
1:B:310:HIS:HE1	2:B:948:HOH:O	2.00	0.45
1:B:564:MSE:HB3	1:B:577:CYS:SG	2.57	0.45
1:A:255:HIS:CD2	1:A:257:ASN:HB2	2.51	0.45
1:A:310:HIS:HE1	2:A:1026:HOH:O	2.00	0.45
1:B:320:ASN:C	1:B:321:ARG:HG2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:C	1:A:496:LEU:HD23	2.37	0.44
1:B:228:GLN:CG	1:B:372:MSE:HE2	2.47	0.44
1:B:548:HIS:HE1	1:B:572:ASP:OD1	1.99	0.44
1:B:228:GLN:HG3	1:B:372:MSE:HE2	1.99	0.44
1:B:68:GLN:O	1:B:72:GLU:HG3	2.18	0.44
1:B:124:LEU:HG	1:B:338:GLY:HA2	2.00	0.44
1:B:142:LEU:C	1:B:142:LEU:HD23	2.38	0.44
1:A:237:TRP:HH2	2:A:835:HOH:O	2.00	0.44
1:B:372:MSE:CG	1:B:373:VAL:N	2.79	0.44
1:B:123:ILE:HG13	1:B:565:PHE:CZ	2.53	0.44
1:B:204:THR:HG23	1:B:282:SER:HB3	1.99	0.44
1:A:192:ASN:C	1:A:192:ASN:HD22	2.21	0.43
1:A:349:PRO:HA	1:A:352:VAL:HG22	2.00	0.43
1:A:109:GLN:NE2	2:A:992:HOH:O	2.51	0.43
1:A:228:GLN:CG	1:A:372:MSE:HG3	2.48	0.43
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.54	0.43
1:A:202:HIS:HE1	1:A:278:SER:O	2.02	0.42
1:B:31:HIS:CE1	1:B:160:VAL:HG11	2.54	0.42
1:B:199:PRO:HA	1:B:200:PRO:HD3	1.89	0.42
1:A:95:GLU:OE1	1:A:461:HIS:HE1	2.02	0.42
1:B:192:ASN:HD22	1:B:192:ASN:C	2.22	0.42
1:B:157:THR:HG22	1:B:157:THR:O	2.19	0.42
1:B:176:ILE:HA	1:B:326:THR:HG21	2.01	0.42
1:A:294:ARG:HG3	1:A:294:ARG:NH1	2.35	0.42
1:B:65:HIS:CE1	1:B:69:LEU:HD11	2.54	0.42
1:A:564:MSE:HB3	1:A:577:CYS:SG	2.60	0.42
1:B:90:ARG:O	1:B:94:MSE:HG2	2.19	0.42
1:B:434:GLN:HG3	1:B:503:HIS:CE1	2.54	0.42
1:B:172:GLN:OE1	1:B:350:PRO:HG2	2.20	0.42
1:B:206:VAL:HG22	1:B:320:ASN:OD1	2.20	0.42
1:A:199:PRO:HA	1:A:200:PRO:HD3	1.92	0.41
1:A:206:VAL:HG22	1:A:211:PHE:CD2	2.55	0.41
1:A:320:ASN:C	1:A:321:ARG:HG2	2.40	0.41
1:B:41:PRO:HA	1:B:42:PRO:HD3	1.95	0.41
1:A:416:HIS:CG	1:A:612:LEU:HD21	2.55	0.41
1:A:535:PRO:C	2:A:990:HOH:O	2.59	0.41
1:B:487:VAL:HA	1:B:488:PRO:HD3	1.88	0.41
1:B:147:LEU:HD11	1:B:216:VAL:HB	2.02	0.41
1:B:192:ASN:ND2	1:B:194:LEU:H	2.19	0.41
1:B:349:PRO:O	1:B:352:VAL:HG22	2.21	0.41
1:B:35:LEU:HA	1:B:36:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:CE1	1:A:153:ILE:HD11	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	594/596 (100%)	578 (97%)	16 (3%)	0	100	100
1	B	594/596 (100%)	578 (97%)	14 (2%)	2 (0%)	37	25
All	All	1188/1192 (100%)	1156 (97%)	30 (2%)	2 (0%)	44	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	624	ALA
1	B	623	ARG

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	524/504 (104%)	520 (99%)	4 (1%)	79	76
1	B	524/504 (104%)	517 (99%)	7 (1%)	65	59
All	All	1048/1008 (104%)	1037 (99%)	11 (1%)	73	68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	192	ASN
1	A	343	HIS
1	A	506	TYR
1	B	132	LEU
1	B	156	GLU
1	B	166	GLN
1	B	192	ASN
1	B	405	GLN
1	B	506	TYR
1	B	615	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	65	HIS
1	A	68	GLN
1	A	84	GLN
1	A	109	GLN
1	A	112	GLN
1	A	135	GLN
1	A	166	GLN
1	A	187	GLN
1	A	192	ASN
1	A	202	HIS
1	A	207	HIS
1	A	210	GLN
1	A	228	GLN
1	A	255	HIS
1	A	277	ASN
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	357	HIS
1	A	461	HIS
1	A	503	HIS
1	A	548	HIS
1	A	550	ASN
1	A	555	GLN
1	A	586	ASN

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Mol	Chain	Res	Type
1	A	619	GLN
1	A	620	ASN
1	B	32	GLN
1	B	65	HIS
1	B	68	GLN
1	B	84	GLN
1	B	109	GLN
1	B	112	GLN
1	B	135	GLN
1	B	187	GLN
1	B	192	ASN
1	B	202	HIS
1	B	207	HIS
1	B	228	GLN
1	B	255	HIS
1	B	307	GLN
1	B	310	HIS
1	B	328	GLN
1	B	357	HIS
1	B	461	HIS
1	B	503	HIS
1	B	548	HIS
1	B	550	ASN
1	B	555	GLN
1	B	586	ASN
1	B	605	HIS
1	B	619	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 [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	576/596 (96%)	-0.13	28 (4%) 36 33	5, 12, 29, 71	0
1	B	576/596 (96%)	0.25	47 (8%) 19 16	8, 17, 41, 70	0
All	All	1152/1192 (96%)	0.06	75 (6%) 26 23	5, 14, 33, 71	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	VAL	9.0
1	A	164	GLY	8.8
1	A	165	GLY	7.6
1	A	371	PRO	7.4
1	B	368	VAL	6.6
1	B	163	LEU	6.3
1	A	367	LEU	6.2
1	A	163	LEU	6.1
1	B	624	ALA	6.0
1	B	625	LYS	5.4
1	A	625	LYS	5.3
1	B	162	PHE	5.3
1	B	373	VAL	5.3
1	A	166	GLN	5.3
1	A	162	PHE	5.3
1	A	369	ARG	5.2
1	B	34	ALA	5.2
1	B	367	LEU	5.1
1	A	132	LEU	4.7
1	B	623	ARG	4.5
1	B	157	THR	4.5
1	B	31	HIS	4.4
1	A	370	SER	4.2
1	B	30	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	237	TRP	4.1
1	B	622	PRO	4.0
1	B	371	PRO	4.0
1	B	156	GLU	3.9
1	B	165	GLY	3.8
1	B	132	LEU	3.6
1	B	155	ASN	3.6
1	B	160	VAL	3.6
1	B	33	ASP	3.6
1	B	32	GLN	3.5
1	B	370	SER	3.5
1	B	346	ALA	3.4
1	B	158	LEU	3.3
1	B	164	GLY	3.2
1	B	161	GLU	3.2
1	B	369	ARG	3.2
1	A	243	SER	3.0
1	B	159	PRO	2.9
1	B	219	SER	2.9
1	A	227	ASP	2.8
1	A	133	GLN	2.8
1	B	365	PRO	2.8
1	A	198	ARG	2.8
1	A	364	LYS	2.7
1	B	364	LYS	2.7
1	B	345	ALA	2.7
1	A	155	ASN	2.7
1	A	33	ASP	2.7
1	A	365	PRO	2.6
1	A	237	TRP	2.6
1	B	366	GLU	2.5
1	A	366	GLU	2.5
1	B	298	ASP	2.5
1	B	490	GLN	2.4
1	A	30	ALA	2.4
1	B	166	GLN	2.4
1	B	68	GLN	2.3
1	A	48	ASP	2.3
1	B	409	ILE	2.2
1	B	273	ARG	2.2
1	A	92	LYS	2.2
1	A	303	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	294	ARG	2.2
1	B	198	ARG	2.1
1	B	297	ASP	2.1
1	B	349	PRO	2.1
1	A	315	LYS	2.1
1	B	268	LYS	2.1
1	B	220	ASP	2.0
1	B	374	PRO	2.0
1	B	488	PRO	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 monosaccharides 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.