



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:43 pm BST

PDB ID : 6NKH
Title : Structure of MalC Reductase/Diels-Alderase from *Malbranchea aurantiaca*
Authors : Dan, Q.; Newmister, S.A.; Smith, J.L.; Sherman, D.H.
Deposited on : 2019-01-07
Resolution : 1.60 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

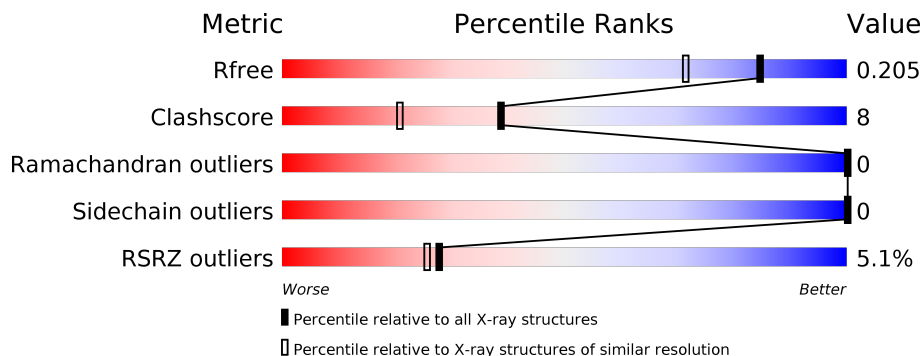
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 $\leq 5\%$. 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	264	
1	B	264	
1	C	264	
1	D	264	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16482 atoms, of which 8007 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	261	3979	1232	2024	343	367	13	0	0	0
1	B	258	3929	1216	1998	340	362	13	0	0	0
1	C	259	3941	1222	2004	338	364	13	0	0	0
1	D	255	3893	1206	1981	337	356	13	0	0	0

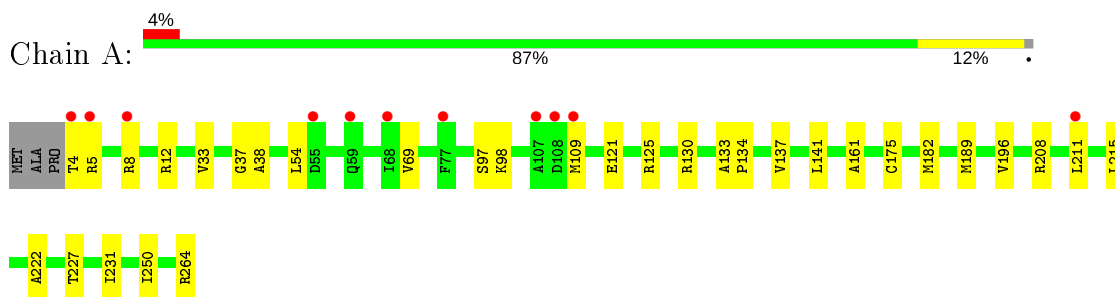
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	167	Total 167	O 167	0	0
2	B	196	Total 196	O 196	0	0
2	C	224	Total 224	O 224	0	0
2	D	153	Total 153	O 153	0	0

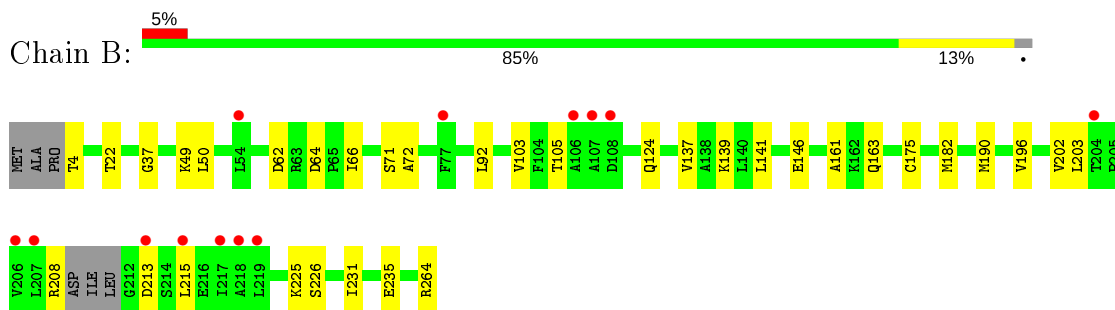
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

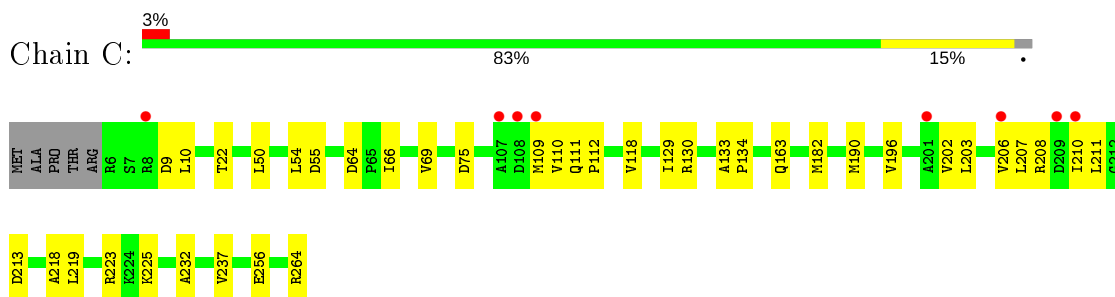
- Molecule 1: Short chain dehydrogenase



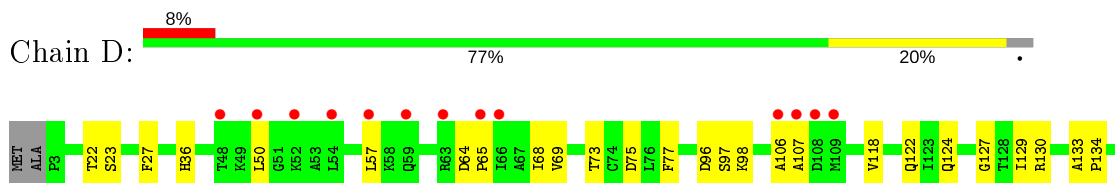
- Molecule 1: Short chain dehydrogenase

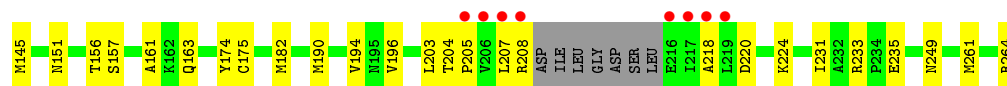


- Molecule 1: Short chain dehydrogenase



- Molecule 1: Short chain dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	79.37Å 79.37Å 133.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.97 – 1.60 42.97 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.97-1.60) 94.1 (42.97-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 1.60Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.166 , 0.199 0.172 , 0.205	Depositor DCC
R_{free} test set	1997 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.350 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16482	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7901e-05.*

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	0.37	0/1986	0.55	0/2696
1	B	0.33	0/1961	0.54	0/2660
1	C	0.35	0/1968	0.56	0/2672
1	D	0.38	0/1943	0.56	0/2636
All	All	0.36	0/7858	0.55	0/10664

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

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	1955	2024	2024	27	0
1	B	1931	1998	1997	28	0
1	C	1937	2004	2004	33	0
1	D	1912	1981	1982	38	0
2	A	167	0	0	4	1
2	B	196	0	0	7	2
2	C	224	0	0	9	2
2	D	153	0	0	7	1
All	All	8475	8007	8007	118	5

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 8.

All (118) 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:107:ALA:HB3	1:D:130:ARG:HD3	1.53	0.90
1:A:264:ARG:NH2	1:B:190:MET:SD	2.49	0.86
1:A:208:ARG:HD3	1:A:215:LEU:HD22	1.57	0.84
1:D:22:THR:HG22	1:D:50:LEU:HD23	1.68	0.76
1:C:55:ASP:OD1	2:C:301:HOH:O	2.07	0.73
1:A:121:GLU:OE2	1:A:125:ARG:NH2	2.22	0.73
1:C:130:ARG:NE	2:C:306:HOH:O	2.22	0.72
1:A:5:ARG:NH2	1:B:62:ASP:OD2	2.23	0.71
1:A:141:LEU:HD22	1:A:189:MET:HE1	1.73	0.71
1:B:208:ARG:HA	1:B:215:LEU:HD23	1.72	0.71
1:B:213:ASP:OD1	2:B:301:HOH:O	2.12	0.68
1:B:146:GLU:OE1	2:B:302:HOH:O	2.12	0.68
1:A:141:LEU:HD22	1:A:189:MET:CE	2.24	0.67
1:D:124:GLN:O	2:D:301:HOH:O	2.13	0.66
1:D:218:ALA:O	2:D:302:HOH:O	2.13	0.65
1:C:75:ASP:O	2:C:302:HOH:O	2.14	0.65
1:D:203:LEU:HD11	1:D:208:ARG:HB2	1.79	0.64
1:D:204:THR:OG1	1:D:205:PRO:HD2	2.00	0.62
1:D:145:MET:HE2	1:D:151:ASN:HB3	1.81	0.61
1:D:204:THR:HG22	1:D:207:LEU:HD12	1.83	0.60
1:C:190:MET:SD	1:D:264:ARG:NH2	2.75	0.59
1:D:106:ALA:HB2	1:D:156:THR:CG2	2.32	0.59
1:B:103:VAL:HG12	1:B:105:THR:HG23	1.82	0.59
1:A:182:MET:HG3	1:A:196:VAL:HG23	1.84	0.59
1:C:9:ASP:HB2	2:C:324:HOH:O	2.01	0.59
1:D:36:HIS:NE2	2:D:305:HOH:O	2.32	0.58
1:C:225:LYS:O	1:C:264:ARG:HD2	2.04	0.58
1:B:226:SER:O	1:B:264:ARG:NH1	2.36	0.58
1:A:8:ARG:HG2	1:A:12:ARG:HD2	1.87	0.57
1:B:202:VAL:HG12	2:B:438:HOH:O	2.03	0.57
1:D:203:LEU:CD1	1:D:208:ARG:HB2	2.35	0.56
1:A:161:ALA:HB2	1:A:175:CYS:HB3	1.88	0.56
1:B:235:GLU:OE2	2:B:303:HOH:O	2.18	0.56
1:C:182:MET:HG3	1:C:196:VAL:HG23	1.89	0.55
1:B:208:ARG:HA	1:B:215:LEU:CD2	2.37	0.54
1:C:206:VAL:O	1:C:210:ILE:HG13	2.07	0.54
1:D:163:GLN:NE2	1:D:261:MET:O	2.40	0.54
1:B:22:THR:HG22	1:B:50:LEU:HD23	1.91	0.53
1:C:112:PRO:HG2	2:C:452:HOH:O	2.09	0.53
1:B:50:LEU:HD22	1:B:71:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:HB2	1:D:231:ILE:HG21	1.90	0.53
1:C:203:LEU:HD12	1:C:207:LEU:HD23	1.90	0.53
1:C:22:THR:HG22	1:C:50:LEU:HD23	1.90	0.52
1:D:22:THR:HG21	2:D:366:HOH:O	2.09	0.52
1:C:264:ARG:NH2	1:D:190:MET:SD	2.83	0.52
1:A:211:LEU:HD12	1:A:215:LEU:HD12	1.92	0.52
1:C:64:ASP:OD2	1:C:66:ILE:HG12	2.10	0.52
1:D:127:GLY:HA2	1:D:174:TYR:CE2	2.45	0.51
1:A:4:THR:N	1:B:4:THR:N	2.59	0.51
1:A:33:VAL:HG13	1:A:38:ALA:HB3	1.93	0.51
1:C:256:GLU:OE1	2:C:304:HOH:O	2.19	0.51
1:A:54:LEU:CD1	1:A:69:VAL:HG12	2.41	0.50
1:D:106:ALA:HB2	1:D:156:THR:HG22	1.93	0.50
1:A:227:THR:HA	1:B:190:MET:HE1	1.95	0.49
1:C:202:VAL:HG21	1:C:237:VAL:HG21	1.95	0.49
1:C:232:ALA:HB2	1:D:249:ASN:CG	2.33	0.49
1:D:133:ALA:HB3	1:D:134:PRO:HD3	1.95	0.49
1:D:50:LEU:HD12	1:D:73:THR:HG22	1.94	0.49
1:D:220:ASP:O	1:D:224:LYS:HG3	2.13	0.49
1:B:203:LEU:HB3	1:B:231:ILE:HG21	1.95	0.49
1:A:130:ARG:NH1	2:A:306:HOH:O	2.39	0.48
1:C:54:LEU:CD1	1:C:69:VAL:HG12	2.43	0.48
1:A:133:ALA:HB3	1:A:134:PRO:HD3	1.95	0.48
2:A:368:HOH:O	1:C:163:GLN:HG3	2.13	0.48
1:D:182:MET:HG3	1:D:196:VAL:HG23	1.97	0.47
1:A:137:VAL:O	1:A:141:LEU:HB2	2.15	0.47
1:B:161:ALA:HB2	1:B:175:CYS:HB3	1.98	0.46
1:D:233:ARG:HB3	1:D:235:GLU:OE1	2.15	0.46
1:D:64:ASP:OD1	1:D:65:PRO:HD2	2.15	0.46
1:B:137:VAL:O	1:B:141:LEU:HB2	2.16	0.46
1:C:133:ALA:HB3	1:C:134:PRO:HD3	1.98	0.46
1:D:96:ASP:OD1	2:D:303:HOH:O	2.20	0.46
1:C:203:LEU:HD11	1:C:208:ARG:CG	2.46	0.46
1:B:124:GLN:HG2	2:B:451:HOH:O	2.16	0.45
1:B:64:ASP:OD2	1:B:66:ILE:HG13	2.17	0.45
1:C:109:MET:HG2	1:C:110:VAL:O	2.16	0.45
1:B:163:GLN:CG	2:B:401:HOH:O	2.64	0.45
1:A:109:MET:HG3	1:A:109:MET:O	2.17	0.44
1:C:219:LEU:O	1:C:223:ARG:HG3	2.17	0.44
1:D:75:ASP:O	1:D:75:ASP:OD1	2.35	0.44
1:B:139:LYS:NZ	1:C:118:VAL:O	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:NE2	1:B:264:ARG:O	2.50	0.44
1:C:110:VAL:HG22	1:C:111:GLN:N	2.33	0.44
1:D:68:ILE:HG22	1:D:69:VAL:N	2.33	0.43
1:D:22:THR:HG22	1:D:50:LEU:CD2	2.44	0.43
1:C:129:ILE:HG23	1:C:130:ARG:HG2	1.99	0.43
1:A:130:ARG:NH1	2:A:317:HOH:O	2.52	0.43
1:C:203:LEU:HD11	1:C:208:ARG:HG3	2.01	0.43
1:B:225:LYS:O	1:B:264:ARG:HD3	2.20	0.42
1:C:54:LEU:HD12	1:C:69:VAL:HG12	2.00	0.42
1:D:97:SER:OG	1:D:98:LYS:N	2.53	0.42
1:D:127:GLY:CA	1:D:174:TYR:CE2	3.03	0.42
1:C:203:LEU:HD21	1:C:208:ARG:HD3	2.02	0.42
1:B:72:ALA:HB2	1:B:92:LEU:HD23	2.02	0.42
1:A:54:LEU:HD12	1:A:69:VAL:HG12	2.02	0.42
1:C:213:ASP:OD2	2:C:305:HOH:O	2.21	0.42
1:B:182:MET:HG3	1:B:196:VAL:HG23	2.01	0.41
1:B:22:THR:HB	1:B:49:LYS:HG2	2.02	0.41
1:D:182:MET:HG2	1:D:194:VAL:HG12	2.03	0.41
1:A:12:ARG:HG2	1:A:37:GLY:HA3	2.02	0.41
1:D:23:SER:N	2:D:307:HOH:O	2.36	0.41
1:D:130:ARG:HH12	1:D:157:SER:HA	1.86	0.41
1:D:161:ALA:HB2	1:D:175:CYS:HB3	2.03	0.41
1:A:125:ARG:HG3	2:A:399:HOH:O	2.21	0.41
1:A:8:ARG:O	1:A:12:ARG:HG3	2.20	0.41
1:B:37:GLY:O	1:B:66:ILE:HD11	2.20	0.41
1:C:211:LEU:HD13	1:C:218:ALA:HB3	2.03	0.41
1:D:77:PHE:CZ	1:D:129:ILE:HD12	2.56	0.41
1:A:211:LEU:CD1	1:A:215:LEU:HD12	2.51	0.41
1:A:97:SER:OG	1:A:98:LYS:N	2.54	0.40
1:B:4:THR:N	2:B:325:HOH:O	2.54	0.40
1:D:118:VAL:HA	1:D:122:GLN:OE1	2.21	0.40
1:A:222:ALA:HB3	1:A:231:ILE:HD11	2.04	0.40
1:A:250:ILE:HG23	1:A:250:ILE:O	2.21	0.40
1:C:206:VAL:HG23	2:C:417:HOH:O	2.21	0.40
1:C:223:ARG:NH1	2:C:329:HOH:O	2.53	0.40
1:C:10:LEU:HD11	2:D:421:HOH:O	2.20	0.40
1:D:27:PHE:CE1	1:D:57:LEU:HG	2.56	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:HOH:O	2:C:487:HOH:O[2_675]	1.87	0.33
2:B:446:HOH:O	2:B:446:HOH:O[2_665]	2.00	0.20
2:C:480:HOH:O	2:C:480:HOH:O[2_675]	2.10	0.10
2:B:439:HOH:O	2:B:455:HOH:O[2_675]	2.11	0.09
2:A:365:HOH:O	2:D:329:HOH:O[3_665]	2.18	0.02

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	259/264 (98%)	256 (99%)	3 (1%)	0	100	100
1	B	254/264 (96%)	247 (97%)	7 (3%)	0	100	100
1	C	257/264 (97%)	253 (98%)	4 (2%)	0	100	100
1	D	251/264 (95%)	243 (97%)	8 (3%)	0	100	100
All	All	1021/1056 (97%)	999 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	213/215 (99%)	213 (100%)	0	100	100
1	B	210/215 (98%)	210 (100%)	0	100	100
1	C	211/215 (98%)	211 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	208/215 (97%)	208 (100%)	0	100	100
All	All	842/860 (98%)	842 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	261/264 (98%)	0.15	11 (4%) 36 33	15, 28, 50, 65	0
1	B	258/264 (97%)	0.06	13 (5%) 28 26	13, 25, 54, 65	0
1	C	259/264 (98%)	-0.03	8 (3%) 49 46	13, 23, 46, 64	0
1	D	255/264 (96%)	0.27	21 (8%) 11 10	14, 29, 62, 78	0
All	All	1033/1056 (97%)	0.11	53 (5%) 28 26	13, 26, 53, 78	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	ALA	7.7
1	A	109	MET	6.5
1	D	107	ALA	6.0
1	D	207	LEU	5.6
1	B	219	LEU	4.8
1	D	217	ILE	4.7
1	D	216	GLU	4.6
1	A	8	ARG	4.5
1	C	108	ASP	4.3
1	D	108	ASP	4.3
1	A	4	THR	4.2
1	C	209	ASP	4.2
1	C	107	ALA	4.1
1	B	54	LEU	3.9
1	A	211	LEU	3.7
1	D	206	VAL	3.7
1	C	109	MET	3.6
1	D	219	LEU	3.6
1	D	48	THR	3.6
1	B	106	ALA	3.4
1	C	8	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	217	ILE	3.4
1	D	205	PRO	3.3
1	D	109	MET	3.3
1	B	107	ALA	3.2
1	A	5	ARG	3.1
1	C	210	ILE	3.0
1	D	106	ALA	3.0
1	A	59	GLN	2.9
1	D	63	ARG	2.9
1	D	50	LEU	2.8
1	B	77	PHE	2.8
1	D	66	ILE	2.7
1	A	77	PHE	2.6
1	B	207	LEU	2.6
1	B	108	ASP	2.5
1	D	208	ARG	2.5
1	D	218	ALA	2.4
1	B	204	THR	2.4
1	D	65	PRO	2.3
1	D	52	LYS	2.3
1	D	54	LEU	2.2
1	A	108	ASP	2.2
1	D	57	LEU	2.2
1	B	206	VAL	2.2
1	D	59	GLN	2.2
1	C	206	VAL	2.1
1	B	213	ASP	2.1
1	A	68	ILE	2.1
1	A	55	ASP	2.1
1	C	201	ALA	2.1
1	B	218	ALA	2.1
1	B	215	LEU	2.1

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 carbohydrates 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.