



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:38 PM UTC

PDB ID : 9WXS / pdb_00009wxs
Title : Silver-bound E.coli Malate dehydrogenase (C251S)
Authors : Wang, H.; Wang, M.; Sun, H.
Deposited on : 2025-09-25
Resolution : 1.56 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

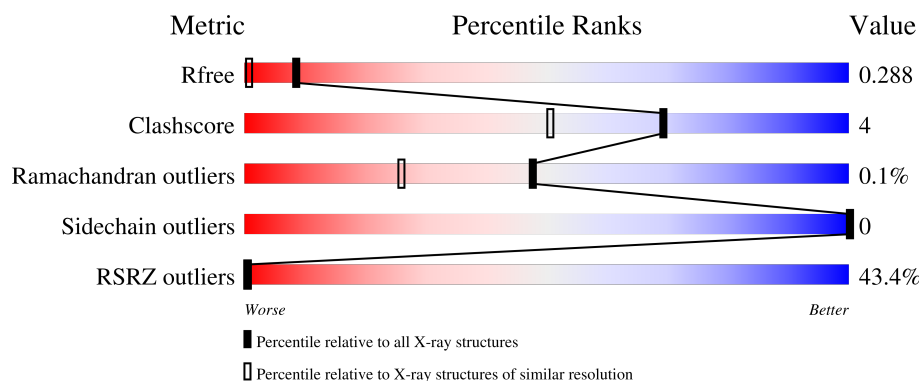
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	312	42% 87% 9% .
1	B	312	40% 91% 6% .
1	C	312	38% 89% 7% .
1	D	312	48% 90% 6% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9327 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2174	1381	365	423	5			
1	B	304	Total	C	N	O	S	0	0	0
			2203	1399	372	427	5			
1	C	301	Total	C	N	O	S	0	0	0
			2179	1384	366	424	5			
1	D	300	Total	C	N	O	S	0	0	0
			2174	1381	365	423	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	SER	CYS	engineered mutation	UNP P61889
B	251	SER	CYS	engineered mutation	UNP P61889
C	251	SER	CYS	engineered mutation	UNP P61889
D	251	SER	CYS	engineered mutation	UNP P61889

- Molecule 2 is SILVER ION (CCD ID: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ag	0	0
			1	1		
2	B	1	Total	Ag	0	0
			1	1		
2	C	1	Total	Ag	0	0
			1	1		
2	D	1	Total	Ag	0	0
			1	1		

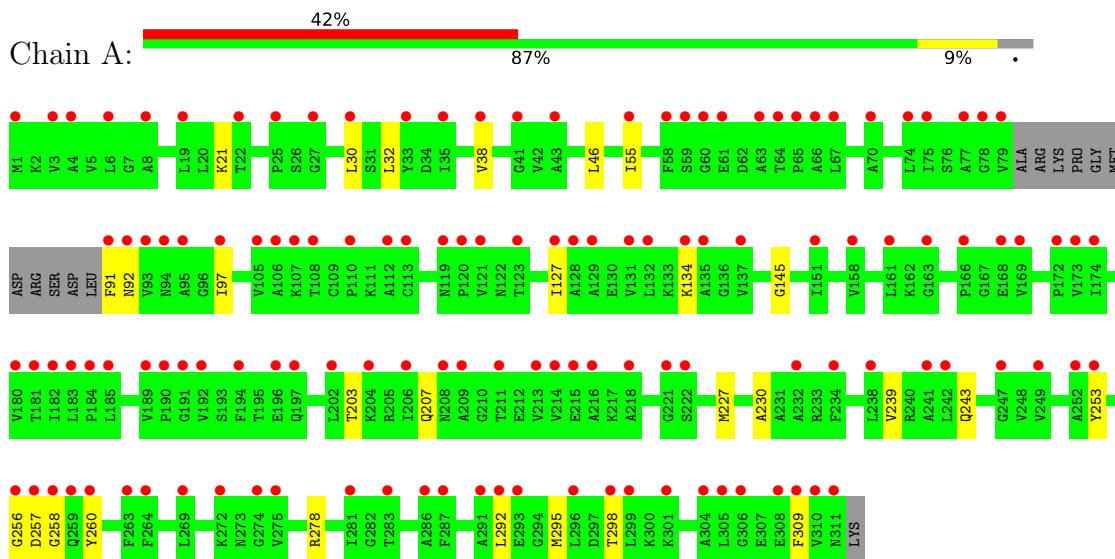
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	151	Total 151	O 151	0	0
3	B	169	Total 169	O 169	0	0
3	C	161	Total 161	O 161	0	0
3	D	112	Total 112	O 112	0	0

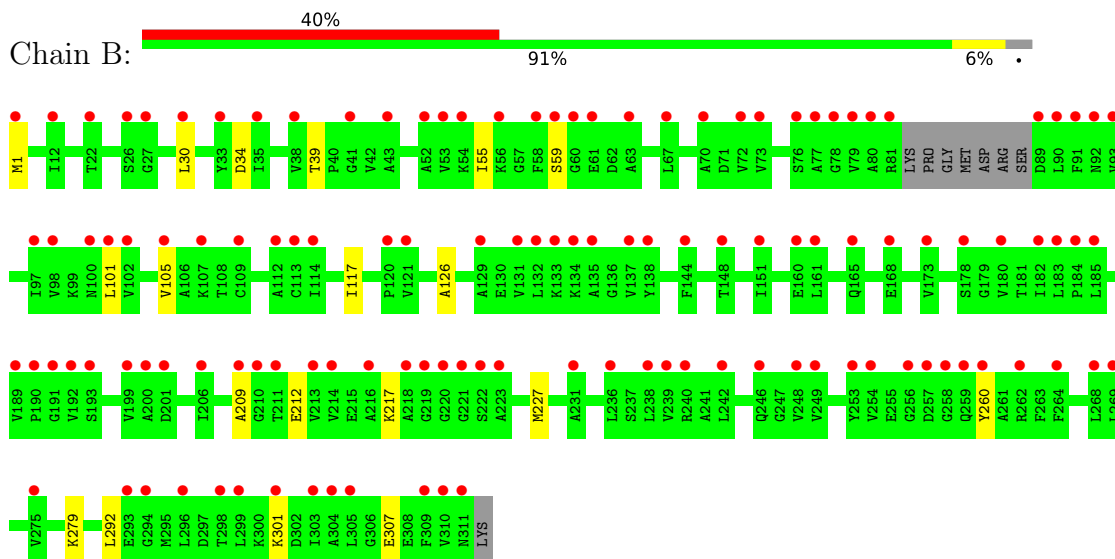
3 Residue-property plots [i](#)

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.

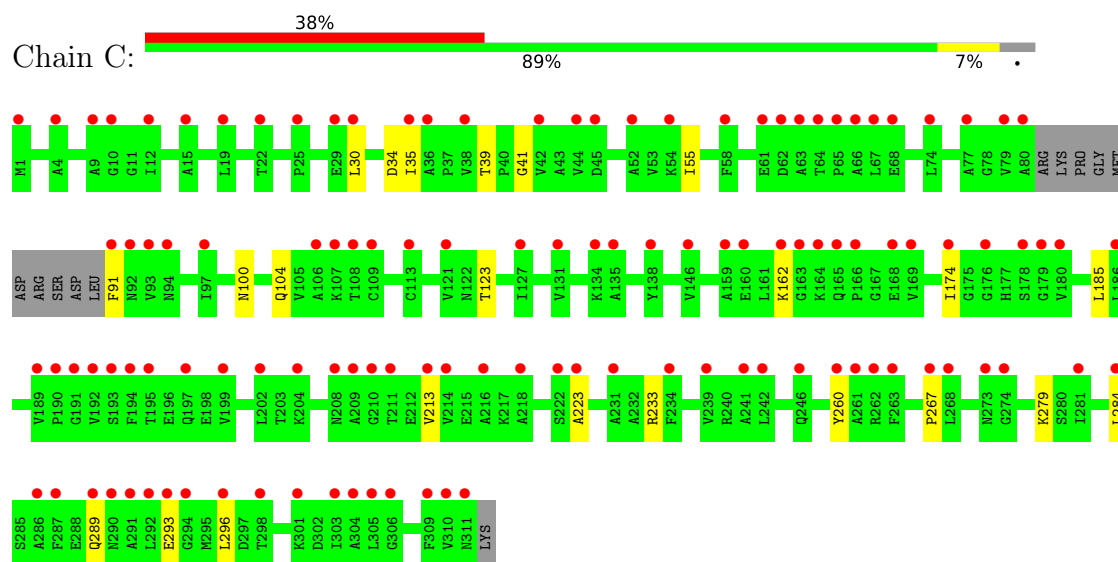
• Molecule 1: Malate dehydrogenase



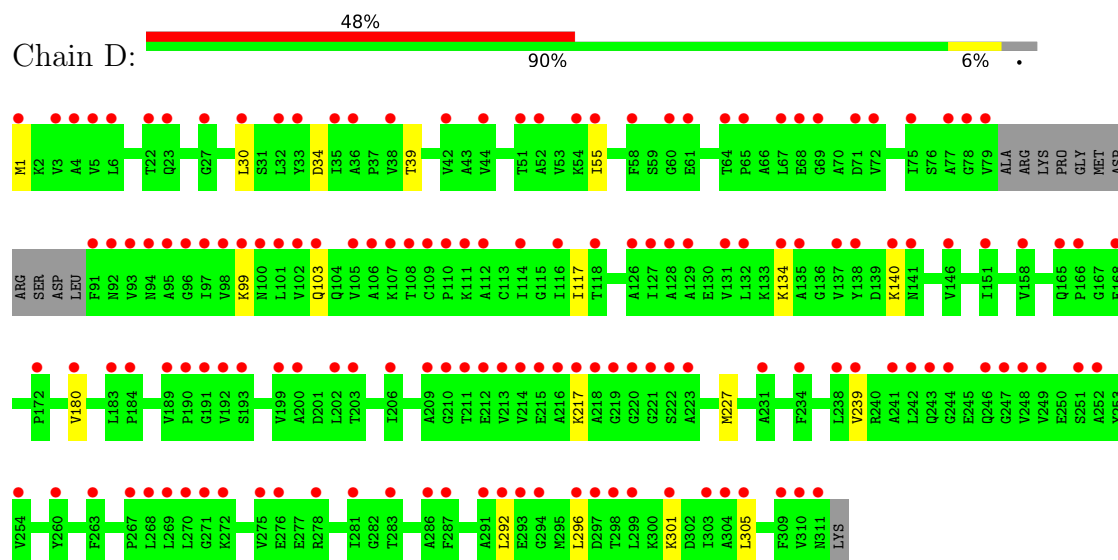
• Molecule 1: Malate dehydrogenase



• Molecule 1: Malate dehydrogenase



• Molecule 1: Malate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.56Å 156.28Å 77.39Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	36.54 – 1.56 36.54 – 1.56	Depositor EDS
% Data completeness (in resolution range)	97.3 (36.54-1.56) 97.4 (36.54-1.56)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.16_3549:000	Depositor
R, R_{free}	0.266 , 0.296 (Not available) , 0.288	Depositor DCC
R_{free} test set	7977 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	1.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9327	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
AG

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	0.26	0/2200	0.50	0/2982
1	B	0.29	0/2229	0.52	0/3021
1	C	0.30	0/2205	0.52	0/2989
1	D	0.24	0/2200	0.46	0/2982
All	All	0.27	0/8834	0.50	0/11974

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	2174	0	2252	21	0
1	B	2203	0	2283	14	0
1	C	2179	0	2257	15	0
1	D	2174	0	2252	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	151	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	169	0	0	4	0
3	C	161	0	0	1	0
3	D	112	0	0	2	0
All	All	9327	0	9044	59	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 4.

All (59) 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:C:35:ILE:H	1:C:35:ILE:HD12	1.64	0.62
1:D:30:LEU:HD23	1:D:55:ILE:HD12	1.83	0.61
1:D:140:LYS:HG3	3:D:549:HOH:O	2.02	0.58
1:A:30:LEU:O	1:A:55:ILE:HA	2.05	0.57
1:A:256:GLY:HA2	1:A:278:ARG:HE	1.71	0.56
1:C:30:LEU:O	1:C:55:ILE:HA	2.06	0.55
1:D:34:ASP:HB3	1:D:39:THR:OG1	2.06	0.55
1:C:233:ARG:HA	3:C:637:HOH:O	2.06	0.54
1:A:295:MET:O	1:A:298:THR:OG1	2.23	0.54
1:A:91:PHE:CE1	1:A:127:ILE:HD11	2.43	0.54
1:C:289:GLN:O	1:C:293:GLU:HG3	2.09	0.53
1:B:301:LYS:HG2	3:B:550:HOH:O	2.09	0.52
1:B:117:ILE:HG23	1:B:227:MET:HE2	1.92	0.52
1:C:34:ASP:HB3	1:C:39:THR:OG1	2.10	0.52
1:D:301:LYS:O	1:D:305:LEU:HG	2.09	0.52
1:B:279:LYS:HE2	3:B:595:HOH:O	2.10	0.51
1:A:30:LEU:HD23	1:A:55:ILE:HD12	1.93	0.51
1:B:209:ALA:O	1:B:212:GLU:HB2	2.11	0.50
1:B:1:MET:N	3:B:501:HOH:O	2.41	0.50
1:D:1:MET:HG2	1:D:239:VAL:HG13	1.94	0.49
1:C:91:PHE:CE1	1:C:123:THR:HG21	2.49	0.48
1:C:41:GLY:HA3	1:D:217:LYS:HG2	1.96	0.47
1:A:97:ILE:HG13	3:A:552:HOH:O	2.14	0.47
1:A:227:MET:HE3	1:A:230:ALA:HB3	1.97	0.46
1:A:256:GLY:HA2	1:A:278:ARG:NE	2.29	0.46
1:C:260:TYR:HB3	1:C:296:LEU:HD21	1.98	0.45
1:C:174:ILE:HD13	1:C:185:LEU:HD11	1.98	0.45
1:B:34:ASP:HB3	1:B:39:THR:OG1	2.17	0.45
1:B:34:ASP:O	1:B:59:SER:HA	2.17	0.44
1:C:267:PRO:HB2	1:C:279:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:TYR:CE1	1:A:292:LEU:HD21	2.52	0.44
1:C:91:PHE:HE1	1:C:123:THR:HG21	1.82	0.44
1:A:91:PHE:HE1	1:A:127:ILE:HD11	1.81	0.44
1:A:32:LEU:HD11	1:A:55:ILE:HD11	2.00	0.44
1:A:145:GLY:HA3	1:A:253:TYR:HB3	2.00	0.44
1:C:284:LEU:HB3	1:C:289:GLN:HG3	1.99	0.44
1:A:256:GLY:HA3	3:A:562:HOH:O	2.19	0.43
1:D:99:LYS:O	1:D:103:GLN:HG3	2.18	0.43
1:D:117:ILE:HG23	1:D:227:MET:HE2	2.00	0.43
1:C:100:ASN:O	1:C:104:GLN:HG3	2.19	0.43
1:A:227:MET:HE3	1:A:227:MET:HA	2.00	0.43
1:C:162:LYS:HD3	1:C:162:LYS:HA	1.62	0.43
1:D:180:VAL:HG22	3:D:556:HOH:O	2.18	0.42
1:B:30:LEU:O	1:B:55:ILE:HA	2.20	0.42
1:A:257:ASP:OD1	1:A:258:GLY:N	2.52	0.42
1:A:38:VAL:HG23	1:B:217:LYS:HB3	2.02	0.42
1:A:239:VAL:O	1:A:243:GLN:HG3	2.20	0.41
1:A:21:LYS:HE3	1:A:46:LEU:O	2.20	0.41
1:B:126:ALA:HB1	1:B:307:GLU:HG3	2.02	0.41
1:D:292:LEU:O	1:D:296:LEU:HG	2.21	0.41
1:A:203:THR:O	1:A:207:GLN:HG3	2.20	0.41
1:B:260:TYR:CE1	1:B:292:LEU:HD21	2.56	0.41
1:C:213:VAL:HG21	1:C:223:ALA:HB2	2.03	0.41
1:D:134:LYS:HE3	1:D:134:LYS:HB2	1.76	0.41
1:A:134:LYS:HG3	3:A:571:HOH:O	2.21	0.41
1:A:91:PHE:HZ	1:A:309:PHE:HB2	1.86	0.40
1:B:30:LEU:HD23	1:B:55:ILE:HD12	2.04	0.40
1:B:101:LEU:O	1:B:105:VAL:HG23	2.22	0.40
1:B:1:MET:HB3	3:B:584:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	296/312 (95%)	292 (99%)	3 (1%)	1 (0%)	36	18
1	B	300/312 (96%)	297 (99%)	3 (1%)	0	100	100
1	C	297/312 (95%)	295 (99%)	2 (1%)	0	100	100
1	D	296/312 (95%)	293 (99%)	3 (1%)	0	100	100
All	All	1189/1248 (95%)	1177 (99%)	11 (1%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASN

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	230/241 (95%)	230 (100%)	0	100	100
1	B	232/241 (96%)	232 (100%)	0	100	100
1	C	230/241 (95%)	230 (100%)	0	100	100
1	D	230/241 (95%)	230 (100%)	0	100	100
All	All	922/964 (96%)	922 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	ASN
1	B	290	ASN
1	D	100	ASN
1	D	229	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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	300/312 (96%)	1.99	130 (43%) 0 0	15, 23, 37, 65	0
1	B	304/312 (97%)	1.91	124 (40%) 0 0	13, 22, 34, 55	0
1	C	301/312 (96%)	1.90	119 (39%) 1 0	14, 22, 36, 66	0
1	D	300/312 (96%)	2.26	150 (50%) 0 0	13, 25, 44, 96	0
All	All	1205/1248 (96%)	2.01	523 (43%) 0 0	13, 23, 38, 96	0

All (523) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91	PHE	11.5
1	D	93	VAL	10.6
1	D	79	VAL	10.1
1	A	91	PHE	9.9
1	D	214	VAL	9.2
1	C	80	ALA	9.1
1	D	92	ASN	8.1
1	D	211	THR	7.5
1	D	218	ALA	7.3
1	C	192	VAL	7.3
1	C	91	PHE	7.2
1	D	216	ALA	7.0
1	A	93	VAL	6.6
1	A	79	VAL	6.5
1	C	311	ASN	6.5
1	A	92	ASN	6.1
1	B	80	ALA	6.1
1	D	213	VAL	6.0
1	A	214	VAL	5.6
1	C	93	VAL	5.6
1	D	305	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	310	VAL	5.1
1	D	215	GLU	5.1
1	A	183	LEU	5.1
1	C	35	ILE	5.0
1	D	210	GLY	4.8
1	C	92	ASN	4.8
1	B	92	ASN	4.7
1	C	287	PHE	4.7
1	A	196	GLU	4.7
1	D	247	GLY	4.6
1	D	100	ASN	4.5
1	A	192	VAL	4.5
1	D	61	GLU	4.5
1	C	79	VAL	4.4
1	D	309	PHE	4.4
1	A	257	ASP	4.4
1	B	79	VAL	4.4
1	A	211	THR	4.3
1	C	296	LEU	4.2
1	B	93	VAL	4.2
1	C	190	PRO	4.2
1	D	304	ALA	4.2
1	D	219	GLY	4.1
1	D	52	ALA	4.1
1	D	97	ILE	4.1
1	C	163	GLY	4.1
1	A	310	VAL	4.1
1	B	301	LYS	4.0
1	B	81	ARG	4.0
1	A	309	PHE	4.0
1	B	249	VAL	4.0
1	D	108	THR	4.0
1	D	311	ASN	3.9
1	B	214	VAL	3.9
1	C	213	VAL	3.9
1	B	35	ILE	3.9
1	B	178	SER	3.9
1	A	283	THR	3.9
1	B	135	ALA	3.9
1	B	293	GLU	3.8
1	D	222	SER	3.8
1	C	211	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	211	THR	3.8
1	C	286	ALA	3.7
1	B	218	ALA	3.7
1	D	223	ALA	3.7
1	B	89	ASP	3.6
1	A	304	ALA	3.6
1	B	131	VAL	3.6
1	B	213	VAL	3.6
1	D	310	VAL	3.6
1	B	223	ALA	3.6
1	C	77	ALA	3.6
1	D	95	ALA	3.6
1	B	114	ILE	3.5
1	C	189	VAL	3.5
1	A	190	PRO	3.5
1	D	244	GLY	3.5
1	D	242	LEU	3.5
1	A	127	ILE	3.5
1	D	35	ILE	3.5
1	B	60	GLY	3.5
1	D	55	ILE	3.5
1	C	194	PHE	3.4
1	B	219	GLY	3.4
1	A	107	LYS	3.4
1	D	114	ILE	3.4
1	C	214	VAL	3.4
1	D	275	VAL	3.4
1	A	151	ILE	3.3
1	B	97	ILE	3.3
1	B	180	VAL	3.3
1	D	137	VAL	3.3
1	A	184	PRO	3.3
1	C	290	ASN	3.3
1	D	138	TYR	3.3
1	A	242	LEU	3.3
1	D	77	ALA	3.3
1	D	291	ALA	3.3
1	D	127	ILE	3.3
1	B	191	GLY	3.3
1	D	249	VAL	3.3
1	D	94	ASN	3.3
1	A	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	200	ALA	3.3
1	B	183	LEU	3.2
1	D	296	LEU	3.2
1	D	220	GLY	3.2
1	D	248	VAL	3.2
1	A	63	ALA	3.2
1	B	311	ASN	3.2
1	A	35	ILE	3.2
1	A	61	GLU	3.2
1	A	60	GLY	3.2
1	C	309	PHE	3.2
1	B	238	LEU	3.2
1	B	199	VAL	3.2
1	D	38	VAL	3.2
1	B	209	ALA	3.2
1	D	135	ALA	3.2
1	D	281	ILE	3.1
1	A	258	GLY	3.1
1	B	63	ALA	3.1
1	B	262	ARG	3.1
1	D	268	LEU	3.1
1	B	193	SER	3.1
1	A	112	ALA	3.1
1	A	241	ALA	3.1
1	D	260	TYR	3.1
1	B	101	LEU	3.1
1	C	305	LEU	3.1
1	B	210	GLY	3.1
1	D	54	LYS	3.1
1	D	23	GLN	3.1
1	A	182	ILE	3.1
1	A	64	THR	3.0
1	A	168	GLU	3.0
1	A	213	VAL	3.0
1	A	275	VAL	3.0
1	B	38	VAL	3.0
1	B	222	SER	3.0
1	D	239	VAL	3.0
1	A	305	LEU	3.0
1	A	221	GLY	3.0
1	D	4	ALA	3.0
1	B	298	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	137	VAL	3.0
1	B	192	VAL	3.0
1	D	33	TYR	3.0
1	D	110	PRO	3.0
1	B	296	LEU	3.0
1	B	216	ALA	3.0
1	D	191	GLY	3.0
1	A	137	VAL	3.0
1	C	138	TYR	3.0
1	A	222	SER	3.0
1	B	112	ALA	2.9
1	C	223	ALA	2.9
1	B	78	GLY	2.9
1	B	221	GLY	2.9
1	C	191	GLY	2.9
1	D	3	VAL	2.9
1	C	1	MET	2.9
1	D	168	GLU	2.9
1	D	241	ALA	2.9
1	D	96	GLY	2.9
1	B	165	GLN	2.9
1	C	246	GLN	2.9
1	B	73	VAL	2.9
1	D	278	ARG	2.9
1	A	67	LEU	2.9
1	B	90	LEU	2.9
1	C	268	LEU	2.9
1	D	132	LEU	2.9
1	D	78	GLY	2.9
1	C	291	ALA	2.9
1	C	164	LYS	2.9
1	D	140	LYS	2.9
1	A	120	PRO	2.9
1	C	38	VAL	2.9
1	C	169	VAL	2.9
1	D	301	LYS	2.9
1	B	190	PRO	2.8
1	B	220	GLY	2.8
1	C	193	SER	2.8
1	B	173	VAL	2.8
1	B	189	VAL	2.8
1	C	42	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	304	ALA	2.8
1	C	159	ALA	2.8
1	B	91	PHE	2.8
1	B	59	SER	2.8
1	B	260	TYR	2.8
1	A	249	VAL	2.8
1	B	105	VAL	2.8
1	B	275	VAL	2.8
1	B	1	MET	2.8
1	B	134	LYS	2.8
1	A	191	GLY	2.8
1	A	256	GLY	2.8
1	A	298	THR	2.8
1	A	253	TYR	2.8
1	C	260	TYR	2.8
1	A	238	LEU	2.8
1	D	6	LEU	2.8
1	C	218	ALA	2.7
1	D	102	VAL	2.7
1	D	27	GLY	2.7
1	D	298	THR	2.7
1	D	212	GLU	2.7
1	D	287	PHE	2.7
1	C	134	LYS	2.7
1	D	134	LYS	2.7
1	A	106	ALA	2.7
1	A	218	ALA	2.7
1	A	296	LEU	2.7
1	B	305	LEU	2.7
1	D	297	ASP	2.7
1	D	112	ALA	2.7
1	A	131	VAL	2.7
1	B	98	VAL	2.7
1	D	103	GLN	2.7
1	A	274	GLY	2.7
1	D	64	THR	2.7
1	C	262	ARG	2.7
1	A	174	ILE	2.7
1	A	263	PHE	2.7
1	D	303	ILE	2.7
1	D	246	GLN	2.7
1	C	113	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	19	LEU	2.7
1	A	299	LEU	2.7
1	C	284	LEU	2.7
1	C	292	LEU	2.7
1	D	221	GLY	2.7
1	A	180	VAL	2.7
1	D	192	VAL	2.7
1	C	204	LYS	2.7
1	A	70	ALA	2.6
1	B	52	ALA	2.6
1	A	33	TYR	2.6
1	B	256	GLY	2.6
1	B	107	LYS	2.6
1	A	269	LEU	2.6
1	B	254	VAL	2.6
1	D	146	VAL	2.6
1	C	289	GLN	2.6
1	B	76	SER	2.6
1	D	1	MET	2.6
1	C	303	ILE	2.6
1	A	113	CYS	2.6
1	D	109	CYS	2.6
1	A	77	ALA	2.6
1	A	216	ALA	2.6
1	C	216	ALA	2.6
1	B	67	LEU	2.6
1	C	242	LEU	2.6
1	D	101	LEU	2.6
1	C	199	VAL	2.6
1	C	4	ALA	2.6
1	C	304	ALA	2.6
1	D	283	THR	2.6
1	B	264	PHE	2.6
1	D	270	LEU	2.6
1	A	94	ASN	2.6
1	B	248	VAL	2.6
1	D	254	VAL	2.6
1	D	294	GLY	2.6
1	B	113	CYS	2.5
1	C	9	ALA	2.5
1	C	231	ALA	2.5
1	D	36	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	128	ALA	2.5
1	A	204	LYS	2.5
1	B	54	LYS	2.5
1	D	107	LYS	2.5
1	A	260	TYR	2.5
1	C	58	PHE	2.5
1	C	273	ASN	2.5
1	A	78	GLY	2.5
1	A	38	VAL	2.5
1	A	189	VAL	2.5
1	D	105	VAL	2.5
1	C	63	ALA	2.5
1	C	241	ALA	2.5
1	D	252	ALA	2.5
1	C	208	ASN	2.5
1	A	75	ILE	2.5
1	B	268	LEU	2.5
1	C	30	LEU	2.5
1	D	292	LEU	2.5
1	C	10	GLY	2.5
1	D	65	PRO	2.5
1	A	293	GLU	2.5
1	D	158	VAL	2.5
1	D	165	GLN	2.5
1	A	135	ALA	2.5
1	B	109	CYS	2.5
1	B	12	ILE	2.5
1	B	303	ILE	2.5
1	C	127	ILE	2.5
1	B	299	LEU	2.5
1	C	25	PRO	2.5
1	D	234	PHE	2.5
1	A	259	GLN	2.5
1	A	158	VAL	2.5
1	D	189	VAL	2.5
1	C	209	ALA	2.4
1	B	26	SER	2.4
1	B	258	GLY	2.4
1	D	271	GLY	2.4
1	B	133	LYS	2.4
1	A	65	PRO	2.4
1	B	33	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	67	LEU	2.4
1	D	299	LEU	2.4
1	B	144	PHE	2.4
1	B	309	PHE	2.4
1	A	108	THR	2.4
1	C	64	THR	2.4
1	C	298	THR	2.4
1	D	22	THR	2.4
1	C	239	VAL	2.4
1	A	209	ALA	2.4
1	A	291	ALA	2.4
1	B	77	ALA	2.4
1	D	106	ALA	2.4
1	A	272	LYS	2.4
1	C	179	GLY	2.4
1	D	172	PRO	2.4
1	D	190	PRO	2.4
1	A	292	LEU	2.4
1	B	168	GLU	2.4
1	C	108	THR	2.4
1	D	118	THR	2.4
1	A	234	PHE	2.4
1	C	234	PHE	2.4
1	D	263	PHE	2.4
1	C	107	LYS	2.4
1	D	272	LYS	2.4
1	A	163	GLY	2.4
1	D	231	ALA	2.4
1	C	131	VAL	2.4
1	D	131	VAL	2.4
1	A	308	GLU	2.4
1	C	293	GLU	2.4
1	D	68	GLU	2.4
1	D	184	PRO	2.4
1	B	182	ILE	2.4
1	B	132	LEU	2.4
1	B	161	LEU	2.4
1	A	43	ALA	2.3
1	A	3	VAL	2.3
1	B	184	PRO	2.3
1	C	162	LYS	2.3
1	A	123	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	151	ILE	2.3
1	C	12	ILE	2.3
1	C	97	ILE	2.3
1	D	151	ILE	2.3
1	B	242	LEU	2.3
1	C	61	GLU	2.3
1	D	238	LEU	2.3
1	D	293	GLU	2.3
1	A	208	ASN	2.3
1	A	95	ALA	2.3
1	A	264	PHE	2.3
1	B	58	PHE	2.3
1	D	58	PHE	2.3
1	C	109	CYS	2.3
1	B	56	LYS	2.3
1	B	239	VAL	2.3
1	C	44	VAL	2.3
1	D	72	VAL	2.3
1	D	166	PRO	2.3
1	A	22	THR	2.3
1	A	306	GLY	2.3
1	B	257	ASP	2.3
1	A	6	LEU	2.3
1	A	185	LEU	2.3
1	C	19	LEU	2.3
1	C	15	ALA	2.3
1	C	135	ALA	2.3
1	D	129	ALA	2.3
1	C	68	GLU	2.3
1	A	58	PHE	2.3
1	A	311	ASN	2.3
1	B	100	ASN	2.3
1	B	72	VAL	2.3
1	B	310	VAL	2.3
1	C	180	VAL	2.3
1	D	98	VAL	2.3
1	D	180	VAL	2.3
1	D	51	THR	2.3
1	D	203	THR	2.3
1	A	247	GLY	2.3
1	B	246	GLN	2.3
1	C	301	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	99	LYS	2.3
1	B	206	ILE	2.3
1	C	174	ILE	2.3
1	D	30	LEU	2.3
1	C	29	GLU	2.3
1	A	59	SER	2.3
1	B	253	TYR	2.3
1	B	231	ALA	2.2
1	D	286	ALA	2.2
1	A	172	PRO	2.2
1	C	65	PRO	2.2
1	C	62	ASP	2.2
1	B	240	ARG	2.2
1	C	22	THR	2.2
1	A	41	GLY	2.2
1	B	294	GLY	2.2
1	C	176	GLY	2.2
1	C	274	GLY	2.2
1	D	5	VAL	2.2
1	A	161	LEU	2.2
1	C	74	LEU	2.2
1	D	32	LEU	2.2
1	A	55	ILE	2.2
1	A	206	ILE	2.2
1	D	116	ILE	2.2
1	D	206	ILE	2.2
1	C	94	ASN	2.2
1	A	66	ALA	2.2
1	B	43	ALA	2.2
1	C	106	ALA	2.2
1	D	209	ALA	2.2
1	B	148	THR	2.2
1	C	168	GLU	2.2
1	B	27	GLY	2.2
1	D	60	GLY	2.2
1	C	146	VAL	2.2
1	D	243	GLN	2.2
1	D	202	LEU	2.2
1	A	128	ALA	2.2
1	B	200	ALA	2.2
1	C	261	ALA	2.2
1	D	217	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	210	GLY	2.2
1	C	294	GLY	2.2
1	D	251	SER	2.2
1	C	263	PHE	2.2
1	A	169	VAL	2.2
1	A	173	VAL	2.2
1	C	160	GLU	2.2
1	D	44	VAL	2.2
1	A	301	LYS	2.2
1	C	67	LEU	2.1
1	A	129	ALA	2.1
1	C	36	ALA	2.1
1	D	126	ALA	2.1
1	D	267	PRO	2.1
1	D	75	ILE	2.1
1	D	193	SER	2.1
1	B	53	VAL	2.1
1	B	102	VAL	2.1
1	B	121	VAL	2.1
1	D	42	VAL	2.1
1	B	41	GLY	2.1
1	C	52	ALA	2.1
1	C	267	PRO	2.1
1	D	69	GLY	2.1
1	A	4	ALA	2.1
1	A	74	LEU	2.1
1	A	132	LEU	2.1
1	A	286	ALA	2.1
1	B	30	LEU	2.1
1	B	236	LEU	2.1
1	C	186	LEU	2.1
1	B	61	GLU	2.1
1	D	276	GLU	2.1
1	C	45	ASP	2.1
1	C	281	ILE	2.1
1	D	71	ASP	2.1
1	A	134	LYS	2.1
1	C	54	LYS	2.1
1	C	178	SER	2.1
1	A	105	VAL	2.1
1	C	121	VAL	2.1
1	D	199	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	25	PRO	2.1
1	A	110	PRO	2.1
1	A	119	ASN	2.1
1	C	166	PRO	2.1
1	A	8	ALA	2.1
1	A	181	THR	2.1
1	A	232	ALA	2.1
1	A	252	ALA	2.1
1	B	70	ALA	2.1
1	B	129	ALA	2.1
1	C	66	ALA	2.1
1	A	202	LEU	2.1
1	D	183	LEU	2.1
1	D	269	LEU	2.1
1	A	97	ILE	2.1
1	C	165	GLN	2.1
1	C	197	GLN	2.1
1	A	215	GLU	2.1
1	B	160	GLU	2.1
1	C	222	SER	2.1
1	A	27	GLY	2.1
1	B	201	ASP	2.1
1	D	141	ASN	2.1
1	A	166	PRO	2.1
1	B	120	PRO	2.1
1	B	22	THR	2.0
1	A	121	VAL	2.0
1	A	197	GLN	2.0
1	B	259	GLN	2.0
1	A	281	ILE	2.0
1	B	138	TYR	2.0
1	C	306	GLY	2.0
1	D	111	LYS	2.0
1	C	195	THR	2.0
1	A	194	PHE	2.0
1	A	287	PHE	2.0
1	A	30	LEU	2.0
1	B	185	LEU	2.0
1	B	269	LEU	2.0
1	C	202	LEU	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, 95th 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($\text{\AA}^2$)	Q<0.9
2	AG	A	401	1/1	0.98	0.07	19,19,19,19	1
2	AG	C	401	1/1	0.98	0.05	21,21,21,21	1
2	AG	B	401	1/1	0.99	0.05	20,20,20,20	1
2	AG	D	401	1/1	0.99	0.05	29,29,29,29	1

6.5 Other polymers [i](#)

There are no such residues in this entry.