



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:58 PM UTC

PDB ID : 4PCQ / pdb_00004pcq
Title : Crystal Structure of MtbAldR (Rv2779c)
Authors : Dey, A.; Ramachandran, R.
Deposited on : 2014-04-16
Resolution : 2.95 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

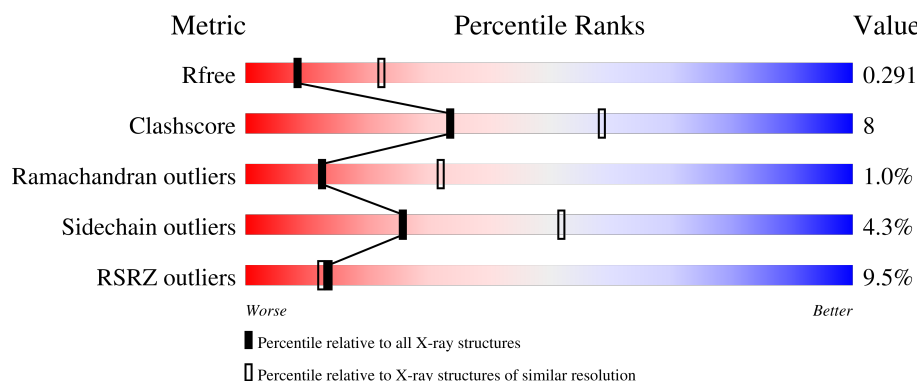
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	190	7% 64% 13% • 22%
1	B	190	9% 61% 16% •• 22%
1	C	190	6% 61% 16% • 23%
1	D	190	7% 59% 17% • 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4254 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 Possible transcriptional regulatory protein (Probably Lrp/AsnC-family).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1060	664	188	204	4			
1	B	149	Total	C	N	O	S	0	0	0
			1064	669	190	201	4			
1	C	147	Total	C	N	O	S	0	0	0
			1037	642	190	201	4			
1	D	145	Total	C	N	O	S	0	0	0
			1060	659	198	199	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ALA	-	expression tag	UNP O33321
A	181	ALA	-	expression tag	UNP O33321
A	182	ALA	-	expression tag	UNP O33321
A	183	LEU	-	expression tag	UNP O33321
A	184	GLY	-	expression tag	UNP O33321
A	185	HIS	-	expression tag	UNP O33321
A	186	HIS	-	expression tag	UNP O33321
A	187	HIS	-	expression tag	UNP O33321
A	188	HIS	-	expression tag	UNP O33321
A	189	HIS	-	expression tag	UNP O33321
A	190	HIS	-	expression tag	UNP O33321
B	180	ALA	-	expression tag	UNP O33321
B	181	ALA	-	expression tag	UNP O33321
B	182	ALA	-	expression tag	UNP O33321
B	183	LEU	-	expression tag	UNP O33321
B	184	GLY	-	expression tag	UNP O33321
B	185	HIS	-	expression tag	UNP O33321
B	186	HIS	-	expression tag	UNP O33321
B	187	HIS	-	expression tag	UNP O33321
B	188	HIS	-	expression tag	UNP O33321

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Chain	Residue	Modelled	Actual	Comment	Reference
B	189	HIS	-	expression tag	UNP O33321
B	190	HIS	-	expression tag	UNP O33321
C	180	ALA	-	expression tag	UNP O33321
C	181	ALA	-	expression tag	UNP O33321
C	182	ALA	-	expression tag	UNP O33321
C	183	LEU	-	expression tag	UNP O33321
C	184	GLY	-	expression tag	UNP O33321
C	185	HIS	-	expression tag	UNP O33321
C	186	HIS	-	expression tag	UNP O33321
C	187	HIS	-	expression tag	UNP O33321
C	188	HIS	-	expression tag	UNP O33321
C	189	HIS	-	expression tag	UNP O33321
C	190	HIS	-	expression tag	UNP O33321
D	180	ALA	-	expression tag	UNP O33321
D	181	ALA	-	expression tag	UNP O33321
D	182	ALA	-	expression tag	UNP O33321
D	183	LEU	-	expression tag	UNP O33321
D	184	GLY	-	expression tag	UNP O33321
D	185	HIS	-	expression tag	UNP O33321
D	186	HIS	-	expression tag	UNP O33321
D	187	HIS	-	expression tag	UNP O33321
D	188	HIS	-	expression tag	UNP O33321
D	189	HIS	-	expression tag	UNP O33321
D	190	HIS	-	expression tag	UNP O33321

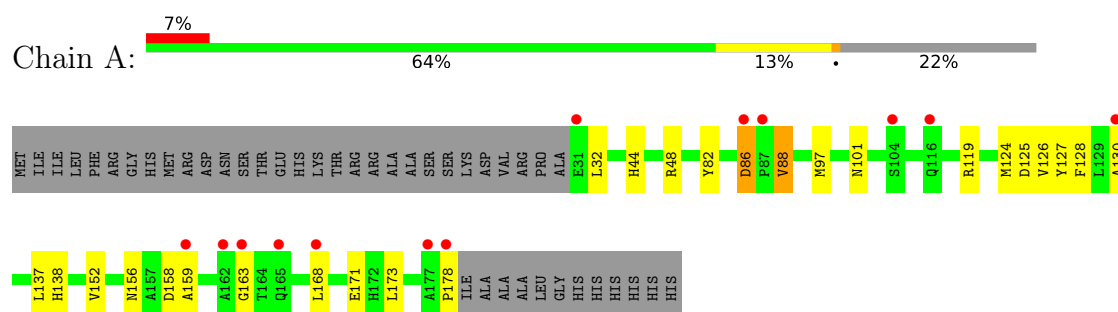
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	6	Total O 6 6	0	0
2	C	14	Total O 14 14	0	0
2	D	6	Total O 6 6	0	0

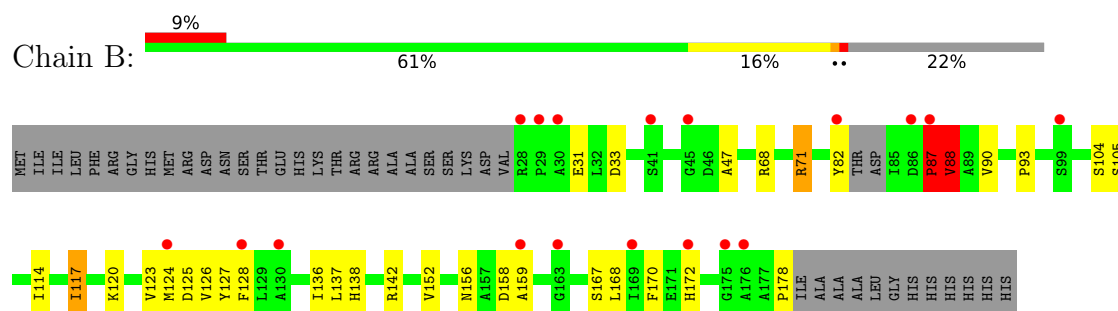
3 Residue-property plots [i](#)

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.

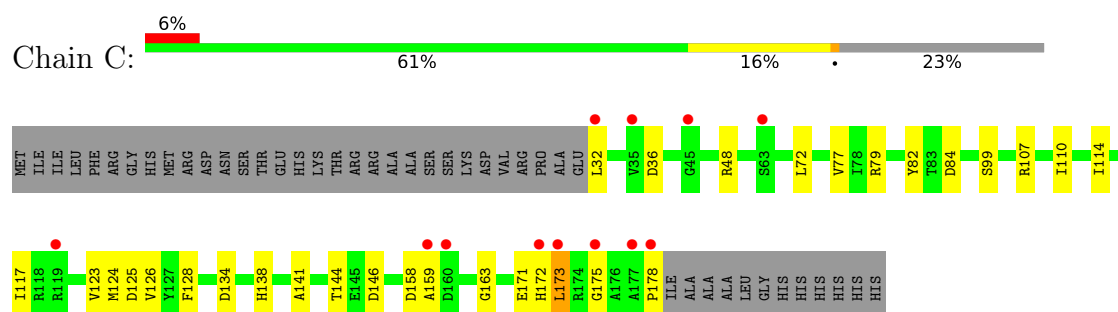
- Molecule 1: Possible transcriptional regulatory protein (Probably Lrp/AsnC-family)



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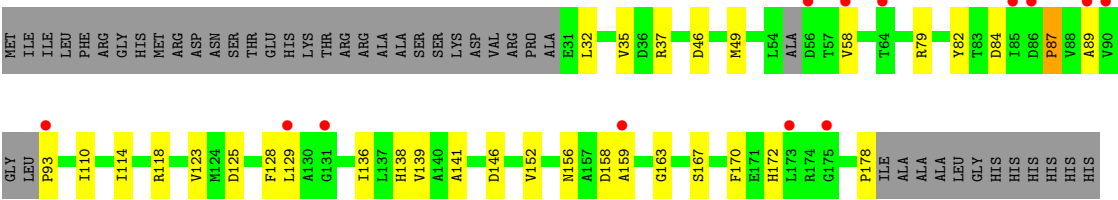


- Molecule 1: Possible transcriptional regulatory protein (Probably Lrp/AsnC-family)



- Molecule 1: Possible transcriptional regulatory protein (Probably Lrp/AsnC-family)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.74Å 146.10Å 49.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.19 – 2.95 27.19 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.19-2.95) 95.5 (27.19-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.263 , 0.299 0.265 , 0.291	Depositor DCC
R_{free} test set	940 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4254	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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	0.40	0/1074	0.85	0/1464
1	B	0.40	0/1077	0.91	2/1466 (0.1%)
1	C	0.41	0/1050	0.87	1/1432 (0.1%)
1	D	0.37	0/1071	0.85	3/1450 (0.2%)
All	All	0.39	0/4272	0.87	6/5812 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	PRO	N-CA-CB	7.63	111.39	103.00
1	D	87	PRO	N-CA-CB	7.33	110.95	103.25
1	B	87	PRO	N-CA-CB	7.01	110.61	103.25
1	D	178	PRO	N-CA-CB	6.84	110.52	103.00
1	D	93	PRO	N-CA-CB	6.69	110.36	103.00
1	B	178	PRO	N-CA-CB	6.66	110.32	103.00

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	1060	0	1008	17	0
1	B	1064	0	1006	23	0
1	C	1037	0	941	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1060	0	992	19	0
2	A	7	0	0	2	1
2	B	6	0	0	0	0
2	C	14	0	0	0	1
2	D	6	0	0	1	0
All	All	4254	0	3947	63	1

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 (63) 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:173:LEU:HB2	1:D:79:ARG:HD2	1.59	0.85
1:D:125:ASP:HB2	1:D:138:HIS:HB3	1.63	0.81
1:C:48:ARG:NH2	1:D:49:MET:O	2.15	0.80
1:B:71:ARG:HH11	1:B:71:ARG:HB3	1.48	0.77
1:C:32:LEU:O	1:C:36:ASP:HB2	1.89	0.73
1:A:125:ASP:HB2	1:A:138:HIS:HB3	1.71	0.72
1:D:129:LEU:HD11	1:D:136:ILE:HG13	1.74	0.70
1:B:93:PRO:HD2	1:B:142:ARG:HA	1.75	0.69
1:B:125:ASP:HB2	1:B:138:HIS:HB3	1.76	0.68
1:C:84:ASP:OD2	1:D:79:ARG:NE	2.28	0.66
1:A:128:PHE:CD1	1:B:170:PHE:HB2	2.33	0.63
1:C:107:ARG:NH2	1:C:134:ASP:OD2	2.32	0.62
1:B:114:ILE:HA	1:B:117:ILE:HG22	1.82	0.61
1:A:130:ALA:HB3	1:B:167:SER:HB3	1.82	0.61
1:C:125:ASP:HB2	1:C:138:HIS:HB3	1.83	0.59
1:A:126:VAL:HB	1:B:172:HIS:HB2	1.85	0.58
1:A:32:LEU:HD22	1:B:90:VAL:HG11	1.86	0.57
1:A:158:ASP:OD1	1:A:159:ALA:N	2.32	0.56
1:C:114:ILE:HG13	1:C:128:PHE:HZ	1.71	0.56
1:D:163:GLY:HA3	2:D:206:HOH:O	2.06	0.55
1:B:114:ILE:HG13	1:B:128:PHE:CZ	2.42	0.55
1:A:86:ASP:C	1:A:88:VAL:H	2.15	0.54
1:B:152:VAL:HA	1:B:156:ASN:HB2	1.89	0.54
1:B:158:ASP:OD1	1:B:159:ALA:N	2.34	0.54
1:A:163:GLY:HA3	2:A:207:HOH:O	2.09	0.53
1:D:158:ASP:OD1	1:D:159:ALA:N	2.36	0.53
1:C:128:PHE:CD1	1:D:170:PHE:HB3	2.44	0.53
1:B:33:ASP:OD2	1:B:68:ARG:NH2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:HB	1:D:172:HIS:HB2	1.91	0.52
1:B:71:ARG:HH11	1:B:71:ARG:CB	2.21	0.51
1:C:158:ASP:OD1	1:C:159:ALA:N	2.36	0.50
1:D:46:ASP:HB3	1:D:49:MET:HE3	1.93	0.50
1:D:114:ILE:HG13	1:D:128:PHE:CZ	2.47	0.50
1:C:171:GLU:HG2	1:C:172:HIS:N	2.27	0.50
1:A:168:LEU:HD21	1:B:127:TYR:HB3	1.92	0.49
1:A:159:ALA:HB3	2:A:206:HOH:O	2.12	0.49
1:A:44:HIS:ND1	1:A:178:PRO:HD3	2.28	0.48
1:C:141:ALA:HB1	1:C:146:ASP:HB3	1.96	0.47
1:A:171:GLU:HG3	1:B:127:TYR:CE2	2.50	0.47
1:C:114:ILE:HA	1:C:117:ILE:HG22	1.97	0.47
1:D:32:LEU:O	1:D:37:ARG:NH2	2.48	0.47
1:B:120:LYS:O	1:B:123:VAL:HG22	2.15	0.47
1:C:79:ARG:N	1:D:84:ASP:O	2.46	0.46
1:D:152:VAL:HA	1:D:156:ASN:HB2	1.97	0.46
1:A:82:TYR:HB2	1:B:82:TYR:CZ	2.52	0.44
1:B:114:ILE:HG13	1:B:128:PHE:CE2	2.53	0.44
1:C:72:LEU:O	1:C:77:VAL:HG22	2.16	0.44
1:C:175:GLY:H	1:D:118:ARG:HH22	1.65	0.44
1:A:48:ARG:NH1	1:B:47:ALA:O	2.38	0.44
1:A:127:TYR:HD2	1:B:168:LEU:HD21	1.82	0.43
1:D:123:VAL:HA	1:D:139:VAL:HG12	2.01	0.43
1:D:141:ALA:HB1	1:D:146:ASP:HB3	2.00	0.43
1:C:82:TYR:CZ	1:D:82:TYR:HB2	2.53	0.43
1:C:99:SER:O	1:C:163:GLY:HA2	2.18	0.43
1:D:35:VAL:HG13	1:D:58:VAL:HG11	2.02	0.42
1:B:127:TYR:HB2	1:B:136:ILE:HG12	2.02	0.42
1:C:114:ILE:HG13	1:C:128:PHE:CZ	2.51	0.41
1:B:87:PRO:O	1:B:88:VAL:HG13	2.20	0.41
1:C:171:GLU:HG2	1:C:172:HIS:H	1.84	0.41
1:A:152:VAL:HA	1:A:156:ASN:HB2	2.03	0.41
1:C:123:VAL:O	1:C:124:MET:HE2	2.21	0.41
1:B:126:VAL:HG22	1:B:137:LEU:HD22	2.03	0.41
1:A:119:ARG:HH11	1:A:119:ARG:HD3	1.77	0.40

All (1) 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:A:203:HOH:O	2:C:204:HOH:O[2_655]	2.19	0.01

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	146/190 (77%)	135 (92%)	9 (6%)	2 (1%)	9	24
1	B	145/190 (76%)	136 (94%)	7 (5%)	2 (1%)	9	24
1	C	145/190 (76%)	137 (94%)	8 (6%)	0	100	100
1	D	139/190 (73%)	133 (96%)	4 (3%)	2 (1%)	9	24
All	All	575/760 (76%)	541 (94%)	28 (5%)	6 (1%)	12	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	B	87	PRO
1	B	88	VAL
1	D	87	PRO
1	D	89	ALA
1	A	86	ASP

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	103/156 (66%)	98 (95%)	5 (5%)	22	48
1	B	101/156 (65%)	94 (93%)	7 (7%)	14	35
1	C	94/156 (60%)	91 (97%)	3 (3%)	34	59
1	D	100/156 (64%)	98 (98%)	2 (2%)	48	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	398/624 (64%)	381 (96%)	17 (4%)	26	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	MET
1	A	101	ASN
1	A	124	MET
1	A	137	LEU
1	A	173	LEU
1	B	31	GLU
1	B	71	ARG
1	B	88	VAL
1	B	104	SER
1	B	105	SER
1	B	117	ILE
1	B	124	MET
1	C	110	ILE
1	C	144	THR
1	C	173	LEU
1	D	110	ILE
1	D	167	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	148/190 (77%)	0.82	13 (8%) 15 14	23, 48, 64, 93	0
1	B	149/190 (78%)	0.98	18 (12%) 8 8	22, 43, 67, 81	0
1	C	147/190 (77%)	0.75	12 (8%) 17 15	22, 39, 77, 94	0
1	D	145/190 (76%)	0.82	13 (8%) 15 13	22, 42, 70, 86	0
All	All	589/760 (77%)	0.84	56 (9%) 14 12	22, 44, 72, 94	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	PRO	5.7
1	A	86	ASP	4.5
1	B	159	ALA	4.2
1	B	130	ALA	4.1
1	C	159	ALA	4.1
1	D	89	ALA	3.8
1	B	29	PRO	3.8
1	D	85	ILE	3.6
1	D	159	ALA	3.5
1	B	86	ASP	3.5
1	A	178	PRO	3.4
1	C	32	LEU	3.4
1	D	175	GLY	3.3
1	C	175	GLY	3.3
1	A	159	ALA	3.1
1	D	86	ASP	3.1
1	D	64	THR	3.0
1	B	128	PHE	3.0
1	B	45	GLY	3.0
1	B	169	ILE	3.0
1	B	41	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	175	GLY	2.7
1	A	165	GLN	2.7
1	C	173	LEU	2.7
1	A	31	GLU	2.6
1	A	163	GLY	2.6
1	C	63	SER	2.6
1	B	176	ALA	2.5
1	B	172	HIS	2.5
1	A	130	ALA	2.5
1	B	30	ALA	2.5
1	D	58	VAL	2.5
1	C	160	ASP	2.4
1	A	162	ALA	2.4
1	A	177	ALA	2.4
1	B	87	PRO	2.4
1	D	131	GLY	2.4
1	D	90	VAL	2.3
1	A	168	LEU	2.3
1	D	173	LEU	2.3
1	C	172	HIS	2.3
1	B	99	SER	2.3
1	C	35	VAL	2.2
1	B	163	GLY	2.2
1	B	28	ARG	2.2
1	D	56	ASP	2.2
1	C	178	PRO	2.2
1	C	119	ARG	2.2
1	B	124	MET	2.2
1	D	93	PRO	2.2
1	C	45	GLY	2.1
1	A	104	SER	2.1
1	A	116	GLN	2.0
1	D	129	LEU	2.0
1	C	177	ALA	2.0
1	B	82	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.