



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:52 PM EDT

PDB ID : 3O1N / pdb_00003o1n
Title : 1.03 Angstrom Crystal Structure of Q236A Mutant Type I Dehydroquinase Dehydratase (aroD) from Salmonella typhimurium
Authors : Light, S.H.; Minasov, G.; Shuvalova, L.; Papazisi, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-07-21
Resolution : 1.03 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

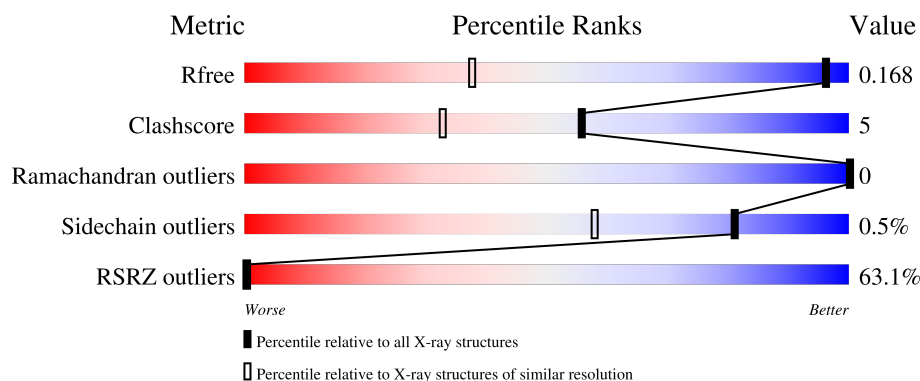
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.03 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	1036 (1.06-1.02)
Clashscore	190562	1063 (1.06-1.02)
Ramachandran outliers	187476	1034 (1.06-1.02)
Sidechain outliers	187428	1035 (1.06-1.02)
RSRZ outliers	180081	1035 (1.06-1.02)

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	276	54% 86% 5% 9%
1	B	276	60% 80% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4951 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 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	22	0
			2102	1326	364	400	12			
1	B	246	Total	C	N	O	S	0	19	0
			1995	1260	334	388	13			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P58687
A	-22	HIS	-	expression tag	UNP P58687
A	-21	HIS	-	expression tag	UNP P58687
A	-20	HIS	-	expression tag	UNP P58687
A	-19	HIS	-	expression tag	UNP P58687
A	-18	HIS	-	expression tag	UNP P58687
A	-17	HIS	-	expression tag	UNP P58687
A	-16	SER	-	expression tag	UNP P58687
A	-15	SER	-	expression tag	UNP P58687
A	-14	GLY	-	expression tag	UNP P58687
A	-13	VAL	-	expression tag	UNP P58687
A	-12	ASP	-	expression tag	UNP P58687
A	-11	LEU	-	expression tag	UNP P58687
A	-10	GLY	-	expression tag	UNP P58687
A	-9	THR	-	expression tag	UNP P58687
A	-8	GLU	-	expression tag	UNP P58687
A	-7	ASN	-	expression tag	UNP P58687
A	-6	LEU	-	expression tag	UNP P58687
A	-5	TYR	-	expression tag	UNP P58687
A	-4	PHE	-	expression tag	UNP P58687
A	-3	GLN	-	expression tag	UNP P58687
A	-2	SER	-	expression tag	UNP P58687
A	-1	ASN	-	expression tag	UNP P58687
A	0	ALA	-	expression tag	UNP P58687
A	236	ALA	GLN	engineered mutation	UNP P58687

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP P58687
B	-22	HIS	-	expression tag	UNP P58687
B	-21	HIS	-	expression tag	UNP P58687
B	-20	HIS	-	expression tag	UNP P58687
B	-19	HIS	-	expression tag	UNP P58687
B	-18	HIS	-	expression tag	UNP P58687
B	-17	HIS	-	expression tag	UNP P58687
B	-16	SER	-	expression tag	UNP P58687
B	-15	SER	-	expression tag	UNP P58687
B	-14	GLY	-	expression tag	UNP P58687
B	-13	VAL	-	expression tag	UNP P58687
B	-12	ASP	-	expression tag	UNP P58687
B	-11	LEU	-	expression tag	UNP P58687
B	-10	GLY	-	expression tag	UNP P58687
B	-9	THR	-	expression tag	UNP P58687
B	-8	GLU	-	expression tag	UNP P58687
B	-7	ASN	-	expression tag	UNP P58687
B	-6	LEU	-	expression tag	UNP P58687
B	-5	TYR	-	expression tag	UNP P58687
B	-4	PHE	-	expression tag	UNP P58687
B	-3	GLN	-	expression tag	UNP P58687
B	-2	SER	-	expression tag	UNP P58687
B	-1	ASN	-	expression tag	UNP P58687
B	0	ALA	-	expression tag	UNP P58687
B	236	ALA	GLN	engineered mutation	UNP P58687

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0

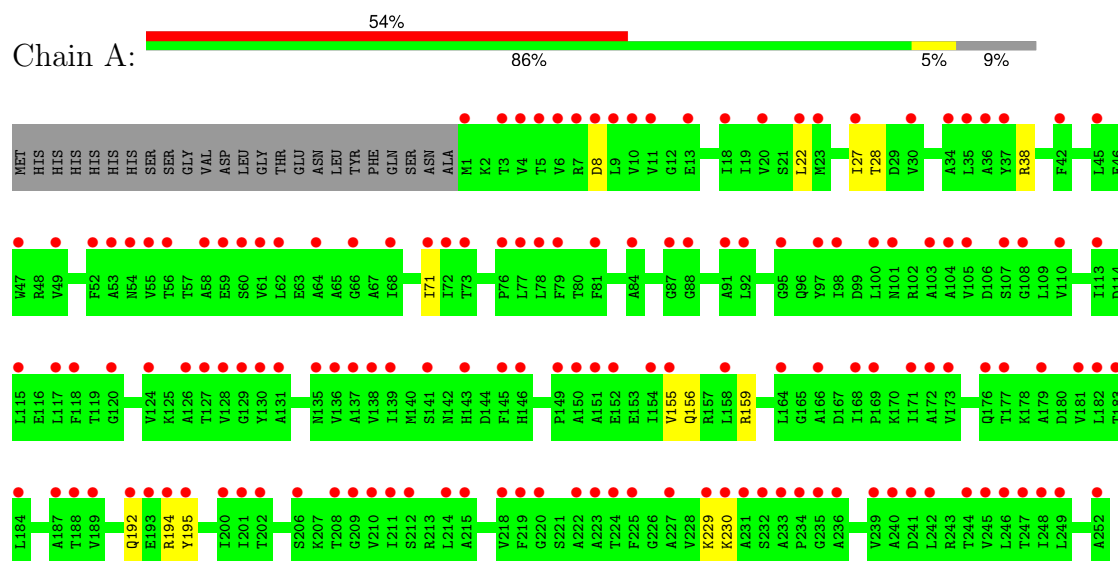
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	418	Total 446	O 446	0	36
4	B	357	Total 403	O 403	0	60

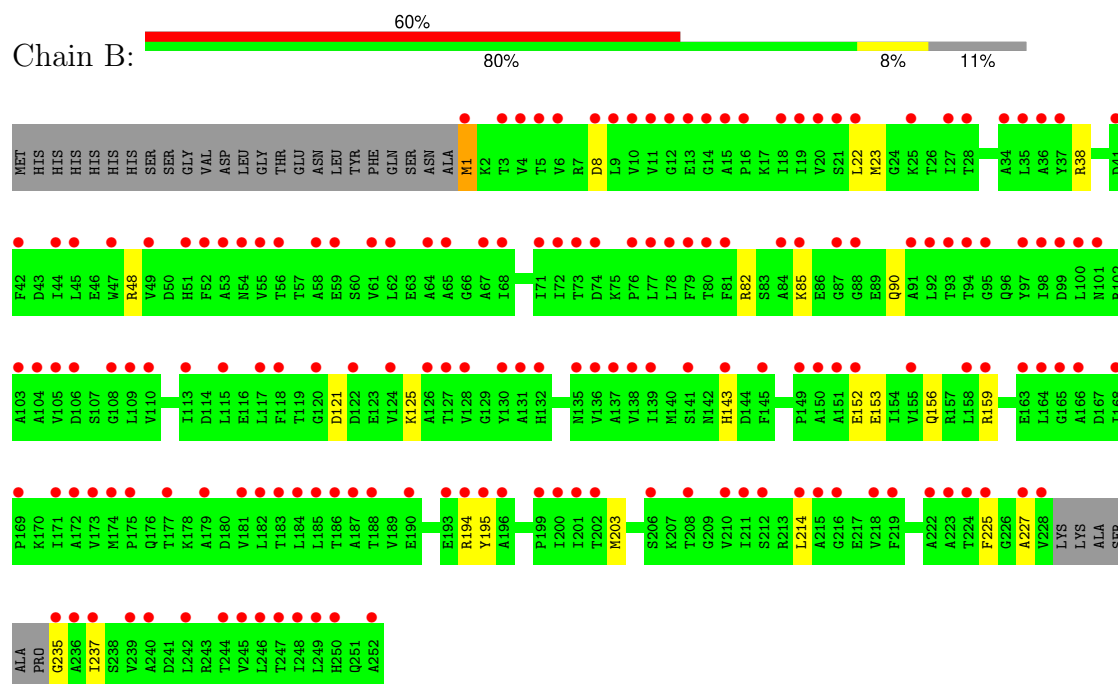
3 Residue-property plots [i](#)

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: 3-dehydroquinate dehydratase



• Molecule 1: 3-dehydroquinate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.43Å 46.48Å 55.79Å 104.23° 97.50° 98.70°	Depositor
Resolution (Å)	26.62 – 1.03 26.62 – 1.03	Depositor EDS
% Data completeness (in resolution range)	92.6 (26.62-1.03) 92.6 (26.62-1.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.03Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.140 , 0.162 0.147 , 0.168	Depositor DCC
R_{free} test set	9868 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4951	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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: CL, MG

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	0.71	0/2138	0.77	0/2887
1	B	0.72	0/2046	0.80	1/2766 (0.0%)
All	All	0.72	0/4184	0.79	1/5653 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ARG	N-CA-C	5.22	116.97	111.28

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	2102	0	2162	17	0
1	B	1995	0	2044	22	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	446	0	0	2	0
4	B	403	0	0	6	0
All	All	4951	0	4206	39	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 5.

All (39) 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:194[B]:ARG:HB2	1:A:195[B]:TYR:CD2	2.22	0.75
1:B:85:LYS:HE3	4:B:471:HOH:O	1.88	0.72
1:A:156:GLN:HE22	1:A:159[B]:ARG:HH11	1.38	0.71
1:A:194[B]:ARG:HB2	1:A:195[B]:TYR:CE2	2.29	0.67
1:B:90:GLN:HB2	4:B:388:HOH:O	1.95	0.67
1:B:156[A]:GLN:HG2	4:B:580:HOH:O	1.99	0.62
1:A:194[B]:ARG:CB	1:A:195[B]:TYR:CE2	2.82	0.62
1:B:1:MET:HE2	4:B:483:HOH:O	2.02	0.59
1:B:90:GLN:CB	4:B:388:HOH:O	2.50	0.58
1:B:194:ARG:NH2	1:B:195:TYR:OH	2.34	0.57
1:A:156:GLN:HE22	1:A:159[B]:ARG:NH1	2.03	0.56
1:A:194[B]:ARG:NH1	4:A:634[B]:HOH:O	2.38	0.56
1:B:194:ARG:NE	1:B:195:TYR:CE2	2.73	0.56
1:B:214:LEU:HD21	1:B:237:ILE:CD1	2.37	0.55
1:A:194[B]:ARG:HB3	1:A:195[B]:TYR:CZ	2.42	0.55
1:B:214:LEU:HD21	1:B:237:ILE:HD13	1.89	0.55
1:B:153[B]:GLU:OE1	1:B:156[B]:GLN:OE1	2.28	0.52
1:A:155:VAL:O	1:A:159[B]:ARG:HG3	2.10	0.52
1:B:23[B]:MET:HE3	1:B:48:ARG:HG3	1.93	0.51
1:B:121:ASP:HB3	1:B:125:LYS:NZ	2.25	0.51
1:B:152:GLU:H	1:B:152:GLU:CD	2.19	0.50
1:B:227:ALA:HB2	1:B:235:GLY:HA3	1.93	0.50
1:B:121:ASP:HB3	1:B:125:LYS:HZ2	1.77	0.49
1:A:27[A]:ILE:HG23	1:A:28:THR:N	2.29	0.48
1:B:156[A]:GLN:HE22	1:B:159:ARG:HH11	1.60	0.47
1:A:194[B]:ARG:CB	1:A:195[B]:TYR:CD2	2.98	0.45
1:B:82:ARG:CZ	1:B:143:HIS:CE1	2.99	0.45
1:B:8:ASP:HB2	4:B:777[B]:HOH:O	2.15	0.45
1:B:1:MET:HE3	1:B:1:MET:HB2	1.77	0.44
1:A:192:GLN:HG2	4:A:576[B]:HOH:O	2.18	0.43
1:B:203[B]:MET:HE1	1:B:225:PHE:HD1	1.84	0.43
1:A:156:GLN:NE2	1:A:159[B]:ARG:HH11	2.11	0.43
1:A:194[B]:ARG:HB3	1:A:195[B]:TYR:CE2	2.55	0.41
1:A:229[A]:LYS:HG2	1:A:230:LYS:HG3	2.03	0.41
1:A:38[A]:ARG:NH2	1:A:71:ILE:O	2.54	0.41
1:B:22:LEU:C	1:B:22:LEU:HD23	2.46	0.41
1:A:38[B]:ARG:HD3	1:A:71:ILE:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:NE	1:B:195:TYR:CZ	2.89	0.40
1:A:22:LEU:HD23	1:A:22:LEU:C	2.45	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	271/276 (98%)	262 (97%)	9 (3%)	0	100	100
1	B	261/276 (95%)	257 (98%)	4 (2%)	0	100	100
All	All	532/552 (96%)	519 (98%)	13 (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	226/225 (100%)	225 (100%)	1 (0%)	84	63
1	B	218/225 (97%)	217 (100%)	1 (0%)	81	58
All	All	444/450 (99%)	442 (100%)	2 (0%)	81	58

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	B	1	MET

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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	252/276 (91%)	2.27	149 (59%) 0 0	6, 13, 19, 27	22 (8%)
1	B	246/276 (89%)	2.31	165 (67%) 0 0	5, 13, 20, 26	19 (7%)
All	All	498/552 (90%)	2.29	314 (63%) 0 0	5, 13, 20, 27	41 (8%)

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	ALA	5.3
1	A	8	ASP	5.2
1	B	236	ALA	4.9
1	B	1	MET	4.7
1	A	6	VAL	4.7
1	A	4	VAL	4.4
1	A	128	VAL	4.3
1	B	195	TYR	4.3
1	A	131	ALA	4.3
1	B	235	GLY	4.3
1	A	10	VAL	4.2
1	A	138	VAL	4.2
1	A	135[A]	ASN	4.1
1	A	234	PRO	4.0
1	B	8	ASP	3.9
1	B	128	VAL	3.9
1	B	145	PHE	3.8
1	A	168	ILE	3.8
1	A	136	VAL	3.8
1	B	228	VAL	3.8
1	A	208[A]	THR	3.7
1	B	55	VAL	3.7
1	B	173	VAL	3.7
1	B	210[A]	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	49	VAL	3.7
1	B	79	PHE	3.7
1	B	135	ASN	3.6
1	A	36	ALA	3.5
1	A	252	ALA	3.5
1	B	54[A]	ASN	3.5
1	B	124	VAL	3.5
1	A	201	ILE	3.5
1	A	73	THR	3.4
1	A	72	ILE	3.4
1	A	139	ILE	3.4
1	A	245	VAL	3.4
1	B	105	VAL	3.4
1	A	58	ALA	3.3
1	B	172	ALA	3.3
1	B	201	ILE	3.3
1	B	237	ILE	3.3
1	B	136	VAL	3.3
1	A	126	ALA	3.3
1	B	150	ALA	3.3
1	B	252	ALA	3.3
1	B	194	ARG	3.3
1	B	115	LEU	3.3
1	A	187	ALA	3.3
1	A	231	ALA	3.3
1	A	232	SER	3.2
1	A	47	TRP	3.2
1	A	233	ALA	3.2
1	B	166	ALA	3.2
1	A	173	VAL	3.2
1	B	193	GLU	3.2
1	A	130	TYR	3.2
1	B	200	ILE	3.2
1	A	129	GLY	3.2
1	B	74	ASP	3.2
1	A	166	ALA	3.2
1	B	28	THR	3.2
1	A	195[A]	TYR	3.2
1	B	52	PHE	3.2
1	B	113	ILE	3.2
1	A	45[A]	LEU	3.1
1	A	100	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	249	LEU	3.1
1	A	150	ALA	3.1
1	A	209	GLY	3.1
1	A	155	VAL	3.1
1	B	218	VAL	3.1
1	A	154	ILE	3.1
1	B	100	LEU	3.1
1	B	84	ALA	3.1
1	A	61	VAL	3.1
1	A	225	PHE	3.1
1	A	230	LYS	3.1
1	B	139	ILE	3.1
1	B	15	ALA	3.1
1	B	104	ALA	3.1
1	B	62[A]	LEU	3.1
1	B	184	LEU	3.1
1	B	247	THR	3.1
1	A	229[A]	LYS	3.0
1	B	12	GLY	3.0
1	A	79	PHE	3.0
1	A	124	VAL	3.0
1	A	218	VAL	3.0
1	B	4	VAL	3.0
1	A	27[A]	ILE	3.0
1	A	248	ILE	3.0
1	B	72	ILE	3.0
1	B	224	THR	3.0
1	B	77	LEU	3.0
1	A	210	VAL	3.0
1	B	239	VAL	3.0
1	A	84	ALA	3.0
1	A	172	ALA	3.0
1	A	236	ALA	3.0
1	B	47	TRP	3.0
1	A	141	SER	3.0
1	A	37	TYR	2.9
1	A	110	VAL	2.9
1	B	6	VAL	2.9
1	A	104	ALA	2.9
1	B	126	ALA	2.9
1	A	171	ILE	2.9
1	B	214	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	199	PRO	2.9
1	B	91	ALA	2.9
1	A	68	ILE	2.9
1	B	98	ILE	2.9
1	A	7[A]	ARG	2.9
1	A	92	LEU	2.9
1	A	146	HIS	2.9
1	A	206	SER	2.9
1	A	5	THR	2.9
1	B	37	TYR	2.9
1	B	130	TYR	2.9
1	B	131	ALA	2.9
1	A	52	PHE	2.9
1	A	81	PHE	2.9
1	A	11	VAL	2.9
1	A	239	VAL	2.9
1	B	245	VAL	2.9
1	A	71	ILE	2.8
1	B	78	LEU	2.8
1	B	127	THR	2.8
1	B	183	THR	2.8
1	B	53	ALA	2.8
1	B	49	VAL	2.8
1	B	138	VAL	2.8
1	B	155	VAL	2.8
1	A	249	LEU	2.8
1	B	92	LEU	2.8
1	B	87	GLY	2.8
1	B	18	ILE	2.8
1	B	68	ILE	2.8
1	B	248	ILE	2.8
1	B	5	THR	2.8
1	B	58	ALA	2.8
1	B	196	ALA	2.8
1	A	118	PHE	2.8
1	A	189	VAL	2.8
1	B	20	VAL	2.8
1	B	181	VAL	2.8
1	B	19	ILE	2.8
1	B	27[A]	ILE	2.8
1	A	91	ALA	2.7
1	B	34	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	118	PHE	2.7
1	A	62	LEU	2.7
1	A	78	LEU	2.7
1	B	35	LEU	2.7
1	A	23[A]	MET	2.7
1	A	20	VAL	2.7
1	A	55	VAL	2.7
1	A	181	VAL	2.7
1	B	149	PRO	2.7
1	A	64	ALA	2.7
1	B	65	ALA	2.7
1	B	99	ASP	2.7
1	A	115	LEU	2.7
1	B	16	PRO	2.7
1	A	3	THR	2.7
1	A	105	VAL	2.7
1	A	212	SER	2.7
1	A	222	ALA	2.7
1	A	97	TYR	2.6
1	A	182	LEU	2.6
1	B	158	LEU	2.6
1	A	145	PHE	2.6
1	A	98	ILE	2.6
1	A	113	ILE	2.6
1	B	44	ILE	2.6
1	A	183	THR	2.6
1	B	208	THR	2.6
1	A	9	LEU	2.6
1	A	214	LEU	2.6
1	B	182	LEU	2.6
1	A	54[A]	ASN	2.6
1	B	42	PHE	2.6
1	A	200[A]	ILE	2.6
1	B	152	GLU	2.6
1	B	227	ALA	2.6
1	A	120	GLY	2.6
1	A	202	THR	2.6
1	B	51	HIS	2.6
1	A	35[A]	LEU	2.5
1	A	42	PHE	2.5
1	B	219	PHE	2.5
1	A	53	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	151	ALA	2.5
1	A	108	GLY	2.5
1	A	235	GLY	2.5
1	B	11	VAL	2.5
1	B	171	ILE	2.5
1	A	101	ASN	2.5
1	B	169	PRO	2.5
1	B	56	THR	2.5
1	A	192	GLN	2.5
1	A	34	ALA	2.5
1	B	81	PHE	2.5
1	B	225	PHE	2.5
1	B	61	VAL	2.5
1	B	211	ILE	2.5
1	A	149	PRO	2.5
1	B	3	THR	2.5
1	B	103	ALA	2.5
1	B	151	ALA	2.5
1	A	169	PRO	2.4
1	A	56	THR	2.4
1	A	247	THR	2.4
1	B	177	THR	2.4
1	A	143	HIS	2.4
1	A	1[A]	MET	2.4
1	A	184	LEU	2.4
1	A	103	ALA	2.4
1	A	240	ALA	2.4
1	B	179	ALA	2.4
1	A	76	PRO	2.4
1	B	94	THR	2.4
1	B	202	THR	2.4
1	A	30	VAL	2.4
1	A	13	GLU	2.4
1	B	163[A]	GLU	2.4
1	B	246	LEU	2.4
1	B	97	TYR	2.4
1	A	219	PHE	2.4
1	B	168	ILE	2.4
1	A	77	LEU	2.3
1	A	164	LEU	2.3
1	B	216	GLY	2.3
1	B	222	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	244	THR	2.3
1	B	244	THR	2.3
1	B	212	SER	2.3
1	A	211	ILE	2.3
1	B	64	ALA	2.3
1	B	67	ALA	2.3
1	B	190	GLU	2.3
1	B	95	GLY	2.3
1	A	137	ALA	2.3
1	A	242	LEU	2.3
1	A	127	THR	2.3
1	A	177	THR	2.3
1	A	224	THR	2.3
1	A	194[A]	ARG	2.2
1	B	159	ARG	2.2
1	B	85	LYS	2.2
1	B	59	GLU	2.2
1	B	250	HIS	2.2
1	B	122[A]	ASP	2.2
1	A	215	ALA	2.2
1	B	137	ALA	2.2
1	B	223	ALA	2.2
1	B	110	VAL	2.2
1	A	246	LEU	2.2
1	B	9	LEU	2.2
1	B	22	LEU	2.2
1	B	117	LEU	2.2
1	B	164	LEU	2.2
1	A	95	GLY	2.2
1	B	108	GLY	2.2
1	A	152	GLU	2.2
1	A	188	THR	2.2
1	B	80	THR	2.2
1	B	186	THR	2.2
1	A	220	GLY	2.2
1	A	107	SER	2.2
1	B	10	VAL	2.2
1	B	185	LEU	2.2
1	A	227	ALA	2.1
1	B	165	GLY	2.1
1	B	187	ALA	2.1
1	A	22	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	117	LEU	2.1
1	B	132	HIS	2.1
1	B	206	SER	2.1
1	B	88	GLY	2.1
1	B	73	THR	2.1
1	B	240	ALA	2.1
1	A	18	ILE	2.1
1	A	59[A]	GLU	2.1
1	B	45	LEU	2.1
1	B	109	LEU	2.1
1	B	242	LEU	2.1
1	A	241	ASP	2.1
1	B	106	ASP	2.1
1	B	141	SER	2.1
1	B	175	PRO	2.1
1	A	66	GLY	2.1
1	A	223	ALA	2.1
1	B	143	HIS	2.1
1	A	158	LEU	2.0
1	B	71	ILE	2.0
1	B	25	LYS	2.0
1	A	87	GLY	2.0
1	A	88	GLY	2.0
1	B	13	GLU	2.0
1	B	120	GLY	2.0
1	B	76	PRO	2.0
1	A	176	GLN	2.0
1	B	93	THR	2.0
1	B	101	ASN	2.0
1	B	188	THR	2.0
1	B	41	ASP	2.0
1	A	60	SER	2.0
1	A	179	ALA	2.0
1	B	21	SER	2.0
1	B	36	ALA	2.0
1	A	193[A]	GLU	2.0
1	B	174	MET	2.0
1	B	14	GLY	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](#)

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	CL	A	253	1/1	0.85	0.11	11,11,11,11	1
3	MG	A	255	1/1	0.85	0.08	18,18,18,18	1
3	MG	B	254	1/1	0.87	0.12	12,12,12,12	1
3	MG	B	253	1/1	0.89	0.12	19,19,19,19	1
3	MG	A	254	1/1	0.93	0.10	20,20,20,20	1

6.5 Other polymers [i](#)

There are no such residues in this entry.