



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:57 AM EDT

PDB ID : 2JAJ / pdb_00002jaj
Title : DDAH1 complexed with L-257
Authors : Murray-Rust, J.; O'Hara, B.P.; Rossiter, S.; Leiper, J.M.; Vallance, P.; McDonald, N.Q.
Deposited on : 2006-11-29
Resolution : 2.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

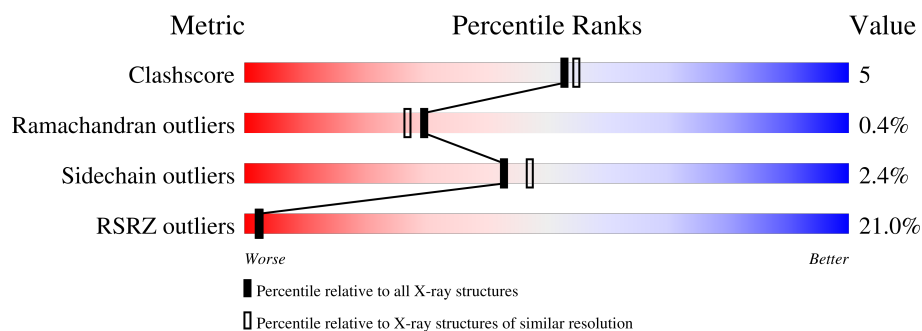
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	289	% 87% 8% 6%
1	B	289	39% 78% 18% • •

2 Entry composition [i](#)

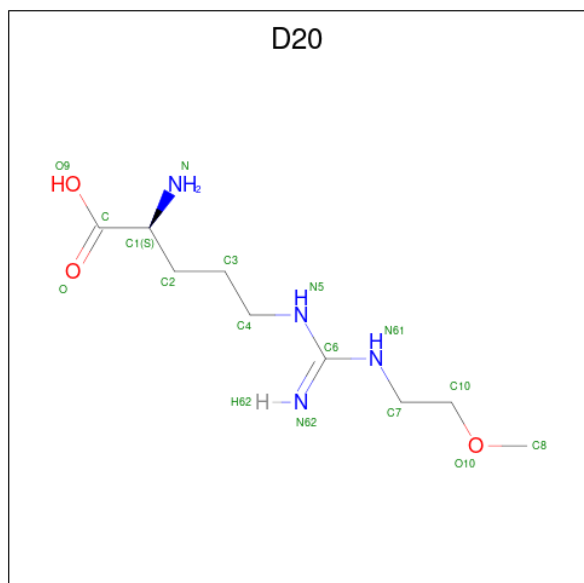
There are 3 unique types of molecules in this entry. The entry contains 4381 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NG, NG-DIMETHYLARGININE DIMETHYLAMINOHYDROLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	2	0
			2054	1292	347	401	14			
1	B	281	Total	C	N	O	S	0	0	0
			2014	1270	344	387	13			

- Molecule 2 is N 5 -{IMINO[(2-METHOXYETHYL)AMINO]METHYL}-L-ORNITHINE (CCD ID: D20) (formula: C₉H₂₀N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	9	4	3		
2	B	1	Total	C	N	O	0	0
			16	9	4	3		

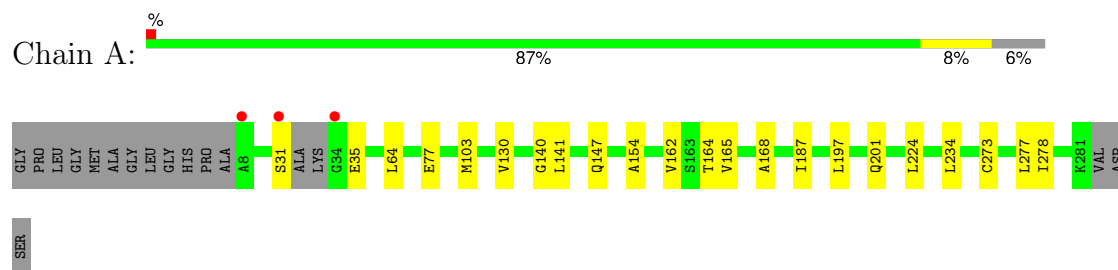
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total 233	O 233	0	0
3	B	48	Total 48	O 48	0	0

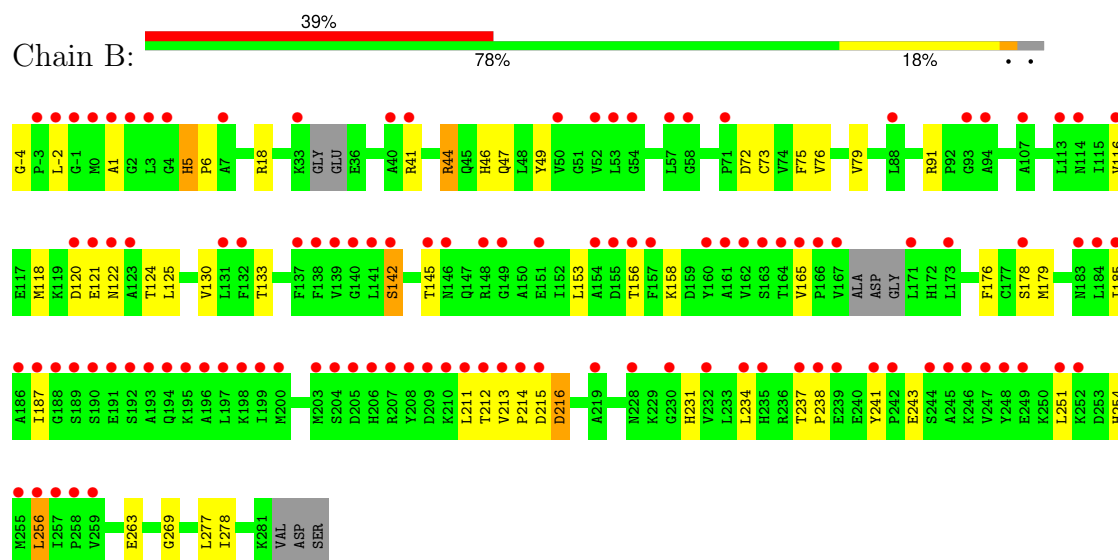
3 Residue-property plots

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: NG, NG-DIMETHYLARGININE DIMETHYLAMINOHYDROLASE 1



- Molecule 1: NG, NG-DIMETHYLARGININE DIMETHYLAMINOHYDROLASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.85Å 46.91Å 147.61Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.00) 93.5 (30.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.263 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4381	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D20

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	1.19	2/2091 (0.1%)	1.10	0/2835
1	B	0.78	0/2047	1.04	8/2792 (0.3%)
All	All	1.01	2/4138 (0.0%)	1.07	8/5627 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	VAL	CA-CB	6.60	1.62	1.54
1	A	140	GLY	C-O	-5.89	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-4	GLY	CA-C-N	6.98	126.95	119.76
1	B	-4	GLY	C-N-CA	6.98	126.95	119.76
1	B	216	ASP	N-CA-C	5.80	118.38	111.71
1	B	142	SER	N-CA-C	5.62	116.50	108.74
1	B	130	VAL	N-CA-C	5.53	116.06	107.99
1	B	1	ALA	N-CA-C	5.33	116.97	110.41
1	B	5	HIS	CA-C-N	5.14	126.27	119.84
1	B	5	HIS	C-N-CA	5.14	126.27	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	ALA	Peptide

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	2054	0	2025	9	0
1	B	2014	0	1902	32	0
2	A	16	0	19	0	0
2	B	16	0	18	1	0
3	A	233	0	0	1	0
3	B	48	0	0	0	0
All	All	4381	0	3964	40	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 (40) 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:B:116:VAL:HG11	1:B:156:THR:OG1	1.90	0.71
1:A:197:LEU:O	1:A:201:GLN:HG3	1.91	0.70
1:B:251:LEU:HB2	1:B:256:LEU:HD21	1.77	0.66
1:B:44:ARG:NH2	1:B:47:GLN:OE1	2.32	0.62
1:B:142:SER:OG	1:B:145:THR:N	2.30	0.60
1:A:224:LEU:HD23	3:A:2002:HOH:O	2.05	0.55
1:B:41:ARG:HB3	1:B:263:GLU:HG3	1.89	0.54
1:B:46:HIS:O	1:B:49:TYR:HB3	2.09	0.52
1:B:251:LEU:HB3	1:B:254:HIS:HB2	1.91	0.51
1:B:75:PHE:CE2	1:B:269:GLY:HA3	2.45	0.51
1:B:215:ASP:CB	1:B:241:TYR:CD2	2.94	0.51
1:B:5:HIS:HB2	1:B:6:PRO:HD2	1.93	0.51
1:B:237:THR:HB	1:B:238:PRO:HD2	1.93	0.50
1:B:214:PRO:HG2	1:B:243:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:C	1:B:278:ILE:HG13	2.37	0.49
1:B:231:HIS:HB3	1:B:254:HIS:CD2	2.48	0.49
1:A:64:LEU:HD13	1:A:103:MET:HG2	1.94	0.48
1:B:215:ASP:CB	1:B:241:TYR:HD2	2.27	0.47
1:B:91:ARG:HB2	1:B:118:MET:HG2	1.97	0.47
1:B:176:PHE:HA	1:B:216:ASP:O	2.15	0.46
1:B:118:MET:HE3	1:B:118:MET:HB2	1.76	0.46
1:B:5:HIS:HB2	1:B:6:PRO:CD	2.46	0.46
1:A:187:ILE:HG12	1:A:197:LEU:HD22	1.99	0.45
1:B:18:ARG:HD3	1:B:73:CYS:HB2	1.97	0.45
1:B:153:LEU:O	1:B:156:THR:HB	2.16	0.45
1:B:215:ASP:HB3	1:B:241:TYR:CD2	2.51	0.45
1:B:185:ILE:O	1:B:211:LEU:N	2.47	0.44
1:A:141:LEU:HG	1:A:164:THR:HB	2.00	0.43
1:B:76:VAL:O	1:B:79:VAL:HG22	2.19	0.43
1:A:147:GLN:HE22	1:B:-2:LEU:HD21	1.84	0.43
1:A:154:ALA:HA	1:A:162:VAL:HG21	2.02	0.42
1:B:178:SER:O	1:B:185:ILE:HG23	2.19	0.42
1:B:120:ASP:C	1:B:122:ASN:H	2.27	0.42
1:B:187:ILE:HG23	1:B:212:THR:HG23	2.01	0.42
1:B:125:LEU:HD12	1:B:145:THR:HG23	2.03	0.41
1:B:237:THR:HB	1:B:238:PRO:CD	2.50	0.41
1:A:277:LEU:C	1:A:278:ILE:HG13	2.46	0.41
1:B:133:THR:HA	1:B:179:MET:SD	2.60	0.41
1:B:72:ASP:OD1	2:B:500:D20:N	2.49	0.41
1:A:77:GLU:HB3	1:A:273:CYS:HA	2.02	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	270/289 (93%)	261 (97%)	8 (3%)	1 (0%)	30	27
1	B	275/289 (95%)	256 (93%)	18 (6%)	1 (0%)	30	27
All	All	545/578 (94%)	517 (95%)	26 (5%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	B	121	GLU

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	220/241 (91%)	217 (99%)	3 (1%)	59	66
1	B	197/241 (82%)	190 (96%)	7 (4%)	31	31
All	All	417/482 (86%)	407 (98%)	10 (2%)	43	47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	165	VAL
1	A	234	LEU
1	B	44	ARG
1	B	124	THR
1	B	158	LYS
1	B	165	VAL
1	B	213	VAL
1	B	234	LEU
1	B	256	LEU

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	202	GLN
1	B	122	ASN
1	B	206	HIS
1	B	228	ASN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	D20	B	500	-	11,15,15	1.17	1 (9%)	14,17,17	0.73	0
2	D20	A	500	-	11,15,15	0.97	0	14,17,17	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D20	B	500	-	-	1/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D20	A	500	-	-	0/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	D20	C2-C1	2.08	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	D20	C2-C3-C4-N5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	D20	1	0

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	272/289 (94%)	0.31	3 (1%) 78 77	20, 31, 40, 52	2 (0%)
1	B	281/289 (97%)	1.88	113 (40%) 0 1	29, 47, 70, 73	0
All	All	553/578 (95%)	1.11	116 (20%) 2 2	20, 37, 68, 73	2 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	VAL	7.4
1	B	163	SER	5.3
1	A	34	GLY	5.1
1	B	188	GLY	5.0
1	B	162	VAL	4.9
1	B	247	VAL	4.7
1	B	193	ALA	4.7
1	B	165	VAL	4.5
1	B	154	ALA	4.4
1	B	211	LEU	4.4
1	B	214	PRO	4.2
1	B	187	ILE	4.2
1	B	141	LEU	4.0
1	B	138	PHE	4.0
1	B	185	ILE	4.0
1	B	189	SER	3.8
1	B	164	THR	3.7
1	B	167	VAL	3.7
1	B	132	PHE	3.6
1	B	209	ASP	3.5
1	B	208	TYR	3.5
1	B	199	ILE	3.4
1	B	131	LEU	3.4
1	B	139	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	40	ALA	3.4
1	B	203	MET	3.3
1	B	232	VAL	3.3
1	B	157	PHE	3.3
1	B	246	LYS	3.3
1	B	238	PRO	3.3
1	B	184	LEU	3.1
1	B	251	LEU	3.1
1	B	123	ALA	3.1
1	B	257	ILE	3.1
1	B	205	ASP	3.1
1	B	186	ALA	3.0
1	B	194	GLN	3.0
1	B	161	ALA	3.0
1	B	245	ALA	3.0
1	B	171	LEU	3.0
1	B	191	GLU	2.9
1	B	244	SER	2.9
1	B	259	VAL	2.9
1	B	166	PRO	2.9
1	B	114	ASN	2.9
1	B	160	TYR	2.9
1	B	156	THR	2.8
1	B	-1	GLY	2.8
1	B	140	GLY	2.8
1	B	178	SER	2.8
1	B	0	MET	2.8
1	B	242	PRO	2.8
1	B	190	SER	2.8
1	B	173	LEU	2.8
1	B	239	GLU	2.7
1	B	4	GLY	2.7
1	B	142	SER	2.7
1	B	197	LEU	2.7
1	B	258	PRO	2.7
1	B	-2	LEU	2.6
1	B	204	SER	2.6
1	B	7	ALA	2.6
1	B	145	THR	2.6
1	B	155	ASP	2.6
1	B	192	SER	2.6
1	B	230	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	116	VAL	2.5
1	B	196	ALA	2.5
1	B	219	ALA	2.5
1	B	210	LYS	2.5
1	B	183	ASN	2.5
1	B	237	THR	2.5
1	B	-3	PRO	2.5
1	B	137	PHE	2.5
1	B	93	GLY	2.5
1	B	215	ASP	2.4
1	B	234	LEU	2.4
1	B	212	THR	2.4
1	A	8	ALA	2.4
1	B	249	GLU	2.4
1	B	235	HIS	2.4
1	B	1	ALA	2.4
1	B	107	ALA	2.4
1	A	31	SER	2.4
1	B	241	TYR	2.3
1	B	53	LEU	2.3
1	B	228	ASN	2.3
1	B	252	LYS	2.3
1	B	200	MET	2.3
1	B	195	LYS	2.2
1	B	88	LEU	2.2
1	B	121	GLU	2.2
1	B	120	ASP	2.2
1	B	3	LEU	2.2
1	B	256	LEU	2.2
1	B	248	TYR	2.2
1	B	207	ARG	2.2
1	B	33	LYS	2.1
1	B	71	PRO	2.1
1	B	50	VAL	2.1
1	B	94	ALA	2.1
1	B	198	LYS	2.1
1	B	122	ASN	2.1
1	B	58	GLY	2.1
1	B	57	LEU	2.1
1	B	113	LEU	2.1
1	B	151	GLU	2.0
1	B	255	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	41	ARG	2.0
1	B	148	ARG	2.0
1	B	206	HIS	2.0
1	B	2	GLY	2.0
1	B	149	GLY	2.0
1	B	52	VAL	2.0
1	B	146	ASN	2.0
1	B	54	GLY	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(Å ²)	Q<0.9
2	D20	B	500	16/16	0.84	0.15	39,41,47,47	0
2	D20	A	500	16/16	0.93	0.10	28,32,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.