



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:02 AM GMT

PDB ID : 2VOA
Title : STRUCTURE OF AN AP ENDONUCLEASE FROM ARCHAEOGLOBUS FULGIDUS
Authors : Kuettner, E.B.; Schmiedel, R.; Greiner-Stoffele, T.; Strater, N.
Deposited on : 2008-02-11
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

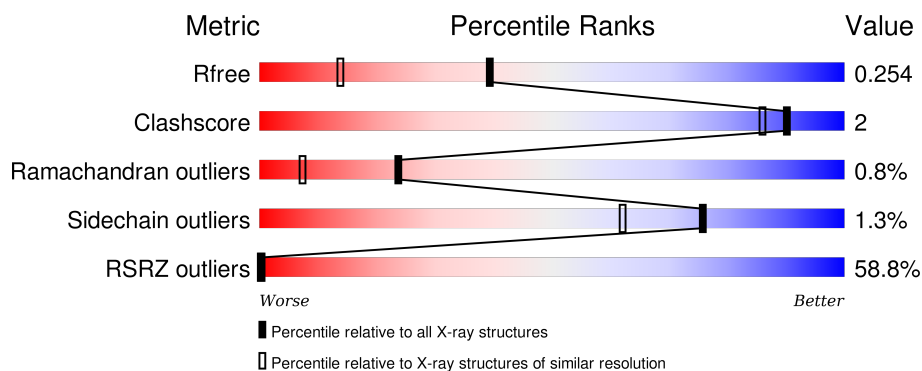
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	257	<div> <div>18%</div> <div> <div>93%</div> <div>7%</div> </div> </div>
1	B	257	<div> <div>100%</div> <div>92%</div> <div>8%</div> </div>
2	C	10	<div> <div>60%</div> <div>50%</div> <div>40%</div> <div>10%</div> </div>
3	D	10	<div> <div>60%</div> <div>60%</div> <div>30%</div> <div>10%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4849 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 EXODEOXYRIBONUCLEASE III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	3	0
			2115	1355	371	380	9			
1	B	257	Total	C	N	O	S	0	2	0
			2110	1352	368	380	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	VAL	ENGINEERED MUTATION	UNP O29675
B	217	GLY	VAL	ENGINEERED MUTATION	UNP O29675

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*GP*TP*AP*GP*CP*CP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			205	97	41	58	9			

- Molecule 3 is a DNA chain called 5'-D(*CP*GP*GP*CP*TP*AP*CP*CP*GP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	P	0	0	0
			199	95	37	58	9			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	65	Total	O	0	0
			65	65		
4	C	7	Total	O	0	0
			7	7		

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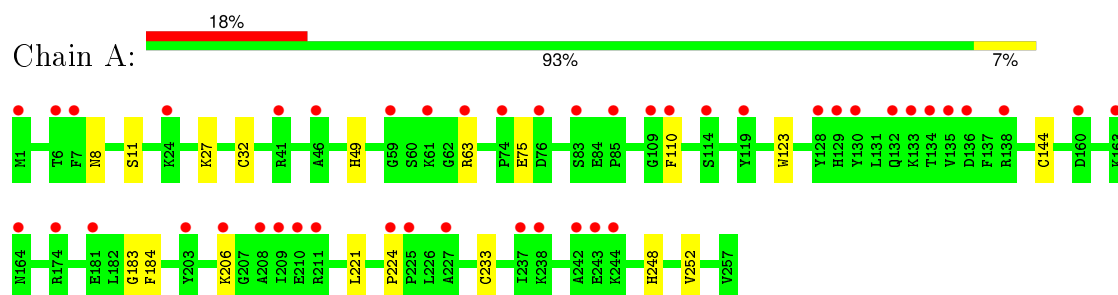
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	O	0	0
			3	3		

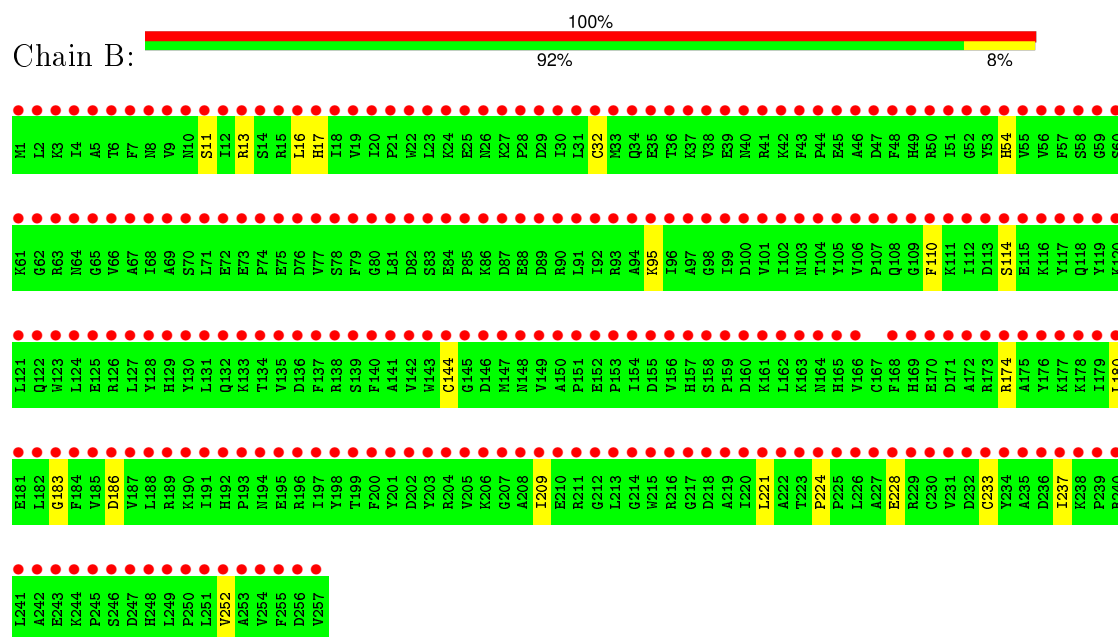
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

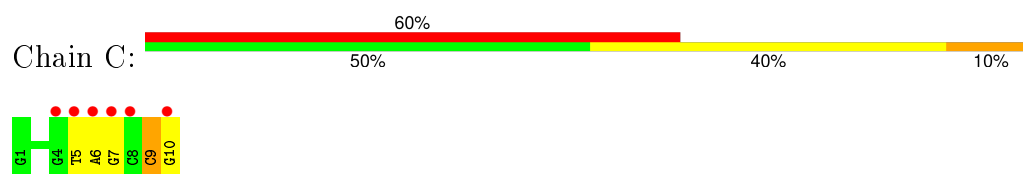
• Molecule 1: EXODEOXYRIBONUCLEASE III



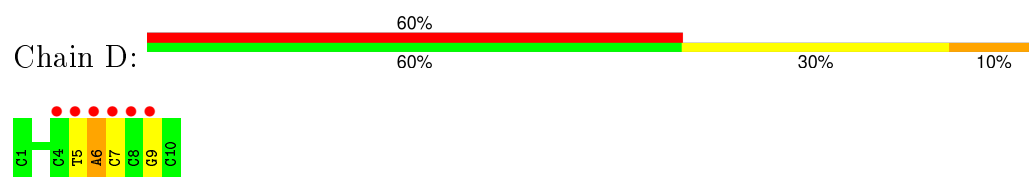
• Molecule 1: EXODEOXYRIBONUCLEASE III



• Molecule 2: 5'-D(*GP*CP*GP*GP*TP*AP*GP*CP*CP*GP)-3'



• Molecule 3: 5'-D(*CP*GP*GP*CP*TP*AP*CP*CP*GP*CP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.79Å 60.82Å 72.35Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	29.60 – 1.70 29.60 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.60-1.70) 100.0 (29.60-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.230 0.234 , 0.254	Depositor DCC
R_{free} test set	1316 reflections (2.03%)	DCC
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.3	EDS
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 64865 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4849	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OCS

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	0.63	0/2170	0.70	0/2934
1	B	0.55	1/2158 (0.0%)	0.66	1/2918 (0.0%)
2	C	0.97	0/230	1.69	4/354 (1.1%)
3	D	0.84	0/222	1.63	5/340 (1.5%)
All	All	0.63	1/4780 (0.0%)	0.84	10/6546 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	SER	C-O	6.22	1.35	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9	DC	O4'-C4'-C3'	-11.74	98.95	106.00
3	D	6	DA	P-O3'-C3'	9.73	131.37	119.70
2	C	9	DC	P-O3'-C3'	7.95	129.25	119.70
3	D	9	DG	O4'-C1'-N9	-7.84	102.51	108.00
3	D	7	DC	O4'-C1'-N1	7.01	112.91	108.00
3	D	6	DA	C4'-C3'-C2'	-6.84	96.95	103.10
1	B	13	ARG	NE-CZ-NH2	-6.44	117.08	120.30
3	D	6	DA	O4'-C1'-N9	5.93	112.15	108.00
2	C	9	DC	C4'-C3'-C2'	-5.46	98.19	103.10
2	C	5	DT	C4-C5-C7	5.24	122.14	119.00

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	2115	0	2108	8	0
1	B	2110	0	2098	9	0
2	C	205	0	113	3	0
3	D	199	0	113	1	0
4	A	145	0	0	2	0
4	B	65	0	0	2	0
4	C	7	0	0	0	0
4	D	3	0	0	0	0
All	All	4849	0	4432	21	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 2.

All (21) 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)
2:C:9:DC:H2'	2:C:10:DG:C8	2.26	0.70
1:A:49:HIS:HE1	4:A:2037:HOH:O	1.82	0.61
1:B:32[A]:CYS:SG	1:B:144[A]:CYS:SG	3.02	0.58
1:B:209:ILE:HG21	1:B:237:ILE:HD11	1.84	0.58
1:A:183:GLY:O	1:A:224:PRO:HD3	2.07	0.55
1:A:184:PHE:HB3	1:A:221:LEU:HB3	1.91	0.53
1:B:17:HIS:HD2	4:B:2003:HOH:O	1.92	0.52
1:B:186:ASP:HA	1:B:221:LEU:HD23	1.91	0.51
2:C:9:DC:H2''	2:C:10:DG:O5'	2.12	0.49
3:D:5:DT:H2''	3:D:6:DA:H5''	1.95	0.49
1:B:183:GLY:O	1:B:224:PRO:HD3	2.13	0.48
1:B:233:CYS:HA	1:B:252:VAL:O	2.14	0.48
2:C:6:DA:H2'	2:C:7:DG:C8	2.49	0.47
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.67	0.46
1:A:32:CYS:SG	1:A:144[B]:CYS:SG	3.12	0.46
1:B:54:HIS:HD2	4:B:2005:HOH:O	1.98	0.45
1:A:27:LYS:HE3	4:A:2013:HOH:O	2.17	0.44
1:A:233:CYS:HA	1:A:252:VAL:O	2.18	0.44
1:B:224:PRO:O	1:B:228:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:CD2	1:B:221:LEU:HD22	2.50	0.41
1:A:8:ASN:HB3	1:A:248:HIS:CG	2.56	0.41

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	257/257 (100%)	253 (98%)	2 (1%)	2 (1%)	24	7
1	B	256/257 (100%)	252 (98%)	2 (1%)	2 (1%)	24	7
All	All	513/514 (100%)	505 (98%)	4 (1%)	4 (1%)	24	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	SER
1	A	11	SER
1	A	110	PHE
1	B	110	PHE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/226 (101%)	226 (99%)	3 (1%)	76	62
1	B	228/226 (101%)	225 (99%)	3 (1%)	76	62
All	All	457/452 (101%)	451 (99%)	6 (1%)	76	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	75	GLU
1	A	123	TRP
1	B	16	LEU
1	B	95	LYS
1	B	174	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	122	GLN
1	B	17	HIS
1	B	49	HIS
1	B	54	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	OCS	A	167	1	7,8,9	1.25	1 (14%)	7,11,13	1.39	1 (14%)
1	OCS	B	167	1	7,8,9	1.21	1 (14%)	7,11,13	2.19	3 (42%)

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
1	OCS	A	167	1	-	0/4/7/9	0/0/0/0
1	OCS	B	167	1	-	0/4/7/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	OCS	CB-SG	2.48	1.81	1.77
1	B	167	OCS	CB-SG	2.53	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	OCS	O-C-CA	-2.14	119.92	125.49
1	B	167	OCS	OD3-SG-CB	2.36	108.93	106.94
1	A	167	OCS	OD1-SG-CB	2.55	109.09	106.94
1	B	167	OCS	OD1-SG-CB	4.38	110.63	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	256/257 (99%)	1.15	45 (17%) 2 2	26, 30, 36, 41	0
1	B	256/257 (99%)	11.30	256 (100%) 0 0	25, 31, 37, 41	0
2	C	10/10 (100%)	2.49	6 (60%) 0 0	29, 31, 33, 35	0
3	D	10/10 (100%)	2.40	6 (60%) 0 0	27, 32, 37, 42	0
All	All	532/534 (99%)	6.08	313 (58%) 0 0	25, 30, 37, 42	0

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144[A]	CYS	37.2
1	B	7	PHE	35.1
1	B	105	TYR	33.7
1	B	220	ILE	33.4
1	B	219	ALA	33.3
1	B	200	PHE	31.6
1	B	32[A]	CYS	31.5
1	B	143	TRP	30.6
1	B	251	LEU	30.4
1	B	9	VAL	28.4
1	B	102	ILE	27.7
1	B	199	THR	27.4
1	B	149	VAL	27.4
1	B	145	GLY	27.2
1	B	6	THR	26.4
1	B	235	ALA	26.4
1	B	33	MET	24.0
1	B	147	MET	23.8
1	B	104	THR	23.0
1	B	218	ASP	22.8
1	B	248	HIS	22.7

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Mol	Chain	Res	Type	RSRZ
1	B	4	ILE	22.5
1	B	92	ILE	22.5
1	B	221	LEU	22.3
1	B	34	GLN	22.3
1	B	31	LEU	22.3
1	B	106	VAL	21.9
1	B	176	TYR	21.3
1	B	101	VAL	21.3
1	B	201	TYR	20.6
1	B	146	ASP	20.0
1	B	250	PRO	19.9
1	B	142	VAL	19.8
1	B	249	LEU	19.2
1	B	5	ALA	18.9
1	B	66	VAL	18.8
1	B	215	TRP	18.8
1	B	103	ASN	18.8
1	B	216	ARG	18.6
1	B	8	ASN	18.4
1	B	237	ILE	18.3
1	B	30	ILE	17.9
1	B	217	GLY	17.8
1	B	198	TYR	17.8
1	B	246	SER	17.7
1	B	36	THR	17.6
1	B	197	ILE	17.5
1	B	188	LEU	17.5
1	B	68	ILE	17.4
1	B	22	TRP	17.1
1	B	91	LEU	16.4
1	B	234	TYR	16.4
1	B	96	ILE	16.3
1	B	141	ALA	16.0
1	B	241	LEU	15.5
1	B	123	TRP	15.3
1	B	90	ARG	15.2
1	B	65	GLY	15.1
1	B	252	VAL	15.0
1	B	35	GLU	14.7
1	B	148	ASN	14.7
1	B	150	ALA	14.1
1	B	213	LEU	14.0

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Mol	Chain	Res	Type	RSRZ
1	B	247	ASP	13.9
1	B	89	ASP	13.9
1	B	184	PHE	13.8
1	B	140	PHE	13.8
1	B	63	ARG	13.6
1	B	64	ASN	13.6
1	B	203	TYR	13.5
1	B	222	ALA	13.3
1	B	60	SER	13.1
1	B	12	ILE	13.1
1	B	10	ASN	13.0
1	B	127	LEU	12.9
1	B	97	ALA	12.7
1	B	180	LEU	12.7
1	B	253	ALA	12.6
1	B	67	ALA	12.5
1	B	59	GLY	12.4
1	B	185	VAL	12.4
1	B	56	VAL	12.1
1	B	151	PRO	12.1
1	B	107	PRO	12.0
1	B	55	VAL	12.0
1	B	214	GLY	12.0
1	B	98	GLY	11.9
1	B	81	LEU	11.8
1	B	233	CYS	11.8
1	B	57	PHE	11.7
1	B	53	TYR	11.6
1	B	79	PHE	11.6
1	B	131	LEU	11.5
1	B	18	ILE	11.3
1	B	255	PHE	11.3
1	B	138	ARG	11.1
1	B	179	ILE	10.9
1	B	71	LEU	10.9
1	B	48	PHE	10.7
1	B	205	VAL	10.7
1	B	130	TYR	10.7
1	B	69	ALA	10.7
1	B	108	GLN	10.7
1	B	124	LEU	10.6
1	B	165	HIS	10.4

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Mol	Chain	Res	Type	RSRZ
1	B	239	PRO	10.3
1	B	202	ASP	10.3
1	B	230	CYS	10.3
1	B	156	VAL	10.3
1	B	110	PHE	10.3
1	B	62	GLY	10.2
1	B	166	VAL	10.2
1	B	77	VAL	10.1
1	B	242	ALA	10.0
1	B	58	SER	9.9
1	B	1	MET	9.9
1	B	209	ILE	9.9
1	B	157	HIS	9.6
1	B	23	LEU	9.6
1	B	43	PHE	9.5
1	B	139	SER	9.4
1	B	162	LEU	9.4
1	B	257	VAL	9.3
1	B	254	VAL	9.3
1	B	19	VAL	9.2
1	B	186	ASP	9.2
1	B	161	LYS	9.2
1	B	236	ASP	9.1
1	B	11	SER	9.0
1	B	174	ARG	8.8
1	B	37	LYS	8.8
1	B	52	GLY	8.7
1	B	134	THR	8.6
1	B	119	TYR	8.5
1	B	128	TYR	8.5
1	B	93	ARG	8.4
1	B	160	ASP	8.4
1	B	154	ILE	8.4
1	B	118	GLN	8.3
1	B	74	PRO	8.3
1	B	226	LEU	8.2
1	B	61	LYS	8.2
1	B	70	SER	8.1
1	B	40	ASN	8.1
1	B	28	PRO	8.1
1	B	117	TYR	8.0
1	B	29	ASP	7.9

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Mol	Chain	Res	Type	RSRZ
1	B	245	PRO	7.8
1	B	87	ASP	7.8
1	B	182	LEU	7.7
1	B	38	VAL	7.7
1	B	112	ILE	7.7
1	B	208	ALA	7.7
1	B	187	VAL	7.7
1	B	54	HIS	7.7
1	B	175	ALA	7.7
1	B	155	ASP	7.6
1	B	2	LEU	7.6
1	B	204	ARG	7.6
1	B	16	LEU	7.5
1	B	88	GLU	7.5
1	B	3	LYS	7.5
1	B	240	ARG	7.4
1	B	80	GLY	7.4
1	B	99	ILE	7.4
1	B	121	LEU	7.4
1	B	206	LYS	7.4
1	B	244	LYS	7.3
1	B	196	ARG	7.2
1	B	231	VAL	7.2
1	B	15	ARG	7.2
1	B	135	VAL	7.2
1	B	190	LYS	7.1
1	B	194	ASN	7.1
1	B	129	HIS	7.0
1	B	85	PRO	7.0
1	B	137	PHE	6.9
1	B	238	LYS	6.9
1	B	94	ALA	6.9
1	B	183	GLY	6.9
1	B	20	ILE	6.8
1	B	95	LYS	6.7
1	B	223	THR	6.7
1	B	228	GLU	6.6
1	B	100	ASP	6.6
1	B	212	GLY	6.5
1	B	211	ARG	6.5
1	B	115	GLU	6.5
1	B	207	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	181	GLU	6.5
1	B	153	PRO	6.4
1	B	26	ASN	6.4
1	B	41	ARG	6.4
1	B	168	PHE	6.4
1	B	72	GLU	6.4
1	B	14	SER	6.1
1	B	193	PRO	6.1
1	B	114	SER	6.1
1	B	191	ILE	6.0
1	B	21	PRO	6.0
1	B	136	ASP	6.0
1	B	189	ARG	6.0
1	B	82	ASP	5.9
1	B	163	LYS	5.8
1	B	195	GLU	5.8
1	B	232	ASP	5.8
1	B	76	ASP	5.7
1	B	164	ASN	5.6
1	B	113	ASP	5.6
1	B	125	GLU	5.6
1	B	172	ALA	5.5
1	B	51	ILE	5.5
1	B	78	SER	5.5
1	B	225	PRO	5.4
1	B	46	ALA	5.3
1	B	17	HIS	5.3
1	B	177	LYS	5.2
1	B	116	LYS	5.2
1	B	192	HIS	5.1
1	B	126	ARG	5.1
1	B	152	GLU	5.1
1	B	210	GLU	5.0
1	A	242	ALA	5.0
1	B	50	ARG	5.0
1	B	132	GLN	5.0
1	B	224	PRO	4.9
2	C	8	DC	4.9
1	B	13	ARG	4.8
1	B	47	ASP	4.8
1	B	111	LYS	4.8
1	B	120	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	119	TYR	4.7
1	B	178	LYS	4.7
1	B	45	GLU	4.7
1	B	83	SER	4.6
1	A	210	GLU	4.5
1	A	59	GLY	4.4
1	B	44	PRO	4.3
1	B	173	ARG	4.3
1	B	84	GLU	4.3
1	B	159	PRO	4.2
1	B	229	ARG	4.1
1	B	75	GLU	4.1
2	C	7	DG	4.0
3	D	6	DA	4.0
1	B	86	LYS	4.0
1	B	122	GLN	3.9
1	B	133	LYS	3.9
1	B	25	GLU	3.9
1	B	24	LYS	3.8
1	B	227	ALA	3.8
1	B	170	GLU	3.8
1	B	27	LYS	3.7
1	B	171	ASP	3.7
3	D	5	DT	3.7
1	B	109	GLY	3.7
1	B	158	SER	3.7
1	B	42	LYS	3.7
1	B	49	HIS	3.7
1	A	135	VAL	3.6
1	B	73	GLU	3.5
1	A	211	ARG	3.4
1	B	243	GLU	3.4
1	B	39	GLU	3.4
1	A	61	LYS	3.4
3	D	7	DC	3.2
1	A	83	SER	3.1
1	A	243	GLU	3.1
1	A	138	ARG	3.0
1	A	133	LYS	3.0
1	A	129	HIS	3.0
3	D	8	DC	3.0
1	A	203	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	169	HIS	2.9
1	A	238	LYS	2.9
1	A	134	THR	2.9
2	C	10	DG	2.8
1	A	85	PRO	2.8
1	A	208	ALA	2.8
1	B	256	ASP	2.8
1	A	6	THR	2.8
1	A	164	ASN	2.7
1	A	130	TYR	2.7
2	C	6	DA	2.7
1	A	244	LYS	2.7
1	A	209	ILE	2.7
1	A	74	PRO	2.7
1	A	237	ILE	2.6
1	A	46	ALA	2.6
1	A	174	ARG	2.6
1	A	41	ARG	2.6
1	A	63	ARG	2.5
1	A	160	ASP	2.5
3	D	9	DG	2.4
1	A	136	ASP	2.4
1	A	24	LYS	2.4
3	D	4	DC	2.4
1	A	114	SER	2.3
1	A	7	PHE	2.3
1	A	163	LYS	2.3
1	A	206	LYS	2.3
1	A	110	PHE	2.3
1	A	181	GLU	2.3
1	A	128	TYR	2.3
1	A	109	GLY	2.3
1	A	227	ALA	2.2
1	A	132	GLN	2.2
1	A	224	PRO	2.2
2	C	5	DT	2.2
1	A	225	PRO	2.1
1	A	76	ASP	2.1
2	C	4	DG	2.1
1	A	1	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	OCS	B	167	9/10	0.34	0.66	-	34,35,40,40	0
1	OCS	A	167	9/10	0.94	0.15	-	30,32,37,37	0

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.