



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:22 pm 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

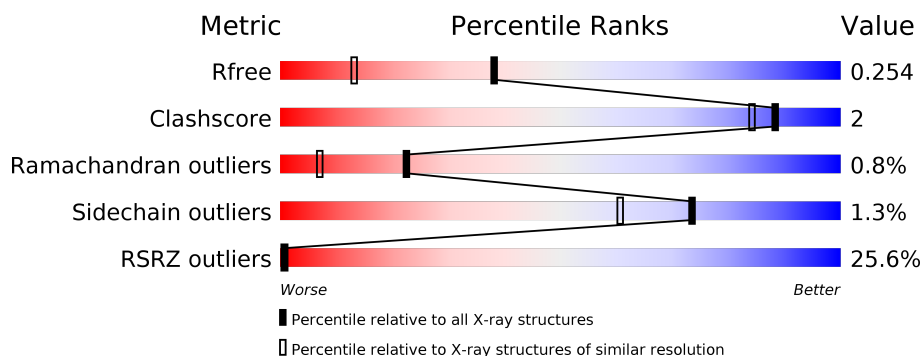
1 Overall quality at a glance

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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (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>25%</div> <div>93%</div> <div>7%</div> </div>
1	B	257	<div> <div>26%</div> <div>92%</div> <div>8%</div> </div>
2	C	10	<div> <div>20%</div> <div>50%</div> <div>40%</div> <div>10%</div> </div>
3	D	10	<div> <div>40%</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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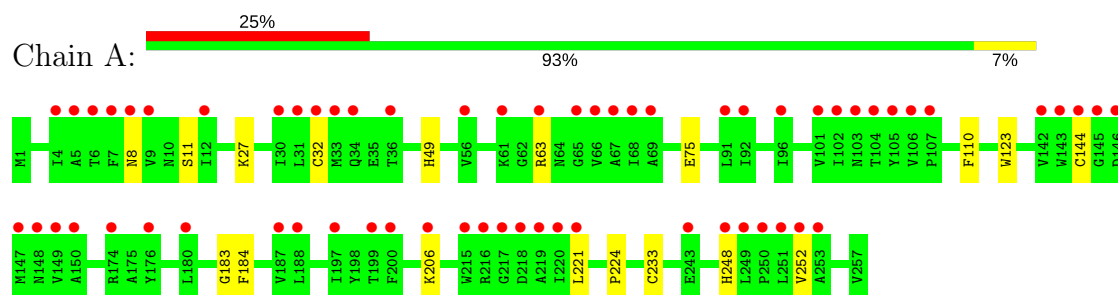
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	O	0	0
			3	3		

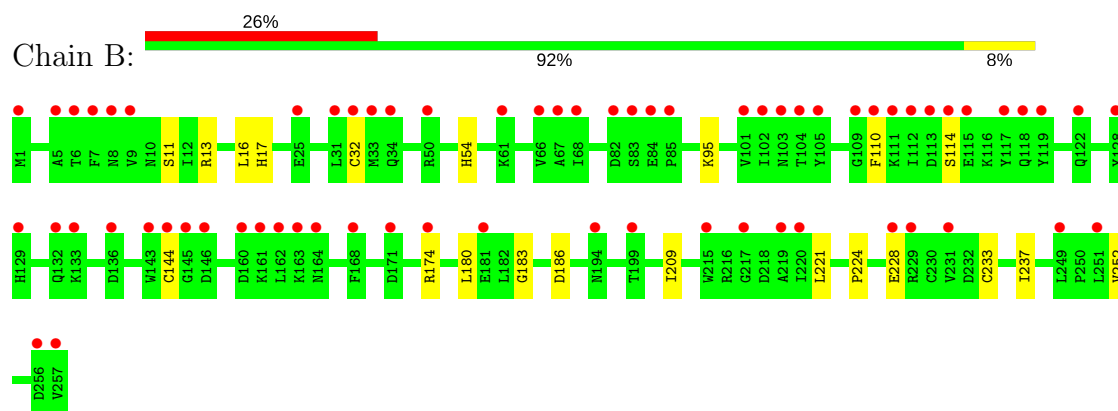
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

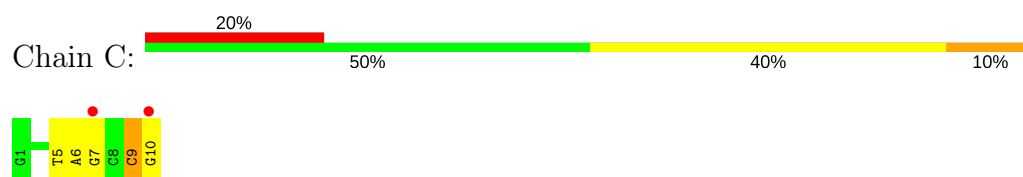
• Molecule 1: EXODEOXYRIBONUCLEASE III



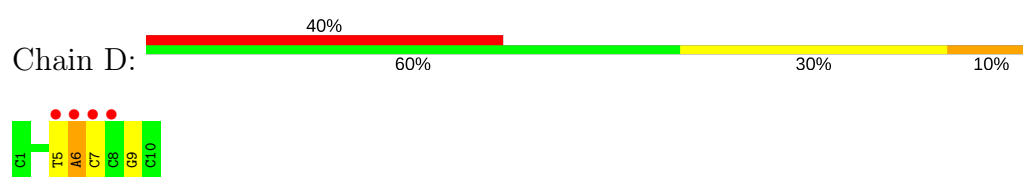
• Molecule 1: EXODEOXYRIBONUCLEASE III



• 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)	0.38 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	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, 0.333 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: 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%)	22	7
1	B	256/257 (100%)	252 (98%)	2 (1%)	2 (1%)	22	7
All	All	513/514 (100%)	505 (98%)	4 (1%)	4 (1%)	22	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%)	73	60
1	B	228/226 (101%)	225 (99%)	3 (1%)	73	60
All	All	457/452 (101%)	451 (99%)	6 (1%)	73	60

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	8,8,9	1.13	1 (12%)	7,11,13	1.99	2 (28%)
1	OCS	B	167	1	8,8,9	1.14	1 (12%)	7,11,13	2.39	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	CA-C	2.02	1.52	1.50
1	B	167	OCS	CA-C	2.33	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	OCS	OD3-SG-CB	2.46	108.93	106.83
1	A	167	OCS	OD1-SG-CB	2.65	109.09	106.83
1	B	167	OCS	OD2-SG-CB	2.66	109.26	106.01
1	A	167	OCS	OD2-SG-CB	3.91	110.78	106.01
1	B	167	OCS	OD1-SG-CB	4.45	110.63	106.83

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%)	1.32	63 (24%) 1 1	26, 30, 36, 41	0
1	B	256/257 (99%)	1.18	67 (26%) 1 0	25, 31, 37, 41	0
2	C	10/10 (100%)	1.14	2 (20%) 1 1	29, 31, 33, 35	0
3	D	10/10 (100%)	1.38	4 (40%) 0 0	27, 32, 37, 42	0
All	All	532/534 (99%)	1.25	136 (25%) 1 1	25, 30, 37, 42	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	PHE	7.7
1	A	144[A]	CYS	6.5
1	A	32	CYS	6.4
1	A	219	ALA	6.3
1	A	7	PHE	6.1
1	B	257	VAL	6.1
1	A	6	THR	6.1
1	B	112	ILE	6.0
1	A	220	ILE	6.0
1	B	113	ASP	5.7
1	A	217	GLY	5.6
1	A	68	ILE	5.6
1	A	147	MET	5.4
1	B	160	ASP	5.3
1	A	251	LEU	5.3
1	A	145	GLY	5.2
1	A	31	LEU	5.1
1	B	1	MET	5.0
1	A	105	TYR	5.0
1	A	143	TRP	5.0
1	A	104	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	119	TYR	4.9
1	A	106	VAL	4.8
1	A	5	ALA	4.8
1	B	7	PHE	4.8
1	B	115	GLU	4.8
1	B	32[A]	CYS	4.7
1	A	9	VAL	4.6
1	A	66	VAL	4.6
2	C	7	DG	4.3
1	A	142[A]	VAL	4.3
1	A	249	LEU	4.2
1	A	67	ALA	4.2
1	B	144[A]	CYS	4.2
1	A	221	LEU	4.2
1	A	8	ASN	4.1
1	A	149	VAL	4.0
1	A	199	THR	4.0
1	B	114	SER	4.0
1	A	218	ASP	4.0
1	A	4	ILE	3.9
1	A	30	ILE	3.9
1	A	102	ILE	3.9
1	B	174	ARG	3.9
1	B	6	THR	3.9
1	A	33	MET	3.8
1	A	146	ASP	3.8
1	A	36	THR	3.8
1	A	101	VAL	3.7
1	B	164	ASN	3.6
1	B	145	GLY	3.6
1	B	163	LYS	3.5
1	A	92	ILE	3.5
1	B	5	ALA	3.5
1	A	34	GLN	3.5
1	A	176	TYR	3.4
1	B	194	ASN	3.3
1	A	250	PRO	3.3
1	B	256	ASP	3.3
1	A	91	LEU	3.2
1	B	122	GLN	3.2
1	B	118	GLN	3.2
3	D	6	DA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	128	TYR	3.2
1	A	103	ASN	3.2
1	A	148	ASN	3.1
1	B	181	GLU	3.1
3	D	5	DT	3.1
1	B	219	ALA	3.1
1	B	129	HIS	3.0
1	B	105	TYR	3.0
1	B	82	ASP	3.0
1	B	8	ASN	3.0
1	A	12	ILE	3.0
1	B	251	LEU	2.9
1	A	216	ARG	2.9
1	B	104	THR	2.9
1	B	67	ALA	2.9
1	B	228	GLU	2.9
1	B	146	ASP	2.8
1	B	162	LEU	2.8
1	A	248	HIS	2.8
1	B	168	PHE	2.8
1	A	150	ALA	2.7
1	A	200	PHE	2.7
1	B	132	GLN	2.7
1	B	66	VAL	2.7
1	B	229	ARG	2.7
1	A	206	LYS	2.6
1	A	180	LEU	2.6
1	A	188	LEU	2.6
1	A	215	TRP	2.6
1	A	253	ALA	2.6
2	C	10	DG	2.6
1	B	68	ILE	2.6
1	B	31	LEU	2.6
1	B	50	ARG	2.5
1	A	65	GLY	2.5
1	B	215	TRP	2.5
1	B	217	GLY	2.5
1	B	84	GLU	2.5
1	B	117	TYR	2.5
1	A	243	GLU	2.5
1	A	197	ILE	2.4
1	B	171	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	61	LYS	2.4
1	B	25	GLU	2.4
1	B	143	TRP	2.4
1	A	107	PRO	2.4
1	B	9	VAL	2.4
1	B	161	LYS	2.4
1	B	85	PRO	2.4
1	A	252	VAL	2.3
1	B	111	LYS	2.3
1	B	101	VAL	2.3
3	D	7	DC	2.3
1	B	109	GLY	2.3
1	B	133	LYS	2.3
1	B	199	THR	2.3
1	B	83	SER	2.2
1	B	34	GLN	2.2
1	B	249	LEU	2.2
1	B	33	MET	2.2
1	B	103	ASN	2.2
1	A	63	ARG	2.2
1	B	102	ILE	2.2
1	A	69	ALA	2.2
1	A	61	LYS	2.1
1	A	96	ILE	2.1
1	B	220	ILE	2.1
1	A	56	VAL	2.1
1	A	187	VAL	2.1
1	B	231	VAL	2.1
1	A	174	ARG	2.0
3	D	8	DC	2.0
1	B	136	ASP	2.0

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

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(\AA^2)	Q<0.9
1	OCS	B	167	9/10	0.95	0.10	-	34,35,40,40	0
1	OCS	A	167	9/10	0.96	0.14	-	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.