



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N7X
Title : Crystal structure of Penaeus stylirostris densovirus capsid
Authors : Kaufmann, B.; Rossmann, M.G.
Deposited on : 2010-05-27
Resolution : 2.50 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

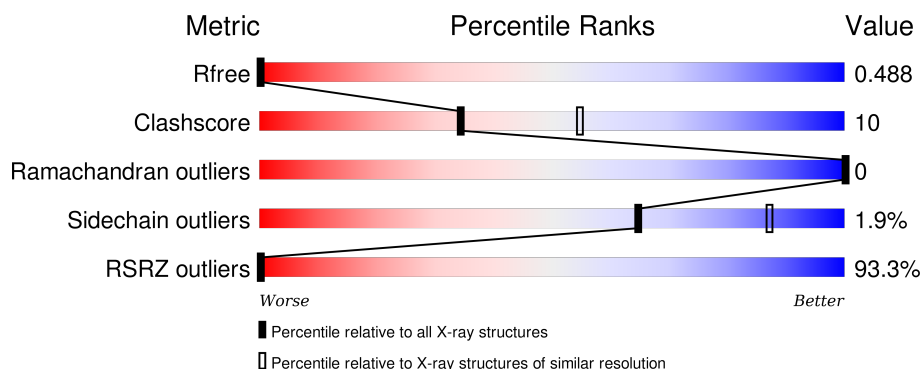
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	329	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	331	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	332	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2558 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2396	1526	410	441	19			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

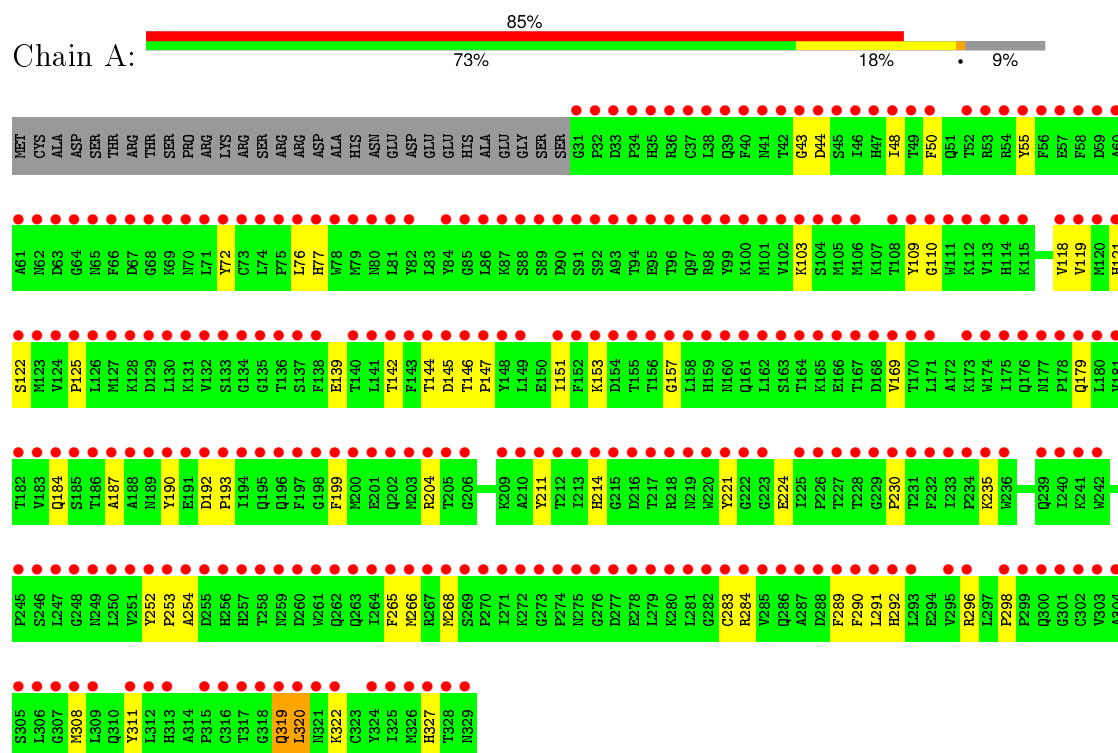
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		

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 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 ($\text{RSRZ} > 2$). 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: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	235.89Å 245.47Å 268.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.98 – 2.51	Depositor EDS
% Data completeness (in resolution range)	63.4 (50.00-2.50) 64.0 (49.98-2.51)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.285 0.488 , 0.488	Depositor DCC
R_{free} test set	16819 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.4	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 337569 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.29	EDS
Total number of atoms	2558	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.36	0/2465	0.66	0/3342

There are no bond length outliers.

There are no bond angle outliers.

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	2396	0	2320	47	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	159	0	0	3	0
All	All	2558	0	2320	47	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 10.

All (47) 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:268:MET:HE2	1:A:268:MET:HA	1.58	0.84
1:A:125:PRO:HB2	1:A:142:THR:HG21	1.63	0.81
1:A:230:PRO:HD3	1:A:320:LEU:HD13	1.61	0.80
1:A:252:TYR:CZ	1:A:254:ALA:HB2	2.33	0.64
1:A:77:HIS:H	1:A:77:HIS:CD2	2.16	0.63
1:A:125:PRO:HB2	1:A:142:THR:CG2	2.30	0.62
1:A:252:TYR:CE2	1:A:254:ALA:HB2	2.35	0.62
1:A:153:LYS:HB2	1:A:199:PHE:HB3	1.82	0.61
1:A:284:ARG:HD2	4:A:355:HOH:O	2.01	0.60
1:A:109:TYR:CE2	1:A:298:PRO:HB3	2.37	0.59
1:A:76:LEU:HD22	1:A:118:VAL:HG23	1.85	0.59
1:A:142:THR:HG23	1:A:144:THR:O	2.05	0.56
1:A:55:TYR:CE1	1:A:284:ARG:NH2	2.74	0.56
1:A:43:GLY:HA2	1:A:296:ARG:NE	2.22	0.55
1:A:118:VAL:HG22	1:A:289:PHE:CD1	2.42	0.54
1:A:145:ASP:HB2	4:A:360:HOH:O	2.08	0.53
1:A:157:GLY:HA2	1:A:327:HIS:CE1	2.43	0.53
1:A:121:HIS:HD2	1:A:122:SER:OG	1.91	0.52
1:A:110:GLY:HA2	1:A:221:TYR:O	2.09	0.51
1:A:118:VAL:HG12	1:A:119:VAL:N	2.26	0.51
1:A:77:HIS:H	1:A:77:HIS:HD2	1.59	0.50
1:A:43:GLY:HA2	1:A:296:ARG:CZ	2.42	0.50
1:A:319:GLN:HE21	1:A:322:LYS:HG3	1.75	0.49
1:A:151:ILE:HG12	1:A:266:MET:HG2	1.95	0.48
1:A:44:ASP:OD1	1:A:44:ASP:N	2.47	0.47
1:A:319:GLN:NE2	1:A:322:LYS:HG3	2.30	0.46
1:A:268:MET:HE1	1:A:283:CYS:SG	2.56	0.46
1:A:76:LEU:HD22	1:A:118:VAL:CG2	2.44	0.45
1:A:50:PHE:O	1:A:290:PHE:HA	2.17	0.45
1:A:268:MET:CE	1:A:283:CYS:SG	3.05	0.45
1:A:72:TYR:O	1:A:265:PHE:HA	2.17	0.43
1:A:268:MET:HE2	1:A:268:MET:CA	2.37	0.43
1:A:184:GLN:HB3	1:A:187:ALA:HB2	1.99	0.43
1:A:291:LEU:HD23	1:A:291:LEU:C	2.39	0.43
1:A:103:LYS:HE2	1:A:224:GLU:OE2	2.19	0.42
1:A:292:HIS:HB3	4:A:416:HOH:O	2.17	0.42
1:A:146:THR:N	1:A:147:PRO:CD	2.82	0.42
1:A:192:ASP:HB3	1:A:193:PRO:HD3	2.01	0.41
1:A:230:PRO:HD3	1:A:320:LEU:CD1	2.43	0.41
1:A:214:HIS:O	1:A:235:LYS:HE2	2.20	0.41
1:A:252:TYR:HB2	1:A:253:PRO:HD2	2.02	0.41
1:A:308:MET:HA	1:A:311:TYR:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:N	1:A:48:ILE:HD12	2.36	0.41
1:A:76:LEU:HD11	1:A:211:TYR:HB2	2.03	0.41
1:A:169:VAL:HG21	1:A:179:GLN:HG3	2.02	0.41
1:A:319:GLN:HE21	1:A:319:GLN:HB2	1.74	0.41
1:A:319:GLN:HE21	1:A:322:LYS:CG	2.34	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	297/329 (90%)	288 (97%)	9 (3%)	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	262/288 (91%)	257 (98%)	5 (2%)	65	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	GLU

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Mol	Chain	Res	Type
1	A	190	TYR
1	A	204	ARG
1	A	319	GLN
1	A	320	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	77	HIS
1	A	121	HIS
1	A	160	ASN
1	A	249	ASN
1	A	262	GLN
1	A	319	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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

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	299/329 (90%)	4.35	279 (93%) 0 0	16, 23, 41, 63	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	GLY	13.2
1	A	135	GLY	11.6
1	A	295	VAL	10.9
1	A	299	PRO	9.8
1	A	31	GLY	9.5
1	A	155	THR	9.2
1	A	101	MET	8.6
1	A	261	TRP	8.5
1	A	325	ILE	8.5
1	A	168	ASP	8.0
1	A	252	TYR	7.9
1	A	276	GLY	7.6
1	A	183	VAL	7.6
1	A	136	THR	7.5
1	A	227	THR	7.2
1	A	99	TYR	7.2
1	A	64	GLY	7.2
1	A	48	ILE	7.2
1	A	248	GLY	7.1
1	A	160	ASN	7.1
1	A	320	LEU	7.1
1	A	220	TRP	7.1
1	A	169	VAL	7.1
1	A	190	TYR	7.0
1	A	133	SER	7.0
1	A	68	GLY	6.9
1	A	78	TRP	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	259	ASN	6.8
1	A	199	PHE	6.8
1	A	137	SER	6.8
1	A	175	ILE	6.7
1	A	319	GLN	6.7
1	A	328	THR	6.6
1	A	43	GLY	6.5
1	A	329	ASN	6.5
1	A	309	LEU	6.5
1	A	260	ASP	6.4
1	A	194	ILE	6.4
1	A	86	LEU	6.4
1	A	178	PRO	6.4
1	A	146	THR	6.4
1	A	74	LEU	6.4
1	A	129	ASP	6.3
1	A	122	SER	6.3
1	A	66	PHE	6.2
1	A	324	TYR	6.2
1	A	283	CYS	6.2
1	A	142	THR	6.2
1	A	140	THR	6.1
1	A	258	THR	6.1
1	A	127	MET	6.1
1	A	205	THR	6.1
1	A	315	PRO	6.1
1	A	195	GLN	6.1
1	A	312	LEU	6.1
1	A	34	PRO	6.0
1	A	213	ILE	6.0
1	A	62	ASN	5.9
1	A	198	GLY	5.9
1	A	193	PRO	5.9
1	A	254	ALA	5.9
1	A	151	ILE	5.8
1	A	145	ASP	5.8
1	A	317	THR	5.8
1	A	326	MET	5.7
1	A	156	THR	5.7
1	A	212	THR	5.7
1	A	40	PHE	5.7
1	A	278	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	73	CYS	5.6
1	A	289	PHE	5.6
1	A	192	ASP	5.6
1	A	96	THR	5.6
1	A	174	TRP	5.5
1	A	58	PHE	5.5
1	A	277	ASP	5.5
1	A	81	LEU	5.5
1	A	149	LEU	5.5
1	A	282	GLY	5.5
1	A	242	TRP	5.5
1	A	164	THR	5.4
1	A	246	SER	5.4
1	A	298	PRO	5.4
1	A	52	THR	5.4
1	A	56	PHE	5.4
1	A	37	CYS	5.4
1	A	253	PRO	5.3
1	A	204	ARG	5.3
1	A	102	VAL	5.3
1	A	103	LYS	5.3
1	A	171	LEU	5.2
1	A	35	HIS	5.2
1	A	302	CYS	5.2
1	A	251	VAL	5.2
1	A	161	GLN	5.2
1	A	157	GLY	5.1
1	A	303	VAL	5.1
1	A	265	PHE	5.1
1	A	304	ALA	5.0
1	A	36	ARG	5.0
1	A	100	LYS	5.0
1	A	185	SER	5.0
1	A	288	ASP	5.0
1	A	170	THR	4.9
1	A	125	PRO	4.9
1	A	166	GLU	4.9
1	A	113	VAL	4.8
1	A	85	GLY	4.8
1	A	228	THR	4.8
1	A	264	ILE	4.8
1	A	44	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	187	ALA	4.8
1	A	211	TYR	4.8
1	A	97	GLN	4.7
1	A	89	SER	4.7
1	A	41	ASN	4.7
1	A	206	GLY	4.7
1	A	218	ARG	4.6
1	A	131	LYS	4.6
1	A	84	TYR	4.6
1	A	119	VAL	4.6
1	A	221	TYR	4.6
1	A	177	ASN	4.6
1	A	262	GLN	4.6
1	A	305	SER	4.6
1	A	72	TYR	4.5
1	A	130	LEU	4.5
1	A	291	LEU	4.5
1	A	50	PHE	4.4
1	A	138	PHE	4.4
1	A	274	PRO	4.4
1	A	281	LEU	4.4
1	A	152	PHE	4.3
1	A	200	MET	4.3
1	A	233	ILE	4.3
1	A	313	HIS	4.3
1	A	327	HIS	4.2
1	A	197	PHE	4.2
1	A	318	GLY	4.2
1	A	273	GLY	4.2
1	A	148	TYR	4.2
1	A	203	MET	4.2
1	A	132	VAL	4.2
1	A	95	GLU	4.2
1	A	275	ASN	4.1
1	A	59	ASP	4.1
1	A	112	LYS	4.1
1	A	202	GLN	4.1
1	A	184	GLN	4.1
1	A	189	ASN	4.1
1	A	90	ASP	4.0
1	A	292	HIS	4.0
1	A	215	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	80	ASN	4.0
1	A	322	LYS	4.0
1	A	159	HIS	4.0
1	A	105	MET	4.0
1	A	300	GLN	3.9
1	A	186	THR	3.9
1	A	108	THR	3.9
1	A	153	LYS	3.8
1	A	67	ASP	3.8
1	A	98	ARG	3.8
1	A	286	GLN	3.8
1	A	82	TYR	3.8
1	A	55	TYR	3.7
1	A	225	ILE	3.7
1	A	162	LEU	3.7
1	A	210	ALA	3.7
1	A	46	ILE	3.7
1	A	255	ASP	3.7
1	A	32	PRO	3.7
1	A	231	THR	3.7
1	A	307	GLY	3.6
1	A	38	LEU	3.6
1	A	91	SER	3.6
1	A	63	ASP	3.6
1	A	223	GLY	3.6
1	A	158	LEU	3.6
1	A	217	THR	3.6
1	A	268	MET	3.6
1	A	93	ALA	3.5
1	A	57	GLU	3.5
1	A	240	ILE	3.5
1	A	165	LYS	3.5
1	A	235	LYS	3.5
1	A	229	GLY	3.5
1	A	191	GLU	3.5
1	A	110	GLY	3.4
1	A	188	ALA	3.4
1	A	176	GLN	3.4
1	A	87	LYS	3.4
1	A	143	PHE	3.4
1	A	61	ALA	3.3
1	A	71	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	144	THR	3.3
1	A	69	LYS	3.3
1	A	115	LYS	3.3
1	A	124	VAL	3.3
1	A	239	GLN	3.3
1	A	141	LEU	3.3
1	A	293	LEU	3.3
1	A	287	ALA	3.3
1	A	106	MET	3.3
1	A	279	LEU	3.2
1	A	267	ARG	3.2
1	A	285	VAL	3.2
1	A	53	ARG	3.2
1	A	111	TRP	3.2
1	A	280	LYS	3.2
1	A	311	TYR	3.2
1	A	128	LYS	3.2
1	A	256	HIS	3.2
1	A	47	HIS	3.1
1	A	266	MET	3.1
1	A	147	PRO	3.1
1	A	70	ASN	3.1
1	A	236	TRP	3.1
1	A	94	THR	3.1
1	A	121	HIS	3.1
1	A	269	SER	3.1
1	A	126	LEU	3.1
1	A	109	TYR	3.0
1	A	114	HIS	3.0
1	A	270	PRO	3.0
1	A	180	LEU	3.0
1	A	104	SER	3.0
1	A	316	CYS	3.0
1	A	179	GLN	3.0
1	A	60	ALA	3.0
1	A	181	VAL	3.0
1	A	65	ASN	3.0
1	A	120	MET	3.0
1	A	250	LEU	3.0
1	A	88	SER	3.0
1	A	234	PRO	3.0
1	A	42	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	290	PHE	2.9
1	A	45	SER	2.9
1	A	226	PRO	2.9
1	A	163	SER	2.8
1	A	79	MET	2.8
1	A	321	ASN	2.8
1	A	245	PRO	2.8
1	A	54	ARG	2.8
1	A	232	PHE	2.7
1	A	271	ILE	2.7
1	A	230	PRO	2.7
1	A	201	GLU	2.7
1	A	222	GLY	2.7
1	A	134	GLY	2.7
1	A	241	LYS	2.7
1	A	306	LEU	2.7
1	A	296	ARG	2.7
1	A	118	VAL	2.7
1	A	257	HIS	2.6
1	A	308	MET	2.6
1	A	92	SER	2.6
1	A	154	ASP	2.6
1	A	173	LYS	2.6
1	A	76	LEU	2.5
1	A	247	LEU	2.5
1	A	123	MET	2.5
1	A	219	ASN	2.5
1	A	167	THR	2.4
1	A	272	LYS	2.3
1	A	77	HIS	2.3
1	A	214	HIS	2.3
1	A	249	ASN	2.2
1	A	196	GLN	2.2
1	A	33	ASP	2.2
1	A	209	LYS	2.2
1	A	263	GLN	2.2
1	A	284	ARG	2.2
1	A	39	GLN	2.1
1	A	182	THR	2.1
1	A	75	PRO	2.1
1	A	216	ASP	2.0
1	A	49	THR	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 carbohydrates 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. 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
3	MG	A	332	1/1	0.66	0.69	4.28	36,36,36,36	0
3	MG	A	331	1/1	0.69	0.55	1.53	5,5,5,5	0
2	CA	A	330	1/1	0.69	0.43	-	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.