



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 04:13 PM EDT

PDB ID : 3N7X
Title : Crystal structure of Penaeus stylirostris densovirus capsid
Authors : Kaufmann, B.; Rossmann, M.G.
Deposited on : unknown
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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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) : rb-20030345

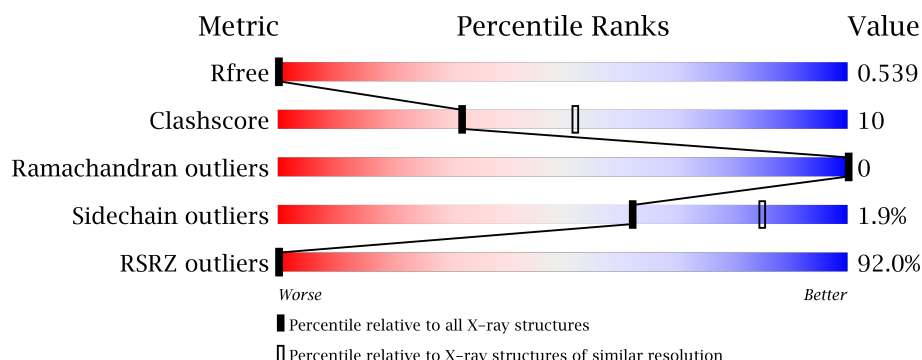
1 Overall quality at a glance

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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	<div> <div>84%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>

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
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		

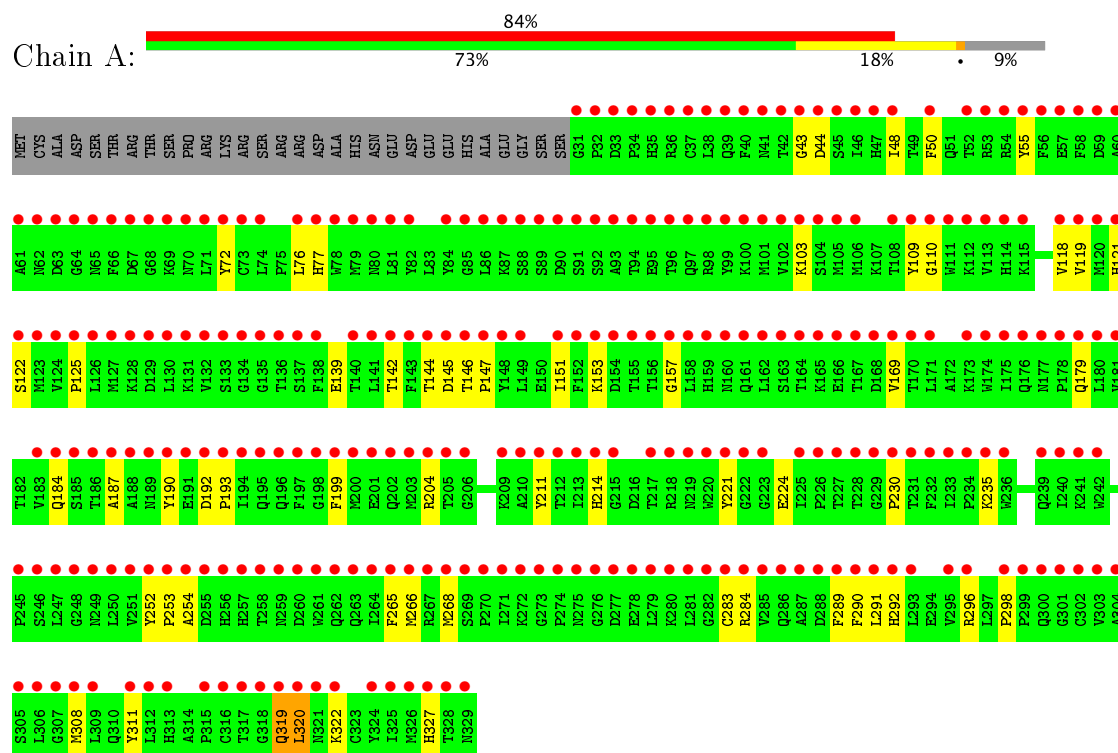
- Molecule 4 is water.

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 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: 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 0.544 , 0.539	Depositor DCC
R_{free} test set	16658 reflections (4.93%)	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
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	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, 0.333 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: 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 [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	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:214:HIS:O	1:A:235:LYS:HE2	2.20	0.41
1:A:230:PRO:HD3	1:A:320:LEU:CD1	2.43	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%)	62 85

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%)	4.17	275 (91%) 0 0	16, 23, 41, 63	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	GLY	12.6
1	A	135	GLY	11.1
1	A	295	VAL	10.4
1	A	299	PRO	9.4
1	A	31	GLY	9.0
1	A	155	THR	8.8
1	A	261	TRP	8.3
1	A	325	ILE	8.2
1	A	101	MET	8.2
1	A	168	ASP	7.7
1	A	252	TYR	7.6
1	A	276	GLY	7.3
1	A	136	THR	7.2
1	A	183	VAL	7.2
1	A	99	TYR	7.0
1	A	227	THR	6.9
1	A	48	ILE	6.9
1	A	220	TRP	6.9
1	A	160	ASN	6.9
1	A	320	LEU	6.9
1	A	64	GLY	6.8
1	A	248	GLY	6.8
1	A	190	TYR	6.8
1	A	169	VAL	6.8
1	A	133	SER	6.7
1	A	78	TRP	6.7
1	A	259	ASN	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	68	GLY	6.6
1	A	199	PHE	6.6
1	A	137	SER	6.5
1	A	175	ILE	6.5
1	A	319	GLN	6.4
1	A	328	THR	6.3
1	A	329	ASN	6.3
1	A	309	LEU	6.2
1	A	43	GLY	6.2
1	A	194	ILE	6.2
1	A	86	LEU	6.2
1	A	260	ASP	6.2
1	A	146	THR	6.1
1	A	74	LEU	6.1
1	A	122	SER	6.1
1	A	178	PRO	6.1
1	A	129	ASP	6.1
1	A	66	PHE	6.0
1	A	324	TYR	6.0
1	A	283	CYS	5.9
1	A	142	THR	5.9
1	A	140	THR	5.9
1	A	195	GLN	5.9
1	A	258	THR	5.9
1	A	205	THR	5.8
1	A	312	LEU	5.8
1	A	315	PRO	5.8
1	A	127	MET	5.8
1	A	213	ILE	5.8
1	A	62	ASN	5.7
1	A	34	PRO	5.7
1	A	198	GLY	5.6
1	A	151	ILE	5.6
1	A	317	THR	5.6
1	A	254	ALA	5.6
1	A	193	PRO	5.6
1	A	145	ASP	5.6
1	A	40	PHE	5.5
1	A	156	THR	5.5
1	A	278	GLU	5.5
1	A	289	PHE	5.5
1	A	212	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	326	MET	5.4
1	A	73	CYS	5.4
1	A	174	TRP	5.3
1	A	192	ASP	5.3
1	A	58	PHE	5.3
1	A	96	THR	5.3
1	A	242	TRP	5.3
1	A	81	LEU	5.3
1	A	149	LEU	5.3
1	A	277	ASP	5.3
1	A	246	SER	5.2
1	A	56	PHE	5.2
1	A	282	GLY	5.2
1	A	164	THR	5.2
1	A	52	THR	5.1
1	A	298	PRO	5.1
1	A	37	CYS	5.1
1	A	103	LYS	5.1
1	A	204	ARG	5.1
1	A	171	LEU	5.0
1	A	35	HIS	5.0
1	A	253	PRO	5.0
1	A	102	VAL	5.0
1	A	161	GLN	5.0
1	A	302	CYS	5.0
1	A	251	VAL	5.0
1	A	265	PHE	4.9
1	A	157	GLY	4.9
1	A	303	VAL	4.9
1	A	36	ARG	4.8
1	A	100	LYS	4.8
1	A	185	SER	4.8
1	A	304	ALA	4.8
1	A	288	ASP	4.7
1	A	166	GLU	4.7
1	A	170	THR	4.7
1	A	125	PRO	4.7
1	A	228	THR	4.6
1	A	264	ILE	4.6
1	A	113	VAL	4.6
1	A	211	TYR	4.6
1	A	85	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	44	ASP	4.6
1	A	187	ALA	4.6
1	A	97	GLN	4.5
1	A	89	SER	4.5
1	A	41	ASN	4.5
1	A	131	LYS	4.5
1	A	218	ARG	4.5
1	A	84	TYR	4.4
1	A	206	GLY	4.4
1	A	221	TYR	4.4
1	A	262	GLN	4.4
1	A	177	ASN	4.4
1	A	305	SER	4.4
1	A	119	VAL	4.4
1	A	72	TYR	4.4
1	A	130	LEU	4.3
1	A	291	LEU	4.3
1	A	50	PHE	4.3
1	A	138	PHE	4.3
1	A	152	PHE	4.2
1	A	274	PRO	4.2
1	A	281	LEU	4.2
1	A	313	HIS	4.1
1	A	233	ILE	4.1
1	A	200	MET	4.1
1	A	197	PHE	4.1
1	A	327	HIS	4.1
1	A	148	TYR	4.0
1	A	318	GLY	4.0
1	A	273	GLY	4.0
1	A	95	GLU	4.0
1	A	275	ASN	4.0
1	A	112	LYS	4.0
1	A	203	MET	4.0
1	A	132	VAL	4.0
1	A	202	GLN	3.9
1	A	59	ASP	3.9
1	A	184	GLN	3.9
1	A	189	ASN	3.9
1	A	292	HIS	3.8
1	A	90	ASP	3.8
1	A	322	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	80	ASN	3.8
1	A	159	HIS	3.8
1	A	300	GLN	3.8
1	A	215	GLY	3.8
1	A	186	THR	3.7
1	A	105	MET	3.7
1	A	108	THR	3.7
1	A	153	LYS	3.7
1	A	98	ARG	3.7
1	A	67	ASP	3.6
1	A	286	GLN	3.6
1	A	82	TYR	3.6
1	A	55	TYR	3.6
1	A	225	ILE	3.5
1	A	162	LEU	3.5
1	A	46	ILE	3.5
1	A	210	ALA	3.5
1	A	231	THR	3.5
1	A	91	SER	3.5
1	A	255	ASP	3.5
1	A	38	LEU	3.5
1	A	32	PRO	3.5
1	A	307	GLY	3.5
1	A	158	LEU	3.4
1	A	63	ASP	3.4
1	A	217	THR	3.4
1	A	223	GLY	3.4
1	A	57	GLU	3.4
1	A	165	LYS	3.4
1	A	235	LYS	3.4
1	A	240	ILE	3.4
1	A	93	ALA	3.4
1	A	268	MET	3.4
1	A	191	GLU	3.3
1	A	229	GLY	3.3
1	A	110	GLY	3.3
1	A	87	LYS	3.3
1	A	176	GLN	3.3
1	A	143	PHE	3.2
1	A	188	ALA	3.2
1	A	69	LYS	3.2
1	A	115	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	LEU	3.2
1	A	61	ALA	3.2
1	A	239	GLN	3.2
1	A	144	THR	3.1
1	A	141	LEU	3.1
1	A	124	VAL	3.1
1	A	293	LEU	3.1
1	A	279	LEU	3.1
1	A	267	ARG	3.1
1	A	287	ALA	3.1
1	A	280	LYS	3.1
1	A	111	TRP	3.1
1	A	106	MET	3.1
1	A	53	ARG	3.1
1	A	311	TYR	3.0
1	A	128	LYS	3.0
1	A	285	VAL	3.0
1	A	256	HIS	3.0
1	A	47	HIS	3.0
1	A	236	TRP	3.0
1	A	70	ASN	3.0
1	A	94	THR	3.0
1	A	147	PRO	3.0
1	A	266	MET	2.9
1	A	121	HIS	2.9
1	A	269	SER	2.9
1	A	109	TYR	2.9
1	A	126	LEU	2.9
1	A	114	HIS	2.9
1	A	180	LEU	2.9
1	A	104	SER	2.9
1	A	179	GLN	2.9
1	A	270	PRO	2.9
1	A	65	ASN	2.8
1	A	88	SER	2.8
1	A	60	ALA	2.8
1	A	316	CYS	2.8
1	A	250	LEU	2.8
1	A	181	VAL	2.8
1	A	290	PHE	2.8
1	A	42	THR	2.8
1	A	120	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	234	PRO	2.8
1	A	45	SER	2.8
1	A	163	SER	2.7
1	A	226	PRO	2.7
1	A	321	ASN	2.7
1	A	79	MET	2.7
1	A	54	ARG	2.6
1	A	232	PHE	2.6
1	A	245	PRO	2.6
1	A	271	ILE	2.6
1	A	201	GLU	2.6
1	A	230	PRO	2.6
1	A	241	LYS	2.6
1	A	296	ARG	2.5
1	A	306	LEU	2.5
1	A	222	GLY	2.5
1	A	257	HIS	2.5
1	A	134	GLY	2.5
1	A	92	SER	2.5
1	A	118	VAL	2.5
1	A	308	MET	2.5
1	A	173	LYS	2.5
1	A	154	ASP	2.4
1	A	76	LEU	2.4
1	A	247	LEU	2.4
1	A	219	ASN	2.4
1	A	123	MET	2.3
1	A	167	THR	2.3
1	A	272	LYS	2.2
1	A	77	HIS	2.2
1	A	214	HIS	2.2
1	A	249	ASN	2.1
1	A	196	GLN	2.1
1	A	209	LYS	2.1
1	A	33	ASP	2.1
1	A	263	GLN	2.1
1	A	284	ARG	2.1
1	A	39	GLN	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 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(\AA^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.