



Full wwPDB X-ray Structure Validation Report

Jul 12, 2014 – 01:13 AM EDT

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 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/ValidationPDFNotes.html>

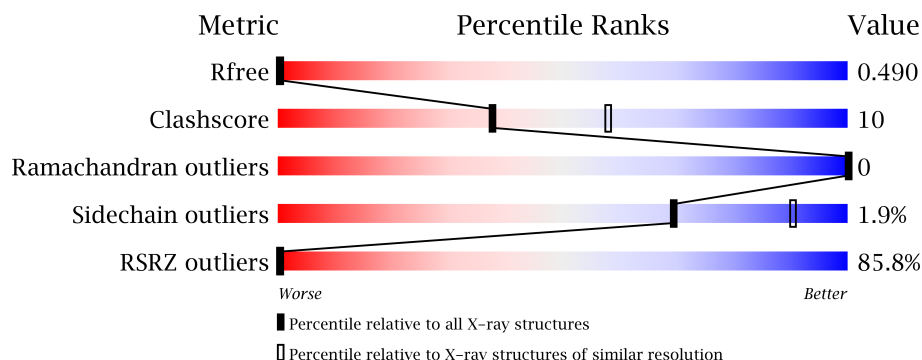
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	329	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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 hydrogen and 0 are deuterium.

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		

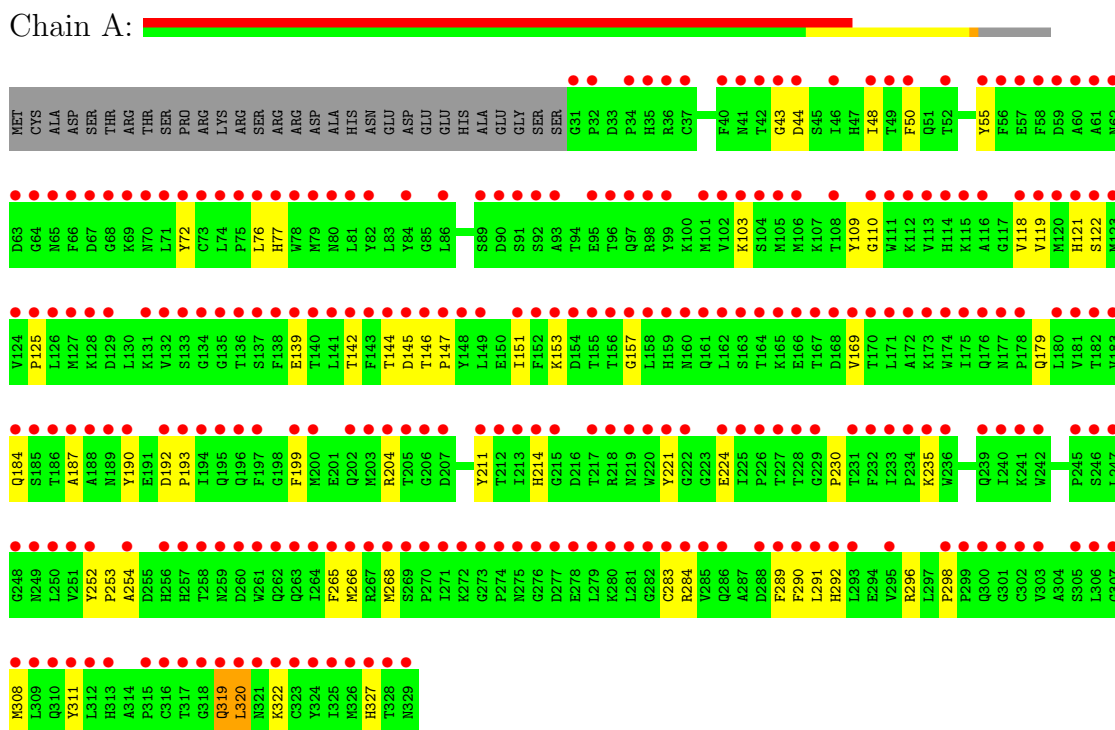
- Molecule 4 is water.

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

3 Residue-property plots

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: 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) 60.5 (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 0.489 , 0.490	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)	0.43 , 203.2	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 337569 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.30	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (47) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:48:ILE:N	1:A:48:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	297/329 (90%)	288 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	262/288 (91%)	257 (98%)	5 (2%)	69	90

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

Mol	Chain	Res	Type
1	A	139	GLU
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 ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

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%)	3.84	258 (86%) 0 0	16, 23, 41, 63	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	ASP	12.2
1	A	133	SER	11.4
1	A	258	THR	11.1
1	A	299	PRO	10.4
1	A	283	CYS	10.0
1	A	81	LEU	9.8
1	A	64	GLY	9.3
1	A	136	THR	9.0
1	A	155	THR	8.7
1	A	52	THR	8.0
1	A	132	VAL	7.9
1	A	50	PHE	7.9
1	A	74	LEU	7.5
1	A	151	ILE	7.4
1	A	152	PHE	7.3
1	A	289	PHE	7.1
1	A	215	GLY	6.9
1	A	232	PHE	6.8
1	A	72	TYR	6.8
1	A	275	ASN	6.8
1	A	135	GLY	6.7
1	A	312	LEU	6.7
1	A	260	ASP	6.6
1	A	171	LEU	6.6
1	A	295	VAL	6.5
1	A	325	ILE	6.5
1	A	114	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	248	GLY	6.4
1	A	203	MET	6.4
1	A	115	LYS	6.4
1	A	324	TYR	6.4
1	A	220	TRP	6.3
1	A	180	LEU	6.2
1	A	138	PHE	6.1
1	A	170	THR	6.1
1	A	78	TRP	6.1
1	A	66	PHE	6.0
1	A	293	LEU	6.0
1	A	329	ASN	6.0
1	A	302	CYS	5.9
1	A	291	LEU	5.8
1	A	146	THR	5.7
1	A	261	TRP	5.7
1	A	166	GLU	5.7
1	A	70	ASN	5.6
1	A	259	ASN	5.6
1	A	149	LEU	5.6
1	A	193	PRO	5.6
1	A	284	ARG	5.6
1	A	282	GLY	5.5
1	A	31	GLY	5.5
1	A	240	ILE	5.5
1	A	62	ASN	5.3
1	A	270	PRO	5.3
1	A	58	PHE	5.3
1	A	122	SER	5.3
1	A	307	GLY	5.3
1	A	73	CYS	5.2
1	A	137	SER	5.2
1	A	305	SER	5.2
1	A	97	GLN	5.2
1	A	127	MET	5.2
1	A	134	GLY	5.1
1	A	211	TYR	5.1
1	A	63	ASP	5.1
1	A	285	VAL	5.0
1	A	57	GLU	5.0
1	A	252	TYR	5.0
1	A	265	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	4.9
1	A	317	THR	4.9
1	A	129	ASP	4.9
1	A	142	THR	4.8
1	A	221	TYR	4.8
1	A	292	HIS	4.8
1	A	84	TYR	4.7
1	A	183	VAL	4.7
1	A	103	LYS	4.7
1	A	162	LEU	4.7
1	A	99	TYR	4.7
1	A	89	SER	4.6
1	A	101	MET	4.6
1	A	298	PRO	4.6
1	A	320	LEU	4.6
1	A	175	ILE	4.6
1	A	169	VAL	4.6
1	A	105	MET	4.6
1	A	124	VAL	4.5
1	A	319	GLN	4.5
1	A	92	SER	4.5
1	A	262	GLN	4.5
1	A	79	MET	4.5
1	A	37	CYS	4.4
1	A	309	LEU	4.4
1	A	174	TRP	4.4
1	A	61	ALA	4.4
1	A	93	ALA	4.4
1	A	141	LEU	4.3
1	A	145	ASP	4.3
1	A	68	GLY	4.3
1	A	308	MET	4.3
1	A	199	PHE	4.3
1	A	40	PHE	4.2
1	A	197	PHE	4.2
1	A	205	THR	4.2
1	A	86	LEU	4.2
1	A	277	ASP	4.2
1	A	189	ASN	4.2
1	A	212	THR	4.2
1	A	226	PRO	4.2
1	A	128	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	158	LEU	4.1
1	A	187	ALA	4.1
1	A	286	GLN	4.1
1	A	123	MET	4.0
1	A	71	LEU	4.0
1	A	273	GLY	4.0
1	A	311	TYR	4.0
1	A	157	GLY	4.0
1	A	207	ASP	4.0
1	A	306	LEU	4.0
1	A	227	THR	4.0
1	A	326	MET	4.0
1	A	190	TYR	3.9
1	A	290	PHE	3.9
1	A	147	PRO	3.9
1	A	186	THR	3.9
1	A	34	PRO	3.9
1	A	315	PRO	3.8
1	A	60	ALA	3.8
1	A	322	LYS	3.8
1	A	218	ARG	3.8
1	A	77	HIS	3.8
1	A	90	ASP	3.8
1	A	194	ILE	3.8
1	A	246	SER	3.8
1	A	140	THR	3.8
1	A	288	ASP	3.7
1	A	239	GLN	3.7
1	A	181	VAL	3.7
1	A	192	ASP	3.7
1	A	188	ALA	3.7
1	A	301	GLY	3.7
1	A	256	HIS	3.6
1	A	143	PHE	3.6
1	A	242	TRP	3.6
1	A	65	ASN	3.6
1	A	213	ILE	3.6
1	A	167	THR	3.6
1	A	160	ASN	3.5
1	A	206	GLY	3.5
1	A	177	ASN	3.5
1	A	245	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	48	ILE	3.5
1	A	271	ILE	3.5
1	A	202	GLN	3.5
1	A	225	ILE	3.5
1	A	156	THR	3.5
1	A	49	THR	3.4
1	A	178	PRO	3.4
1	A	228	THR	3.4
1	A	200	MET	3.3
1	A	35	HIS	3.3
1	A	263	GLN	3.3
1	A	264	ILE	3.3
1	A	69	LYS	3.3
1	A	231	THR	3.2
1	A	121	HIS	3.2
1	A	82	TYR	3.2
1	A	184	GLN	3.2
1	A	163	SER	3.2
1	A	281	LEU	3.2
1	A	164	THR	3.2
1	A	41	ASN	3.1
1	A	148	TYR	3.1
1	A	257	HIS	3.1
1	A	229	GLY	3.1
1	A	80	ASN	3.1
1	A	321	ASN	3.1
1	A	267	ARG	3.1
1	A	280	LYS	3.1
1	A	55	TYR	3.0
1	A	110	GLY	3.0
1	A	276	GLY	3.0
1	A	106	MET	3.0
1	A	153	LYS	3.0
1	A	185	SER	3.0
1	A	316	CYS	3.0
1	A	96	THR	3.0
1	A	327	HIS	3.0
1	A	116	ALA	3.0
1	A	111	TRP	3.0
1	A	234	PRO	3.0
1	A	161	GLN	3.0
1	A	43	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	125	PRO	2.9
1	A	313	HIS	2.9
1	A	118	VAL	2.9
1	A	233	ILE	2.9
1	A	113	VAL	2.9
1	A	214	HIS	2.9
1	A	318	GLY	2.9
1	A	274	PRO	2.8
1	A	91	SER	2.8
1	A	196	GLN	2.8
1	A	269	SER	2.8
1	A	131	LYS	2.8
1	A	32	PRO	2.8
1	A	44	ASP	2.8
1	A	159	HIS	2.8
1	A	279	LEU	2.8
1	A	323	CYS	2.7
1	A	154	ASP	2.7
1	A	144	THR	2.7
1	A	247	LEU	2.7
1	A	119	VAL	2.7
1	A	42	THR	2.7
1	A	250	LEU	2.7
1	A	251	VAL	2.6
1	A	104	SER	2.6
1	A	217	THR	2.5
1	A	165	LYS	2.5
1	A	249	ASN	2.5
1	A	300	GLN	2.4
1	A	108	THR	2.4
1	A	266	MET	2.4
1	A	67	ASP	2.4
1	A	241	LYS	2.4
1	A	236	TRP	2.4
1	A	222	GLY	2.4
1	A	195	GLN	2.4
1	A	59	ASP	2.4
1	A	98	ARG	2.3
1	A	328	THR	2.3
1	A	112	LYS	2.3
1	A	219	ASN	2.3
1	A	120	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	303	VAL	2.3
1	A	102	VAL	2.2
1	A	173	LYS	2.2
1	A	75	PRO	2.2
1	A	268	MET	2.2
1	A	36	ARG	2.2
1	A	204	ARG	2.2
1	A	176	GLN	2.2
1	A	56	PHE	2.2
1	A	278	GLU	2.2
1	A	310	GLN	2.2
1	A	76	LEU	2.1
1	A	182	THR	2.1
1	A	254	ALA	2.1
1	A	224	GLU	2.1
1	A	46	ILE	2.1
1	A	172	ALA	2.1
1	A	95	GLU	2.1
1	A	272	LYS	2.1
1	A	235	LYS	2.0
1	A	139	GLU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	332	1/1	1.41	12.72	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	A	331	1/1	0.29	-1.73	5,5,5,5	0
2	CA	A	330	1/1	0.17	-11.42	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.