



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 04:37 AM UTC

PDB ID : 2J7U / pdb_00002j7u
Title : Dengue virus NS5 RNA dependent RNA polymerase domain
Authors : Yap, T.L.; Xu, T.; Chen, Y.L.; Malet, H.; Egloff, M.P.; Canard, B.; Vasudevan, S.G.; Lescar, J.
Deposited on : 2006-10-17
Resolution : 1.85 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

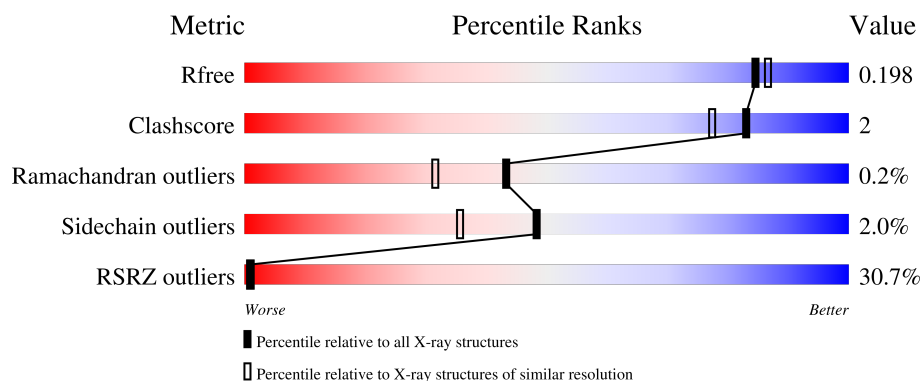
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	635	28% 83% 7% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5220 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 RNA DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	11	0
			4701	2980	842	849	30			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLY	-	expression tag	UNP Q6DLV0
A	267	SER	-	expression tag	UNP Q6DLV0
A	268	HIS	-	expression tag	UNP Q6DLV0
A	269	MET	-	expression tag	UNP Q6DLV0
A	270	LEU	-	expression tag	UNP Q6DLV0
A	271	ASP	-	expression tag	UNP Q6DLV0
A	374	GLU	GLY	conflict	UNP Q6DLV0
A	480	ALA	VAL	conflict	UNP Q6DLV0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

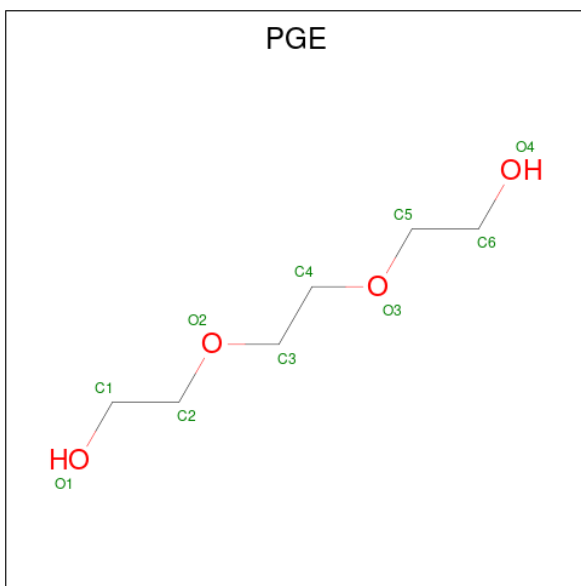
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

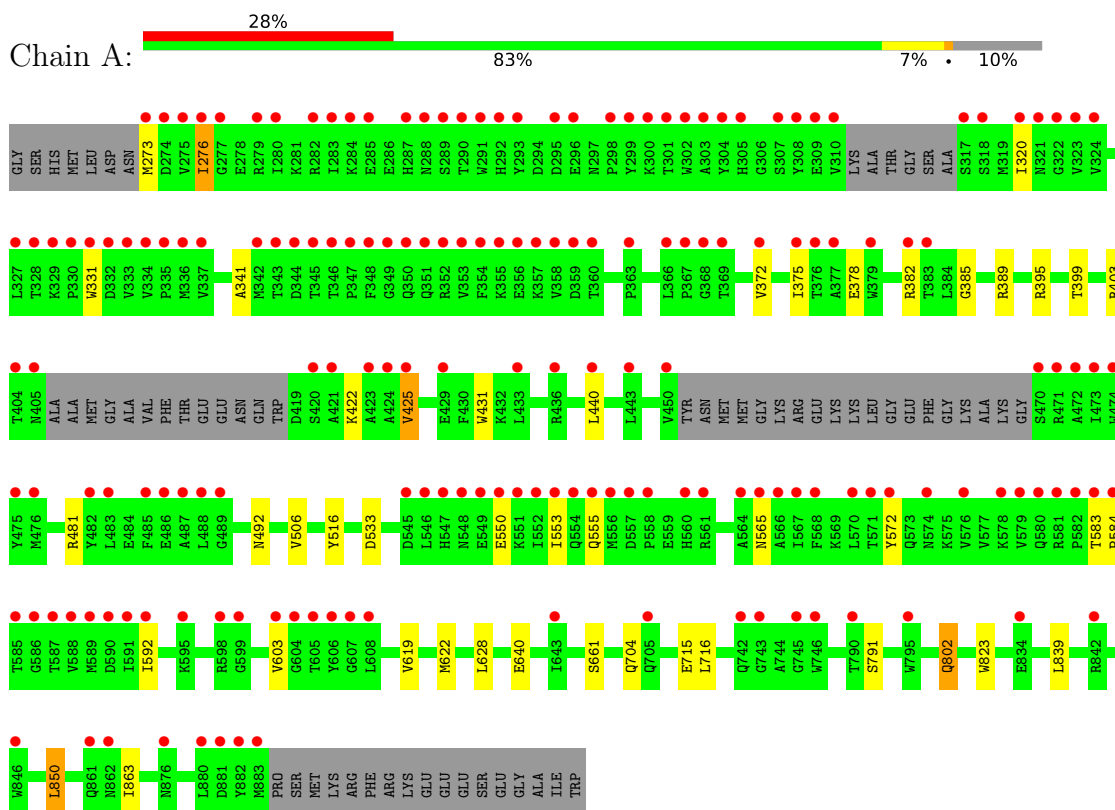
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	505	Total	O	0	0
			505	505		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: RNA DEPENDENT RNA POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	160.15Å 180.48Å 57.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85 20.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.85) 99.8 (20.00-1.85)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.234 0.200 , 0.198	Depositor DCC
R_{free} test set	3601 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, ZN, PGE

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	0.45	0/4854	0.75	0/6576

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	4701	0	4598	22	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	1	0
5	A	10	0	14	0	0
6	A	505	0	0	0	0
All	All	5220	0	4612	22	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 (22) 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:716:LEU:HD21	1:A:839:LEU:HD23	1.60	0.83
1:A:802:GLN:HE21	1:A:802:GLN:H	1.30	0.77
1:A:385:GLY:HA3	1:A:555:GLN:HE22	1.64	0.61
1:A:704:GLN:NE2	1:A:715:GLU:H	2.05	0.55
1:A:403:ARG:HA	1:A:422:LYS:HD3	1.89	0.53
1:A:716:LEU:CD2	1:A:839:LEU:HD23	2.36	0.53
1:A:375:ILE:HD11	1:A:640:GLU:HG2	1.91	0.53
1:A:619:VAL:HA	1:A:622:MET:HE3	1.94	0.49
1:A:273:MET:HB3	1:A:276:ILE:HG22	1.96	0.47
1:A:572:TYR:OH	1:A:603:VAL:O	2.33	0.47
1:A:331:TRP:CE2	1:A:850:LEU:HD22	2.51	0.45
1:A:583:THR:HA	1:A:584:PRO:HD3	1.87	0.44
1:A:399:THR:HG23	1:A:425:VAL:CG1	2.47	0.44
1:A:395:ARG:HG3	1:A:431:TRP:CZ2	2.53	0.43
1:A:320:ILE:HD11	1:A:341:ALA:HB1	2.01	0.43
1:A:378:GLU:O	1:A:382:ARG:HG3	2.19	0.43
1:A:372[A]:VAL:HG11	1:A:628:LEU:HD11	2.00	0.43
1:A:492:ASN:ND2	4:A:1887:CL:CL	2.89	0.42
1:A:506:VAL:CG2	1:A:661[B]:SER:OG	2.68	0.41
1:A:550:GLU:O	1:A:553:ILE:HG12	2.21	0.41
1:A:516:TYR:HB3	1:A:823:TRP:CE2	2.57	0.40

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	576/635 (91%)	553 (96%)	22 (4%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	791	SER

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	502/551 (91%)	492 (98%)	10 (2%)	48 36

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ILE
1	A	389	ARG
1	A	425	VAL
1	A	440	LEU
1	A	481	ARG
1	A	533	ASP
1	A	592	ILE
1	A	802	GLN
1	A	850	LEU
1	A	863	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	A	297	ASN
1	A	339	GLN
1	A	387	ASN
1	A	548	ASN
1	A	555	GLN
1	A	580	GLN
1	A	617	GLN
1	A	621	GLN
1	A	645	GLN
1	A	682	ASN
1	A	704	GLN
1	A	802	GLN
1	A	835	ASN
1	A	868	GLN

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Mol	Chain	Res	Type
1	A	869	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	PGE	A	1888	-	9,9,9	0.43	0	8,8,8	0.60	0

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
5	PGE	A	1888	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1888	PGE	O2-C3-C4-O3
5	A	1888	PGE	O3-C5-C6-O4
5	A	1888	PGE	C6-C5-O3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	573/635 (90%)	1.64	176 (30%) 1 1	19, 35, 42, 51	11 (1%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	THR	12.4
1	A	347	PRO	11.3
1	A	346	THR	9.2
1	A	348	PHE	8.9
1	A	353	VAL	8.4
1	A	343	THR	7.6
1	A	583	THR	7.6
1	A	291	TRP	7.5
1	A	349	GLY	7.3
1	A	280	ILE	7.3
1	A	331	TRP	7.1
1	A	608	LEU	7.0
1	A	330	PRO	6.5
1	A	552	ILE	6.3
1	A	589	MET	6.3
1	A	352	ARG	6.1
1	A	487	ALA	6.0
1	A	310	VAL	6.0
1	A	551	LYS	5.9
1	A	582	PRO	5.9
1	A	547[A]	HIS	5.8
1	A	545	ASP	5.7
1	A	489	GLY	5.7
1	A	358	VAL	5.7
1	A	546	LEU	5.6
1	A	293	TYR	5.6
1	A	548	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	587	THR	5.6
1	A	275	VAL	5.6
1	A	344	ASP	5.4
1	A	303	ALA	5.4
1	A	579	VAL	5.4
1	A	606	TYR	5.3
1	A	354	PHE	5.2
1	A	317	SER	5.1
1	A	355	LYS	5.1
1	A	607	GLY	5.0
1	A	287	HIS	4.9
1	A	283	ILE	4.9
1	A	473	ILE	4.9
1	A	556	MET	4.7
1	A	746	TRP	4.7
1	A	742	GLN	4.6
1	A	335	PRO	4.6
1	A	276	ILE	4.6
1	A	590	ASP	4.6
1	A	743	GLY	4.6
1	A	553	ILE	4.6
1	A	292	HIS	4.5
1	A	876	ASN	4.5
1	A	288	ASN	4.4
1	A	588	VAL	4.4
1	A	305	HIS	4.4
1	A	485	PHE	4.4
1	A	333	VAL	4.2
1	A	882	TYR	4.2
1	A	584	PRO	4.1
1	A	476	MET	4.1
1	A	488	LEU	4.1
1	A	304	TYR	4.0
1	A	880	LEU	4.0
1	A	580	GLN	4.0
1	A	474	TRP	4.0
1	A	290	THR	4.0
1	A	334	VAL	4.0
1	A	586	GLY	3.9
1	A	327	LEU	3.8
1	A	302	TRP	3.8
1	A	560	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	561[A]	ARG	3.8
1	A	342	MET	3.7
1	A	558	PRO	3.7
1	A	295	ASP	3.7
1	A	472	ALA	3.7
1	A	308	TYR	3.6
1	A	572	TYR	3.6
1	A	300	LYS	3.6
1	A	604	GLY	3.5
1	A	296	GLU	3.5
1	A	603	VAL	3.5
1	A	351	GLN	3.5
1	A	483	LEU	3.5
1	A	846	TRP	3.5
1	A	301	THR	3.4
1	A	555	GLN	3.4
1	A	323	VAL	3.4
1	A	318	SER	3.4
1	A	595	LYS	3.3
1	A	372[A]	VAL	3.3
1	A	289	SER	3.3
1	A	299	TYR	3.3
1	A	581	ARG	3.3
1	A	274	ASP	3.3
1	A	285	GLU	3.2
1	A	337	VAL	3.2
1	A	554	GLN	3.2
1	A	591	ILE	3.1
1	A	425	VAL	3.1
1	A	436	ARG	3.1
1	A	440	LEU	3.1
1	A	350	GLN	3.0
1	A	357	LYS	3.0
1	A	356	GLU	3.0
1	A	549	GLU	3.0
1	A	433	LEU	3.0
1	A	328	THR	3.0
1	A	277	GLY	3.0
1	A	424	ALA	3.0
1	A	284	LYS	2.9
1	A	745	GLY	2.9
1	A	790	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	443	LEU	2.8
1	A	578	LYS	2.8
1	A	576	VAL	2.8
1	A	363	PRO	2.8
1	A	557	ASP	2.8
1	A	571	THR	2.7
1	A	282	ARG	2.7
1	A	309	GLU	2.7
1	A	861	GLN	2.7
1	A	568	PHE	2.7
1	A	585	THR	2.7
1	A	566	ALA	2.6
1	A	883	MET	2.6
1	A	881	ASP	2.6
1	A	375	ILE	2.6
1	A	550	GLU	2.6
1	A	366	LEU	2.6
1	A	429	GLU	2.6
1	A	421	ALA	2.6
1	A	475	TYR	2.6
1	A	834	GLU	2.6
1	A	423	ALA	2.6
1	A	273	MET	2.5
1	A	298	PRO	2.5
1	A	570	LEU	2.5
1	A	599	GLY	2.5
1	A	592	ILE	2.5
1	A	486	GLU	2.5
1	A	360	THR	2.5
1	A	482	TYR	2.4
1	A	574	ASN	2.4
1	A	324	VAL	2.4
1	A	377	ALA	2.4
1	A	598	ARG	2.3
1	A	567	ILE	2.3
1	A	405	ASN	2.3
1	A	322	GLY	2.3
1	A	369	THR	2.3
1	A	336	MET	2.3
1	A	279	ARG	2.2
1	A	379	TRP	2.2
1	A	404	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	605	THR	2.2
1	A	705	GLN	2.2
1	A	795	TRP	2.2
1	A	842	ARG	2.2
1	A	376	THR	2.2
1	A	382	ARG	2.2
1	A	862	ASN	2.1
1	A	368	GLY	2.1
1	A	450	VAL	2.1
1	A	565	ASN	2.1
1	A	643	ILE	2.1
1	A	420	SER	2.1
1	A	329	LYS	2.1
1	A	321	ASN	2.1
1	A	564	ALA	2.1
1	A	359	ASP	2.1
1	A	320	ILE	2.0
1	A	383	THR	2.0
1	A	332	ASP	2.0
1	A	307	SER	2.0
1	A	470	SER	2.0
1	A	367	PRO	2.0
1	A	471	ARG	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 oligosaccharides 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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PGE	A	1888	10/10	0.85	0.13	48,49,50,50	0
3	MG	A	1886	1/1	0.89	0.23	47,47,47,47	0
4	CL	A	1887	1/1	0.91	0.27	51,51,51,51	0
2	ZN	A	1885	1/1	0.98	0.11	31,31,31,31	1
2	ZN	A	1884	1/1	0.99	0.11	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.