Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:17 PM GMT

PDB ID	:	4C11
Title	:	Dengue virus RNA dependent RNA polymerase with residues from the NS5 linker region
Authors	:	Lim, S.P.; Lescar, J.
Deposited on	:	2013-08-09
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

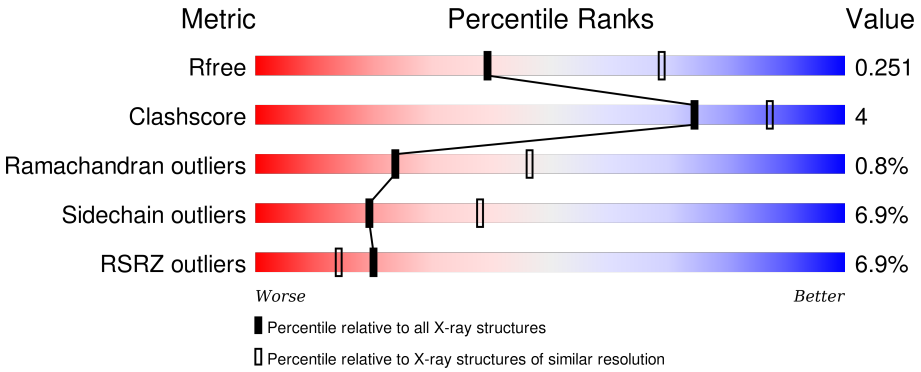
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	638	5% 80% 12% • 7%
2	B	638	8% 81% 12% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10134 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 DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	593	4842	3057	872	882	31	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	GLU	GLY	CONFLICT	UNP Q6DLV0
A	454	LYS	MET	CONFLICT	UNP Q6DLV0

- Molecule 2 is a protein called DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	603	4864	3068	871	893	32	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	GLU	GLY	CONFLICT	UNP Q6DLV0
B	409	ALA	GLY	CONFLICT	UNP Q6DLV0
B	455	ALA	GLY	CONFLICT	UNP Q6DLV0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

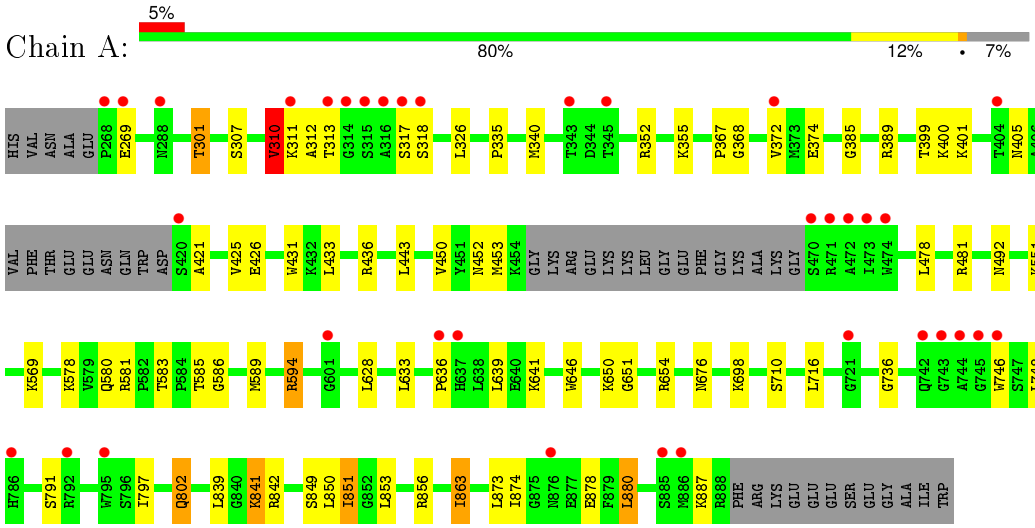
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	236	Total O 236 236	0	0
4	B	188	Total O 188 188	0	0

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 (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.

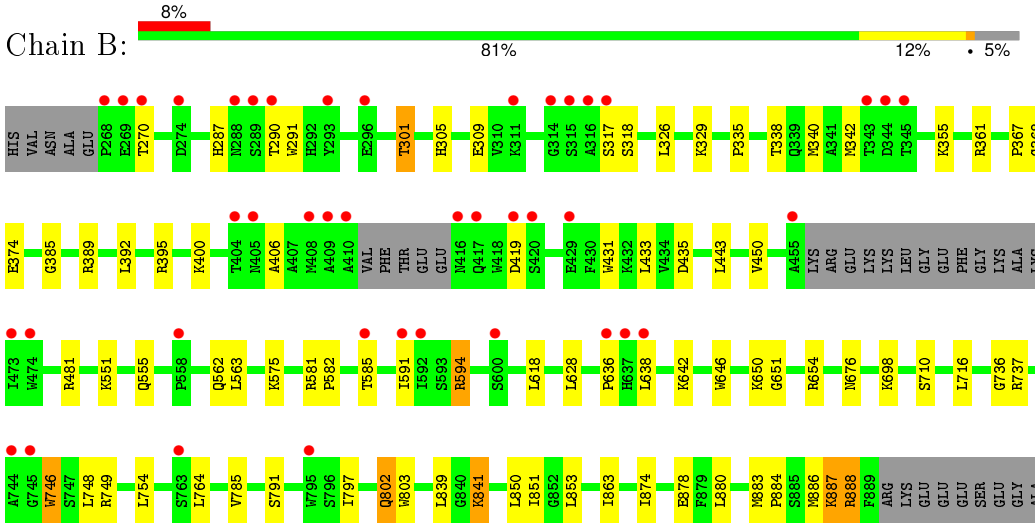
- Molecule 1: DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE

Chain A:



- Molecule 2: DENGUE VIRUS TYPE 3 RNA DEPENDENT RNA POLYMERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.99Å 136.05Å 103.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.94-2.60) 98.0 (19.93-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.192 , 0.245 0.198 , 0.251	Depositor DCC
R_{free} test set	2676 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 87.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 52736 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10134	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	0.52	0/4974	0.73	1/6737 (0.0%)
2	B	0.51	0/4987	0.72	3/6760 (0.0%)
All	All	0.51	0/9961	0.72	4/13497 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	886	MET	C-N-CA	6.74	138.54	121.70
1	A	310	VAL	C-N-CA	6.44	137.79	121.70
2	B	887	LYS	N-CA-C	5.61	126.14	111.00
2	B	746	TRP	N-CA-CB	5.12	119.81	110.60

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	4842	0	4748	43	0
2	B	4864	0	4723	35	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	236	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	188	0	0	1	0
All	All	10134	0	9471	77	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 4.

All (77) 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:311:LYS:HB2	1:A:312:ALA:HA	1.44	0.95
2:B:802:GLN:HE21	2:B:802:GLN:H	1.19	0.89
2:B:301:THR:CG2	2:B:594:ARG:HH12	1.88	0.87
1:A:802:GLN:H	1:A:802:GLN:HE21	1.19	0.87
1:A:301:THR:CG2	1:A:594:ARG:HH12	1.88	0.85
2:B:301:THR:HG23	2:B:594:ARG:HH12	1.49	0.77
1:A:313:THR:HB	1:A:580:GLN:HE22	1.49	0.76
1:A:301:THR:HG23	1:A:594:ARG:HH12	1.52	0.75
2:B:385:GLY:HA3	2:B:555:GLN:HE22	1.52	0.74
1:A:385:GLY:HA3	1:A:555:GLN:HE22	1.52	0.74
2:B:883:MET:HB3	2:B:888:ARG:HD3	1.68	0.74
2:B:716:LEU:HD21	2:B:839:LEU:HD23	1.71	0.73
1:A:452:ASN:HB3	1:A:578:LYS:HG2	1.78	0.66
1:A:310:VAL:HB	1:A:311:LYS:HA	1.79	0.65
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.79	0.65
1:A:311:LYS:CB	1:A:312:ALA:HA	2.25	0.62
1:A:797:ILE:H	1:A:797:ILE:HD12	1.66	0.61
2:B:301:THR:HG23	2:B:594:ARG:NH1	2.15	0.60
2:B:797:ILE:HD12	2:B:797:ILE:H	1.67	0.59
1:A:301:THR:HG23	1:A:594:ARG:NH1	2.16	0.59
2:B:368:GLY:O	2:B:372:VAL:HG23	2.03	0.59
2:B:737:ARG:HA	2:B:740:ILE:HD12	1.85	0.58
2:B:841:LYS:HG2	2:B:851:ILE:HD12	1.84	0.58
2:B:372:VAL:HG11	2:B:628:LEU:HD11	1.88	0.56
1:A:269:GLU:HG3	1:A:594:ARG:HA	1.87	0.55
1:A:335:PRO:HG3	2:B:335:PRO:HG3	1.89	0.54
1:A:421:ALA:O	1:A:425:VAL:HG23	2.07	0.54
1:A:785:VAL:HG11	1:A:880:LEU:HD13	1.89	0.54
1:A:372:VAL:HG11	1:A:628:LEU:HD11	1.88	0.54
1:A:802:GLN:H	1:A:802:GLN:NE2	1.99	0.52
1:A:849:SER:OG	1:A:851:ILE:HG13	2.09	0.52
2:B:340:MET:HG3	2:B:736:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:VAL:CG1	1:A:880:LEU:HB2	2.40	0.52
2:B:802:GLN:H	2:B:802:GLN:NE2	1.99	0.51
1:A:425:VAL:HG13	1:A:431:TRP:HZ2	1.76	0.51
1:A:583:THR:HG23	1:A:586:GLY:H	1.77	0.50
2:B:290:THR:HG21	2:B:309:GLU:HG2	1.94	0.50
2:B:371:LYS:HG2	2:B:638:LEU:HB3	1.94	0.50
2:B:785:VAL:HG11	2:B:880:LEU:HB2	1.93	0.49
2:B:748:LEU:HD21	2:B:874:ILE:HA	1.93	0.48
1:A:841:LYS:HD3	1:A:851:ILE:HD13	1.95	0.48
2:B:742:GLN:HG3	2:B:754:LEU:HD21	1.94	0.48
1:A:797:ILE:H	1:A:797:ILE:CD1	2.26	0.48
4:A:2231:HOH:O	2:B:582:PRO:HD2	2.14	0.47
2:B:392:LEU:HD21	2:B:563:LEU:HD12	1.96	0.47
1:A:583:THR:CG2	1:A:586:GLY:H	2.27	0.47
1:A:748:LEU:HD21	1:A:874:ILE:HA	1.96	0.47
2:B:287:HIS:O	2:B:291:TRP:HB2	2.15	0.47
1:A:367:PRO:HB2	1:A:636:PRO:HA	1.96	0.47
1:A:399:THR:HA	1:A:425:VAL:HG11	1.97	0.47
1:A:340:MET:HG3	1:A:736:GLY:HA3	1.97	0.47
1:A:746:TRP:HE3	1:A:750:GLU:HB3	1.79	0.47
2:B:841:LYS:HG2	2:B:851:ILE:CD1	2.46	0.46
2:B:367:PRO:HB2	2:B:636:PRO:HA	1.97	0.46
2:B:305:HIS:HB2	2:B:591:ILE:HG22	1.98	0.46
2:B:887:LYS:N	2:B:888:ARG:HA	2.31	0.46
1:A:628:LEU:HD13	1:A:633:LEU:HD21	1.97	0.46
2:B:797:ILE:CD1	2:B:797:ILE:H	2.28	0.45
1:A:565:ASN:O	1:A:569:LYS:HB2	2.16	0.45
1:A:785:VAL:HG11	1:A:880:LEU:HB2	1.97	0.45
2:B:850:LEU:O	2:B:853:LEU:HB2	2.16	0.44
1:A:850:LEU:O	1:A:853:LEU:HB2	2.16	0.44
1:A:401:LYS:O	1:A:405:ASN:HB2	2.17	0.43
1:A:310:VAL:HB	1:A:311:LYS:CA	2.48	0.43
2:B:764:LEU:HD12	2:B:803:TRP:HB3	2.01	0.43
2:B:395:ARG:HG3	2:B:431:TRP:CZ2	2.54	0.42
1:A:301:THR:CG2	1:A:594:ARG:NH1	2.68	0.42
2:B:884:PRO:HA	2:B:887:LYS:HA	2.01	0.42
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.55	0.41
2:B:618:LEU:HA	2:B:618:LEU:HD23	1.96	0.41
1:A:307:SER:HA	1:A:589:MET:O	2.20	0.41
1:A:368:GLY:O	1:A:372:VAL:HG23	2.21	0.41
1:A:433:LEU:HD23	1:A:436:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:ILE:HA	1:A:863:ILE:HD13	2.00	0.41
1:A:851:ILE:HG23	1:A:856:ARG:CZ	2.51	0.41
2:B:646:TRP:CZ2	2:B:654:ARG:HG3	2.56	0.41
2:B:562:GLN:HG3	4:B:2030:HOH:O	2.22	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	590/638 (92%)	564 (96%)	22 (4%)	4 (1%)	26	51
2	B	597/638 (94%)	576 (96%)	15 (2%)	6 (1%)	19	39
All	All	1187/1276 (93%)	1140 (96%)	37 (3%)	10 (1%)	24	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	742	GLN
1	A	310	VAL
1	A	651	GLY
2	B	651	GLY
2	B	743	GLY
1	A	551	LYS
2	B	551	LYS
2	B	791	SER
1	A	791	SER
2	B	406	ALA

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	520/555 (94%)	483 (93%)	37 (7%)	18 36
2	B	516/555 (93%)	481 (93%)	35 (7%)	20 39
All	All	1036/1110 (93%)	964 (93%)	72 (7%)	19 38

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	THR
1	A	310	VAL
1	A	317	SER
1	A	318	SER
1	A	326	LEU
1	A	352	ARG
1	A	355	LYS
1	A	374	GLU
1	A	389[A]	ARG
1	A	389[B]	ARG
1	A	400	LYS
1	A	426	GLU
1	A	443	LEU
1	A	450	VAL
1	A	453	MET
1	A	478	LEU
1	A	481	ARG
1	A	492	ASN
1	A	581	ARG
1	A	585	THR
1	A	594	ARG
1	A	639	LEU
1	A	641	LYS
1	A	650	LYS
1	A	676	ASN
1	A	698	LYS
1	A	710	SER

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Mol	Chain	Res	Type
1	A	749	ARG
1	A	802	GLN
1	A	841	LYS
1	A	842	ARG
1	A	851	ILE
1	A	863	ILE
1	A	873	LEU
1	A	878	GLU
1	A	880	LEU
1	A	887	LYS
2	B	270	THR
2	B	301	THR
2	B	317	SER
2	B	318	SER
2	B	326	LEU
2	B	329	LYS
2	B	338	THR
2	B	342	MET
2	B	355	LYS
2	B	361	ARG
2	B	374	GLU
2	B	389	ARG
2	B	400	LYS
2	B	419	ASP
2	B	433	LEU
2	B	435	ASP
2	B	443	LEU
2	B	450	VAL
2	B	481	ARG
2	B	575	LYS
2	B	581	ARG
2	B	585	THR
2	B	594	ARG
2	B	642	LYS
2	B	650	LYS
2	B	676	ASN
2	B	698	LYS
2	B	710	SER
2	B	746	TRP
2	B	749	ARG
2	B	802	GLN
2	B	841	LYS

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Mol	Chain	Res	Type
2	B	863	ILE
2	B	878	GLU
2	B	888	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	555	GLN
1	A	562	GLN
1	A	621	GLN
1	A	682	ASN
1	A	704	GLN
1	A	760	GLN
1	A	768	HIS
1	A	802	GLN
1	A	835	ASN
2	B	339	GLN
2	B	452	ASN
2	B	548	ASN
2	B	555	GLN
2	B	621	GLN
2	B	682	ASN
2	B	704	GLN
2	B	742	GLN
2	B	760	GLN
2	B	768	HIS
2	B	802	GLN
2	B	835	ASN

5.3.3 RNA

There are no RNA molecules 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 4 ligands modelled in this entry, 4 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, 95^{th} 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	593/638 (92%)	-0.08	35 (5%)	26	19	28, 55, 98, 152	11 (1%)
2	B	603/638 (94%)	0.17	48 (7%)	15	10	32, 66, 118, 155	11 (1%)
All	All	1196/1276 (93%)	0.04	83 (6%)	20	14	28, 60, 111, 155	22 (1%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	455	ALA	9.4
2	B	637	HIS	8.2
2	B	470	SER	6.8
1	A	472	ALA	6.8
1	A	746	TRP	6.4
2	B	317	SER	6.2
2	B	744	ALA	5.8
2	B	316	ALA	5.8
1	A	744	ALA	5.7
1	A	313	THR	5.5
2	B	638	LEU	5.3
2	B	410	ALA	5.1
1	A	317	SER	5.1
2	B	416	ASN	5.1
2	B	472	ALA	5.1
1	A	473	ILE	5.0
1	A	474	TRP	5.0
2	B	745	GLY	4.9
1	A	470	SER	4.8
2	B	473	ILE	4.7
1	A	315	SER	4.5
2	B	409	ALA	4.5
1	A	316	ALA	4.4
2	B	743	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	636	PRO	4.2
1	A	795	TRP	4.2
2	B	296	GLU	4.1
1	A	743	GLY	3.8
2	B	417	GLN	3.8
2	B	419	ASP	3.8
1	A	268	PRO	3.8
2	B	269	GLU	3.7
1	A	745	GLY	3.7
2	B	420	SER	3.6
2	B	315	SER	3.5
2	B	344	ASP	3.4
2	B	585	THR	3.4
2	B	288	ASN	3.4
2	B	274	ASP	3.3
1	A	314	GLY	3.3
2	B	429	GLU	3.3
1	A	343	THR	3.3
2	B	268	PRO	3.3
2	B	763	SER	3.2
2	B	591	ILE	3.0
1	A	876	ASN	2.9
2	B	289	SER	2.8
2	B	474	TRP	2.8
1	A	637	HIS	2.8
2	B	600	SER	2.7
2	B	345	THR	2.7
1	A	471	ARG	2.7
2	B	742	GLN	2.6
1	A	311	LYS	2.6
1	A	792	ARG	2.6
1	A	318	SER	2.5
1	A	886	MET	2.5
1	A	742	GLN	2.5
2	B	270	THR	2.5
2	B	343	THR	2.5
2	B	293	TYR	2.5
1	A	636	PRO	2.4
2	B	290	THR	2.4
2	B	471	ARG	2.4
1	A	885	SER	2.4
1	A	721	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	795	TRP	2.3
2	B	592	ILE	2.3
2	B	408	MET	2.3
1	A	786	HIS	2.3
2	B	314	GLY	2.3
1	A	288	ASN	2.2
2	B	372	VAL	2.2
1	A	420	SER	2.1
1	A	372	VAL	2.1
1	A	601	GLY	2.1
2	B	404	THR	2.1
2	B	405	ASN	2.1
1	A	345	THR	2.1
1	A	269	GLU	2.1
2	B	558	PRO	2.0
2	B	311	LYS	2.0
1	A	404	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, 95^{th} 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	ZN	A	1890	1/1	0.99	0.08	-0.73	49,49,49,49	0
3	ZN	B	1891	1/1	0.99	0.05	-1.83	73,73,73,73	0
3	ZN	A	1889	1/1	0.99	0.05	-2.34	53,53,53,53	0
3	ZN	B	1890	1/1	0.99	0.06	-3.85	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.