



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:15 AM GMT

PDB ID : 2WHX
Title : A SECOND CONFORMATION OF THE NS3 PROTEASE-HELICASE
FROM DENGUE VIRUS
Authors : Luo, D.; Lescar, J.
Deposited on : 2009-05-07
Resolution : 2.20 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

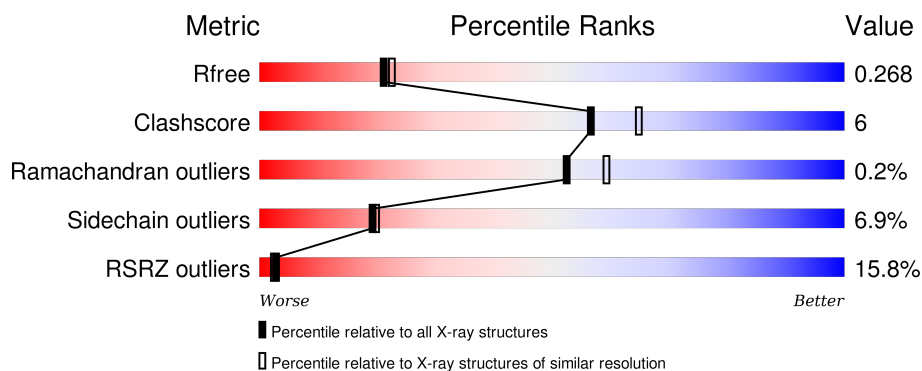
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	618	<div> <div>14%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div> </div>
2	C	14	<div> <div>50%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4860 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 SERINE PROTEASE/NTPASE/HELICASE NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4584	2897	820	846	21			

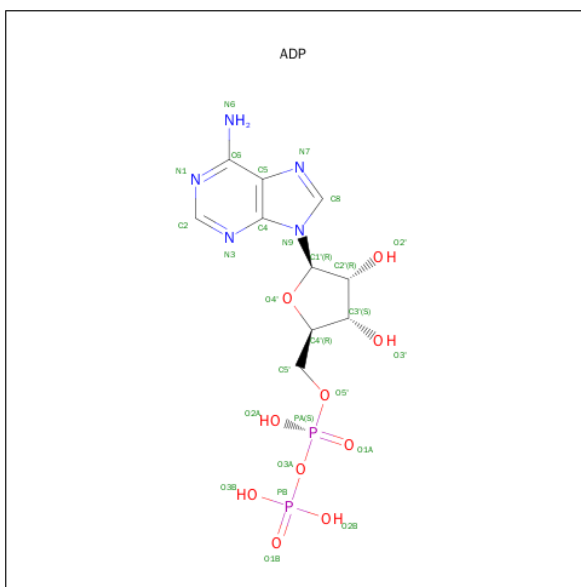
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	LYS	ARG	CONFLICT	UNP Q2YHF0
A	250	ASP	GLU	CONFLICT	UNP Q2YHF0
A	292	CYS	SER	CONFLICT	UNP Q2YHF0
A	321	SER	THR	CONFLICT	UNP Q2YHF0
A	381	ARG	LYS	CONFLICT	UNP Q2YHF0
A	480	LYS	ARG	CONFLICT	UNP Q2YHF0

- Molecule 2 is a protein called SERINE PROTEASE SUBUNIT NS2B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	0	0	0
			109	68	18	23			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

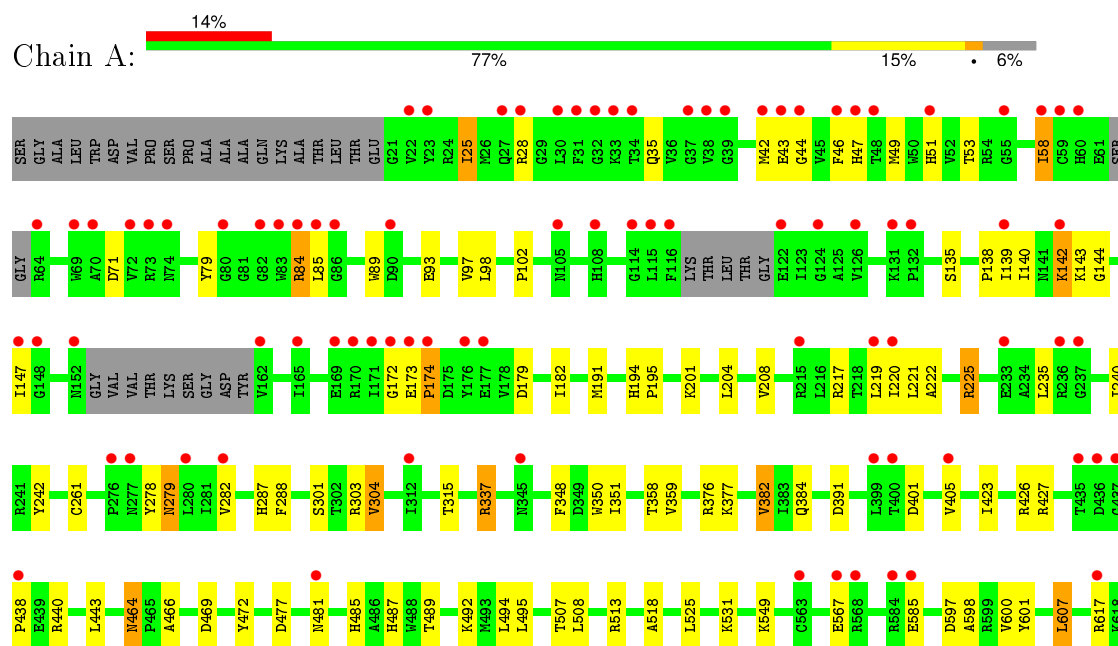
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	137	Total	O	0	0
			137	137		

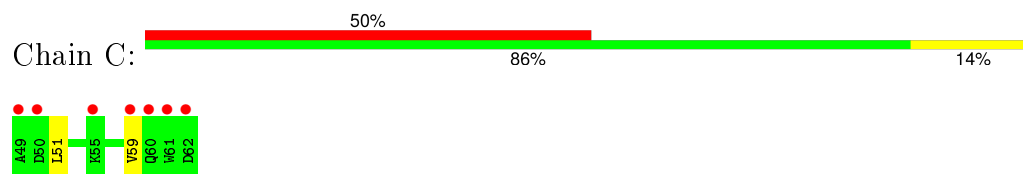
3 Residue-property plots

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: SERINE PROTEASE/NTPASE/HELICASE NS3



- Molecule 2: SERINE PROTEASE SUBUNIT NS2B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.42Å 87.72Å 75.78Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	19.87 – 2.20 19.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.87-2.20) 90.4 (19.87-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.228 , 0.272 0.226 , 0.268	Depositor DCC
R_{free} test set	1555 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31302 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4860	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, ADP, CL

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	0.39	0/4687	0.56	0/6346
2	C	0.38	0/110	0.57	0/149
All	All	0.39	0/4797	0.56	0/6495

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	4584	0	4534	57	0
2	C	109	0	101	2	0
3	A	27	0	12	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	137	0	0	2	0
All	All	4860	0	4647	57	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 6.

All (57) 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:43:GLU:CB	1:A:44:GLY:HA2	1.90	1.00
1:A:47:HIS:HE1	1:A:84:ARG:H	1.29	0.80
1:A:58:ILE:HG22	2:C:51:LEU:HB3	1.71	0.73
1:A:278:TYR:O	1:A:303:ARG:NH2	2.22	0.72
1:A:93:GLU:CB	1:A:142:LYS:HE3	2.22	0.70
1:A:492:LYS:HE3	6:A:2109:HOH:O	1.90	0.70
1:A:301:SER:O	1:A:304:VAL:HG12	1.92	0.70
1:A:47:HIS:CE1	1:A:84:ARG:H	2.09	0.68
1:A:485:HIS:HD2	1:A:487:HIS:H	1.39	0.68
1:A:217:ARG:H	1:A:279:ASN:HD21	1.41	0.67
1:A:43:GLU:CB	1:A:44:GLY:CA	2.72	0.63
1:A:97:VAL:HG22	1:A:139:ILE:HG12	1.84	0.60
1:A:337:ARG:HD2	1:A:350:TRP:CE2	2.37	0.58
1:A:89:TRP:HB2	1:A:147:ILE:HD13	1.84	0.58
1:A:438:PRO:O	1:A:440:ARG:NH1	2.37	0.57
1:A:597:ASP:O	1:A:600:VAL:HG22	2.06	0.56
1:A:235:LEU:HB2	1:A:240:ILE:HD13	1.87	0.56
1:A:98:LEU:HB3	1:A:138:PRO:HG2	1.87	0.55
1:A:179:ASP:O	1:A:182:ILE:HG12	2.07	0.55
1:A:49:MET:CE	1:A:135:SER:HB3	2.37	0.55
1:A:598:ALA:HA	1:A:601:TYR:CE1	2.43	0.54
1:A:601:TYR:HA	1:A:607:LEU:HG	1.89	0.53
1:A:464:ASN:HD22	1:A:464:ASN:C	2.12	0.53
1:A:426:ARG:HD2	1:A:472:TYR:OH	2.09	0.52
1:A:348:PHE:HB3	1:A:351:ILE:HD12	1.93	0.51
1:A:35:GLN:HB3	1:A:102:PRO:HB3	1.92	0.50
1:A:49:MET:HE1	1:A:135:SER:HB3	1.94	0.50
1:A:208:VAL:HG21	1:A:220:ILE:HD11	1.95	0.49
1:A:287:HIS:CD2	1:A:287:HIS:H	2.31	0.48
1:A:194:HIS:HD2	1:A:195:PRO:O	1.97	0.48
1:A:358:THR:HG21	1:A:423:ILE:HD12	1.94	0.48
1:A:204:LEU:HD13	1:A:282:VAL:HG11	1.96	0.48
1:A:173:GLU:HB2	1:A:174:PRO:O	2.14	0.47
1:A:222:ALA:O	1:A:261:CYS:HA	2.14	0.47
1:A:287:HIS:CD2	1:A:315:THR:OG1	2.68	0.46
1:A:140:ILE:HD12	2:C:59:VAL:HG13	1.96	0.46
1:A:172:GLY:HA3	1:A:173:GLU:HA	1.59	0.45
1:A:359:VAL:HG22	1:A:405:VAL:CG2	2.45	0.45
1:A:49:MET:HE3	1:A:51:HIS:HE1	1.81	0.45
1:A:47:HIS:HE1	1:A:84:ARG:N	2.07	0.45
1:A:469:ASP:HA	6:A:2099:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HG2	1:A:242:TYR:OH	2.16	0.44
1:A:376:ARG:HH12	1:A:384:GLN:HE21	1.66	0.44
1:A:217:ARG:N	1:A:279:ASN:HD21	2.12	0.44
1:A:464:ASN:ND2	1:A:466:ALA:H	2.16	0.43
1:A:143:LYS:HA	1:A:144:GLY:HA2	1.85	0.43
1:A:46:PHE:HB3	1:A:79:TYR:HB2	2.00	0.43
1:A:464:ASN:HD22	1:A:466:ALA:H	1.67	0.43
1:A:287:HIS:HD2	1:A:315:THR:OG1	2.01	0.43
1:A:219:LEU:HD21	1:A:221:LEU:HD21	2.01	0.42
1:A:507:THR:OG1	1:A:513:ARG:NH1	2.53	0.42
1:A:492:LYS:HD3	1:A:518:ALA:HB3	2.00	0.42
1:A:25:ILE:CD1	1:A:53:THR:HG22	2.50	0.42
1:A:173:GLU:N	1:A:174:PRO:HA	2.35	0.42
1:A:337:ARG:HD2	1:A:350:TRP:CZ2	2.55	0.41
1:A:42:MET:H	1:A:43:GLU:HA	1.86	0.40
1:A:376:ARG:HG3	1:A:382:VAL:HG13	2.02	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	574/618 (93%)	549 (96%)	24 (4%)	1 (0%)	52	59
2	C	12/14 (86%)	10 (83%)	2 (17%)	0	100	100
All	All	586/632 (93%)	559 (95%)	26 (4%)	1 (0%)	52	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	PRO

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	484/523 (92%)	450 (93%)	34 (7%)	19	19
2	C	11/11 (100%)	11 (100%)	0	100	100
All	All	495/534 (93%)	461 (93%)	34 (7%)	19	20

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	28	ARG
1	A	58	ILE
1	A	71	ASP
1	A	84	ARG
1	A	85	LEU
1	A	142	LYS
1	A	191	MET
1	A	201	LYS
1	A	225	ARG
1	A	279	ASN
1	A	288	PHE
1	A	304	VAL
1	A	337	ARG
1	A	377	LYS
1	A	382	VAL
1	A	391	ASP
1	A	401	ASP
1	A	427	ARG
1	A	443	LEU
1	A	464	ASN
1	A	477	ASP
1	A	481	ASN
1	A	489	THR
1	A	494	LEU
1	A	495	LEU
1	A	508	LEU

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Mol	Chain	Res	Type
1	A	525	LEU
1	A	531	LYS
1	A	549	LYS
1	A	567	GLU
1	A	585	GLU
1	A	607	LEU
1	A	617	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	51	HIS
1	A	141	ASN
1	A	194	HIS
1	A	279	ASN
1	A	287	HIS
1	A	329	ASN
1	A	384	GLN
1	A	456	GLN
1	A	464	ASN
1	A	471	GLN
1	A	481	ASN
1	A	485	HIS
1	A	576	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, 3 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	$\# Z > 2$
3	ADP	A	1619	4	22,29,29	1.08	1 (4%)	27,45,45	1.96	4 (14%)

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
3	ADP	A	1619	4	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1619	ADP	C5-C4	3.18	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1619	ADP	N3-C2-N1	-8.01	122.76	128.89
3	A	1619	ADP	C4-C5-N7	-3.29	106.45	109.48
3	A	1619	ADP	PA-O3A-PB	-2.55	124.11	132.67
3	A	1619	ADP	C1'-N9-C4	-2.25	123.55	126.94

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 [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	582/618 (94%)	0.72	87 (14%) 3 3	14, 20, 26, 34	0
2	C	14/14 (100%)	2.02	7 (50%) 0 0	23, 24, 25, 26	0
All	All	596/632 (94%)	0.75	94 (15%) 3 2	14, 20, 26, 34	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	MET	7.5
1	A	116	PHE	5.6
1	A	82	GLY	5.6
1	A	399	LEU	5.4
1	A	80	GLY	5.2
1	A	172	GLY	5.2
1	A	44	GLY	5.0
1	A	177	GLU	4.9
1	A	55	GLY	4.7
1	A	585	GLU	4.7
1	A	27	GLN	4.6
1	A	122	GLU	4.6
1	A	400	THR	4.6
1	A	126	VAL	4.6
1	A	132	PRO	4.5
1	A	69	TRP	4.4
1	A	58	ILE	4.4
1	A	584	ARG	4.4
1	A	171	ILE	4.4
1	A	85	LEU	4.3
1	A	72	VAL	4.3
1	A	70	ALA	4.3
1	A	236	ARG	4.2
1	A	173	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	174	PRO	4.0
1	A	131	LYS	3.9
1	A	73	ARG	3.9
2	C	50	ASP	3.7
1	A	31	PHE	3.7
1	A	176	TYR	3.6
1	A	86	GLY	3.6
1	A	43	GLU	3.5
2	C	61	TRP	3.5
1	A	165	ILE	3.5
1	A	568	ARG	3.5
1	A	30	LEU	3.5
1	A	28	ARG	3.4
1	A	170	ARG	3.4
1	A	90	ASP	3.3
1	A	147	ILE	3.2
1	A	59	CYS	3.2
1	A	32	GLY	3.2
1	A	84	ARG	3.2
1	A	237	GLY	3.1
1	A	83	TRP	3.0
1	A	60	HIS	3.0
1	A	114	GLY	3.0
1	A	277	ASN	3.0
2	C	62	ASP	2.9
1	A	162	VAL	2.9
1	A	105	ASN	2.9
1	A	169	GLU	2.9
2	C	60	GLN	2.9
1	A	39	GLY	2.9
1	A	233	GLU	2.8
2	C	49	ALA	2.8
1	A	280	LEU	2.8
1	A	115	LEU	2.7
2	C	55	LYS	2.7
1	A	567	GLU	2.7
1	A	282	VAL	2.7
1	A	124	GLY	2.7
1	A	435	THR	2.7
1	A	23	TYR	2.6
1	A	312	ILE	2.6
1	A	22	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	33	LYS	2.6
1	A	481	ASN	2.6
1	A	219	LEU	2.5
1	A	563	CYS	2.5
1	A	437	GLY	2.5
1	A	276	PRO	2.5
1	A	46	PHE	2.5
1	A	617	ARG	2.4
1	A	139	ILE	2.4
1	A	220	ILE	2.4
1	A	142	LYS	2.4
2	C	59	VAL	2.3
1	A	152	ASN	2.3
1	A	38	VAL	2.3
1	A	345	ASN	2.3
1	A	436	ASP	2.3
1	A	64	ARG	2.3
1	A	74	ASN	2.2
1	A	405	VAL	2.1
1	A	438	PRO	2.1
1	A	108	HIS	2.1
1	A	37	GLY	2.1
1	A	51	HIS	2.1
1	A	47	HIS	2.0
1	A	148	GLY	2.0
1	A	215	ARG	2.0
1	A	34	THR	2.0
1	A	48	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	ADP	A	1619	27/27	0.90	0.17	0.72	26,36,46,46	0
4	MN	A	1620	1/1	1.00	0.12	-1.31	25,25,25,25	0
5	CL	A	1621	1/1	0.99	0.06	-2.08	37,37,37,37	0
5	CL	A	1622	1/1	0.98	0.07	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.