Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2022 – 08:10 PM JST

PDB ID	:	7XDS
Title	:	Crystal structure of wheat stem rust effector AvrSr35
Authors	:	Ouyang, S.Y.; Zhao, Y.B.
Deposited on	:	2022-03-28
Resolution	:	2.06 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:

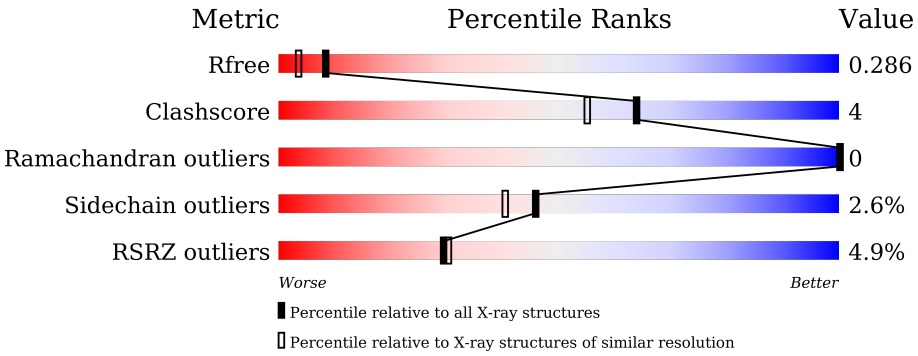
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.06 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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	575	2% 57% 7% 36%
1	B	575	4% 59% 6% 35%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6188 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 AvrSr35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	Se	0	0	0
			3039	1951	496	583	2	7			
1	B	375	Total	C	N	O	S	Se	0	0	0
			3092	1988	506	589	2	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	HIS	-	expression tag	UNP A0A5B0N367
A	5	HIS	-	expression tag	UNP A0A5B0N367
A	6	HIS	-	expression tag	UNP A0A5B0N367
A	7	HIS	-	expression tag	UNP A0A5B0N367
A	8	HIS	-	expression tag	UNP A0A5B0N367
A	9	HIS	-	expression tag	UNP A0A5B0N367
A	10	SER	-	expression tag	UNP A0A5B0N367
A	11	SER	-	expression tag	UNP A0A5B0N367
A	12	GLY	-	expression tag	UNP A0A5B0N367
A	13	VAL	-	expression tag	UNP A0A5B0N367
A	14	ASP	-	expression tag	UNP A0A5B0N367
A	15	LEU	-	expression tag	UNP A0A5B0N367
A	16	GLY	-	expression tag	UNP A0A5B0N367
A	17	THR	-	expression tag	UNP A0A5B0N367
A	18	GLU	-	expression tag	UNP A0A5B0N367
A	19	ASN	-	expression tag	UNP A0A5B0N367
A	20	LEU	-	expression tag	UNP A0A5B0N367
A	21	TYR	-	expression tag	UNP A0A5B0N367
A	22	PHE	-	expression tag	UNP A0A5B0N367
A	23	GLN	-	expression tag	UNP A0A5B0N367
A	24	SER	-	expression tag	UNP A0A5B0N367
A	25	ASN	-	expression tag	UNP A0A5B0N367
B	4	HIS	-	expression tag	UNP A0A5B0N367
B	5	HIS	-	expression tag	UNP A0A5B0N367
B	6	HIS	-	expression tag	UNP A0A5B0N367

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP A0A5B0N367
B	8	HIS	-	expression tag	UNP A0A5B0N367
B	9	HIS	-	expression tag	UNP A0A5B0N367
B	10	SER	-	expression tag	UNP A0A5B0N367
B	11	SER	-	expression tag	UNP A0A5B0N367
B	12	GLY	-	expression tag	UNP A0A5B0N367
B	13	VAL	-	expression tag	UNP A0A5B0N367
B	14	ASP	-	expression tag	UNP A0A5B0N367
B	15	LEU	-	expression tag	UNP A0A5B0N367
B	16	GLY	-	expression tag	UNP A0A5B0N367
B	17	THR	-	expression tag	UNP A0A5B0N367
B	18	GLU	-	expression tag	UNP A0A5B0N367
B	19	ASN	-	expression tag	UNP A0A5B0N367
B	20	LEU	-	expression tag	UNP A0A5B0N367
B	21	TYR	-	expression tag	UNP A0A5B0N367
B	22	PHE	-	expression tag	UNP A0A5B0N367
B	23	GLN	-	expression tag	UNP A0A5B0N367
B	24	SER	-	expression tag	UNP A0A5B0N367
B	25	ASN	-	expression tag	UNP A0A5B0N367

- Molecule 2 is water.

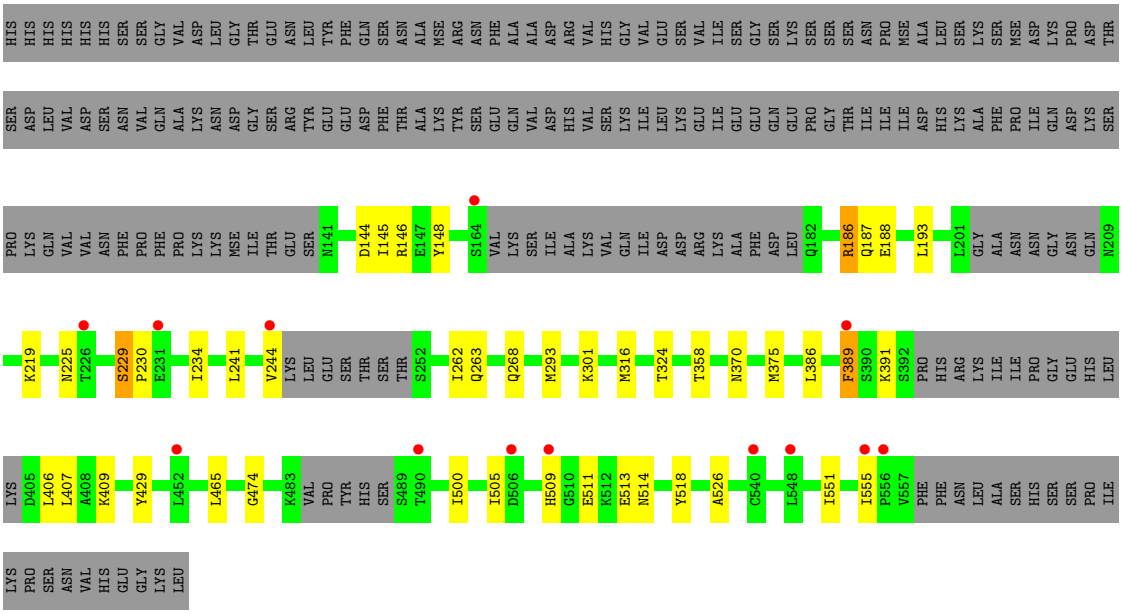
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	B	31	Total O 31 31	0	0

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.

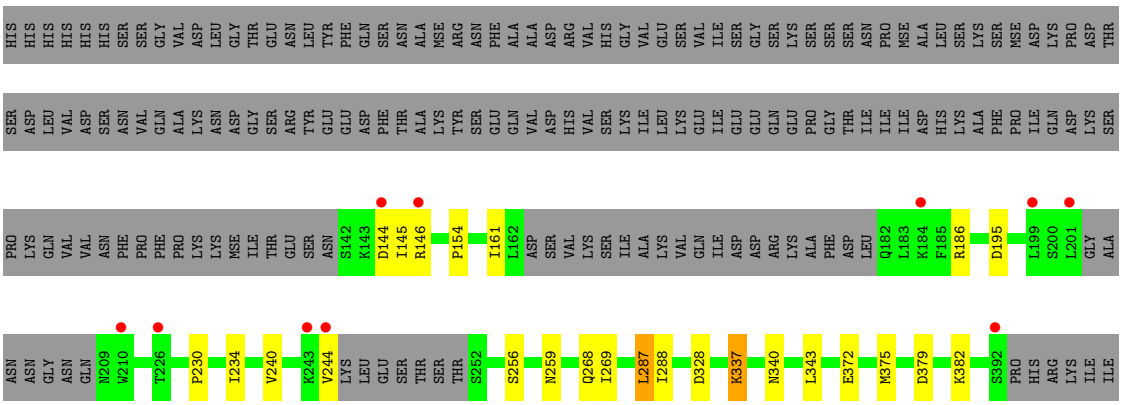
- Molecule 1: AvrSr35

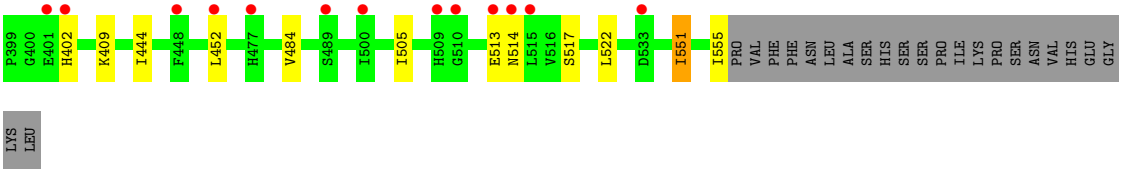
Chain A:



- Molecule 1: AvrSr35

Chain B:




P399
G400
E401
H402
K409
I444
F448
L452
H477
V484
S489
I500
I505
H509
G510
E513
N514
L515
V516
S517
L522
D533
I551
I555
PRO
VAL
PHE
PHE
ASN
LEU
ALA
SER
HIS
SER
SER
PRO
ILE
LYS
PRO
SER
ASN
VAL
HIS
GLU
GLY

LYS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.12Å 115.27Å 143.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.89 – 2.06 44.89 – 2.06	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.89-2.06) 97.8 (44.89-2.06)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.257 , 0.287 0.256 , 0.286	Depositor DCC
R_{free} test set	2758 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6188	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.58	0/3088	0.68	0/4137
1	B	0.53	0/3146	0.65	0/4216
All	All	0.55	0/6234	0.67	0/8353

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ARG	Sidechain
1	A	186	ARG	Sidechain

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	3039	0	3036	27	0
1	B	3092	0	3091	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	26	0	0	0	0
2	B	31	0	0	0	0
All	All	6188	0	6127	52	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 (52) 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:B:145:ILE:CD1	1:B:517:SER:HB3	1.74	1.18
1:B:145:ILE:HD11	1:B:517:SER:CB	1.80	1.11
1:B:186:ARG:HE	1:B:268:GLN:HB3	1.44	0.81
1:A:193:LEU:HD21	1:A:262:ILE:HD13	1.70	0.71
1:B:240:VAL:O	1:B:244:VAL:HG23	1.91	0.71
1:B:145:ILE:HD11	1:B:517:SER:HB3	0.85	0.70
1:B:161:ILE:HD11	1:B:522:LEU:HD23	1.76	0.66
1:B:328:ASP:OD2	1:B:337:LYS:HE2	1.96	0.65
1:B:551:ILE:HD13	1:B:555:ILE:HD11	1.77	0.65
1:B:145:ILE:HD13	1:B:514:ASN:O	1.97	0.64
1:B:244:VAL:HG13	1:B:259:ASN:ND2	2.14	0.63
1:A:551:ILE:O	1:A:555:ILE:HG12	2.01	0.60
1:B:379:ASP:HB3	1:B:382:LYS:HD2	1.85	0.58
1:B:337:LYS:NZ	1:B:340:ASN:HD22	2.02	0.58
1:B:328:ASP:CG	1:B:337:LYS:HE2	2.25	0.56
1:B:145:ILE:CD1	1:B:517:SER:CB	2.59	0.56
1:A:386:LEU:HD23	1:A:406:LEU:HD21	1.87	0.56
1:A:193:LEU:HD21	1:A:262:ILE:CD1	2.35	0.55
1:B:337:LYS:O	1:B:337:LYS:HD3	2.07	0.54
1:B:186:ARG:NE	1:B:268:GLN:HB3	2.21	0.54
1:A:241:LEU:HD13	1:A:293:MSE:SE	2.58	0.53
1:B:230:PRO:O	1:B:234:ILE:HG12	2.09	0.53
1:B:186:ARG:HD3	1:B:269:ILE:HD13	1.90	0.53
1:A:230:PRO:O	1:A:234:ILE:HG12	2.09	0.52
1:A:188:GLU:OE2	1:A:500:ILE:HD12	2.11	0.52
1:A:145:ILE:HD11	1:A:518:TYR:HB2	1.93	0.50
1:A:375:MSE:HB3	1:A:409:LYS:HD2	1.94	0.49
1:A:513:GLU:H	1:A:513:GLU:CD	2.15	0.49
1:B:161:ILE:HD11	1:B:522:LEU:CD2	2.43	0.48
1:A:186:ARG:NE	1:A:268:GLN:HB3	2.31	0.46
1:A:316:MSE:SE	1:A:474:GLY:HA2	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:CE1	1:A:511:GLU:HG3	2.51	0.46
1:B:375:MSE:HB3	1:B:409:LYS:HD3	1.99	0.45
1:A:389:PHE:CD1	1:A:389:PHE:O	2.70	0.45
1:A:244:VAL:HG11	1:A:263:GLN:HG3	2.00	0.44
1:A:389:PHE:CD1	1:A:389:PHE:C	2.91	0.43
1:B:244:VAL:HG13	1:B:259:ASN:HD21	1.81	0.43
1:A:391:LYS:HA	1:A:391:LYS:HD2	1.72	0.43
1:A:370:ASN:HB2	1:A:429:TYR:CD2	2.53	0.43
1:A:465:LEU:HD11	1:A:526:ALA:HA	2.00	0.42
1:B:484:VAL:O	1:B:505:ILE:HD13	2.19	0.42
1:A:324:THR:CG2	1:A:358:THR:HG22	2.49	0.42
1:A:187:GLN:HE22	1:A:225:ASN:HB3	1.85	0.42
1:A:219:LYS:HA	1:A:219:LYS:HD3	1.85	0.42
1:A:244:VAL:CG1	1:A:263:GLN:HG3	2.50	0.41
1:A:229:SER:O	1:A:230:PRO:C	2.59	0.41
1:A:144:ASP:HB3	1:A:514:ASN:HD21	1.86	0.41
1:B:551:ILE:CD1	1:B:555:ILE:HD11	2.46	0.41
1:B:234:ILE:HG23	1:B:287:LEU:HG	2.02	0.41
1:A:145:ILE:HD13	1:A:514:ASN:O	2.21	0.40
1:A:301:LYS:HE2	1:A:358:THR:HG21	2.03	0.40
1:B:288:ILE:HD12	1:B:343:LEU:HG	2.04	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	357/575 (62%)	349 (98%)	8 (2%)	0	100	100
1	B	365/575 (64%)	360 (99%)	5 (1%)	0	100	100
All	All	722/1150 (63%)	709 (98%)	13 (2%)	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	346/520 (66%)	341 (99%)	5 (1%)	67	64
1	B	351/520 (68%)	338 (96%)	13 (4%)	34	27
All	All	697/1040 (67%)	679 (97%)	18 (3%)	46	40

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	SER
1	A	389	PHE
1	A	407	LEU
1	A	505	ILE
1	A	509	HIS
1	B	144	ASP
1	B	146	ARG
1	B	154	PRO
1	B	195	ASP
1	B	256	SER
1	B	287	LEU
1	B	337	LYS
1	B	372	GLU
1	B	402	HIS
1	B	444	ILE
1	B	452	LEU
1	B	513	GLU
1	B	551	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN

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Mol	Chain	Res	Type
1	A	189	ASN
1	A	218	ASN
1	A	257	GLN
1	A	281	GLN
1	A	319	ASN
1	A	468	GLN
1	A	471	GLN
1	A	514	ASN
1	B	182	GLN
1	B	187	GLN
1	B	189	ASN
1	B	259	ASN
1	B	278	GLN
1	B	340	ASN
1	B	378	GLN
1	B	477	HIS
1	B	514	ASN
1	B	545	GLN
1	B	549	ASN
1	B	554	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	362/575 (62%)	0.49	13 (3%)	42	45	7, 27, 53, 81	0
1	B	368/575 (64%)	0.57	23 (6%)	20	20	8, 28, 56, 90	0
All	All	730/1150 (63%)	0.53	36 (4%)	29	30	7, 27, 54, 90	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	SER	5.5
1	B	244	VAL	4.8
1	B	452	LEU	3.8
1	B	477	HIS	3.6
1	B	448	PHE	3.5
1	A	555	ILE	3.5
1	B	515	LEU	3.2
1	B	510	GLY	3.0
1	A	226	THR	3.0
1	A	452	LEU	3.0
1	B	509	HIS	2.9
1	B	513	GLU	2.9
1	B	392	SER	2.9
1	A	506	ASP	2.6
1	B	146	ARG	2.6
1	B	533	ASP	2.6
1	A	540	CYS	2.5
1	B	201	LEU	2.5
1	B	199	LEU	2.4
1	B	144	ASP	2.4
1	B	210	TRP	2.3
1	B	489	SER	2.3
1	B	500	ILE	2.2
1	B	226	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	389	PHE	2.2
1	B	402	HIS	2.2
1	B	184	LYS	2.2
1	B	514	ASN	2.2
1	A	556	PRO	2.2
1	A	548	LEU	2.1
1	B	243	LYS	2.1
1	A	231	GLU	2.1
1	A	244	VAL	2.1
1	A	490	THR	2.1
1	A	509	HIS	2.1
1	B	401	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.