W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:19 PM GMT

PDB ID	:	4L51
Title	:	Crystal structures of the LsrR proteins complexed with phospho-AI-2 and its two different analogs reveal distinct mechanisms for ligand recognition
Authors	:	Ryu, K.S.; Ha, J.H.; Eo, Y.
Deposited on	:	2013-06-10
Resolution	:	1.90 Å(reported)

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

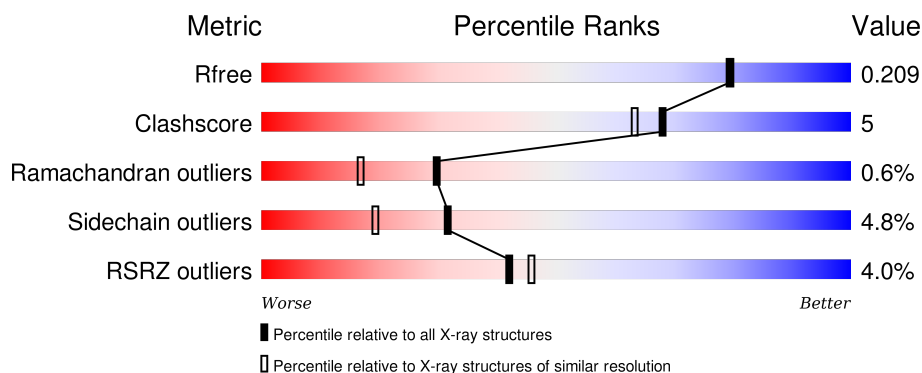|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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:
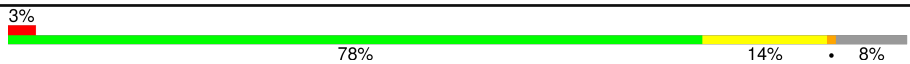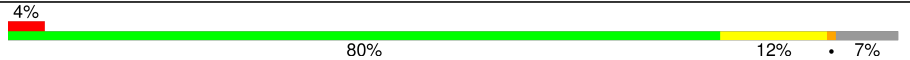*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Rfree		0.209
Clashscore		5
Ramachandran outliers		0.6%
Sidechain outliers		4.8%
RSRZ outliers		4.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	266	3% 78% 14% • 8%
1	B	266	4% 80% 12% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4005 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 Transcriptional regulator LsrR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	2	0
			1814	1135	325	344	10			
1	B	248	Total	C	N	O	S	0	3	0
			1835	1150	328	347	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	SER	-	EXPRESSION TAG	UNP P76141
B	52	SER	-	EXPRESSION TAG	UNP P76141

- Molecule 2 is SUGAR (5-O-PHOSPHONO-ALPHA-D-RIBOFURANOSE) (three-letter code: HSX) (formula: $C_5H_{11}O_8P$).

HSX
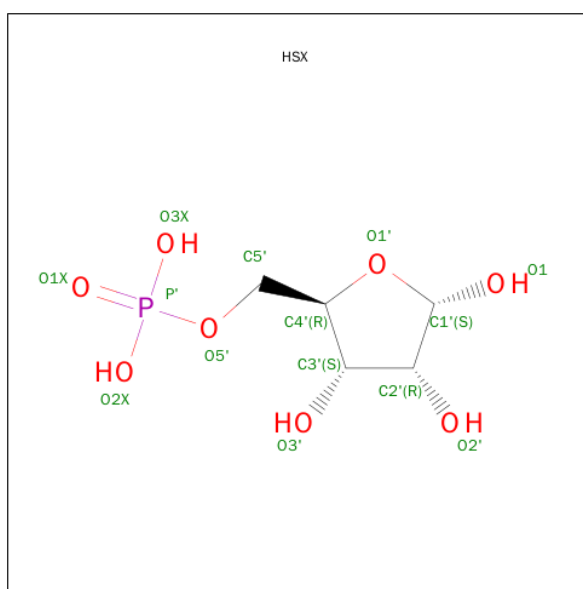
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			14	5	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 14	C 5	O 8	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total 161	O 161	0	0
3	B	167	Total 167	O 167	0	0

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: Transcriptional regulator LsrR

Chain A:

- Molecule 1: Transcriptional regulator LsrR

Chain B:
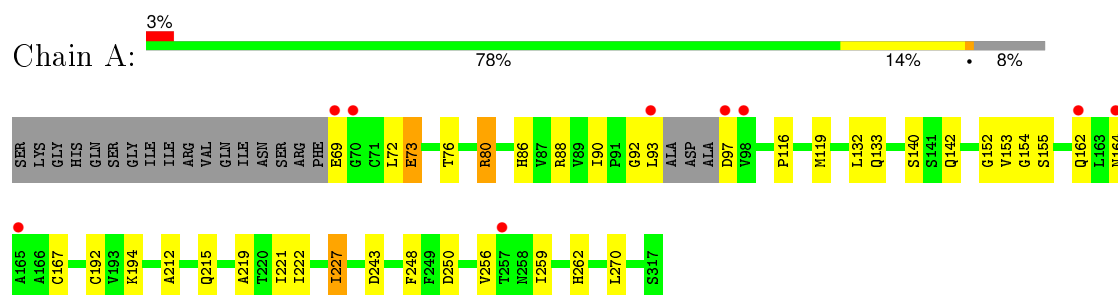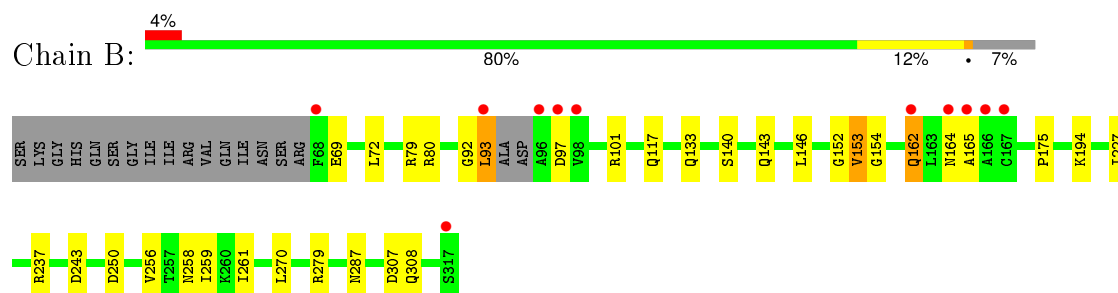
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	116.61Å　116.61Å　79.74Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	42.70　–　1.90 42.66　–　1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.70-1.90) 99.3 (42.66-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.53 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.166　,　0.204 0.175　,　0.209	Depositor DCC
R_{free} test set	2454 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.2	EDS
Estimated twinning fraction	0.040 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	0 of 48280 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4005	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 3.64% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HSX

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	0.91	0/1834	0.99	3/2474 (0.1%)
1	B	0.93	1/1859 (0.1%)	1.05	11/2508 (0.4%)
All	All	0.92	1/3693 (0.0%)	1.02	14/4982 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	VAL	CB-CG2	5.20	1.63	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	B	80	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	80	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	B	101	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	80	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	93	LEU	CA-CB-CG	5.93	128.94	115.30
1	B	79	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	80	ARG	CB-CG-CD	5.42	125.69	111.60
1	B	279	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	153	VAL	N-CA-CB	-5.24	99.98	111.50
1	A	119	MET	CG-SD-CE	5.21	108.53	100.20
1	A	250	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	B	250	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	B	307	ASP	CB-CG-OD1	5.06	122.86	118.30

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	1814	0	1874	22	0
1	B	1835	0	1894	14	0
2	A	14	0	9	0	0
2	B	14	0	8	1	0
3	A	161	0	0	4	0
3	B	167	0	0	3	0
All	All	4005	0	3785	35	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 5.

All (35) 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)
2:B:401:HSX:C1'	2:B:401:HSX:O1'	1.67	1.34
1:B:133:GLN:HG2	1:B:162:GLN:HG3	1.52	0.92
1:A:133:GLN:HG2	1:A:162:GLN:HG3	1.59	0.84
1:B:237[B]:ARG:CZ	3:B:664:HOH:O	2.29	0.80
1:A:248:PHE:H	1:A:262:HIS:CE1	2.01	0.79
1:B:237[B]:ARG:NH1	3:B:664:HOH:O	2.24	0.70
1:A:69:GLU:O	1:A:73:GLU:OE1	2.15	0.64
1:A:194:LYS:HG3	3:A:760:HOH:O	1.96	0.64
1:A:86:HIS:HE1	3:A:614:HOH:O	1.81	0.63
1:A:248:PHE:H	1:A:262:HIS:HE1	1.46	0.61
1:A:133:GLN:HG2	1:A:162:GLN:CG	2.33	0.57
1:A:212:ALA:H	1:A:215:GLN:HE21	1.53	0.56
1:A:116:PRO:HG3	1:A:142:GLN:NE2	2.23	0.53
1:B:140:SER:OG	1:B:164:ASN:ND2	2.41	0.53
1:A:76:THR:O	1:A:80:ARG:HG3	2.10	0.52
1:B:152[A]:GLY:O	1:B:154:GLY:N	2.44	0.51
1:B:227:ILE:HG22	1:B:261:ILE:HD12	1.94	0.50
1:A:133:GLN:CG	1:A:162:GLN:HG3	2.37	0.50
1:B:194:LYS:HG3	3:B:520:HOH:O	2.12	0.50
1:A:162:GLN:HG2	1:B:165:ALA:HB2	1.94	0.48
1:A:140:SER:OG	1:A:164:ASN:ND2	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:VAL:HB	1:A:259:ILE:HD12	1.95	0.47
1:A:227:ILE:HD13	1:A:227:ILE:O	2.16	0.45
1:A:92:GLY:HA2	3:A:728:HOH:O	2.16	0.45
1:A:152[B]:GLY:O	1:A:155:SER:OG	2.31	0.45
1:B:92:GLY:H	1:B:308:GLN:HE21	1.63	0.45
1:A:219:ALA:O	1:A:222:ILE:HG22	2.16	0.44
1:A:192:CYS:SG	1:B:175:PRO:HB3	2.58	0.44
1:B:256:VAL:HB	1:B:259:ILE:HD12	2.01	0.43
1:A:132:LEU:HA	1:A:132:LEU:HD23	1.78	0.42
1:B:117:GLN:HA	1:B:143:GLN:O	2.19	0.42
1:A:167:CYS:HA	3:A:691:HOH:O	2.20	0.42
1:B:258:ASN:OD1	1:B:258:ASN:N	2.50	0.42
1:A:152[A]:GLY:O	1:A:154:GLY:N	2.53	0.41
1:B:162:GLN:HE21	1:B:162:GLN:HA	1.85	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	244/266 (92%)	240 (98%)	3 (1%)	1 (0%)	39	27
1	B	247/266 (93%)	245 (99%)	0	2 (1%)	24	11
All	All	491/532 (92%)	485 (99%)	3 (1%)	3 (1%)	30	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	VAL
1	B	69	GLU
1	B	153	VAL

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	188/203 (93%)	178 (95%)	10 (5%)	28	16
1	B	190/203 (94%)	182 (96%)	8 (4%)	36	24
All	All	378/406 (93%)	360 (95%)	18 (5%)	31	19

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

Mol	Chain	Res	Type
1	A	72	LEU
1	A	73	GLU
1	A	88	ARG
1	A	90	ILE
1	A	93	LEU
1	A	97	ASP
1	A	221	ILE
1	A	227	ILE
1	A	243	ASP
1	A	270	LEU
1	B	72	LEU
1	B	93	LEU
1	B	97	ASP
1	B	146	LEU
1	B	162	GLN
1	B	243	ASP
1	B	270	LEU
1	B	287	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	142	GLN
1	A	191	ASN
1	A	201	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	215	GLN
1	A	229	GLN
1	A	262	HIS
1	B	115	GLN
1	B	142	GLN
1	B	162	GLN
1	B	191	ASN
1	B	287	ASN
1	B	308	GLN

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 ⓘ

2 ligands are modelled in this entry.

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	#$|Z| > 2$
2	HSX	A	501	-	14,14,14	2.82	7 (50%)	18,21,21	2.21	6 (33%)
2	HSX	B	401	-	14,14,14	6.58	8 (57%)	18,21,21	3.03	6 (33%)

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
2	HSX	A	501	-	-	0/6/22/22	0/1/1/1
2	HSX	B	401	-	-	0/6/22/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HSX	C1'-C2'	-6.03	1.46	1.52
2	A	501	HSX	C1'-C2'	-5.28	1.47	1.52
2	B	401	HSX	O3'-C3'	-4.55	1.32	1.43
2	A	501	HSX	C2'-C3'	-4.10	1.42	1.53
2	B	401	HSX	O1'-C4'	-4.08	1.35	1.45
2	B	401	HSX	C2'-C3'	-3.73	1.43	1.53
2	A	501	HSX	O1'-C4'	-3.14	1.37	1.45
2	B	401	HSX	P'-O3X	-2.22	1.46	1.54
2	B	401	HSX	O5'-C5'	-2.21	1.35	1.44
2	A	501	HSX	P'-O1X	2.11	1.58	1.51
2	A	501	HSX	C3'-C4'	2.20	1.58	1.53
2	A	501	HSX	O1-C1'	3.18	1.50	1.39
2	B	401	HSX	O1-C1'	3.57	1.52	1.39
2	A	501	HSX	O1'-C1'	4.98	1.48	1.42
2	B	401	HSX	O1'-C1'	21.92	1.67	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HSX	C1'-C2'-C3'	-5.24	95.52	102.45
2	A	501	HSX	O3'-C3'-C2'	-3.63	100.03	111.83
2	A	501	HSX	O1'-C4'-C5'	-3.31	97.49	109.32
2	A	501	HSX	O2'-C2'-C3'	-2.67	103.13	111.83
2	B	401	HSX	O3'-C3'-C2'	-2.41	103.98	111.83
2	B	401	HSX	O2'-C2'-C3'	-2.10	105.00	111.83
2	B	401	HSX	C2'-C3'-C4'	2.44	107.63	102.61
2	A	501	HSX	O3'-C3'-C4'	2.85	119.59	111.05
2	B	401	HSX	O2'-C2'-C1'	3.01	119.81	111.62
2	A	501	HSX	O2'-C2'-C1'	3.45	121.00	111.62
2	A	501	HSX	O1-C1'-O1'	4.99	117.77	111.22
2	B	401	HSX	O1-C1'-O1'	9.80	124.09	111.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HSX	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	246/266 (92%)	-0.27	9 (3%)	45	49	12, 21, 49, 83	0
1	B	248/266 (93%)	-0.30	11 (4%)	38	41	12, 20, 45, 86	1 (0%)
All	All	494/532 (92%)	-0.29	20 (4%)	42	46	12, 21, 49, 86	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	ALA	9.9
1	B	68	PHE	6.9
1	A	69	GLU	4.6
1	B	93	LEU	4.5
1	A	93	LEU	3.9
1	B	165	ALA	3.9
1	A	98	VAL	3.8
1	A	97	ASP	3.7
1	B	166	ALA	3.5
1	A	165	ALA	3.4
1	B	97	ASP	3.3
1	B	317	SER	3.3
1	A	162	GLN	2.8
1	B	98	VAL	2.4
1	A	257	THR	2.4
1	B	167	CYS	2.3
1	B	162	GLN	2.2
1	A	70	GLY	2.2
1	B	164	ASN	2.1
1	A	164	ASN	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
2	HSX	A	501	14/14	0.98	0.09	0.42	16,24,38,38	0
2	HSX	B	401	14/14	0.97	0.07	-0.05	16,28,36,37	0

6.5 Other polymers (i)

There are no such residues in this entry.