



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 10:08 AM JST

PDB ID : 8XAS
Title : Crystal structure of AtARR1-DBD in complex with a DNA fragment
Authors : Li, J.X.; Zhou, C.M.; zhang, P.; Wang, J.W.
Deposited on : 2023-12-05
Resolution : 2.35 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)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

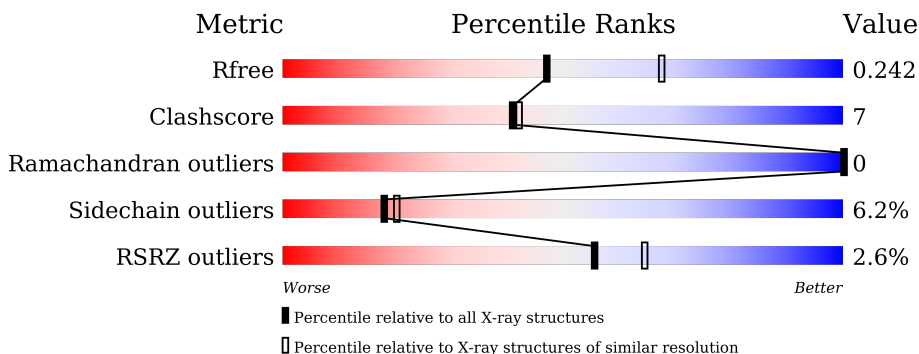
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	81	 % 62% 10% 27%
1	B	81	 2% 63% 12% 23%
1	C	81	 7% 65% 11% 22%
1	D	81	 % 59% 15% 26%
1	E	81	 % 53% 16% 27%
1	F	81	 2% 63% 11% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	X	25	 64% 36%
2	Y	25	 76% 24%
3	G	25	 76% 24%
3	H	25	 80% 20%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5285 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 Two-component response regulator ARR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	59	484	313	91	79	1	0	0	0
1	B	62	499	322	94	82	1	0	0	0
1	C	63	505	325	95	84	1	0	0	0
1	D	60	488	315	92	80	1	0	0	0
1	E	59	484	313	91	79	1	0	0	0
1	F	62	501	323	95	82	1	0	0	0

- Molecule 2 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	X	25	506	244	89	148	25	0	0	0
2	Y	25	506	244	89	148	25	0	0	0

- Molecule 3 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	G	25	519	249	93	152	25	0	0	0
3	H	25	519	249	93	152	25	0	0	0

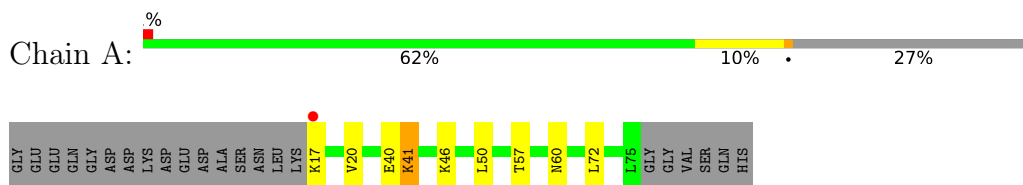
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	21	Total O 21 21	0	0
4	C	22	Total O 22 22	0	0
4	D	19	Total O 19 19	0	0
4	E	21	Total O 21 21	0	0
4	F	26	Total O 26 26	0	0
4	X	36	Total O 36 36	0	0
4	G	37	Total O 37 37	0	0
4	Y	32	Total O 32 32	0	0
4	H	35	Total O 35 35	0	0

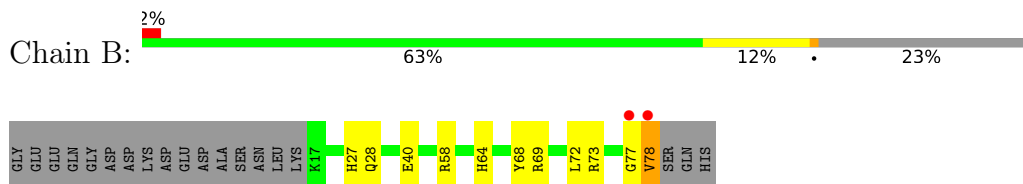
3 Residue-property plots [i](#)

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.

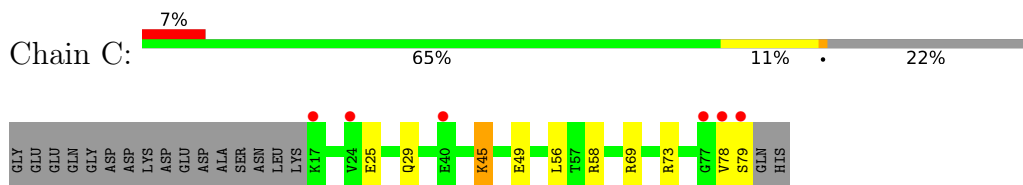
- Molecule 1: Two-component response regulator ARR1



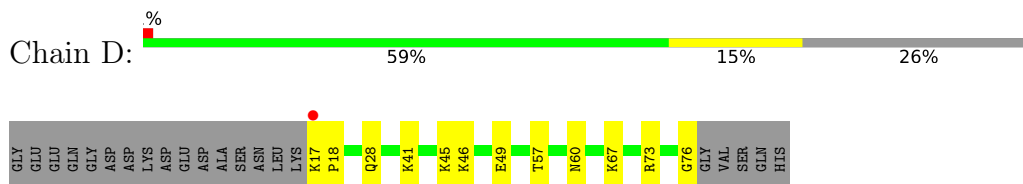
- Molecule 1: Two-component response regulator ARR1



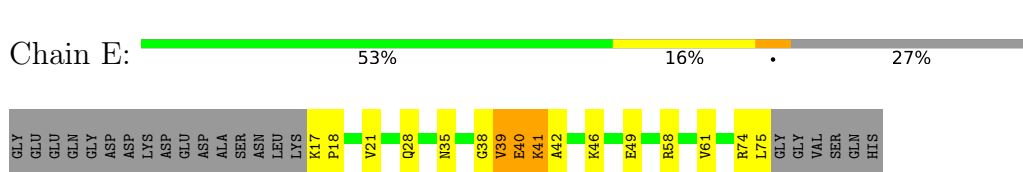
- Molecule 1: Two-component response regulator ARR1



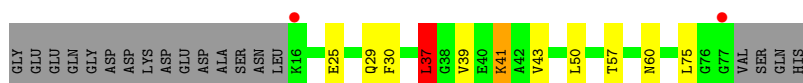
- Molecule 1: Two-component response regulator ARR1



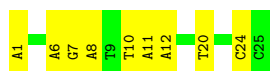
- Molecule 1: Two-component response regulator ARR1



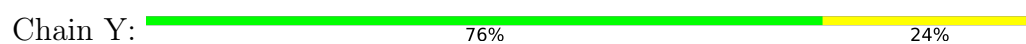
- Molecule 1: Two-component response regulator ARR1



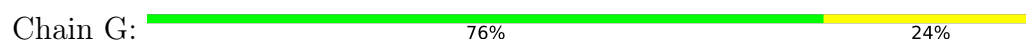
- Molecule 2: DNA (50-MER)



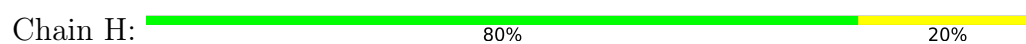
- Molecule 2: DNA (50-MER)



- Molecule 3: DNA (50-MER)



- Molecule 3: DNA (50-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.83Å 79.11Å 162.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.23 – 2.35 39.56 – 2.35	Depositor EDS
% Data completeness (in resolution range)	81.2 (38.23-2.35) 83.7 (39.56-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.197 , 0.242 0.197 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (5.51%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtrriage
Anisotropy	0.234	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5285	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3072e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.68	0/492	0.64	0/663
1	B	0.87	0/507	0.67	0/683
1	C	0.39	0/513	0.54	0/691
1	D	0.62	0/496	0.64	0/668
1	E	0.87	0/492	0.70	0/663
1	F	0.69	0/509	0.74	1/684 (0.1%)
2	X	1.02	1/566 (0.2%)	0.98	0/869
2	Y	0.98	1/566 (0.2%)	1.03	0/869
3	G	0.89	0/582	1.01	1/898 (0.1%)
3	H	0.90	0/582	1.08	0/898
All	All	0.82	2/5305 (0.0%)	0.85	2/7586 (0.0%)

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	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	1	DA	O3'-P	-5.69	1.54	1.61
2	X	12	DA	O3'-P	-5.11	1.55	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	37	LEU	CA-CB-CG	5.66	128.32	115.30
3	G	64	DT	OP2-P-O3'	5.18	116.59	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	40	GLU	Peptide

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	484	0	518	5	0
1	B	499	0	533	7	0
1	C	505	0	538	7	0
1	D	488	0	521	9	0
1	E	484	0	518	11	0
1	F	501	0	537	6	0
2	X	506	0	284	9	0
2	Y	506	0	284	9	0
3	G	519	0	286	4	0
3	H	519	0	286	8	0
4	A	25	0	0	2	0
4	B	21	0	0	0	0
4	C	22	0	0	2	0
4	D	19	0	0	2	0
4	E	21	0	0	0	0
4	F	26	0	0	1	0
4	G	37	0	0	1	0
4	H	35	0	0	1	1
4	X	36	0	0	3	0
4	Y	32	0	0	0	0
All	All	5285	0	4305	63	1

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 7.

All (63) 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:Y:25:DC:O2	3:H:55:DG:N2	1.68	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LYS:N	1:D:18:PRO:HD3	1.68	1.06
2:Y:25:DC:C2	3:H:55:DG:N2	2.22	0.99
2:X:10:DT:OP2	4:X:101:HOH:O	1.83	0.97
1:A:41:LYS:HE3	4:A:123:HOH:O	1.62	0.97
2:X:6:DA:H4'	2:X:7:DG:OP1	1.69	0.91
2:X:20:DT:OP2	4:X:102:HOH:O	1.88	0.90
1:D:17:LYS:N	1:D:18:PRO:CD	2.40	0.84
1:C:79:SER:O	4:C:102:HOH:O	2.11	0.69
1:E:41:LYS:O	1:E:41:LYS:HG3	1.93	0.68
2:X:24:DC:OP2	4:X:103:HOH:O	2.12	0.68
1:A:57:THR:H	1:A:60:ASN:HD22	1.43	0.66
1:D:57:THR:H	1:D:60:ASN:ND2	1.94	0.65
1:C:58:ARG:NH2	4:C:103:HOH:O	2.30	0.64
2:Y:25:DC:N3	3:H:55:DG:N1	2.46	0.63
1:B:27:HIS:HD2	1:B:64:HIS:NE2	1.97	0.63
1:F:57:THR:H	1:F:60:ASN:HD22	1.49	0.60
3:H:66:DG:OP2	4:H:101:HOH:O	2.17	0.58
1:B:69:ARG:O	1:B:73:ARG:HG3	2.03	0.58
2:X:6:DA:C4'	2:X:7:DG:OP1	2.47	0.58
1:C:73:ARG:HG2	1:C:78:VAL:HG13	1.85	0.57
2:Y:6:DA:H2''	2:Y:7:DG:O5'	2.08	0.54
1:E:46:LYS:NZ	1:E:49:GLU:OE1	2.38	0.53
2:X:11:DA:C2	3:G:70:DA:C2	2.97	0.53
1:C:25:GLU:HG2	1:C:29:GLN:HE21	1.73	0.53
2:X:1:DA:C8	2:X:1:DA:H5'	2.45	0.52
1:C:69:ARG:O	1:C:73:ARG:HG3	2.10	0.51
2:X:1:DA:H5'	2:X:1:DA:H8	1.74	0.51
1:D:57:THR:H	1:D:60:ASN:HD22	1.60	0.50
1:D:67:LYS:NZ	3:G:56:DG:O6	2.38	0.49
1:F:43:VAL:HB	2:Y:14:DC:H5''	1.94	0.49
2:Y:25:DC:N3	3:H:55:DG:C2	2.79	0.49
1:E:39:VAL:HG13	1:E:42:ALA:HB3	1.95	0.48
1:C:45:LYS:O	1:C:49:GLU:HG3	2.13	0.48
1:F:75:LEU:HA	4:F:101:HOH:O	2.14	0.47
1:D:45:LYS:O	1:D:49:GLU:HG2	2.13	0.47
1:E:17:LYS:N	1:E:18:PRO:HD2	2.30	0.47
1:D:73:ARG:NH1	4:D:101:HOH:O	2.13	0.47
1:F:25:GLU:O	1:F:29:GLN:HG3	2.15	0.47
1:A:20:VAL:O	3:H:56:DG:H5''	2.16	0.46
1:B:27:HIS:CD2	1:B:64:HIS:NE2	2.82	0.46
1:D:73:ARG:HD2	4:D:101:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:VAL:HG12	1:E:40:GLU:HG2	1.98	0.46
2:Y:6:DA:H2'	2:Y:7:DG:C8	2.51	0.45
3:G:74:DT:H2''	3:G:75:DG:N7	2.31	0.45
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.69	0.45
1:E:58:ARG:HD2	2:Y:9:DT:OP2	2.16	0.45
2:Y:25:DC:O2	3:H:55:DG:H22	1.23	0.45
1:F:41:LYS:HB2	1:F:41:LYS:HE2	1.57	0.44
1:B:77:GLY:HA3	1:B:78:VAL:HA	1.51	0.44
1:A:46:LYS:HE2	4:A:102:HOH:O	2.17	0.43
1:E:39:VAL:HA	1:E:40:GLU:HA	1.69	0.43
1:F:37:LEU:HD13	1:F:50:LEU:HD11	1.99	0.43
3:G:66:DG:OP2	4:G:101:HOH:O	2.22	0.43
1:B:40:GLU:H	1:B:40:GLU:CD	2.23	0.42
1:E:38:GLY:O	1:E:41:LYS:N	2.49	0.41
3:H:74:DT:H2''	3:H:75:DG:N7	2.34	0.41
1:E:35:ASN:HD22	1:E:35:ASN:HA	1.68	0.41
1:E:40:GLU:HA	1:E:42:ALA:H	1.84	0.41
1:B:68:TYR:CZ	1:B:72:LEU:HD11	2.56	0.41
1:B:58:ARG:NH2	2:X:8:DA:H3'	2.35	0.41
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.83	0.40
1:D:76:GLY:HA3	1:E:21:VAL:HB	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:119:HOH:O	4:H:135:HOH:O[2_454]	2.15	0.05

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	57/81 (70%)	56 (98%)	1 (2%)	0	100	100
1	B	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
1	C	61/81 (75%)	59 (97%)	2 (3%)	0	100	100
1	D	58/81 (72%)	56 (97%)	2 (3%)	0	100	100
1	E	57/81 (70%)	56 (98%)	1 (2%)	0	100	100
1	F	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
All	All	353/486 (73%)	345 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	53/69 (77%)	49 (92%)	4 (8%)	13	14
1	B	54/69 (78%)	52 (96%)	2 (4%)	34	43
1	C	55/69 (80%)	54 (98%)	1 (2%)	59	70
1	D	53/69 (77%)	50 (94%)	3 (6%)	20	24
1	E	53/69 (77%)	47 (89%)	6 (11%)	6	5
1	F	54/69 (78%)	50 (93%)	4 (7%)	13	14
All	All	322/414 (78%)	302 (94%)	20 (6%)	18	20

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	40	GLU
1	A	41	LYS
1	A	50	LEU
1	B	28	GLN
1	B	78	VAL
1	C	45	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	28	GLN
1	D	41	LYS
1	D	46	LYS
1	E	28	GLN
1	E	39	VAL
1	E	41	LYS
1	E	61	VAL
1	E	74	ARG
1	E	75	LEU
1	F	30	PHE
1	F	37	LEU
1	F	39	VAL
1	F	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	B	27	HIS
1	C	29	GLN
1	D	60	ASN
1	E	35	ASN
1	E	36	GLN
1	F	36	GLN
1	F	60	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 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	58/81 (71%)	-0.02	1 (1%) 70 78	22, 31, 54, 75	0
1	B	61/81 (75%)	-0.00	2 (3%) 46 57	22, 33, 56, 78	0
1	C	62/81 (76%)	0.26	6 (9%) 7 12	22, 31, 66, 78	0
1	D	59/81 (72%)	0.02	1 (1%) 70 78	23, 37, 57, 84	0
1	E	58/81 (71%)	0.05	0 100 100	26, 35, 63, 76	0
1	F	61/81 (75%)	0.16	2 (3%) 46 57	21, 30, 65, 75	0
2	X	25/25 (100%)	-0.02	0 100 100	26, 35, 74, 76	0
2	Y	25/25 (100%)	-0.09	0 100 100	26, 39, 70, 79	0
3	G	25/25 (100%)	-0.25	0 100 100	25, 38, 72, 74	0
3	H	25/25 (100%)	-0.12	0 100 100	24, 37, 73, 75	0
All	All	459/586 (78%)	0.04	12 (2%) 56 64	21, 34, 70, 84	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	GLY	5.5
1	A	17	LYS	4.9
1	C	77	GLY	4.2
1	C	79	SER	4.2
1	C	17	LYS	3.6
1	C	78	VAL	3.3
1	F	77	GLY	3.1
1	B	78	VAL	3.0
1	C	24	VAL	2.4
1	F	16	LYS	2.4
1	C	40	GLU	2.3
1	D	17	LYS	2.3

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.