WORLDWIDE PDB PROTEIN DATA BANK

Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Jul 30, 2019 – 12:38 PM EDT

Deposition ID : D_1000240321
PDB ID : *(not yet assigned)*

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

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

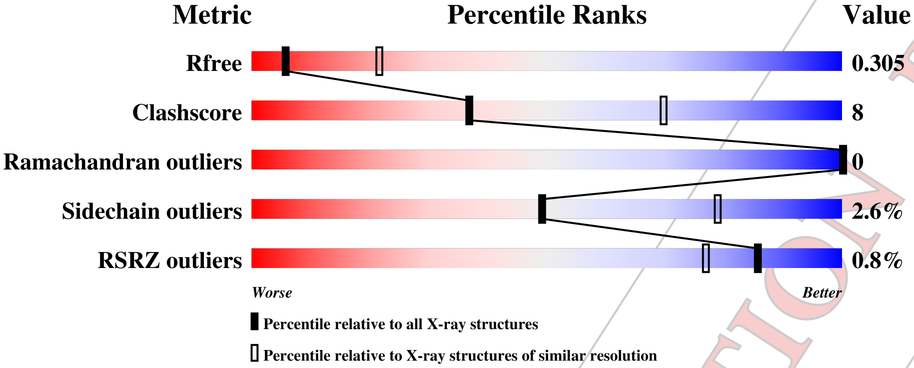
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance (i)

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

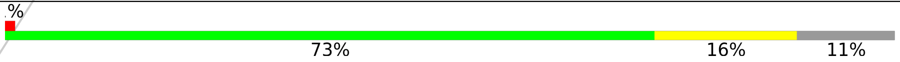
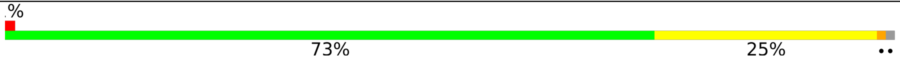
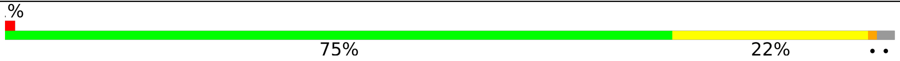
The reported resolution of this entry is 3.17 Å.

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}	111664	1235 (3.20-3.16)
Clashscore	122126	1362 (3.20-3.16)
Ramachandran outliers	120053	1340 (3.20-3.16)
Sidechain outliers	120020	1339 (3.20-3.16)
RSRZ outliers	108989	1193 (3.20-3.16)

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	178	
1	C	178	
2	B	156	
2	D	156	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4920 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1254	812	208	230	4	0	0	0
1	C	159	1254	812	208	230	4	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	SER	-	expression tag	UNP A0A191KWA2
A	171	GLY	-	expression tag	UNP A0A191KWA2
A	172	SER	-	expression tag	UNP A0A191KWA2
A	173	HIS	-	expression tag	UNP A0A191KWA2
A	174	HIS	-	expression tag	UNP A0A191KWA2
A	175	HIS	-	expression tag	UNP A0A191KWA2
A	176	HIS	-	expression tag	UNP A0A191KWA2
A	177	HIS	-	expression tag	UNP A0A191KWA2
A	178	HIS	-	expression tag	UNP A0A191KWA2
C	170	SER	-	expression tag	UNP A0A191KWA2
C	171	GLY	-	expression tag	UNP A0A191KWA2
C	172	SER	-	expression tag	UNP A0A191KWA2
C	173	HIS	-	expression tag	UNP A0A191KWA2
C	174	HIS	-	expression tag	UNP A0A191KWA2
C	175	HIS	-	expression tag	UNP A0A191KWA2
C	176	HIS	-	expression tag	UNP A0A191KWA2
C	177	HIS	-	expression tag	UNP A0A191KWA2
C	178	HIS	-	expression tag	UNP A0A191KWA2

- Molecule 2 is a protein called Interferon stimulated gene 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	155	1210	759	216	227	8	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	153	1202	755	214	225	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

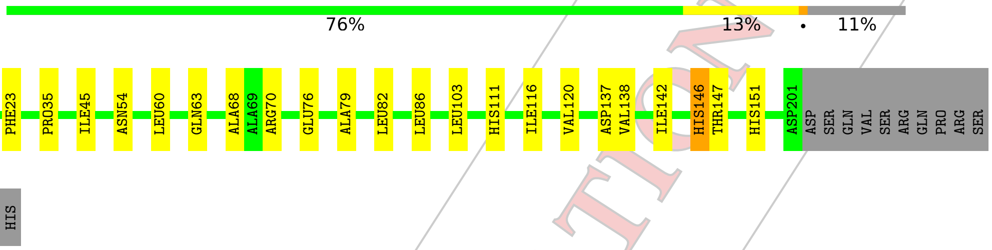
Chain	Residue	Modelled	Actual	Comment	Reference
B	78	SER	CYS	conflict	UNP Q9GKP4
D	78	SER	CYS	conflict	UNP Q9GKP4

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

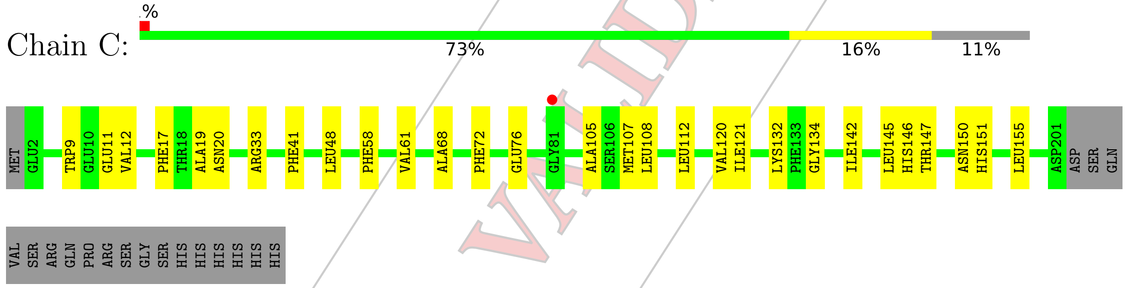
- Molecule 1: RNA-dependent RNA polymerase

Chain A:



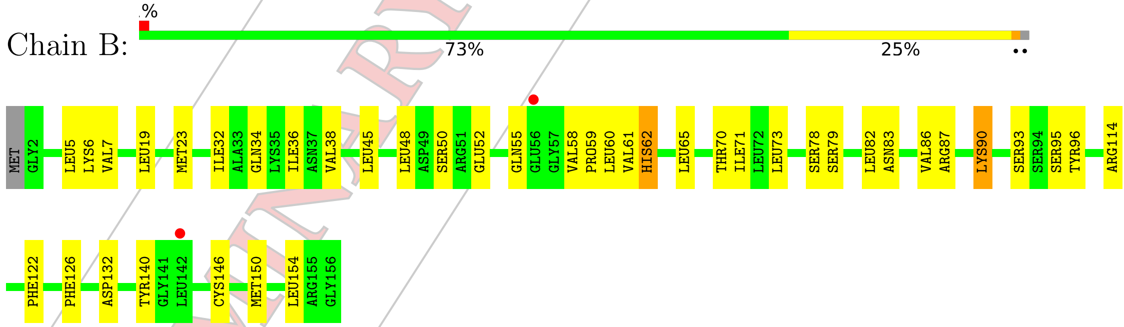
- Molecule 1: RNA-dependent RNA polymerase

Chain C:



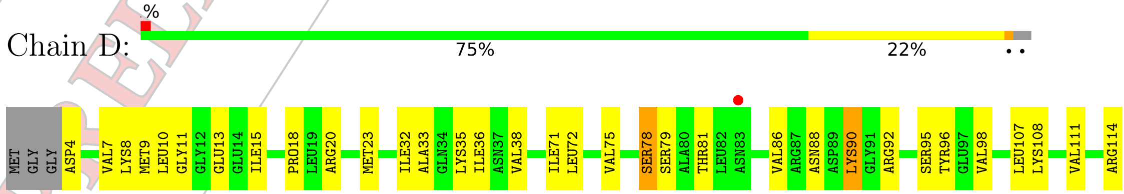
- Molecule 2: Interferon stimulated gene 17

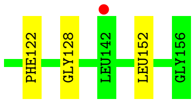
Chain B:



- Molecule 2: Interferon stimulated gene 17

Chain D:




PHE122
GLY128
LEU142
LEU152
GLY156

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	55.39Å 55.39Å 497.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.44 – 3.17 44.75 – 3.17	Depositor EDS
% Data completeness (in resolution range)	83.8 (41.44-3.17) 76.3 (44.75-3.17)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.19Å)	Xtriage
Refinement program	phenix.refine 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.253 , 0.305 0.253 , 0.305	Depositor DCC
R_{free} test set	1241 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	88.3	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.170 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.25	0/1283	0.42	0/1742
1	C	0.25	0/1283	0.42	0/1742
2	B	0.26	0/1226	0.51	0/1651
2	D	0.25	0/1218	0.46	0/1641
All	All	0.25	0/5010	0.45	0/6776

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	1254	0	1209	13	0
1	C	1254	0	1209	20	0
2	B	1210	0	1237	27	0
2	D	1202	0	1231	27	0
All	All	4920	0	4886	83	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 8.

All (83) 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:D:88:ASN:ND2	2:D:92:ARG:O	2.11	0.84
2:D:95:SER:O	2:D:114:ARG:NH1	2.17	0.77
2:D:20:ARG:HB2	2:D:23:MET:HB2	1.70	0.73
2:B:5:LEU:HB2	2:B:19:LEU:HD23	1.72	0.72
1:A:60:LEU:O	1:A:63:GLN:HB2	1.93	0.69
1:C:132:LYS:NZ	1:C:134:GLY:O	2.25	0.68
1:C:145:LEU:HD12	1:C:155:LEU:HD21	1.77	0.66
2:B:61:VAL:HG23	2:B:62:HIS:H	1.60	0.65
2:D:90:LYS:H	2:D:90:LYS:HD2	1.62	0.64
1:A:147:THR:HG23	1:A:151:HIS:HB3	1.81	0.63
2:D:78:SER:OG	2:D:79:SER:N	2.32	0.62
2:D:10:LEU:HD23	2:D:11:GLY:H	1.65	0.62
2:B:6:LYS:O	2:B:70:THR:HA	2.00	0.60
2:B:6:LYS:HB2	2:B:70:THR:HG22	1.84	0.60
1:C:48:LEU:HD12	1:C:142:ILE:HG23	1.83	0.59
1:C:17:PHE:HB2	1:C:132:LYS:HB3	1.85	0.58
1:A:45:ILE:HA	1:A:142:ILE:HD11	1.87	0.56
2:B:78:SER:N	2:B:79:SER:HA	2.21	0.55
1:A:10:GLU:OE2	2:B:87:ARG:NH2	2.39	0.54
2:B:45:LEU:HD21	2:B:73:LEU:HD12	1.90	0.54
2:D:7:VAL:HG12	2:D:15:ILE:HG12	1.91	0.53
1:A:137:ASP:OD1	1:A:138:VAL:N	2.42	0.53
1:C:9:TRP:CZ3	1:C:132:LYS:HB2	2.44	0.53
2:B:7:VAL:HG23	2:B:71:ILE:HG13	1.91	0.52
1:C:41:PHE:HZ	1:C:105:ALA:HB2	1.75	0.51
1:C:9:TRP:CE3	1:C:19:ALA:HB2	2.46	0.50
1:A:146:HIS:HD2	2:B:154:LEU:HD22	1.75	0.50
2:D:32:ILE:O	2:D:36:ILE:HG12	2.13	0.49
1:A:70:ARG:HA	1:A:86:LEU:HD11	1.95	0.49
1:C:150:ASN:OD1	1:C:150:ASN:N	2.46	0.49
2:B:86:VAL:O	2:B:93:SER:HA	2.12	0.49
2:D:122:PHE:HB3	2:D:152:LEU:HA	1.93	0.49
2:D:75:VAL:O	2:D:75:VAL:HG13	2.13	0.49
2:D:7:VAL:HG23	2:D:71:ILE:HG13	1.95	0.48
2:B:50:SER:HB3	2:B:52:GLU:HG3	1.95	0.48
2:D:4:ASP:HA	2:D:18:PRO:HA	1.95	0.48
2:B:48:LEU:HD11	2:B:70:THR:OG1	2.15	0.47
2:B:87:ARG:HA	2:B:93:SER:HA	1.97	0.46
2:D:8:LYS:HB3	2:D:72:LEU:HD23	1.96	0.46
1:A:35:PRO:HB3	1:C:33:ARG:CZ	2.45	0.46
2:B:32:ILE:O	2:B:36:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:PHE:HB3	2:D:152:LEU:HD23	1.97	0.46
2:B:126:PHE:HE1	2:B:146:CYS:HB2	1.79	0.46
2:B:122:PHE:CD1	2:B:150:MET:HG3	2.50	0.46
1:C:9:TRP:CH2	1:C:132:LYS:HD3	2.51	0.46
1:C:9:TRP:CZ3	1:C:132:LYS:HD3	2.51	0.46
1:A:76:GLU:HG2	1:A:103:LEU:HD12	1.98	0.46
2:B:86:VAL:HB	2:B:96:TYR:CE2	2.51	0.46
2:D:86:VAL:HB	2:D:96:TYR:HE2	1.80	0.46
2:B:55:GLN:HB2	2:B:58:VAL:HG11	1.97	0.45
1:A:120:VAL:HA	1:A:146:HIS:HB3	1.99	0.45
1:A:79:ALA:HA	1:A:82:LEU:HD12	1.98	0.45
1:A:68:ALA:HB2	1:A:111:HIS:HB2	1.99	0.43
2:B:96:TYR:CZ	2:B:114:ARG:HD2	2.53	0.43
1:C:41:PHE:CZ	1:C:105:ALA:HB2	2.53	0.43
2:D:114:ARG:HE	2:D:114:ARG:HB2	1.65	0.43
2:B:90:LYS:HE2	2:B:90:LYS:HB2	1.71	0.43
2:D:10:LEU:HD23	2:D:11:GLY:N	2.33	0.43
2:D:81:THR:HG23	2:D:98:VAL:O	2.18	0.43
1:A:116:ILE:HA	1:A:142:ILE:HG23	2.01	0.43
1:C:68:ALA:HB1	1:C:107:MET:HB3	2.01	0.43
1:C:11:GLU:HG2	1:C:11:GLU:H	1.67	0.42
2:D:96:TYR:CZ	2:D:111:VAL:HG12	2.54	0.42
2:B:132:ASP:N	2:B:140:TYR:OH	2.49	0.42
2:D:86:VAL:HB	2:D:96:TYR:CE2	2.54	0.42
2:B:55:GLN:HB2	2:B:58:VAL:CG1	2.50	0.42
2:D:15:ILE:HD11	2:D:32:ILE:HG13	2.01	0.42
1:C:121:ILE:HG12	1:C:147:THR:HA	2.00	0.42
1:C:58:PHE:O	1:C:61:VAL:HG12	2.20	0.42
2:B:36:ILE:HG13	2:B:38:VAL:HG22	2.02	0.42
1:C:120:VAL:HA	1:C:146:HIS:HB3	2.01	0.42
2:D:33:ALA:HB1	2:D:38:VAL:O	2.19	0.42
2:B:59:PRO:HB2	2:B:61:VAL:HG22	2.01	0.42
1:C:72:PHE:O	1:C:76:GLU:N	2.52	0.41
2:B:95:SER:O	2:B:114:ARG:NH2	2.41	0.41
2:D:9:MET:HB2	2:D:13:GLU:HG2	2.01	0.41
1:C:108:LEU:O	1:C:112:LEU:HB2	2.20	0.41
2:B:154:LEU:HD23	2:B:154:LEU:HA	1.92	0.41
2:B:60:LEU:HD12	2:B:65:LEU:HG	2.03	0.41
2:D:35:LYS:HG3	2:D:36:ILE:HG23	2.02	0.41
2:D:108:LYS:HA	2:D:111:VAL:HG22	2.03	0.41
2:D:98:VAL:HG21	2:D:107:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:O	2:D:128:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	156/178 (88%)	147 (94%)	9 (6%)	0	100	100
1	C	156/178 (88%)	149 (96%)	7 (4%)	0	100	100
2	B	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
2	D	151/156 (97%)	141 (93%)	10 (7%)	0	100	100
All	All	616/668 (92%)	585 (95%)	31 (5%)	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	131/150 (87%)	127 (97%)	4 (3%)	43	75
1	C	131/150 (87%)	129 (98%)	2 (2%)	67	88
2	B	135/136 (99%)	129 (96%)	6 (4%)	31	66
2	D	135/136 (99%)	133 (98%)	2 (2%)	67	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	532/572 (93%)	518 (97%)	14 (3%)	49	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	23	PHE
1	A	54	ASN
1	A	146	HIS
2	B	23	MET
2	B	34	GLN
2	B	62	HIS
2	B	82	LEU
2	B	83	ASN
2	B	90	LYS
1	C	20	ASN
1	C	151	HIS
2	D	78	SER
2	D	90	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	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 ⓘ

There are no ligands in this entry.

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 (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	158/178 (88%)	-0.27	0	100	100	72, 105, 135, 156	0
1	C	158/178 (88%)	-0.26	1 (0%)	89	83	75, 110, 145, 153	1 (0%)
2	B	155/156 (99%)	-0.23	2 (1%)	77	64	81, 119, 155, 180	0
2	D	153/156 (98%)	-0.10	2 (1%)	77	64	85, 133, 154, 181	0
All	All	624/668 (93%)	-0.22	5 (0%)	86	77	72, 118, 151, 181	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	142	LEU	4.9
2	D	83	ASN	3.5
2	B	56	GLU	2.6
2	B	142	LEU	2.3
1	C	81	GLY	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.