



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 08:08 AM UTC

PDB ID : 7V5V / pdb_00007v5v
Title : LysR family transcriptional regulator RipR from Salmonella Typhimurium
Authors : Ki, N.; Ha, N.-C.
Deposited on : 2021-08-18
Resolution : 2.37 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

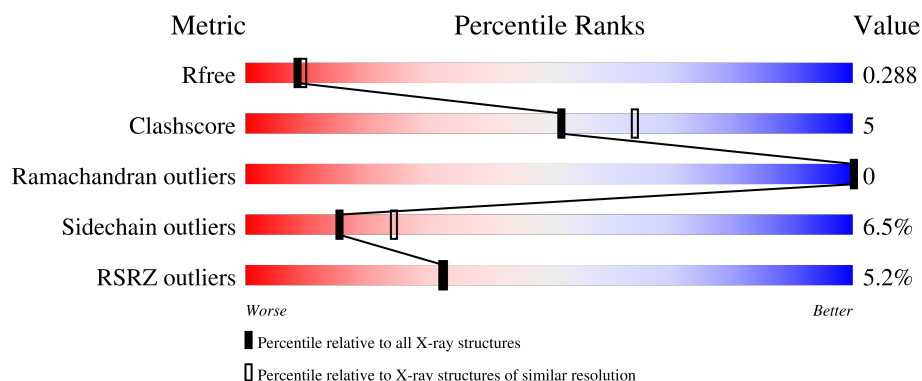
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	208	8% 85% 13% .
1	B	208	6% 88% 11% .
1	C	208	3% 80% 15% ..
1	D	208	3% 71% 26% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6309 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 RipR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1580	1008	275	290	7			
1	B	207	Total	C	N	O	S	0	0	0
			1584	1011	275	290	8			
1	C	203	Total	C	N	O	S	0	0	0
			1551	992	268	284	7			
1	D	205	Total	C	N	O	S	0	0	0
			1564	999	270	288	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	MET	-	initiating methionine	UNP Q93DX4
B	85	MET	-	initiating methionine	UNP Q93DX4
C	85	MET	-	initiating methionine	UNP Q93DX4
D	85	MET	-	initiating methionine	UNP Q93DX4

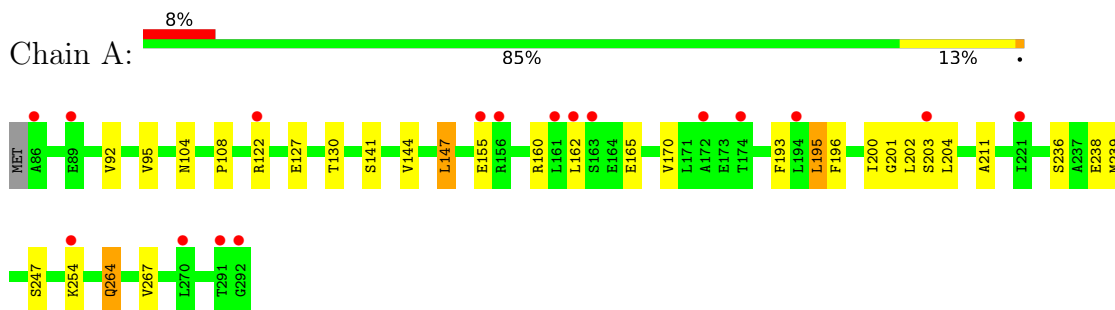
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	10	Total	O	0	0
			10	10		
2	C	8	Total	O	0	0
			8	8		
2	D	8	Total	O	0	0
			8	8		

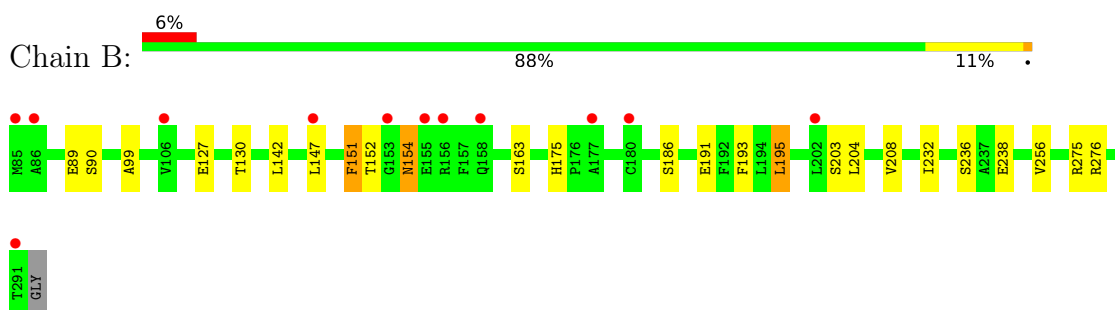
3 Residue-property plots [i](#)

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.

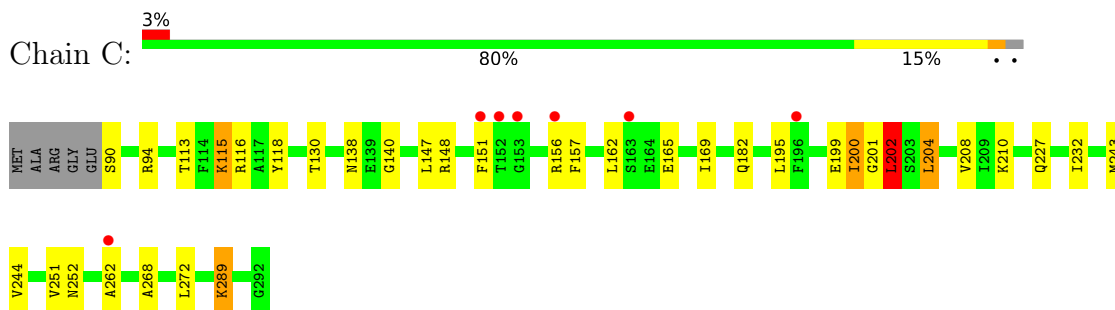
• Molecule 1: RipR



• Molecule 1: RipR

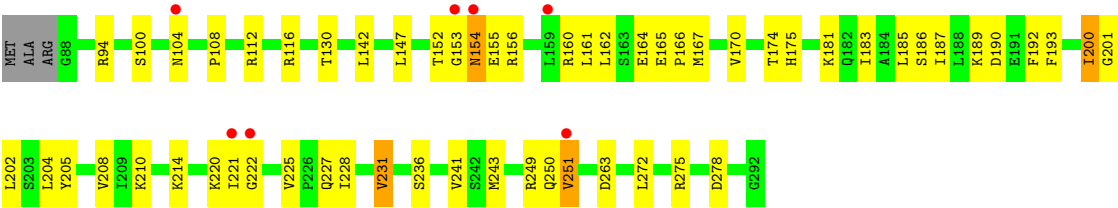


• Molecule 1: RipR



• Molecule 1: RipR





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.41Å 72.42Å 91.61Å 90.00° 104.62° 90.00°	Depositor
Resolution (Å)	39.26 – 2.37 39.26 – 2.37	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.26-2.37) 95.8 (39.26-2.37)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.236 , 0.295 0.235 , 0.288	Depositor DCC
R_{free} test set	1575 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6309	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.64% 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, 0.333 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	0.45	1/1607 (0.1%)	0.49	1/2176 (0.0%)
1	B	0.27	0/1611	0.40	0/2181
1	C	0.53	1/1578 (0.1%)	0.66	9/2138 (0.4%)
1	D	1.01	7/1591 (0.4%)	0.93	11/2155 (0.5%)
All	All	0.63	9/6387 (0.1%)	0.65	21/8650 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	183	ILE	C-O	-6.65	1.17	1.24
1	C	202	LEU	C-O	-6.24	1.18	1.24
1	D	174	THR	C-O	-5.78	1.16	1.24
1	D	166	PRO	C-O	-5.72	1.17	1.23
1	D	161	LEU	C-O	-5.43	1.17	1.23
1	D	202	LEU	C-O	-5.30	1.19	1.24
1	A	162	LEU	N-CA	-5.25	1.39	1.45
1	D	165	GLU	C-O	-5.10	1.17	1.24
1	D	189	LYS	C-O	-5.04	1.18	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	VAL	N-CA-C	-16.57	85.77	109.63
1	C	251	VAL	N-CA-C	-11.72	94.66	109.30
1	D	251	VAL	CB-CA-C	10.63	128.66	111.32
1	D	201	GLY	N-CA-C	9.19	124.54	112.77
1	C	201	GLY	N-CA-C	8.95	124.22	112.77
1	A	201	GLY	N-CA-C	7.78	121.91	112.49
1	C	251	VAL	CB-CA-C	6.85	121.54	111.33
1	D	175	HIS	CA-C-N	6.85	126.65	119.05
1	D	175	HIS	C-N-CA	6.85	126.65	119.05
1	C	118	TYR	CA-C-N	6.71	126.67	119.28
1	C	118	TYR	C-N-CA	6.71	126.67	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	GLU	N-CA-C	-5.84	99.00	108.52
1	C	252	ASN	N-CA-CB	5.46	119.58	111.23
1	D	183	ILE	N-CA-C	5.42	115.70	108.11
1	C	252	ASN	N-CA-C	-5.22	99.87	108.49
1	C	200	ILE	CA-C-N	5.22	125.74	120.00
1	C	200	ILE	C-N-CA	5.22	125.74	120.00
1	D	154	ASN	N-CA-CB	5.16	119.88	112.08
1	D	200	ILE	CA-C-N	5.16	125.67	120.00
1	D	200	ILE	C-N-CA	5.16	125.67	120.00
1	D	185	LEU	N-CA-C	5.12	117.60	111.71

There are no chirality outliers.

There are no planarity outliers.

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	1580	0	1628	14	0
1	B	1584	0	1634	14	0
1	C	1551	0	1601	20	2
1	D	1564	0	1610	22	2
2	A	4	0	0	0	0
2	B	10	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
All	All	6309	0	6473	65	2

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 (65) 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:238:GLU:O	1:C:115:LYS:NZ	2.12	0.83
1:D:193:PHE:O	1:D:222:GLY:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:HD11	1:D:272:LEU:HB2	1.63	0.80
1:C:202:LEU:N	1:C:202:LEU:HD23	1.97	0.78
1:D:249:ARG:O	1:D:251:VAL:O	2.06	0.73
1:C:130:THR:HG23	1:C:147:LEU:HB2	1.73	0.71
1:C:138:ASN:HD21	1:C:156:ARG:HG3	1.62	0.65
1:A:127:GLU:OE2	1:D:227:GLN:NE2	2.29	0.62
1:C:202:LEU:HD23	1:C:202:LEU:H	1.64	0.60
1:A:254:LYS:HA	1:A:254:LYS:HE3	1.84	0.59
1:A:238:GLU:OE2	1:D:116:ARG:NH2	2.36	0.58
1:C:232:ILE:HD11	1:C:244:VAL:HG11	1.86	0.57
1:B:193:PHE:HB3	1:B:195:LEU:HD23	1.87	0.56
1:D:104:ASN:O	1:D:108:PRO:HD2	2.06	0.55
1:C:156:ARG:HA	1:C:156:ARG:NE	2.22	0.55
1:D:156:ARG:O	1:D:156:ARG:HG2	2.08	0.54
1:C:169:ILE:HD13	1:C:243:MET:HG3	1.89	0.54
1:B:130:THR:HG23	1:B:147:LEU:HB2	1.91	0.53
1:C:113:THR:HG22	1:C:289:LYS:HD3	1.91	0.53
1:A:193:PHE:HB3	1:A:195:LEU:HD13	1.90	0.53
1:C:148:ARG:HD2	1:C:204:LEU:HD13	1.89	0.52
1:B:99:ALA:HB2	1:C:227:GLN:NE2	2.24	0.52
1:C:165:GLU:HG2	1:C:268:ALA:HB3	1.92	0.51
1:B:152:THR:O	1:B:152:THR:OG1	2.26	0.51
1:D:94:ARG:HB3	1:D:142:LEU:HD23	1.93	0.50
1:B:151:PHE:CD1	1:B:151:PHE:N	2.72	0.50
1:D:275:ARG:NH1	1:D:278:ASP:OD2	2.43	0.50
1:A:130:THR:HG23	1:A:147:LEU:HB2	1.92	0.50
1:C:208:VAL:HG13	1:C:243:MET:HE3	1.94	0.50
1:A:95:VAL:HG13	1:A:144:VAL:HG13	1.96	0.47
1:A:165:GLU:OE2	1:A:247:SER:N	2.47	0.47
1:B:151:PHE:H	1:B:151:PHE:HD1	1.57	0.47
1:A:211:ALA:HA	1:A:264:GLN:OE1	2.14	0.47
1:C:162:LEU:HD11	1:C:272:LEU:HB2	1.96	0.47
1:B:232:ILE:HG23	1:B:256:VAL:HG11	1.98	0.46
1:B:175:HIS:NE2	1:B:191:GLU:OE2	2.46	0.46
1:D:108:PRO:O	1:D:112:ARG:HB2	2.15	0.46
1:D:205:TYR:CD1	1:D:205:TYR:C	2.94	0.45
1:C:151:PHE:HA	1:C:202:LEU:HD13	1.99	0.45
1:D:208:VAL:HA	1:D:243:MET:HE2	1.98	0.45
1:C:94:ARG:NH1	1:C:140:GLY:O	2.49	0.44
1:D:153:GLY:C	1:D:155:GLU:N	2.73	0.44
1:C:182:GLN:HB2	1:C:262:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:MET:HB3	1:A:239:MET:HE3	1.79	0.44
1:D:130:THR:HG23	1:D:147:LEU:HB2	1.98	0.44
1:D:250:GLN:O	1:D:251:VAL:C	2.58	0.43
1:B:127:GLU:CD	1:C:227:GLN:HE22	2.26	0.43
1:A:122:ARG:HE	1:A:122:ARG:HB3	1.50	0.43
1:B:142:LEU:O	1:B:275:ARG:NH1	2.41	0.43
1:D:100:SER:HB3	1:D:228:ILE:HD12	2.01	0.42
1:D:208:VAL:HG22	1:D:243:MET:HE2	2.02	0.42
1:A:165:GLU:OE2	1:A:247:SER:HB3	2.19	0.42
1:B:154:ASN:OD1	1:B:154:ASN:N	2.53	0.42
1:D:210:LYS:HD3	1:D:214:LYS:HE3	2.02	0.42
1:A:204:LEU:HD12	1:A:204:LEU:N	2.35	0.41
1:A:92:VAL:CG2	1:A:122:ARG:HH21	2.33	0.41
1:D:263:ASP:OD1	1:D:263:ASP:N	2.54	0.41
1:D:225:VAL:HG12	1:D:231:VAL:HG23	2.02	0.41
1:D:192:PHE:HA	1:D:220:LYS:O	2.21	0.41
1:B:204:LEU:O	1:B:208:VAL:HG23	2.21	0.41
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.87	0.41
1:D:221:ILE:H	1:D:221:ILE:HD12	1.86	0.41
1:B:276:ARG:HE	1:B:276:ARG:HB2	1.66	0.40
1:C:210:LYS:HD2	1:C:210:LYS:N	2.35	0.40
1:A:104:ASN:O	1:A:108:PRO:HD2	2.22	0.40

All (2) 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)
1:C:156:ARG:NH2	1:D:221:ILE:O[2_645]	1.72	0.48
1:C:289:LYS:O	1:D:181:LYS:NZ[1_545]	1.92	0.28

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	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
1	B	205/208 (99%)	199 (97%)	6 (3%)	0	100	100
1	C	201/208 (97%)	197 (98%)	4 (2%)	0	100	100
1	D	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
All	All	814/832 (98%)	792 (97%)	22 (3%)	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	170/171 (99%)	157 (92%)	13 (8%)	12	19
1	B	171/171 (100%)	162 (95%)	9 (5%)	20	33
1	C	168/171 (98%)	159 (95%)	9 (5%)	20	32
1	D	169/171 (99%)	156 (92%)	13 (8%)	12	18
All	All	678/684 (99%)	634 (94%)	44 (6%)	15	24

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	A	147	LEU
1	A	155	GLU
1	A	160	ARG
1	A	170	VAL
1	A	195	LEU
1	A	196	PHE
1	A	200	ILE
1	A	202	LEU
1	A	203	SER
1	A	236	SER
1	A	264	GLN
1	A	267	VAL

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Mol	Chain	Res	Type
1	B	89	GLU
1	B	90	SER
1	B	151	PHE
1	B	154	ASN
1	B	163	SER
1	B	186	SER
1	B	195	LEU
1	B	203	SER
1	B	236	SER
1	C	90	SER
1	C	115	LYS
1	C	116	ARG
1	C	157	PHE
1	C	199	GLU
1	C	200	ILE
1	C	202	LEU
1	C	204	LEU
1	C	289	LYS
1	D	152	THR
1	D	154	ASN
1	D	160	ARG
1	D	167	MET
1	D	170	VAL
1	D	186	SER
1	D	187	ILE
1	D	190	ASP
1	D	200	ILE
1	D	204	LEU
1	D	231	VAL
1	D	236	SER
1	D	241	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	B	252	ASN
1	C	129	ASN
1	D	129	ASN
1	D	154	ASN
1	D	158	GLN

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 oligosaccharides 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

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	207/208 (99%)	0.88	17 (8%) 17 16	27, 40, 61, 159	0
1	B	207/208 (99%)	0.77	12 (5%) 29 28	26, 39, 63, 113	0
1	C	203/208 (97%)	0.58	7 (3%) 48 48	24, 37, 55, 71	0
1	D	205/208 (98%)	0.52	7 (3%) 48 48	23, 34, 54, 122	0
All	All	822/832 (98%)	0.68	43 (5%) 33 32	23, 38, 59, 159	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	SER	9.1
1	D	154	ASN	4.6
1	D	222	GLY	4.5
1	A	162	LEU	4.5
1	B	86	ALA	4.2
1	A	292	GLY	4.0
1	D	221	ILE	4.0
1	D	153	GLY	3.6
1	B	85	MET	3.5
1	C	156	ARG	3.4
1	A	270	LEU	3.4
1	C	153	GLY	3.2
1	C	152	THR	3.2
1	B	291	THR	3.2
1	A	203	SER	3.1
1	A	86	ALA	2.9
1	C	151	PHE	2.7
1	D	159	LEU	2.7
1	A	291	THR	2.7
1	B	158	GLN	2.6
1	C	163	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	104	ASN	2.6
1	A	122	ARG	2.6
1	B	156	ARG	2.6
1	B	147	LEU	2.5
1	C	196	PHE	2.5
1	A	172	ALA	2.5
1	B	153	GLY	2.5
1	A	194	LEU	2.4
1	A	174	THR	2.3
1	A	254	LYS	2.3
1	A	156	ARG	2.3
1	B	155	GLU	2.3
1	A	155	GLU	2.2
1	A	221	ILE	2.2
1	A	161	LEU	2.2
1	B	202	LEU	2.1
1	D	251	VAL	2.1
1	B	177	ALA	2.1
1	C	262	ALA	2.1
1	A	89	GLU	2.1
1	B	106	VAL	2.1
1	B	180	CYS	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 oligosaccharides 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.