



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:58 AM UTC

PDB ID : 2AN1 / pdb_00002an1
Title : Structural Genomics, The crystal structure of a putative kinase from Salmonella typhimurim LT2
Authors : Zhang, R.; Zhou, M.; Holzle, D.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2005-08-10
Resolution : 2.00 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

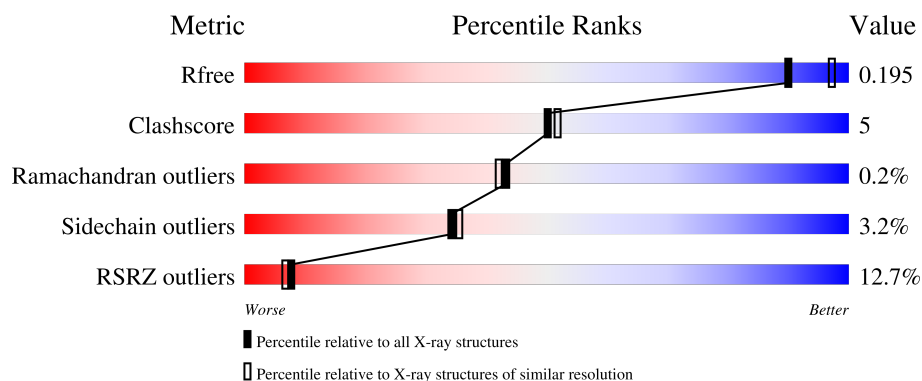
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	292	6% 81% 11% • 6%
1	B	292	10% 88% 9% •
1	C	292	20% 78% 14% • 7%
1	D	292	13% 82% 8% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9108 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 putative kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2149	1364	368	408	9			
1	B	281	Total	C	N	O	S	0	0	0
			2205	1394	384	418	9			
1	C	271	Total	C	N	O	S	0	0	0
			2115	1337	363	406	9			
1	D	268	Total	C	N	O	S	0	0	0
			2097	1330	361	397	9			

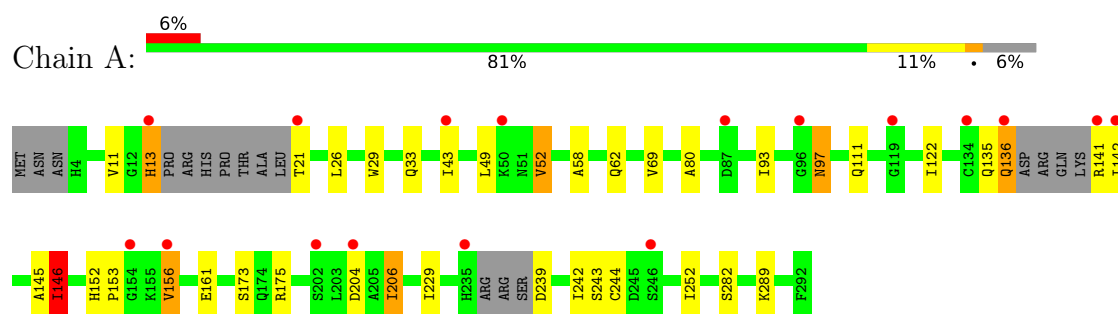
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	151	Total	O	0	0
			151	151		
2	B	170	Total	O	0	0
			170	170		
2	C	104	Total	O	0	0
			104	104		
2	D	117	Total	O	0	0
			117	117		

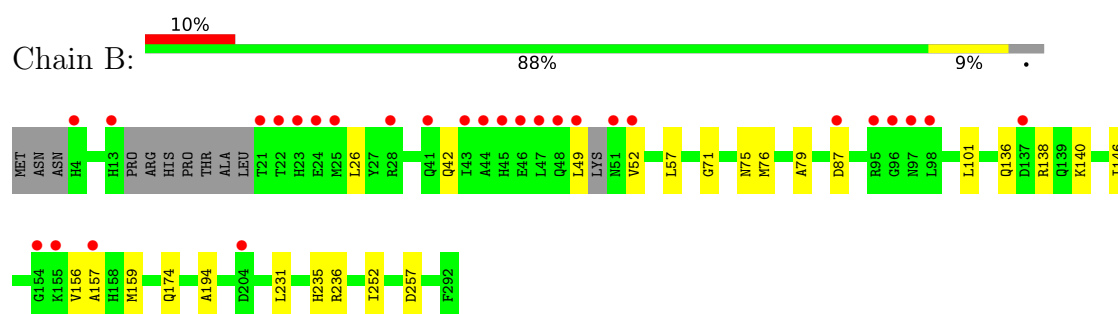
3 Residue-property plots [i](#)

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.

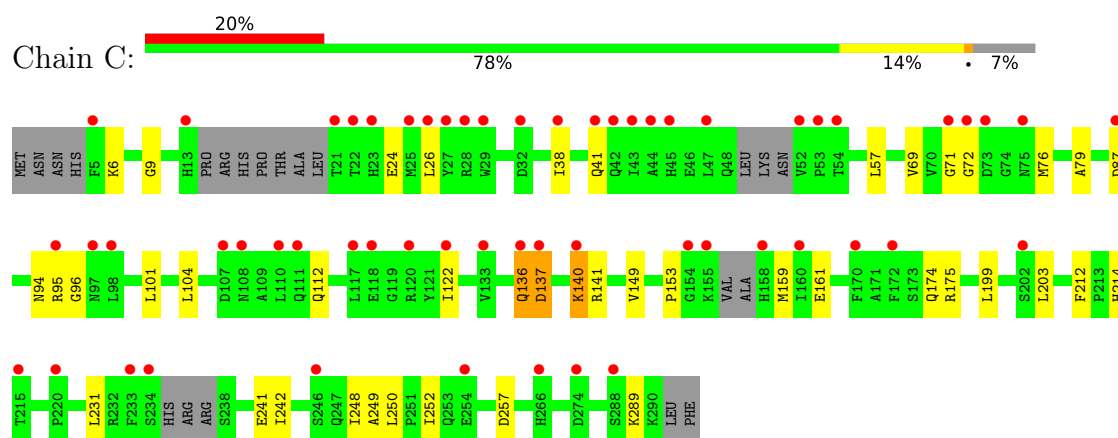
- Molecule 1: putative kinase



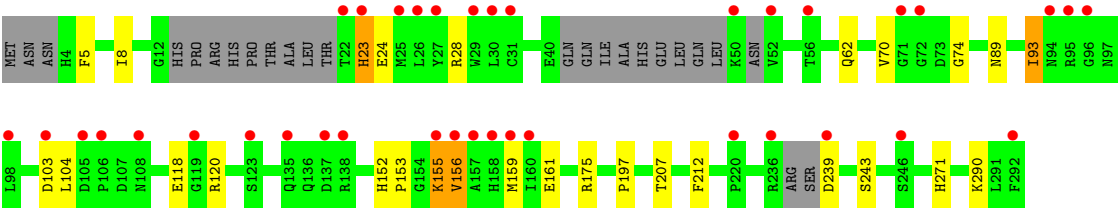
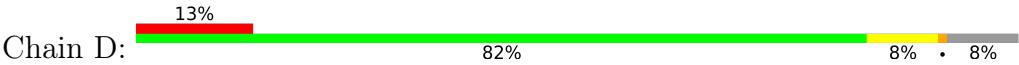
- Molecule 1: putative kinase



- Molecule 1: putative kinase



- Molecule 1: putative kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.53Å 99.32Å 144.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.00) 97.7 (50.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.233 0.202 , 0.195	Depositor DCC
R_{free} test set	4763 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9108	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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.*

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	0.61	0/2189	0.82	1/2968 (0.0%)
1	B	0.65	0/2246	0.82	0/3044
1	C	0.55	0/2151	0.77	0/2914
1	D	0.60	0/2134	0.79	1/2888 (0.0%)
All	All	0.60	0/8720	0.80	2/11814 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ILE	CB-CA-C	-7.55	101.00	111.65
1	D	156	VAL	N-CA-C	6.43	117.06	110.05

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	2149	0	2138	33	0
1	B	2205	0	2195	14	0
1	C	2115	0	2102	22	0
1	D	2097	0	2093	26	0
2	A	151	0	0	7	0
2	B	170	0	0	4	0
2	C	104	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	117	0	0	9	0
All	All	9108	0	8528	91	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 (91) 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:A:13:HIS:HB3	1:A:43:ILE:HG22	1.51	0.92
1:A:161:GLU:HG2	1:A:175:ARG:HG2	1.52	0.91
1:D:155:LYS:HE3	1:D:155:LYS:H	1.45	0.81
1:D:8:ILE:HG12	2:D:548:HOH:O	1.81	0.81
1:C:289:LYS:HD3	2:C:622:HOH:O	1.80	0.80
1:C:136:GLN:O	1:C:137:ASP:HB2	1.79	0.79
1:A:97:ASN:HD22	1:A:97:ASN:H	1.29	0.77
1:B:146:ILE:HB	2:B:673:HOH:O	1.86	0.75
1:D:103:ASP:OD2	1:D:271:HIS:ND1	2.20	0.71
1:A:58:ALA:O	1:A:62:GLN:HG2	1.92	0.68
1:D:239:ASP:N	2:D:561:HOH:O	2.27	0.68
1:D:118:GLU:OE1	1:D:120:ARG:NH2	2.23	0.68
1:A:156:VAL:HG11	1:C:153:PRO:O	1.95	0.67
1:A:242:ILE:HG12	1:A:252:ILE:HD11	1.77	0.66
1:A:97:ASN:HD22	1:A:97:ASN:N	1.90	0.66
1:A:135:GLN:O	1:A:136:GLN:HB3	1.96	0.66
1:C:212:PHE:CD2	2:C:610:HOH:O	2.48	0.65
1:A:206:ILE:HD11	1:A:229:ILE:HD11	1.79	0.65
1:D:74:GLY:HA3	2:D:549:HOH:O	1.94	0.65
1:B:49:LEU:H	1:B:49:LEU:HD12	1.64	0.62
1:B:57:LEU:HD21	1:B:79:ALA:HA	1.79	0.62
1:B:87:ASP:OD1	1:B:87:ASP:C	2.40	0.62
1:C:161:GLU:HG2	1:C:175:ARG:HG2	1.82	0.62
1:C:174:GLN:NE2	2:C:604:HOH:O	2.32	0.62
1:B:236:ARG:NH1	2:B:604:HOH:O	2.33	0.61
1:D:24:GLU:HB3	1:D:28:ARG:HH21	1.66	0.61
1:A:173:SER:OG	1:D:290:LYS:O	2.15	0.60
1:A:97:ASN:H	1:A:97:ASN:ND2	1.99	0.59
1:D:8:ILE:CG1	2:D:548:HOH:O	2.46	0.59
1:B:235:HIS:HD2	2:B:669:HOH:O	1.85	0.59
1:B:138:ARG:HH12	1:B:140:LYS:HZ3	1.51	0.58
1:A:239:ASP:N	2:A:637:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:PHE:HE1	1:D:89:ASN:HD22	1.52	0.57
1:A:49:LEU:CB	1:A:52:VAL:HG11	2.34	0.57
1:A:206:ILE:HD11	1:A:229:ILE:CD1	2.35	0.57
1:C:231:LEU:O	1:C:257:ASP:HB2	2.05	0.56
1:A:49:LEU:HB3	1:A:52:VAL:HG11	1.88	0.56
1:A:152:HIS:HD2	1:A:153:PRO:O	1.89	0.56
1:A:161:GLU:CG	1:A:175:ARG:HG2	2.30	0.56
1:C:242:ILE:HG12	1:C:252:ILE:HD11	1.87	0.55
1:D:161:GLU:HG2	1:D:175:ARG:HG2	1.88	0.54
1:A:152:HIS:HE1	1:A:243:SER:OG	1.91	0.54
1:D:152:HIS:HE1	1:D:243:SER:OG	1.91	0.54
1:A:26:LEU:HD11	1:A:93:ILE:HD11	1.88	0.53
1:C:136:GLN:O	1:C:137:ASP:CB	2.56	0.53
1:B:71:GLY:HA3	1:B:75:ASN:HD22	1.72	0.53
1:D:23:HIS:HD2	1:D:70:VAL:HG11	1.72	0.53
1:D:5:PHE:CB	2:D:548:HOH:O	2.58	0.52
1:D:24:GLU:H	1:D:24:GLU:CD	2.18	0.51
1:C:140:LYS:O	1:C:141:ARG:HG3	2.10	0.51
1:D:239:ASP:HA	2:D:542:HOH:O	2.10	0.51
1:A:141:ARG:HD3	2:A:574:HOH:O	2.11	0.51
1:D:5:PHE:HB3	2:D:548:HOH:O	2.13	0.49
1:D:155:LYS:HE2	1:D:239:ASP:OD2	2.12	0.49
1:C:241:GLU:HB3	1:C:249:ALA:HB1	1.95	0.48
1:D:24:GLU:O	1:D:28:ARG:HG3	2.14	0.48
1:A:11:VAL:CG2	1:A:69:VAL:HG22	2.43	0.47
1:A:204:ASP:HB2	2:A:621:HOH:O	2.12	0.47
1:D:197:PRO:HD2	1:D:207:THR:HG21	1.97	0.47
1:C:71:GLY:HA2	1:C:95:ARG:HH11	1.80	0.47
1:C:159:MET:CE	1:C:214:HIS:HB2	2.44	0.47
1:B:236:ARG:NH2	1:B:252:ILE:O	2.49	0.46
1:A:62:GLN:NE2	2:A:536:HOH:O	2.49	0.46
1:A:141:ARG:C	1:A:142:ILE:HD12	2.40	0.46
1:D:152:HIS:HD2	1:D:153:PRO:O	1.97	0.46
1:A:26:LEU:HD11	1:A:93:ILE:CD1	2.46	0.45
1:C:149:VAL:HG13	1:C:242:ILE:HG23	1.98	0.45
1:C:159:MET:HE1	1:C:214:HIS:CD2	2.52	0.44
1:B:76:MET:HG2	1:B:101:LEU:HB3	2.00	0.44
1:C:72:GLY:HA2	1:C:94:ASN:HA	2.00	0.44
1:A:145:ALA:HB2	1:A:244:CYS:HB3	2.00	0.44
1:A:21:THR:N	2:A:606:HOH:O	2.52	0.43
1:C:76:MET:HG2	1:C:101:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:SER:OG	1:A:289:LYS:HE2	2.18	0.43
1:B:157:ALA:N	1:D:156:VAL:HG11	2.34	0.43
1:A:62:GLN:NE2	2:A:522:HOH:O	2.34	0.43
1:C:199:LEU:HG	1:C:203:LEU:HD23	2.00	0.43
1:A:141:ARG:N	2:A:590:HOH:O	2.52	0.42
1:D:5:PHE:HB2	2:D:548:HOH:O	2.20	0.42
1:B:231:LEU:O	1:B:257:ASP:HB2	2.20	0.42
1:A:80:ALA:HB3	1:A:146:ILE:HD12	2.02	0.42
1:A:152:HIS:HB2	1:A:153:PRO:HD2	2.01	0.42
1:D:159:MET:HE3	2:D:606:HOH:O	2.18	0.42
1:D:93:ILE:HD12	1:D:104:LEU:O	2.19	0.42
1:A:29:TRP:O	1:A:33:GLN:HG2	2.20	0.42
1:C:57:LEU:HD21	1:C:79:ALA:HA	2.02	0.41
1:C:212:PHE:CE2	2:C:610:HOH:O	2.72	0.41
1:B:174:GLN:NE2	2:B:617:HOH:O	2.54	0.40
1:B:194:ALA:HA	1:D:212:PHE:CD1	2.56	0.40
1:C:104:LEU:HD22	1:C:112:GLN:HB3	2.02	0.40
1:C:9:GLY:HA2	1:C:38:ILE:O	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	267/292 (91%)	260 (97%)	7 (3%)	0	100	100
1	B	275/292 (94%)	269 (98%)	6 (2%)	0	100	100
1	C	261/292 (89%)	253 (97%)	6 (2%)	2 (1%)	16	11
1	D	259/292 (89%)	248 (96%)	11 (4%)	0	100	100
All	All	1062/1168 (91%)	1030 (97%)	30 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	ASP
1	C	96	GLY

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	238/254 (94%)	229 (96%)	9 (4%)	29	29
1	B	244/254 (96%)	238 (98%)	6 (2%)	42	45
1	C	235/254 (92%)	224 (95%)	11 (5%)	23	22
1	D	232/254 (91%)	228 (98%)	4 (2%)	53	60
All	All	949/1016 (93%)	919 (97%)	30 (3%)	34	35

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	52	VAL
1	A	97	ASN
1	A	111	GLN
1	A	122	ILE
1	A	136	GLN
1	A	146	ILE
1	A	156	VAL
1	A	206	ILE
1	B	26	LEU
1	B	42	GLN
1	B	52	VAL
1	B	136	GLN
1	B	156	VAL
1	B	159	MET
1	C	6	LYS
1	C	24	GLU
1	C	26	LEU
1	C	41	GLN
1	C	69	VAL

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Mol	Chain	Res	Type
1	C	87	ASP
1	C	122	ILE
1	C	136	GLN
1	C	140	LYS
1	C	248	ILE
1	C	250	LEU
1	D	23	HIS
1	D	62	GLN
1	D	93	ILE
1	D	155	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	13	HIS
1	A	62	GLN
1	A	89	ASN
1	A	97	ASN
1	A	111	GLN
1	A	152	HIS
1	A	158	HIS
1	A	214	HIS
1	A	268	ASN
1	B	13	HIS
1	B	45	HIS
1	B	63	GLN
1	B	75	ASN
1	B	147	ASN
1	B	158	HIS
1	B	174	GLN
1	B	279	ASN
1	C	41	GLN
1	C	48	GLN
1	C	75	ASN
1	C	89	ASN
1	C	94	ASN
1	C	136	GLN
1	C	147	ASN
1	C	214	HIS
1	C	247	GLN
1	C	253	GLN

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Mol	Chain	Res	Type
1	C	266	HIS
1	C	268	ASN
1	D	89	ASN
1	D	97	ASN
1	D	108	ASN
1	D	112	GLN
1	D	147	ASN
1	D	152	HIS
1	D	158	HIS
1	D	235	HIS
1	D	247	GLN
1	D	266	HIS

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	275/292 (94%)	0.35	17 (6%) 26 25	21, 29, 46, 53	0
1	B	281/292 (96%)	0.47	28 (9%) 12 11	21, 30, 50, 80	0
1	C	271/292 (92%)	1.29	57 (21%) 2 2	24, 38, 62, 80	0
1	D	268/292 (91%)	0.88	37 (13%) 6 6	23, 35, 53, 90	0
All	All	1095/1168 (93%)	0.74	139 (12%) 8 7	21, 32, 56, 90	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	6.3
1	B	47	LEU	4.9
1	B	154	GLY	4.7
1	B	155	LYS	4.6
1	D	156	VAL	4.5
1	D	157	ALA	4.4
1	B	43	ILE	4.4
1	C	43	ILE	4.3
1	D	239	ASP	4.3
1	D	22	THR	4.2
1	C	47	LEU	4.1
1	B	13	HIS	4.1
1	C	41	GLN	4.0
1	C	27	TYR	3.9
1	D	52	VAL	3.8
1	C	26	LEU	3.8
1	C	158	HIS	3.7
1	B	46	GLU	3.6
1	D	23	HIS	3.6
1	B	96	GLY	3.5
1	D	27	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	155	LYS	3.4
1	A	13	HIS	3.4
1	B	48	GLN	3.4
1	B	44	ALA	3.3
1	D	155	LYS	3.3
1	D	96	GLY	3.3
1	B	157	ALA	3.3
1	D	106	PRO	3.2
1	C	23	HIS	3.2
1	D	95	ARG	3.2
1	C	111	GLN	3.2
1	A	141	ARG	3.1
1	B	23	HIS	3.1
1	C	5	PHE	3.1
1	D	71	GLY	3.1
1	C	107	ASP	3.1
1	C	21	THR	3.0
1	D	50	LYS	3.0
1	D	246	SER	3.0
1	B	22	THR	3.0
1	C	25	MET	3.0
1	B	98	LEU	2.9
1	C	133	VAL	2.9
1	C	160	ILE	2.9
1	B	45	HIS	2.9
1	B	21	THR	2.9
1	B	87	ASP	2.8
1	C	98	LEU	2.8
1	B	51	ASN	2.8
1	C	136	GLN	2.8
1	A	142	ILE	2.8
1	D	123	SER	2.8
1	C	29	TRP	2.8
1	D	236	ARG	2.7
1	C	202	SER	2.7
1	A	154	GLY	2.7
1	C	44	ALA	2.7
1	D	26	LEU	2.7
1	C	13	HIS	2.7
1	D	31	CYS	2.7
1	B	97	ASN	2.7
1	C	120	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	202	SER	2.6
1	C	71	GLY	2.6
1	C	45	HIS	2.6
1	C	172	PHE	2.6
1	C	170	PHE	2.5
1	C	137	ASP	2.5
1	D	105	ASP	2.5
1	D	25	MET	2.5
1	C	233	PHE	2.5
1	C	42	GLN	2.4
1	C	87	ASP	2.4
1	B	25	MET	2.4
1	D	158	HIS	2.4
1	D	72	GLY	2.4
1	D	94	ASN	2.4
1	B	52	VAL	2.4
1	C	122	ILE	2.4
1	D	29	TRP	2.4
1	B	137	ASP	2.4
1	C	73	ASP	2.4
1	C	234	SER	2.4
1	C	28	ARG	2.4
1	C	266	HIS	2.4
1	C	274	ASP	2.4
1	D	137	ASP	2.4
1	D	138	ARG	2.4
1	D	56	THR	2.4
1	C	97	ASN	2.3
1	C	72	GLY	2.3
1	C	118	GLU	2.3
1	C	117	LEU	2.3
1	D	98	LEU	2.3
1	B	4	HIS	2.3
1	C	38	ILE	2.3
1	C	52	VAL	2.3
1	A	21	THR	2.3
1	A	204	ASP	2.3
1	C	95	ARG	2.3
1	A	134	CYS	2.3
1	B	24	GLU	2.2
1	C	254	GLU	2.2
1	D	160	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	156	VAL	2.2
1	C	108	ASN	2.2
1	B	28	ARG	2.2
1	C	22	THR	2.2
1	A	96	GLY	2.2
1	C	154	GLY	2.2
1	A	50	LYS	2.2
1	C	140	LYS	2.2
1	C	220	PRO	2.1
1	B	41	GLN	2.1
1	C	246	SER	2.1
1	C	288	SER	2.1
1	C	75	ASN	2.1
1	D	159	MET	2.1
1	B	204	ASP	2.1
1	A	136	GLN	2.1
1	C	53	PRO	2.1
1	C	54	THR	2.1
1	A	43	ILE	2.1
1	D	292	PHE	2.1
1	A	246	SER	2.1
1	C	32	ASP	2.1
1	D	103	ASP	2.1
1	A	235	HIS	2.1
1	C	215	THR	2.1
1	D	119	GLY	2.1
1	A	87	ASP	2.0
1	D	135	GLN	2.0
1	B	95	ARG	2.0
1	D	220	PRO	2.0
1	A	119	GLY	2.0
1	D	108	ASN	2.0
1	C	110	LEU	2.0
1	D	30	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.