Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 01:31 AM EDT

PDB ID	:	2AN1
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 (i) 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 (1)) were used in the production of this report:

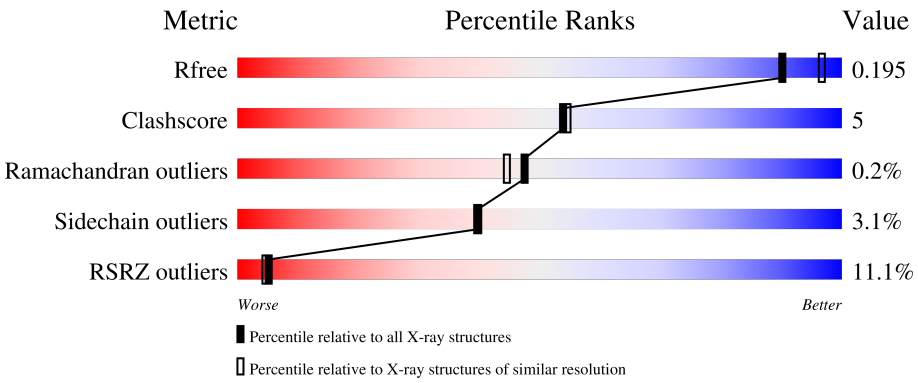
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	3%, 81%, 11%, • 6%
1	B	292	8%, 87%, 10%, •
1	C	292	16%, 79%, 13%, • 7%
1	D	292	13%, 82%, 9%, • 8%

2 Entry composition (i)

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

- Molecule 2 is water.

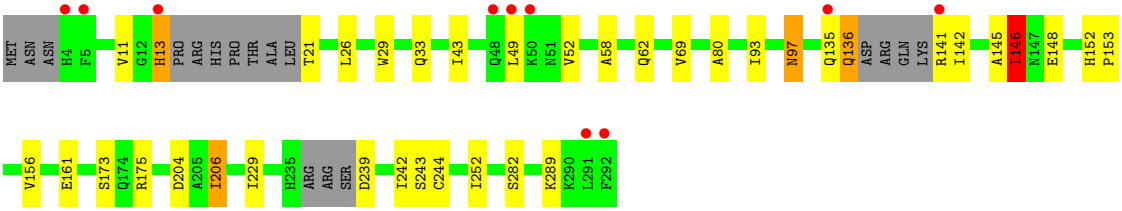
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	151	151	151	0	0
2	B	170	170	170	0	0
2	C	104	104	104	0	0
2	D	117	117	117	0	0

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.

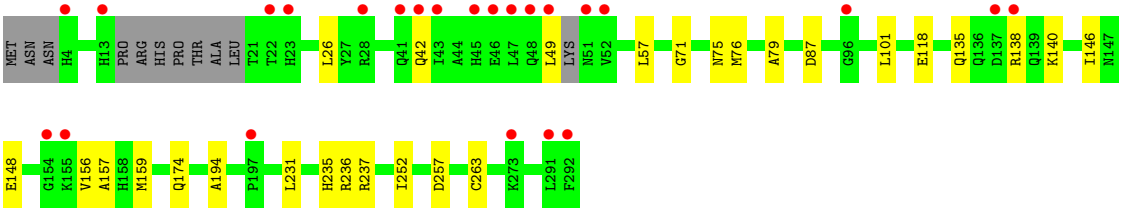
- Molecule 1: putative kinase

Chain A:



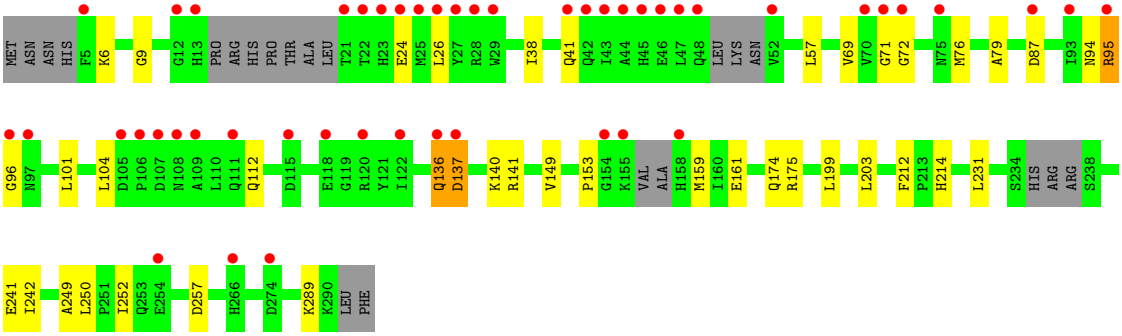
- Molecule 1: putative kinase

Chain B:



- Molecule 1: putative kinase

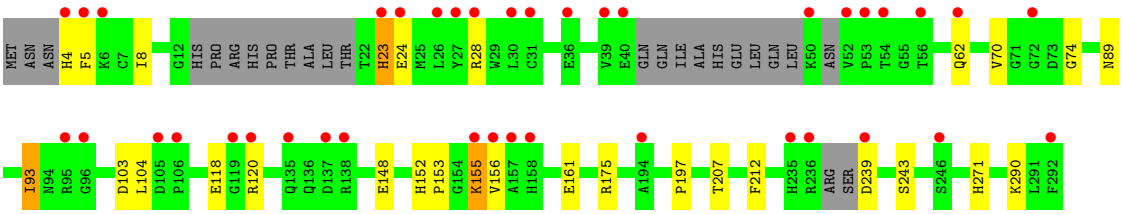
Chain C:



- Molecule 1: putative kinase

Chain D:

13%
82%
9%
8%


MET ASN ASN H4 F5 K6 C7 I8 G12 HIS PRO ARG HIS PRO THR ALA LEU THR T22 H23 E24 M25 L26 Y27 R28 W29 L30 C31 E36 V39 E40 GLN GLN GLN ILE ALA HIS GLU LEU GLN LEU K50 ASN V52 P53 T54 G55 T56 Q62 V70 G71 G72 D73 G74 N89
I93 N94 R95 G96 D103 L104 D105 P106 E118 G119 R120 Q135 Q136 D137 R138 E148 H152 P153 G154 K155 V156 A157 H158 E161 R175 A194 P197 T207 F212 H235 R236 ARG SER D239 S243 S246 H271 K290 L291 F292

4 Data and refinement statistics (i)

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 40.96 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.00) 97.2 (40.96-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.04%)	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)	0.37 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.50	0/2189	0.63	1/2968 (0.0%)
1	B	0.52	1/2246 (0.0%)	0.65	0/3044
1	C	0.44	0/2151	0.58	0/2914
1	D	0.48	0/2134	0.59	0/2888
All	All	0.49	1/8720 (0.0%)	0.61	1/11814 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	CYS	CB-SG	-6.82	1.70	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ILE	CB-CA-C	-5.30	101.00	111.60

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	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	151	0	0	7	0
2	B	170	0	0	4	0
2	C	104	0	0	4	0
2	D	117	0	0	8	0
All	All	9108	0	8528	90	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 (90) 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:C:159:MET:HE2	1:C:214:HIS:HB2	1.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:HD2	2:B:669:HOH:O	1.85	0.59
1:B:87:ASP:OD1	1:B:87:ASP:C	2.40	0.58
1:A:239:ASP:N	2:A:637:HOH:O	2.35	0.58
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:B:138:ARG:HH12	1:B:140:LYS:HZ3	1.52	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: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: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:D:24:GLU:H	1:D:24:GLU:CD	2.18	0.46
1:D:152:HIS:HD2	1:D:153:PRO:O	1.97	0.46
1:C:159:MET:CE	1:C:214:HIS:HB2	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:141:ARG:C	1:A:142:ILE:HD12	2.40	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 (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	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%)	19	13
1	D	259/292 (89%)	248 (96%)	11 (4%)	0	100	100
All	All	1062/1168 (91%)	1030 (97%)	30 (3%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

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

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	238/254 (94%)	232 (98%)	6 (2%)	47	49
1	B	244/254 (96%)	236 (97%)	8 (3%)	38	37
1	C	235/254 (92%)	226 (96%)	9 (4%)	33	31
1	D	232/254 (91%)	226 (97%)	6 (3%)	46	48
All	All	949/1016 (93%)	920 (97%)	29 (3%)	40	40

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	97	ASN
1	A	136	GLN
1	A	146	ILE
1	A	148	GLU
1	A	206	ILE
1	B	26	LEU
1	B	42	GLN
1	B	118	GLU
1	B	135	GLN
1	B	148	GLU
1	B	156	VAL
1	B	159	MET
1	B	237	ARG
1	C	6	LYS
1	C	24	GLU
1	C	26	LEU
1	C	41	GLN

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Mol	Chain	Res	Type
1	C	69	VAL
1	C	87	ASP
1	C	95	ARG
1	C	136	GLN
1	C	250	LEU
1	D	4	HIS
1	D	23	HIS
1	D	62	GLN
1	D	93	ILE
1	D	148	GLU
1	D	155	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	152	HIS
1	A	158	HIS
1	A	268	ASN
1	B	13	HIS
1	B	45	HIS
1	B	75	ASN
1	B	132	GLN
1	B	147	ASN
1	B	158	HIS
1	B	174	GLN
1	B	279	ASN
1	C	41	GLN
1	C	89	ASN
1	C	136	GLN
1	C	147	ASN
1	C	158	HIS
1	C	214	HIS
1	C	247	GLN
1	C	253	GLN
1	C	266	HIS
1	C	268	ASN
1	D	89	ASN

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Mol	Chain	Res	Type
1	D	108	ASN
1	D	147	ASN
1	D	152	HIS
1	D	158	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 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	275/292 (94%)	0.34	10 (3%)	42	42	21, 29, 46, 53	0
1	B	281/292 (96%)	0.51	24 (8%)	10	10	21, 30, 50, 80	0
1	C	271/292 (92%)	1.03	48 (17%)	1	1	24, 38, 62, 80	0
1	D	268/292 (91%)	0.79	39 (14%)	2	2	23, 35, 53, 90	0
All	All	1095/1168 (93%)	0.66	121 (11%)	5	4	21, 32, 56, 90	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	ILE	7.7
1	C	45	HIS	7.5
1	B	48	GLN	6.9
1	D	52	VAL	6.6
1	B	46	GLU	6.5
1	C	42	GLN	6.5
1	C	23	HIS	6.5
1	C	41	GLN	6.3
1	B	45	HIS	5.7
1	C	47	LEU	5.6
1	D	4	HIS	5.5
1	C	52	VAL	5.2
1	C	44	ALA	5.2
1	D	95	ARG	5.1
1	D	27	TYR	5.0
1	C	13	HIS	5.0
1	C	21	THR	5.0
1	C	107	ASP	5.0
1	B	155	LYS	4.8
1	D	157	ALA	4.6
1	C	46	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	28	ARG	4.5
1	C	48	GLN	4.4
1	C	24	GLU	4.4
1	C	136	GLN	4.3
1	C	25	MET	4.3
1	C	120	ARG	4.3
1	B	47	LEU	4.1
1	D	50	LYS	4.1
1	C	95	ARG	4.1
1	C	22	THR	4.0
1	D	239	ASP	4.0
1	C	72	GLY	4.0
1	C	105	ASP	4.0
1	D	156	VAL	3.9
1	D	56	THR	3.9
1	C	108	ASN	3.8
1	C	27	TYR	3.8
1	C	26	LEU	3.8
1	D	53	PRO	3.7
1	B	4	HIS	3.5
1	B	96	GLY	3.5
1	C	29	TRP	3.5
1	D	236	ARG	3.5
1	C	111	GLN	3.5
1	C	106	PRO	3.4
1	A	4	HIS	3.4
1	A	141	ARG	3.3
1	D	292	PHE	3.3
1	B	23	HIS	3.3
1	D	31	CYS	3.3
1	D	28	ARG	3.2
1	C	5	PHE	3.2
1	D	137	ASP	3.2
1	C	118	GLU	3.2
1	B	41	GLN	3.2
1	B	13	HIS	3.1
1	D	23	HIS	3.1
1	B	49	LEU	3.1
1	D	54	THR	3.0
1	C	254	GLU	3.0
1	A	292	PHE	3.0
1	D	155	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	50	LYS	3.0
1	D	246	SER	3.0
1	B	154	GLY	2.9
1	B	51	ASN	2.9
1	C	109	ALA	2.9
1	D	158	HIS	2.9
1	B	138	ARG	2.9
1	D	135	GLN	2.9
1	D	106	PRO	2.9
1	D	24	GLU	2.9
1	D	26	LEU	2.8
1	C	158	HIS	2.8
1	C	96	GLY	2.8
1	C	97	ASN	2.8
1	D	105	ASP	2.8
1	D	6	LYS	2.8
1	C	12	GLY	2.7
1	B	292	PHE	2.7
1	D	119	GLY	2.7
1	A	13	HIS	2.6
1	D	235	HIS	2.6
1	B	22	THR	2.6
1	B	43	ILE	2.6
1	D	120	ARG	2.5
1	D	96	GLY	2.5
1	C	93	ILE	2.5
1	B	273	LYS	2.5
1	A	135	GLN	2.5
1	C	115	ASP	2.5
1	D	62	GLN	2.4
1	C	87	ASP	2.4
1	D	138	ARG	2.4
1	C	75	ASN	2.4
1	C	266	HIS	2.3
1	B	52	VAL	2.3
1	A	291	LEU	2.3
1	B	28	ARG	2.2
1	C	122	ILE	2.2
1	B	197	PRO	2.2
1	C	274	ASP	2.2
1	D	36	GLU	2.1
1	D	39	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	155	LYS	2.1
1	D	40	GLU	2.1
1	A	5	PHE	2.1
1	C	70	VAL	2.1
1	C	71	GLY	2.1
1	C	154	GLY	2.1
1	D	72	GLY	2.1
1	A	49	LEU	2.1
1	C	137	ASP	2.0
1	A	48	GLN	2.0
1	B	42	GLN	2.0
1	B	137	ASP	2.0
1	B	291	LEU	2.0
1	D	30	LEU	2.0
1	D	5	PHE	2.0
1	D	194	ALA	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 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.