



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:40 PM UTC

PDB ID : 2VBX / pdb_00002vbx
Title : Feast or famine regulatory protein (Rv3291c) from *M. tuberculosis* complexed with L-Phenylalanine
Authors : Shrivastava, T.; Ramachandran, R.
Deposited on : 2007-09-18
Resolution : 2.75 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
Mogul : 2022.3.0, CSD as543be (2022)
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

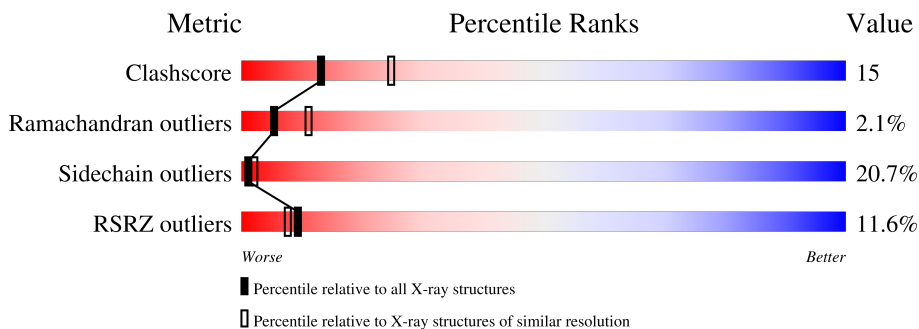
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	150	
1	B	150	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HIS	A	1152	-	-	X	-

2 Entry composition [i](#)

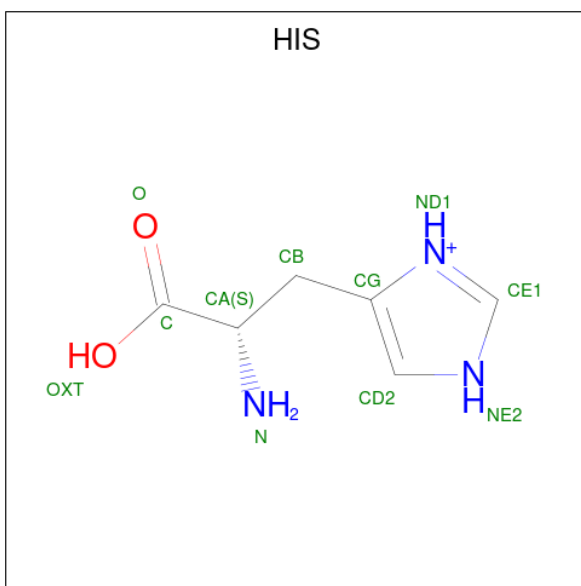
There are 3 unique types of molecules in this entry. The entry contains 2292 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSCRIPTIONAL REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	147	Total	C	N	O	S	0	0	0
			1127	697	209	220	1			
1	B	147	Total	C	N	O	S	0	0	0
			1111	689	203	218	1			

- Molecule 2 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			11	6	3	2		
2	A	1	Total	C	N	O	0	0
			11	6	3	2		

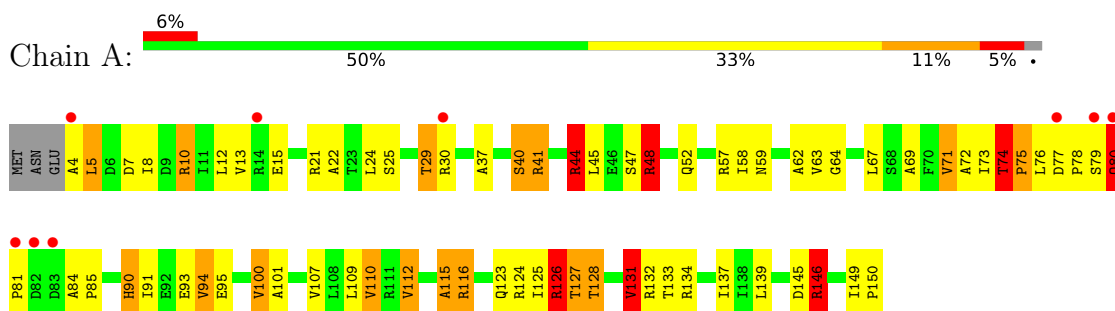
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total 16	O 16	0	0
3	B	16	Total 16	O 16	0	0

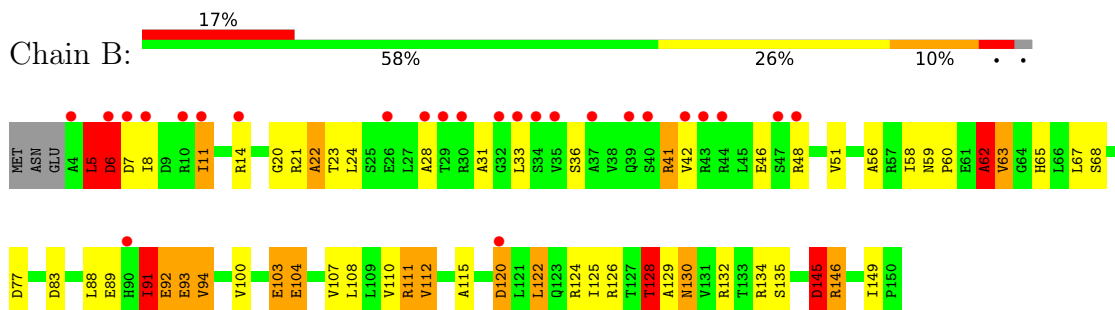
3 Residue-property plots [i](#)

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: TRANSCRIPTIONAL REGULATORY PROTEIN



- Molecule 1: TRANSCRIPTIONAL REGULATORY PROTEIN



4 Data and refinement statistics i

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.90Å 100.90Å 99.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.43 – 2.75 71.35 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.6 (71.43-2.75) 97.6 (71.35-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.226 , 0.270 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-l,-k 0.010 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2292	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 6.53% 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	1.86	14/1141 (1.2%)	1.90	35/1552 (2.3%)
1	B	1.75	11/1125 (1.0%)	1.85	31/1533 (2.0%)
All	All	1.81	25/2266 (1.1%)	1.88	66/3085 (2.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ILE	CA-CB	8.59	1.64	1.53
1	B	111	ARG	N-CA	7.50	1.55	1.45
1	B	104	GLU	N-CA	7.34	1.55	1.45
1	A	101	ALA	CA-CB	-6.63	1.42	1.53
1	A	74	THR	CA-C	6.57	1.58	1.52
1	B	94	VAL	C-O	-6.49	1.15	1.23
1	A	57	ARG	CA-CB	6.46	1.60	1.52
1	A	100	VAL	C-N	6.45	1.42	1.33
1	A	115	ALA	CA-CB	-6.25	1.43	1.53
1	B	112	VAL	C-O	6.24	1.32	1.24
1	A	44	ARG	CA-C	5.92	1.60	1.52
1	A	100	VAL	CA-C	5.71	1.59	1.52
1	B	62	ALA	C-O	-5.70	1.16	1.24
1	A	72	ALA	CA-C	5.70	1.60	1.52
1	B	149	ILE	CA-C	-5.65	1.48	1.53
1	A	116	ARG	CB-CG	5.62	1.69	1.52
1	A	63	VAL	CA-CB	5.58	1.60	1.54
1	B	107	VAL	CA-CB	-5.58	1.47	1.54
1	B	149	ILE	N-CA	-5.57	1.42	1.46
1	A	91	ILE	CA-CB	-5.55	1.47	1.54
1	B	91	ILE	CA-C	5.39	1.58	1.52
1	A	110	VAL	CA-CB	-5.33	1.47	1.55
1	A	37	ALA	CA-CB	-5.26	1.45	1.53
1	A	69	ALA	CA-CB	-5.08	1.44	1.53
1	B	103	GLU	N-CA	5.03	1.52	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLN	CA-C-N	-11.16	107.98	119.92
1	A	80	GLN	C-N-CA	-11.16	107.98	119.92
1	B	104	GLU	N-CA-CB	-9.92	96.17	111.05
1	B	91	ILE	CB-CA-C	9.41	123.94	111.33
1	B	129	ALA	CA-C-N	-9.17	109.18	123.12
1	B	129	ALA	C-N-CA	-9.17	109.18	123.12
1	B	112	VAL	CB-CA-C	8.90	120.11	111.74
1	B	103	GLU	CA-C-N	-8.33	108.12	123.03
1	B	103	GLU	C-N-CA	-8.33	108.12	123.03
1	B	128	THR	N-CA-C	7.95	119.86	111.03
1	B	130	ASN	CB-CA-C	7.81	123.84	111.73
1	A	145	ASP	CA-C-N	-7.80	108.59	122.32
1	A	145	ASP	C-N-CA	-7.80	108.59	122.32
1	A	64	GLY	N-CA-C	7.70	126.13	115.27
1	A	74	THR	CA-C-N	7.65	128.12	119.93
1	A	74	THR	C-N-CA	7.65	128.12	119.93
1	B	129	ALA	N-CA-C	-7.58	100.75	110.53
1	B	103	GLU	O-C-N	7.23	132.37	122.46
1	B	145	ASP	N-CA-C	7.06	125.84	110.80
1	B	120	ASP	N-CA-C	6.76	118.31	111.07
1	B	111	ARG	CD-NE-CZ	-6.42	115.41	124.40
1	B	33	LEU	N-CA-C	6.40	116.31	107.73
1	B	77	ASP	CA-C-N	-6.40	113.02	120.12
1	B	77	ASP	C-N-CA	-6.40	113.02	120.12
1	B	91	ILE	N-CA-CB	6.38	117.90	110.82
1	A	48	ARG	CA-C-N	-6.38	108.91	121.41
1	A	48	ARG	C-N-CA	-6.38	108.91	121.41
1	A	131	VAL	N-CA-CB	-6.26	100.21	111.92
1	B	134	ARG	CA-C-N	-6.25	112.99	122.81
1	B	134	ARG	C-N-CA	-6.25	112.99	122.81
1	B	41	ARG	N-CA-C	-6.23	104.18	110.97
1	B	91	ILE	CA-CB-CG2	6.22	121.07	110.50
1	A	100	VAL	N-CA-CB	-6.11	101.34	111.36
1	A	126	ARG	CG-CD-NE	-6.08	98.62	112.00
1	A	78	PRO	N-CA-C	6.02	120.94	114.68
1	A	62	ALA	N-CA-C	5.97	118.55	111.33
1	B	48	ARG	N-CA-C	-5.95	101.50	110.24
1	A	146	ARG	CD-NE-CZ	5.92	132.69	124.40
1	B	111	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	B	122	LEU	N-CA-C	5.84	117.65	111.28
1	A	71	VAL	CB-CA-C	5.83	119.05	110.77
1	A	116	ARG	N-CA-CB	5.75	118.69	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	N-CA-C	-5.74	105.02	111.28
1	B	135	SER	CA-CB-OG	-5.64	99.82	111.10
1	A	112	VAL	N-CA-CB	-5.62	103.06	112.06
1	A	44	ARG	CA-C-N	5.61	129.23	120.82
1	A	44	ARG	C-N-CA	5.61	129.23	120.82
1	A	58	ILE	N-CA-C	5.60	116.83	109.21
1	A	139	LEU	N-CA-C	-5.60	104.67	112.45
1	B	94	VAL	N-CA-CB	5.59	117.94	111.90
1	B	5	LEU	N-CA-C	-5.58	98.92	110.80
1	A	48	ARG	N-CA-C	-5.55	98.98	110.80
1	B	14	ARG	N-CA-CB	5.45	117.91	110.01
1	A	59	ASN	CA-C-N	-5.36	113.51	119.19
1	A	59	ASN	C-N-CA	-5.36	113.51	119.19
1	A	48	ARG	O-C-N	-5.35	115.48	122.59
1	A	101	ALA	N-CA-C	-5.27	103.43	110.55
1	A	126	ARG	N-CA-CB	5.26	117.85	110.12
1	A	94	VAL	CB-CA-C	5.25	117.91	111.25
1	B	56	ALA	N-CA-C	-5.22	102.02	110.32
1	A	12	LEU	CA-C-O	-5.14	115.41	120.70
1	A	37	ALA	N-CA-C	-5.12	105.69	111.28
1	A	100	VAL	CA-C-O	5.10	126.36	120.90
1	B	63	VAL	N-CA-C	-5.10	107.74	112.43
1	A	40	SER	N-CA-C	5.07	117.20	111.02
1	A	146	ARG	NE-CZ-NH1	5.03	126.53	121.50

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	1127	0	1130	30	0
1	B	1111	0	1104	35	0
2	A	22	0	12	7	0
3	A	16	0	0	10	0
3	B	16	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2292	0	2246	67	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 15.

All (67) 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:132:ARG:HD3	3:B:2012:HOH:O	1.47	1.11
1:B:91:ILE:HD11	1:B:93:GLU:HG2	1.50	0.93
1:A:124:ARG:O	1:A:128:THR:HG23	1.77	0.84
1:A:8:ILE:HB	1:A:41:ARG:NH2	2.00	0.76
2:A:1152:HIS:HA	3:A:2015:HOH:O	1.85	0.76
1:B:21:ARG:O	1:B:22:ALA:C	2.30	0.74
1:B:21:ARG:O	1:B:22:ALA:O	2.07	0.73
1:A:134:ARG:HH12	2:A:1152:HIS:N	1.87	0.72
2:A:1152:HIS:CG	3:A:2015:HOH:O	2.43	0.71
1:A:21:ARG:NH1	1:B:20:GLY:O	2.25	0.69
1:A:15:GLU:OE1	1:A:30:ARG:NH1	2.25	0.68
1:B:63:VAL:O	1:B:63:VAL:HG12	1.94	0.68
2:A:1152:HIS:ND1	3:A:2015:HOH:O	2.27	0.67
1:B:28:ALA:HA	1:B:31:ALA:HB3	1.77	0.65
1:A:134:ARG:NH2	3:A:2011:HOH:O	2.32	0.62
1:B:124:ARG:HD3	3:B:2009:HOH:O	2.00	0.61
1:B:68:SER:OG	1:B:111:ARG:HD3	2.01	0.60
1:A:47:SER:C	1:A:48:ARG:O	2.44	0.58
2:A:1152:HIS:CG	3:A:2011:HOH:O	2.57	0.57
2:A:1152:HIS:ND1	3:A:2011:HOH:O	2.33	0.57
1:B:91:ILE:CD1	1:B:93:GLU:HG2	2.30	0.57
2:A:1152:HIS:ND1	3:A:2009:HOH:O	2.27	0.56
3:A:2010:HOH:O	1:B:103:GLU:HG3	2.04	0.56
1:A:84:ALA:HB3	1:A:85:PRO:HD3	1.94	0.50
1:B:42:VAL:O	1:B:46:GLU:HG3	2.12	0.50
1:B:60:PRO:O	1:B:65:HIS:HB2	2.12	0.49
1:B:59:ASN:HD22	1:B:62:ALA:HB2	1.78	0.49
1:A:77:ASP:OD2	1:A:79:SER:OG	2.31	0.48
1:B:67:LEU:HD12	1:B:115:ALA:HA	1.95	0.48
1:A:146:ARG:NH2	1:B:89:GLU:O	2.40	0.48
1:A:73:ILE:HG22	1:A:133:THR:HG22	1.95	0.48
1:A:10:ARG:NH1	1:A:150:PRO:O	2.47	0.47
1:B:91:ILE:HD12	1:B:92:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:HG2	1:B:145:ASP:HA	1.97	0.46
1:A:44:ARG:NH2	3:A:2004:HOH:O	2.48	0.46
1:B:63:VAL:O	1:B:63:VAL:CG1	2.64	0.45
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.82	0.45
1:B:122:LEU:O	1:B:126:ARG:HG3	2.17	0.45
1:B:128:THR:HG21	3:B:2001:HOH:O	2.17	0.44
1:A:90:HIS:CD2	1:A:90:HIS:C	2.95	0.44
1:A:123:GLN:O	1:A:127:THR:HG23	2.17	0.44
1:B:11:ILE:H	1:B:11:ILE:HG12	1.59	0.44
1:A:8:ILE:CB	1:A:41:ARG:NH2	2.78	0.44
1:A:115:ALA:O	1:A:116:ARG:C	2.61	0.43
1:B:59:ASN:ND2	1:B:62:ALA:HB2	2.33	0.43
1:A:21:ARG:O	1:A:22:ALA:C	2.62	0.43
1:A:76:LEU:HD21	1:A:132:ARG:HG3	2.00	0.43
1:B:91:ILE:HD12	1:B:91:ILE:C	2.44	0.43
1:B:146:ARG:HH11	1:B:146:ARG:HB2	1.83	0.43
1:A:134:ARG:NH2	3:A:2009:HOH:O	2.24	0.43
1:A:149:ILE:HG23	1:B:63:VAL:CG1	2.49	0.43
1:A:4:ALA:O	1:A:5:LEU:HD23	2.19	0.42
1:A:80:GLN:O	1:A:81:PRO:C	2.58	0.42
1:A:149:ILE:HA	1:A:150:PRO:HD3	1.81	0.42
1:B:111:ARG:HD3	1:B:111:ARG:HH11	1.55	0.42
1:A:131:VAL:HG13	1:A:132:ARG:O	2.20	0.42
1:B:83:ASP:OD2	1:B:83:ASP:N	2.49	0.41
1:B:124:ARG:O	1:B:128:THR:HG23	2.20	0.41
1:B:124:ARG:O	1:B:125:ILE:C	2.62	0.41
1:A:25:SER:O	1:A:29:THR:HG23	2.19	0.41
1:B:58:ILE:HG21	1:B:63:VAL:HG21	2.01	0.41
1:B:6:ASP:OD1	1:B:7:ASP:N	2.54	0.41
1:B:8:ILE:HB	1:B:41:ARG:HH21	1.85	0.41
1:B:67:LEU:HD23	1:B:67:LEU:HA	1.87	0.41
1:B:88:LEU:HD13	1:B:108:LEU:HD11	2.02	0.41
1:A:125:ILE:O	1:A:126:ARG:C	2.63	0.41
1:A:74:THR:HA	1:A:75:PRO:HD3	1.87	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	145/150 (97%)	140 (97%)	4 (3%)	1 (1%)	18	34
1	B	145/150 (97%)	126 (87%)	14 (10%)	5 (3%)	3	5
All	All	290/300 (97%)	266 (92%)	18 (6%)	6 (2%)	5	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	LEU
1	B	6	ASP
1	B	22	ALA
1	B	145	ASP
1	B	62	ALA
1	A	48	ARG

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	121/126 (96%)	91 (75%)	30 (25%)	1	1
1	B	118/126 (94%)	98 (83%)	20 (17%)	2	3
All	All	239/252 (95%)	189 (79%)	50 (21%)	1	2

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	ASP
1	A	10	ARG
1	A	13	VAL
1	A	24	LEU
1	A	29	THR
1	A	40	SER
1	A	41	ARG
1	A	44	ARG
1	A	45	LEU
1	A	52	GLN
1	A	67	LEU
1	A	71	VAL
1	A	74	THR
1	A	75	PRO
1	A	80	GLN
1	A	90	HIS
1	A	93	GLU
1	A	94	VAL
1	A	100	VAL
1	A	107	VAL
1	A	109	LEU
1	A	110	VAL
1	A	112	VAL
1	A	126	ARG
1	A	127	THR
1	A	128	THR
1	A	131	VAL
1	A	137	ILE
1	A	146	ARG
1	B	5	LEU
1	B	6	ASP
1	B	11	ILE
1	B	23	THR
1	B	24	LEU
1	B	36	SER
1	B	51	VAL
1	B	91	ILE
1	B	92	GLU
1	B	93	GLU
1	B	94	VAL
1	B	100	VAL
1	B	104	GLU

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Mol	Chain	Res	Type
1	B	110	VAL
1	B	112	VAL
1	B	120	ASP
1	B	128	THR
1	B	130	ASN
1	B	145	ASP
1	B	146	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	80	GLN
1	A	90	HIS
1	A	130	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HIS	A	1152	-	10,11,11	0.74	0	10,14,14	1.62	1 (10%)
2	HIS	A	1151	-	10,11,11	0.76	1 (10%)	10,14,14	1.78	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIS	A	1152	-	-	6/8/8/8	0/1/1/1
2	HIS	A	1151	-	-	1/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1151	HIS	OXT-C	-2.25	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1151	HIS	OXT-C-O	-4.84	113.09	124.08
2	A	1152	HIS	OXT-C-O	-3.91	115.20	124.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1152	HIS	OXT-C-CA-CB
2	A	1152	HIS	CA-CB-CG-ND1
2	A	1152	HIS	O-C-CA-CB
2	A	1152	HIS	C-CA-CB-CG
2	A	1152	HIS	CA-CB-CG-CD2
2	A	1152	HIS	OXT-C-CA-N
2	A	1151	HIS	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1152	HIS	7	0

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	147/150 (98%)	0.20	9 (6%) 27 27	10, 30, 58, 79	0
1	B	147/150 (98%)	0.69	25 (17%) 4 3	9, 34, 91, 94	0
All	All	294/300 (98%)	0.44	34 (11%) 9 8	9, 32, 85, 94	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	VAL	5.9
1	B	48	ARG	5.7
1	A	80	GLN	5.0
1	A	81	PRO	4.4
1	A	4	ALA	4.0
1	B	4	ALA	3.8
1	B	44	ARG	3.8
1	B	40	SER	3.6
1	B	29	THR	3.5
1	B	43	ARG	3.5
1	B	37	ALA	3.4
1	B	30	ARG	3.3
1	B	90	HIS	3.1
1	B	26	GLU	2.9
1	B	33	LEU	2.8
1	A	77	ASP	2.8
1	B	47	SER	2.8
1	B	32	GLY	2.7
1	A	83	ASP	2.7
1	B	34	SER	2.7
1	A	79	SER	2.6
1	B	10	ARG	2.5
1	B	14	ARG	2.5
1	B	11	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	42	VAL	2.5
1	A	82	ASP	2.4
1	B	120	ASP	2.4
1	B	8	ILE	2.4
1	A	30	ARG	2.3
1	B	39	GLN	2.2
1	B	7	ASP	2.2
1	A	14	ARG	2.1
1	B	28	ALA	2.1
1	B	6	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HIS	A	1152	11/11	0.89	0.13	47,50,53,54	0
2	HIS	A	1151	11/11	0.91	0.15	51,52,59,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.