



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 3HUU / pdb_00003huu
Title : Crystal structure of transcription regulator like protein from *Staphylococcus haemolyticus*
Authors : Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-06-15
Resolution : 1.95 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

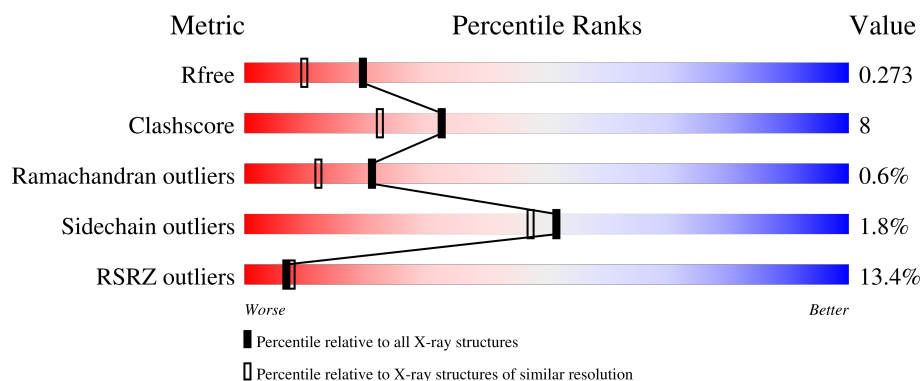
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	305	
1	B	305	
1	C	305	
1	D	305	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8497 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 Transcription regulator like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2100	1325	354	412	9			
1	B	260	Total	C	N	O	S	0	0	0
			2059	1302	342	406	9			
1	C	267	Total	C	N	O	S	0	0	0
			2115	1333	358	415	9			
1	D	265	Total	C	N	O	S	0	0	0
			2095	1321	353	412	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q4L6K9
A	0	SER	-	expression tag	UNP Q4L6K9
A	1	LEU	-	expression tag	UNP Q4L6K9
A	296	GLU	-	expression tag	UNP Q4L6K9
A	297	GLY	-	expression tag	UNP Q4L6K9
A	298	HIS	-	expression tag	UNP Q4L6K9
A	299	HIS	-	expression tag	UNP Q4L6K9
A	300	HIS	-	expression tag	UNP Q4L6K9
A	301	HIS	-	expression tag	UNP Q4L6K9
A	302	HIS	-	expression tag	UNP Q4L6K9
A	303	HIS	-	expression tag	UNP Q4L6K9
B	-1	MET	-	expression tag	UNP Q4L6K9
B	0	SER	-	expression tag	UNP Q4L6K9
B	1	LEU	-	expression tag	UNP Q4L6K9
B	296	GLU	-	expression tag	UNP Q4L6K9
B	297	GLY	-	expression tag	UNP Q4L6K9
B	298	HIS	-	expression tag	UNP Q4L6K9
B	299	HIS	-	expression tag	UNP Q4L6K9
B	300	HIS	-	expression tag	UNP Q4L6K9
B	301	HIS	-	expression tag	UNP Q4L6K9
B	302	HIS	-	expression tag	UNP Q4L6K9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP Q4L6K9
C	-1	MET	-	expression tag	UNP Q4L6K9
C	0	SER	-	expression tag	UNP Q4L6K9
C	1	LEU	-	expression tag	UNP Q4L6K9
C	296	GLU	-	expression tag	UNP Q4L6K9
C	297	GLY	-	expression tag	UNP Q4L6K9
C	298	HIS	-	expression tag	UNP Q4L6K9
C	299	HIS	-	expression tag	UNP Q4L6K9
C	300	HIS	-	expression tag	UNP Q4L6K9
C	301	HIS	-	expression tag	UNP Q4L6K9
C	302	HIS	-	expression tag	UNP Q4L6K9
C	303	HIS	-	expression tag	UNP Q4L6K9
D	-1	MET	-	expression tag	UNP Q4L6K9
D	0	SER	-	expression tag	UNP Q4L6K9
D	1	LEU	-	expression tag	UNP Q4L6K9
D	296	GLU	-	expression tag	UNP Q4L6K9
D	297	GLY	-	expression tag	UNP Q4L6K9
D	298	HIS	-	expression tag	UNP Q4L6K9
D	299	HIS	-	expression tag	UNP Q4L6K9
D	300	HIS	-	expression tag	UNP Q4L6K9
D	301	HIS	-	expression tag	UNP Q4L6K9
D	302	HIS	-	expression tag	UNP Q4L6K9
D	303	HIS	-	expression tag	UNP Q4L6K9

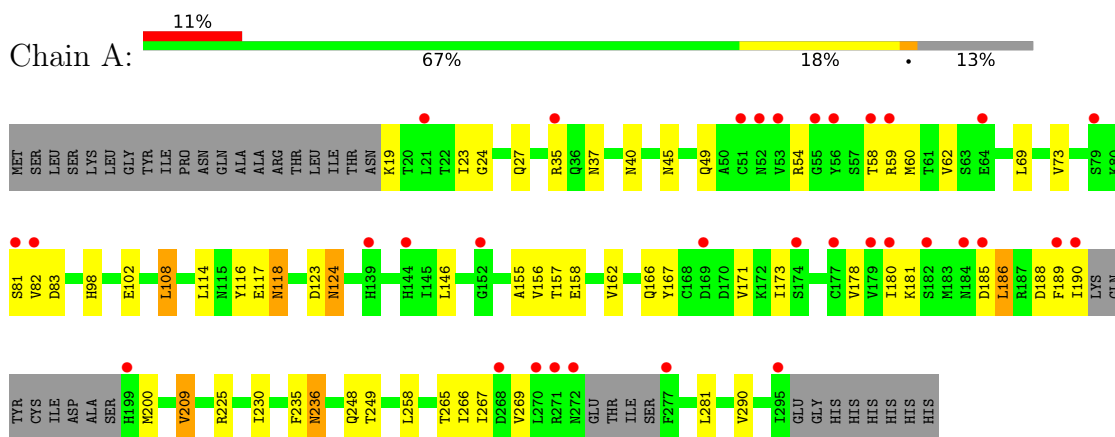
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	38	Total O 38 38	0	0
2	B	30	Total O 30 30	0	0
2	C	26	Total O 26 26	0	0
2	D	34	Total O 34 34	0	0

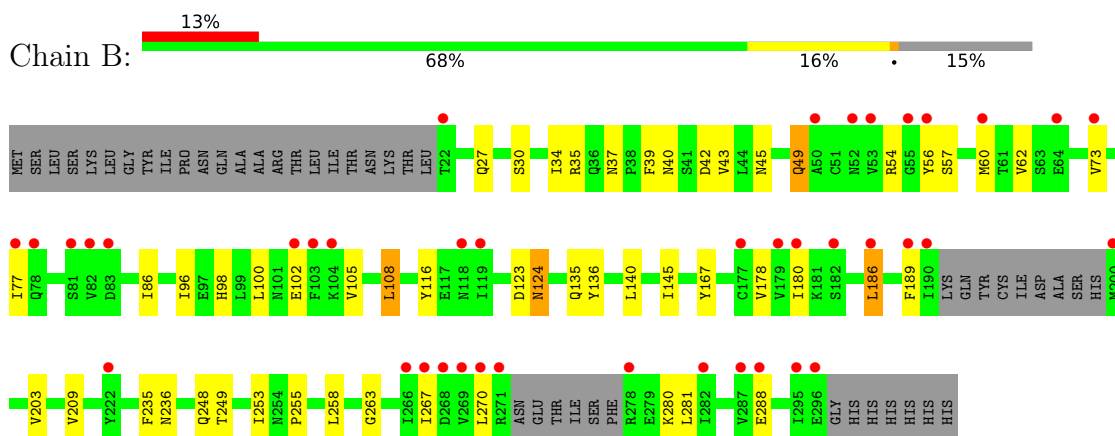
3 Residue-property plots [i](#)

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.

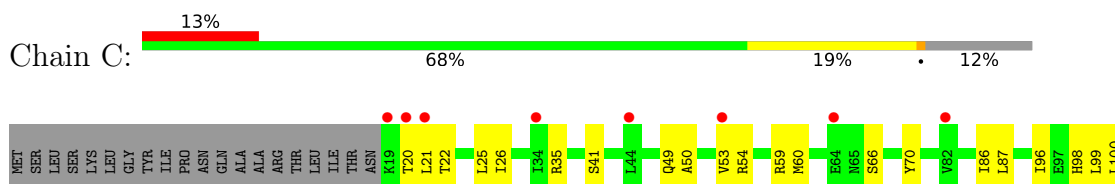
- Molecule 1: Transcription regulator like protein

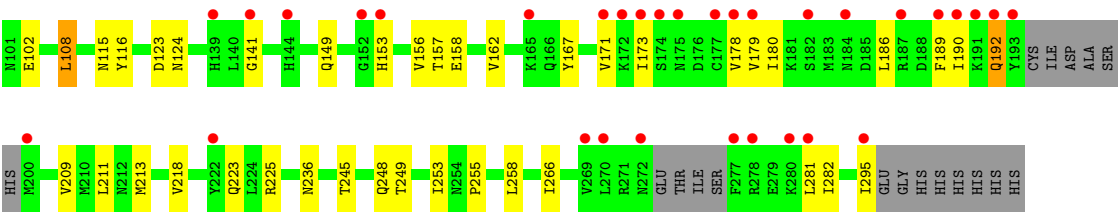


- Molecule 1: Transcription regulator like protein

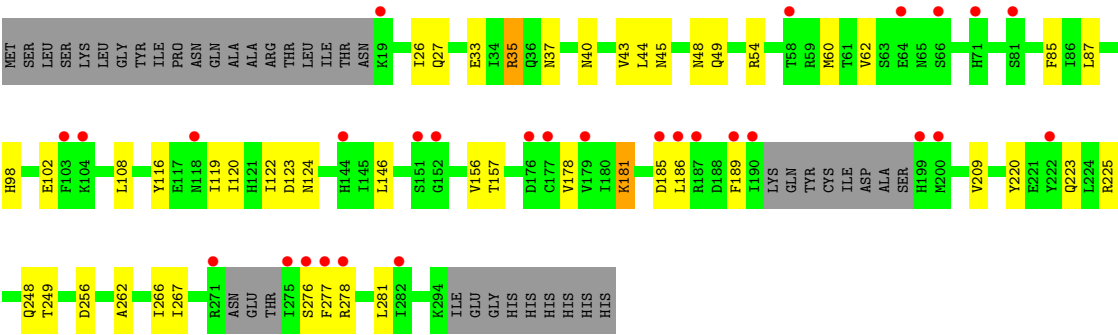


- Molecule 1: Transcription regulator like protein





● Molecule 1: Transcription regulator like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.87Å 68.08Å 97.83Å 82.42° 75.95° 79.39°	Depositor
Resolution (Å)	43.76 – 1.95 43.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	84.2 (43.76-1.95) 84.3 (43.76-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.68 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.274 0.238 , 0.273	Depositor DCC
R_{free} test set	2336 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8497	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2846e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.39	0/2133	0.90	5/2892 (0.2%)
1	B	0.40	0/2092	0.88	5/2840 (0.2%)
1	C	0.48	2/2148 (0.1%)	0.94	8/2912 (0.3%)
1	D	0.41	0/2128	0.93	6/2886 (0.2%)
All	All	0.42	2/8501 (0.0%)	0.91	24/11530 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	ILE	C-N	-9.09	1.20	1.33
1	C	179	VAL	C-N	-7.43	1.23	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	ASN	N-CA-C	-8.94	96.28	110.14
1	D	124	ASN	N-CA-C	-7.90	98.77	110.46
1	A	124	ASN	N-CA-C	-7.87	98.58	110.14
1	D	209	VAL	N-CA-C	6.87	117.63	110.62
1	C	192	GLN	N-CA-C	-6.76	103.20	113.89
1	C	209	VAL	N-CA-C	6.48	117.23	110.62
1	C	248	GLN	N-CA-C	6.32	119.54	109.24
1	A	209	VAL	N-CA-C	6.19	116.94	110.62
1	B	249	THR	N-CA-C	-5.92	101.09	109.96
1	B	209	VAL	N-CA-C	5.86	116.59	110.62
1	B	124	ASN	N-CA-C	-5.75	101.51	110.42
1	A	290	VAL	N-CA-C	5.61	118.06	111.05
1	A	248	GLN	N-CA-C	5.61	118.38	109.24
1	D	119	ILE	N-CA-C	-5.58	100.39	108.87
1	B	140	LEU	N-CA-C	-5.48	106.59	113.28
1	A	249	THR	N-CA-C	-5.46	101.77	109.96
1	D	249	THR	N-CA-C	-5.46	101.77	109.96
1	B	248	GLN	N-CA-C	5.40	118.04	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	GLN	N-CA-C	5.30	118.89	111.74
1	C	211	LEU	N-CA-C	-5.27	105.71	111.82
1	C	66	SER	N-CA-C	5.25	117.01	111.28
1	D	248	GLN	N-CA-C	5.19	117.70	109.24
1	C	249	THR	N-CA-C	-5.13	102.26	109.96
1	C	115	ASN	N-CA-C	5.09	120.14	113.88

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	2100	0	2078	42	0
1	B	2059	0	2032	33	0
1	C	2115	0	2087	40	0
1	D	2095	0	2066	27	0
2	A	38	0	0	0	0
2	B	30	0	0	2	0
2	C	26	0	0	1	0
2	D	34	0	0	1	0
All	All	8497	0	8263	131	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 (131) 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:62:VAL:HG11	1:B:49:GLN:HG3	1.39	1.05
1:C:86:ILE:HG12	1:C:108:LEU:HD11	1.55	0.88
1:A:59:ARG:HD3	1:B:57:SER:HA	1.56	0.87
1:A:49:GLN:HG2	1:B:62:VAL:HG21	1.57	0.87
1:B:86:ILE:HG12	1:B:108:LEU:HD21	1.65	0.79
1:A:146:LEU:HD21	1:A:189:PHE:HE2	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD12	1:C:266:ILE:HD13	1.67	0.75
1:C:49:GLN:CG	1:D:62:VAL:HG21	2.23	0.68
1:A:27:GLN:HE22	1:A:60:MET:HE3	1.57	0.68
1:A:24:GLY:N	1:A:82:VAL:HG21	2.09	0.67
1:C:49:GLN:HG2	1:D:62:VAL:HG21	1.77	0.66
1:D:120:ILE:HG12	1:D:277:PHE:O	1.96	0.64
1:B:263:GLY:O	1:B:267:ILE:HG12	1.97	0.63
1:C:25:LEU:HB2	1:C:60:MET:HG3	1.79	0.63
1:B:178:VAL:HG21	1:B:189:PHE:CZ	2.34	0.61
1:C:253:ILE:HG13	1:C:255:PRO:HD3	1.83	0.60
1:C:53:VAL:HG23	1:C:54:ARG:HG3	1.84	0.59
1:C:59:ARG:HH11	1:C:59:ARG:HG3	1.68	0.59
1:C:213:MET:HG2	2:C:324:HOH:O	2.03	0.58
1:A:27:GLN:NE2	1:A:60:MET:HE3	2.18	0.58
1:B:56:TYR:CD2	1:B:267:ILE:HD12	2.38	0.58
1:A:54:ARG:HD2	1:A:267:ILE:HG21	1.87	0.56
1:D:37:ASN:HB3	1:D:40:ASN:HD22	1.69	0.56
1:D:45:ASN:O	1:D:49:GLN:HG3	2.06	0.56
1:C:86:ILE:HG12	1:C:108:LEU:CD1	2.33	0.56
1:C:186:LEU:O	1:C:190:ILE:HG12	2.06	0.55
1:A:98:HIS:HD2	1:A:116:TYR:OH	1.91	0.53
1:C:258:LEU:HD23	1:C:282:ILE:HD13	1.89	0.53
1:A:178:VAL:HG21	1:A:189:PHE:CE1	2.43	0.53
1:D:26:ILE:HB	1:D:87:LEU:HD12	1.91	0.53
1:A:162:VAL:O	1:A:166:GLN:HG3	2.08	0.53
1:D:27:GLN:HE21	1:D:60:MET:HG2	1.73	0.53
1:D:181:LYS:N	1:D:181:LYS:HD3	2.24	0.53
1:A:265:THR:O	1:A:269:VAL:HG23	2.09	0.53
1:A:200:MET:HE1	1:A:230:ILE:HB	1.90	0.52
1:A:146:LEU:HD21	1:A:189:PHE:CE2	2.38	0.52
1:D:225:ARG:HH11	1:D:225:ARG:HG2	1.74	0.52
1:B:34:ILE:HD12	1:B:34:ILE:N	2.25	0.52
1:B:54:ARG:HD2	1:B:267:ILE:HG21	1.92	0.51
1:B:56:TYR:CE2	1:B:267:ILE:HD12	2.45	0.51
1:B:255:PRO:HA	1:B:258:LEU:HD12	1.92	0.51
1:A:108:LEU:C	1:A:108:LEU:HD23	2.35	0.51
1:A:235:PHE:O	1:A:236:ASN:HB3	2.11	0.51
1:A:37:ASN:HB3	1:A:40:ASN:HD22	1.76	0.51
1:C:20:THR:O	1:C:22:THR:N	2.41	0.51
1:B:27:GLN:NE2	1:B:60:MET:HE2	2.26	0.50
1:D:98:HIS:O	1:D:102:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:HIS:O	1:A:102:GLU:HG2	2.12	0.49
1:A:188:ASP:O	1:A:190:ILE:HG13	2.12	0.49
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.78	0.49
1:C:49:GLN:HG3	1:D:62:VAL:HG21	1.94	0.49
1:C:149:GLN:HG2	1:C:157:THR:CG2	2.43	0.48
1:D:98:HIS:HE1	2:D:306:HOH:O	1.97	0.48
1:C:171:VAL:HG23	1:C:173:ILE:HG12	1.94	0.48
1:C:149:GLN:HG2	1:C:157:THR:HG22	1.95	0.48
1:C:178:VAL:HG11	1:C:189:PHE:CE2	2.48	0.48
1:B:235:PHE:O	1:B:236:ASN:HB3	2.14	0.47
1:D:156:VAL:HG13	1:D:157:THR:N	2.29	0.47
1:D:85:PHE:O	1:D:266:ILE:HD12	2.13	0.47
1:A:82:VAL:HG22	1:A:83:ASP:N	2.28	0.47
1:A:19:LYS:N	1:A:19:LYS:HD2	2.29	0.47
1:A:59:ARG:HH22	1:A:81:SER:HB2	1.80	0.47
1:A:181:LYS:HB2	1:A:185:ASP:OD1	2.15	0.47
1:A:209:VAL:HG13	1:A:235:PHE:O	2.15	0.47
1:B:280:LYS:HD2	1:B:280:LYS:N	2.29	0.47
1:D:62:VAL:O	1:D:62:VAL:HG22	2.14	0.47
1:D:146:LEU:HD21	1:D:189:PHE:HE2	1.79	0.47
1:D:178:VAL:HG21	1:D:189:PHE:CZ	2.50	0.47
1:C:123:ASP:O	1:C:281:LEU:HA	2.15	0.47
1:D:54:ARG:HD2	1:D:267:ILE:HG21	1.97	0.46
1:D:256:ASP:OD1	1:D:256:ASP:N	2.47	0.46
1:C:98:HIS:HD2	1:C:116:TYR:OH	1.98	0.46
1:C:108:LEU:C	1:C:108:LEU:HD22	2.39	0.46
1:A:45:ASN:O	1:A:49:GLN:HG3	2.15	0.46
1:B:98:HIS:O	1:B:102:GLU:HG3	2.15	0.46
1:B:98:HIS:HD2	1:B:116:TYR:OH	1.99	0.46
1:B:86:ILE:HG12	1:B:108:LEU:CD2	2.42	0.46
1:A:114:LEU:HD11	1:A:155:ALA:HB2	1.98	0.46
1:A:180:ILE:HG21	1:A:186:LEU:HG	1.98	0.46
1:A:189:PHE:O	1:A:190:ILE:HB	2.16	0.46
1:C:141:GLY:O	1:C:295:ILE:HD11	2.15	0.46
1:C:190:ILE:C	1:C:192:GLN:H	2.24	0.46
1:B:98:HIS:HE1	2:B:306:HOH:O	1.99	0.45
1:B:100:LEU:HD22	1:B:105:VAL:HG21	1.98	0.45
1:B:135:GLN:HA	1:B:167:TYR:CZ	2.51	0.45
1:B:180:ILE:HG21	1:B:186:LEU:HG	1.99	0.45
1:B:39:PHE:O	1:B:43:VAL:HG23	2.17	0.45
1:C:282:ILE:N	1:C:282:ILE:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:MET:HE3	1:A:230:ILE:HD12	1.99	0.45
1:C:59:ARG:HG3	1:C:59:ARG:NH1	2.32	0.45
1:B:96:ILE:O	1:B:100:LEU:HG	2.17	0.45
1:B:123:ASP:O	1:B:281:LEU:HA	2.17	0.44
1:C:98:HIS:O	1:C:102:GLU:HG2	2.17	0.44
1:C:50:ALA:O	1:C:53:VAL:HG22	2.18	0.44
1:D:27:GLN:NE2	1:D:60:MET:HG2	2.33	0.44
1:D:123:ASP:O	1:D:281:LEU:HA	2.17	0.44
1:A:124:ASN:HD21	1:A:258:LEU:HD11	1.83	0.43
1:A:59:ARG:NH2	1:A:81:SER:HB2	2.33	0.43
1:B:73:VAL:O	1:B:77:ILE:HG13	2.18	0.43
1:C:190:ILE:HG13	1:C:218:VAL:HG11	1.99	0.43
1:C:60:MET:H	1:D:48:ASN:ND2	2.16	0.43
1:C:158:GLU:O	1:C:162:VAL:HG23	2.18	0.43
1:C:96:ILE:O	1:C:100:LEU:HG	2.18	0.43
1:C:26:ILE:HB	1:C:87:LEU:HD12	2.01	0.43
1:A:23:ILE:HG23	1:A:266:ILE:HD13	2.01	0.43
1:C:41:SER:OG	1:D:35:ARG:HD2	2.18	0.43
1:C:186:LEU:HD12	1:C:218:VAL:HG21	2.01	0.43
1:C:167:TYR:O	1:C:171:VAL:HG22	2.18	0.42
1:A:69:LEU:O	1:A:73:VAL:HG23	2.19	0.42
1:B:124:ASN:ND2	1:B:253:ILE:HB	2.34	0.42
1:B:136:TYR:OH	1:B:288:GLU:HG2	2.19	0.42
1:C:70:TYR:CZ	1:C:99:LEU:HD13	2.55	0.42
1:C:156:VAL:HG13	1:C:157:THR:N	2.35	0.42
1:D:98:HIS:HD2	1:D:116:TYR:OH	2.02	0.42
1:D:122:ILE:CD1	1:D:262:ALA:HA	2.50	0.42
1:A:123:ASP:O	1:A:281:LEU:HA	2.19	0.42
1:A:171:VAL:HG23	1:A:173:ILE:HG12	2.00	0.42
1:A:117:GLU:O	1:A:118:ASN:OD1	2.37	0.42
1:A:167:TYR:O	1:A:171:VAL:HG22	2.20	0.42
1:A:35:ARG:NH1	1:B:42:ASP:OD1	2.53	0.41
1:C:141:GLY:C	1:C:295:ILE:HD11	2.45	0.41
1:D:43:VAL:HG13	1:D:44:LEU:N	2.35	0.41
1:A:158:GLU:O	1:A:162:VAL:HG23	2.20	0.41
1:B:37:ASN:HB3	1:B:40:ASN:HD22	1.85	0.41
1:C:225:ARG:HH11	1:C:225:ARG:HG2	1.85	0.41
1:A:35:ARG:HD3	1:B:45:ASN:HB2	2.03	0.41
1:A:156:VAL:HG13	1:A:157:THR:N	2.35	0.41
1:C:245:THR:HG23	1:D:220:TYR:CG	2.56	0.40
1:B:30:SER:O	1:B:35:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ILE:HG12	1:B:203:VAL:CG1	2.51	0.40
1:B:98:HIS:CE1	2:B:306:HOH:O	2.74	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	259/305 (85%)	254 (98%)	4 (2%)	1 (0%)	30	21
1	B	254/305 (83%)	248 (98%)	5 (2%)	1 (0%)	30	21
1	C	261/305 (86%)	250 (96%)	9 (3%)	2 (1%)	16	8
1	D	259/305 (85%)	252 (97%)	5 (2%)	2 (1%)	16	8
All	All	1033/1220 (85%)	1004 (97%)	23 (2%)	6 (1%)	21	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	21	LEU
1	D	276	SER
1	A	236	ASN
1	C	236	ASN
1	D	278	ARG
1	B	270	LEU

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	242/281 (86%)	238 (98%)	4 (2%)	53	49
1	B	238/281 (85%)	235 (99%)	3 (1%)	61	58
1	C	243/281 (86%)	239 (98%)	4 (2%)	55	52
1	D	241/281 (86%)	235 (98%)	6 (2%)	42	34
All	All	964/1124 (86%)	947 (98%)	17 (2%)	51	47

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	108	LEU
1	A	118	ASN
1	A	186	LEU
1	B	49	GLN
1	B	108	LEU
1	B	186	LEU
1	C	35	ARG
1	C	108	LEU
1	C	153	HIS
1	C	223	GLN
1	D	33	GLU
1	D	35	ARG
1	D	108	LEU
1	D	181	LYS
1	D	185	ASP
1	D	186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	40	ASN
1	A	98	HIS
1	A	118	ASN
1	A	124	ASN
1	A	149	GLN
1	A	184	ASN
1	A	248	GLN

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Mol	Chain	Res	Type
1	A	254	ASN
1	A	285	GLN
1	B	27	GLN
1	B	40	ASN
1	B	49	GLN
1	B	52	ASN
1	B	98	HIS
1	B	118	ASN
1	B	124	ASN
1	B	184	ASN
1	B	214	GLN
1	B	248	GLN
1	C	40	ASN
1	C	98	HIS
1	C	118	ASN
1	C	124	ASN
1	C	135	GLN
1	C	192	GLN
1	C	248	GLN
1	C	272	ASN
1	D	27	GLN
1	D	40	ASN
1	D	48	ASN
1	D	98	HIS
1	D	124	ASN
1	D	166	GLN
1	D	212	ASN
1	D	252	ASN
1	D	254	ASN

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 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	265/305 (86%)	0.82	33 (12%) 8 9	19, 28, 45, 56	0
1	B	260/305 (85%)	1.04	40 (15%) 5 5	18, 30, 47, 57	0
1	C	267/305 (87%)	1.03	40 (14%) 5 6	20, 31, 52, 66	0
1	D	265/305 (86%)	0.84	29 (10%) 10 12	18, 28, 47, 64	0
All	All	1057/1220 (86%)	0.93	142 (13%) 7 8	18, 29, 47, 66	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	PHE	12.5
1	C	277	PHE	11.2
1	A	190	ILE	8.0
1	D	199	HIS	6.8
1	D	189	PHE	6.4
1	D	190	ILE	6.0
1	C	189	PHE	6.0
1	C	191	LYS	5.6
1	B	271	ARG	5.2
1	D	276	SER	5.0
1	A	272	ASN	4.9
1	B	189	PHE	4.9
1	A	199	HIS	4.9
1	A	189	PHE	4.7
1	D	118	ASN	4.7
1	C	192	GLN	4.6
1	D	278	ARG	4.3
1	C	20	THR	4.3
1	D	275	ILE	4.3
1	B	190	ILE	4.2
1	C	193	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	102	GLU	3.8
1	B	270	LEU	3.8
1	C	177	CYS	3.8
1	B	118	ASN	3.8
1	B	55	GLY	3.8
1	A	144	HIS	3.7
1	B	269	VAL	3.7
1	B	53	VAL	3.7
1	D	200	MET	3.6
1	D	271	ARG	3.6
1	C	139	HIS	3.6
1	D	144	HIS	3.6
1	C	19	LYS	3.6
1	C	173	ILE	3.5
1	C	144	HIS	3.5
1	C	174	SER	3.4
1	A	295	ILE	3.4
1	C	295	ILE	3.4
1	B	22	THR	3.4
1	C	178	VAL	3.2
1	D	186	LEU	3.2
1	B	266	ILE	3.2
1	D	177	CYS	3.2
1	C	175	ASN	3.1
1	B	278	ARG	3.1
1	A	82	VAL	3.1
1	A	55	GLY	3.1
1	C	172	LYS	3.0
1	A	139	HIS	3.0
1	A	64	GLU	3.0
1	C	171	VAL	2.9
1	D	179	VAL	2.9
1	B	104	LYS	2.9
1	B	267	ILE	2.9
1	C	278	ARG	2.9
1	C	53	VAL	2.9
1	D	185	ASP	2.9
1	B	82	VAL	2.8
1	B	296	GLU	2.8
1	C	152	GLY	2.8
1	B	200	MET	2.8
1	C	190	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	182	SER	2.7
1	B	182	SER	2.7
1	C	21	LEU	2.7
1	A	56	TYR	2.6
1	B	56	TYR	2.6
1	D	66	SER	2.6
1	B	50	ALA	2.6
1	C	182	SER	2.6
1	A	81	SER	2.6
1	A	180	ILE	2.6
1	C	153	HIS	2.5
1	D	64	GLU	2.5
1	B	73	VAL	2.5
1	A	270	LEU	2.5
1	A	59	ARG	2.5
1	B	77	ILE	2.5
1	D	81	SER	2.5
1	B	78	GLN	2.5
1	B	288	GLU	2.5
1	B	52	ASN	2.4
1	C	222	TYR	2.4
1	C	34	ILE	2.4
1	C	184	ASN	2.4
1	A	152	GLY	2.4
1	C	165	LYS	2.4
1	B	295	ILE	2.3
1	A	79	SER	2.3
1	A	174	SER	2.3
1	A	169	ASP	2.3
1	D	187	ARG	2.3
1	D	19	LYS	2.3
1	C	187	ARG	2.3
1	B	287	VAL	2.3
1	D	222	TYR	2.3
1	A	268	ASP	2.3
1	B	179	VAL	2.3
1	A	52	ASN	2.3
1	B	177	CYS	2.3
1	D	71	HIS	2.3
1	B	103	PHE	2.2
1	A	185	ASP	2.2
1	A	184	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	272	ASN	2.2
1	B	60	MET	2.2
1	A	58	THR	2.2
1	A	21	LEU	2.2
1	B	186	LEU	2.2
1	B	180	ILE	2.2
1	C	82	VAL	2.2
1	C	64	GLU	2.2
1	C	270	LEU	2.2
1	B	81	SER	2.2
1	D	176	ASP	2.2
1	B	222	TYR	2.2
1	C	280	LYS	2.2
1	D	152	GLY	2.2
1	A	277	PHE	2.1
1	B	119	ILE	2.1
1	D	282	ILE	2.1
1	A	53	VAL	2.1
1	A	35	ARG	2.1
1	C	44	LEU	2.1
1	D	58	THR	2.1
1	D	151	SER	2.1
1	A	271	ARG	2.1
1	D	104	LYS	2.1
1	A	177	CYS	2.1
1	C	200	MET	2.1
1	B	64	GLU	2.1
1	C	179	VAL	2.1
1	A	51	CYS	2.1
1	B	282	ILE	2.0
1	D	103	PHE	2.0
1	C	141	GLY	2.0
1	A	179	VAL	2.0
1	C	281	LEU	2.0
1	B	83	ASP	2.0
1	B	268	ASP	2.0
1	C	269	VAL	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.