



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:06 AM UTC

PDB ID : 1VHK / pdb_00001vhk
Title : Crystal structure of an hypothetical protein
Authors : Structural GenomiX
Deposited on : 2003-12-01
Resolution : 2.60 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

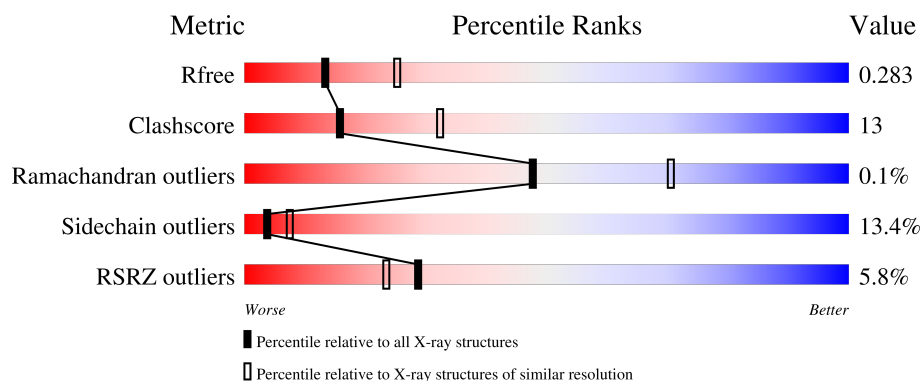
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	268	5% 55% 26% 6% 12%
1	B	268	4% 47% 21% 5% 27%
1	C	268	% 49% 34% 7% 9%
1	D	268	8% 47% 17% • 34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6788 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 Hypothetical protein yqeU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	Se	0	0	0
			1847	1168	314	355	6	4			
1	B	196	Total	C	N	O	S	Se	0	0	0
			1534	975	262	289	6	2			
1	C	244	Total	C	N	O	S	Se	0	1	0
			1923	1216	331	366	6	4			
1	D	178	Total	C	N	O	S	Se	0	0	0
			1397	886	241	264	4	2			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP P54461
A	0	SER	-	cloning artifact	UNP P54461
A	1	LEU	-	cloning artifact	UNP P54461
A	33	MSE	MET	modified residue	UNP P54461
A	35	MSE	MET	modified residue	UNP P54461
A	152	MSE	MET	modified residue	UNP P54461
A	164	MSE	MET	modified residue	UNP P54461
A	257	GLU	-	cloning artifact	UNP P54461
A	258	GLY	-	cloning artifact	UNP P54461
A	259	GLY	-	cloning artifact	UNP P54461
A	260	SER	-	cloning artifact	UNP P54461
A	261	HIS	-	cloning artifact	UNP P54461
A	262	HIS	-	cloning artifact	UNP P54461
A	263	HIS	-	cloning artifact	UNP P54461
A	264	HIS	-	cloning artifact	UNP P54461
A	265	HIS	-	cloning artifact	UNP P54461
A	266	HIS	-	cloning artifact	UNP P54461
B	-1	MSE	-	cloning artifact	UNP P54461
B	0	SER	-	cloning artifact	UNP P54461
B	1	LEU	-	cloning artifact	UNP P54461
B	33	MSE	MET	modified residue	UNP P54461

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Chain	Residue	Modelled	Actual	Comment	Reference
B	35	MSE	MET	modified residue	UNP P54461
B	152	MSE	MET	modified residue	UNP P54461
B	164	MSE	MET	modified residue	UNP P54461
B	257	GLU	-	cloning artifact	UNP P54461
B	258	GLY	-	cloning artifact	UNP P54461
B	259	GLY	-	cloning artifact	UNP P54461
B	260	SER	-	cloning artifact	UNP P54461
B	261	HIS	-	cloning artifact	UNP P54461
B	262	HIS	-	cloning artifact	UNP P54461
B	263	HIS	-	cloning artifact	UNP P54461
B	264	HIS	-	cloning artifact	UNP P54461
B	265	HIS	-	cloning artifact	UNP P54461
B	266	HIS	-	cloning artifact	UNP P54461
C	-1	MSE	-	cloning artifact	UNP P54461
C	0	SER	-	cloning artifact	UNP P54461
C	1	LEU	-	cloning artifact	UNP P54461
C	33	MSE	MET	modified residue	UNP P54461
C	35	MSE	MET	modified residue	UNP P54461
C	152	MSE	MET	modified residue	UNP P54461
C	164	MSE	MET	modified residue	UNP P54461
C	257	GLU	-	cloning artifact	UNP P54461
C	258	GLY	-	cloning artifact	UNP P54461
C	259	GLY	-	cloning artifact	UNP P54461
C	260	SER	-	cloning artifact	UNP P54461
C	261	HIS	-	cloning artifact	UNP P54461
C	262	HIS	-	cloning artifact	UNP P54461
C	263	HIS	-	cloning artifact	UNP P54461
C	264	HIS	-	cloning artifact	UNP P54461
C	265	HIS	-	cloning artifact	UNP P54461
C	266	HIS	-	cloning artifact	UNP P54461
D	-1	MSE	-	cloning artifact	UNP P54461
D	0	SER	-	cloning artifact	UNP P54461
D	1	LEU	-	cloning artifact	UNP P54461
D	33	MSE	MET	modified residue	UNP P54461
D	35	MSE	MET	modified residue	UNP P54461
D	152	MSE	MET	modified residue	UNP P54461
D	164	MSE	MET	modified residue	UNP P54461
D	257	GLU	-	cloning artifact	UNP P54461
D	258	GLY	-	cloning artifact	UNP P54461
D	259	GLY	-	cloning artifact	UNP P54461
D	260	SER	-	cloning artifact	UNP P54461
D	261	HIS	-	cloning artifact	UNP P54461

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Chain	Residue	Modelled	Actual	Comment	Reference
D	262	HIS	-	cloning artifact	UNP P54461
D	263	HIS	-	cloning artifact	UNP P54461
D	264	HIS	-	cloning artifact	UNP P54461
D	265	HIS	-	cloning artifact	UNP P54461
D	266	HIS	-	cloning artifact	UNP P54461

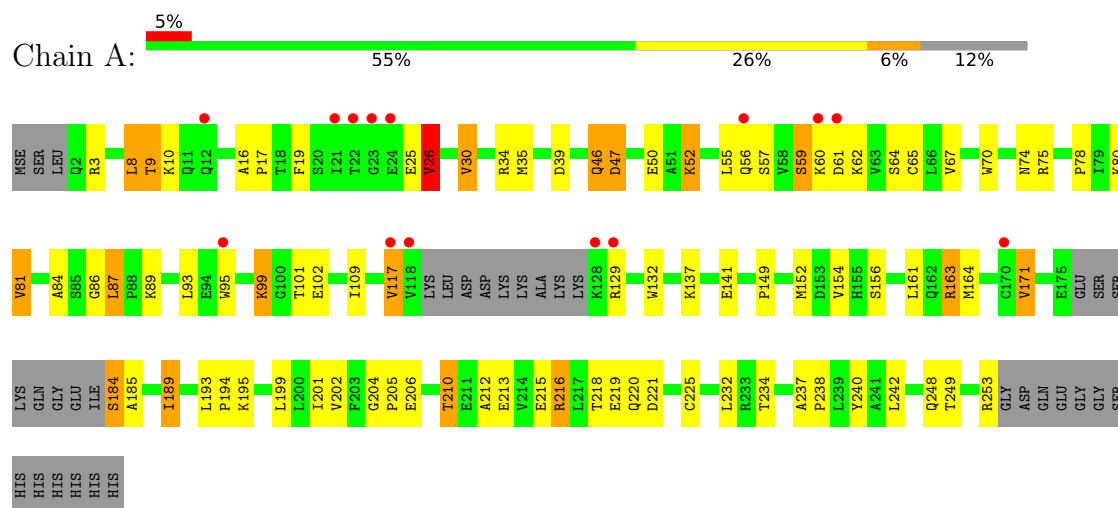
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	24	Total	O	0	0
			24	24		
2	C	32	Total	O	0	0
			32	32		
2	D	10	Total	O	0	0
			10	10		

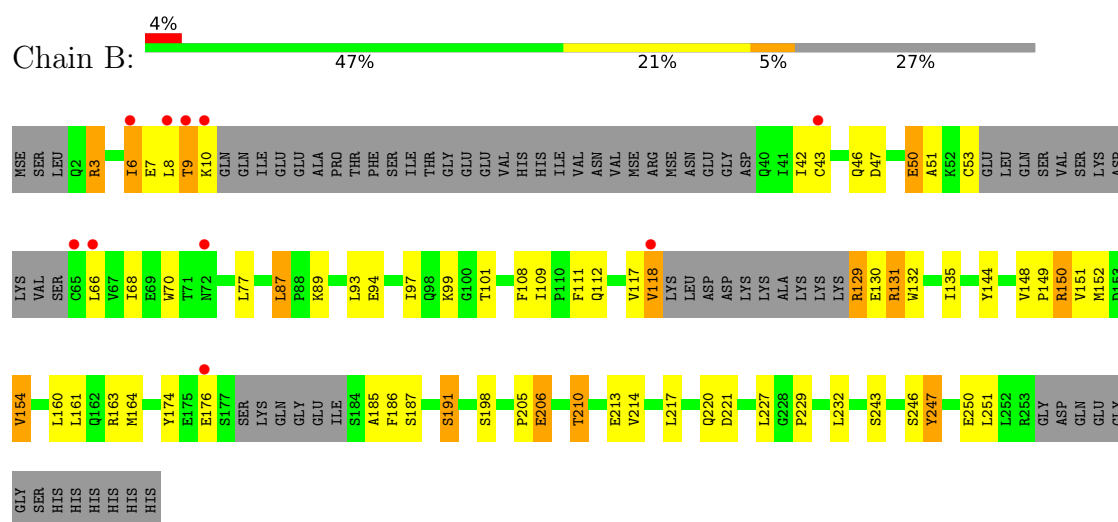
3 Residue-property plots [i](#)

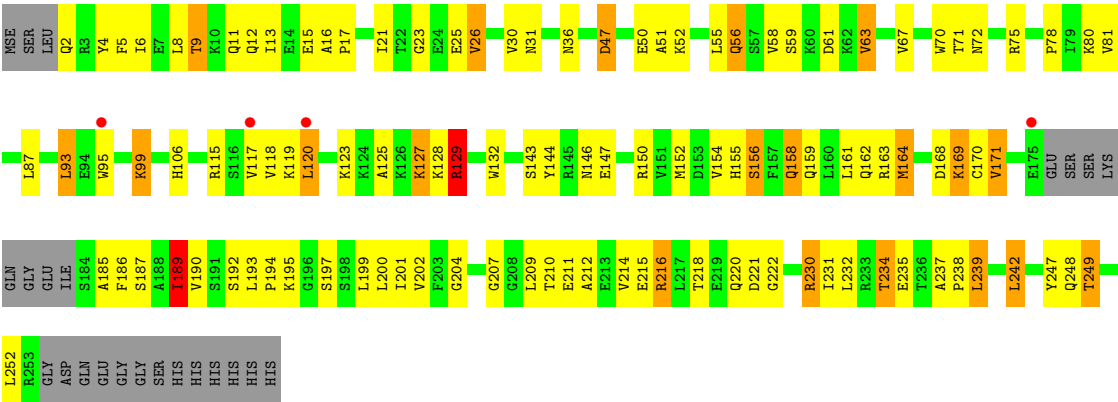
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hypothetical protein yqeU

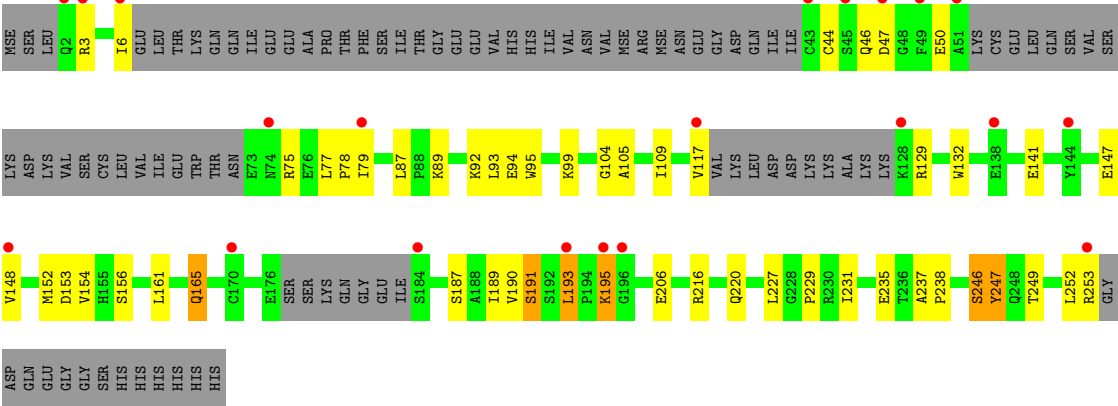


• Molecule 1: Hypothetical protein yqeU





● Molecule 1: Hypothetical protein yqeU



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.71Å 145.05Å 66.01Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	38.19 – 2.60 38.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.19-2.60) 99.5 (38.19-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.61Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.270 , 0.327 (Not available) , 0.283	Depositor DCC
R_{free} test set	1684 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6788	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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

5.1 Standard geometry

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	0.76	0/1874	1.42	10/2524 (0.4%)
1	B	0.83	0/1557	1.48	14/2099 (0.7%)
1	C	0.81	0/1956	1.44	12/2631 (0.5%)
1	D	0.74	0/1418	1.33	7/1907 (0.4%)
All	All	0.79	0/6805	1.42	43/9161 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	CA-CB-CG	7.91	120.51	112.60
1	A	30	VAL	N-CA-C	7.22	117.20	110.42
1	C	31	ASN	CA-CB-CG	-6.69	105.91	112.60
1	C	99	LYS	CA-C-N	6.65	127.36	119.98
1	C	99	LYS	C-N-CA	6.65	127.36	119.98
1	A	80	LYS	CA-C-N	-6.59	115.01	123.19
1	A	80	LYS	C-N-CA	-6.59	115.01	123.19
1	C	47	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	186	PHE	CA-CB-CG	6.41	120.21	113.80
1	D	247	TYR	CA-C-N	6.31	128.64	120.44
1	D	247	TYR	C-N-CA	6.31	128.64	120.44
1	A	156	SER	N-CA-C	-5.80	102.87	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	TYR	CA-C-N	5.77	128.27	120.65
1	B	247	TYR	C-N-CA	5.77	128.27	120.65
1	B	47	ASP	CA-CB-CG	5.77	118.37	112.60
1	D	94	GLU	CB-CG-CD	5.77	122.40	112.60
1	C	252	LEU	N-CA-C	-5.75	104.62	111.69
1	D	47	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	50	GLU	CB-CG-CD	5.52	121.99	112.60
1	D	156	SER	N-CA-C	-5.50	103.12	110.55
1	B	53	CYS	CA-C-O	5.49	130.13	120.80
1	C	30	VAL	N-CA-C	5.46	115.71	110.74
1	B	206	GLU	CA-C-N	-5.45	114.76	123.31
1	B	206	GLU	C-N-CA	-5.45	114.76	123.31
1	A	46	GLN	CA-CB-CG	5.41	124.93	114.10
1	A	26	VAL	N-CA-CB	5.38	116.85	110.55
1	C	156	SER	N-CA-C	-5.38	103.59	110.53
1	B	154	VAL	N-CA-CB	5.37	117.32	110.13
1	C	234	THR	N-CA-CB	5.36	117.99	110.12
1	A	74	ASN	CA-CB-CG	-5.32	107.28	112.60
1	C	129	ARG	CD-NE-CZ	5.31	131.84	124.40
1	B	148	VAL	O-C-N	5.25	124.68	121.37
1	A	9	THR	CA-C-O	-5.21	115.57	121.72
1	D	231	ILE	N-CA-CB	5.09	116.65	110.95
1	C	189	ILE	N-CA-CB	5.08	119.05	110.56
1	C	5	PHE	CA-CB-CG	-5.08	108.72	113.80
1	C	230	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	A	184	SER	CA-C-O	5.06	129.40	120.80
1	B	131	ARG	CA-C-N	5.04	127.04	120.28
1	B	131	ARG	C-N-CA	5.04	127.04	120.28
1	B	185	ALA	CA-C-N	5.03	126.98	120.44
1	B	185	ALA	C-N-CA	5.03	126.98	120.44
1	D	252	LEU	N-CA-C	-5.02	105.47	112.45

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	VAL	Mainchain
1	C	201	ILE	Mainchain

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	1847	0	1837	58	0
1	B	1534	0	1521	42	0
1	C	1923	0	1932	56	0
1	D	1397	0	1383	29	0
2	A	21	0	0	2	0
2	B	24	0	0	1	0
2	C	32	0	0	1	0
2	D	10	0	0	1	0
All	All	6788	0	6673	178	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 13.

All (178) 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:C:75:ARG:HG2	1:D:229:PRO:HB2	1.39	1.01
1:A:57:SER:HB3	1:A:64:SER:HB2	1.46	0.94
1:C:9:THR:HG22	1:C:12:GLN:H	1.40	0.84
1:B:210:THR:HG22	1:B:213:GLU:H	1.42	0.83
1:B:6:ILE:HD11	1:B:43:CYS:HB3	1.61	0.83
1:C:171:VAL:HG12	1:C:199:LEU:HD11	1.65	0.76
1:A:210:THR:HG22	1:A:213:GLU:H	1.49	0.76
1:C:170:CYS:SG	1:C:200:LEU:HD23	2.25	0.76
1:A:35:MSE:HE2	1:A:39:ASP:HB3	1.66	0.76
1:B:129:ARG:NH2	1:B:129:ARG:HB2	2.06	0.71
1:A:78:PRO:HG2	1:A:249:THR:HB	1.73	0.71
1:A:184:SER:HA	2:A:272:HOH:O	1.91	0.70
1:C:58:VAL:HA	1:C:63:VAL:HG22	1.74	0.69
1:A:171:VAL:HG13	1:A:199:LEU:HD11	1.74	0.68
1:B:3:ARG:HH11	1:B:144:TYR:HD1	1.43	0.66
1:C:4:TYR:HD2	1:C:25:GLU:HG3	1.59	0.66
1:C:212:ALA:O	1:C:216:ARG:HG2	1.95	0.66
1:A:152:MSE:HE1	1:A:163:ARG:NH2	2.11	0.66
1:A:171:VAL:HG22	1:A:201:ILE:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LYS:HD2	1:D:253:ARG:NH2	2.12	0.64
1:C:4:TYR:CD2	1:C:25:GLU:HG3	2.33	0.64
1:C:16:ALA:HB1	1:C:17:PRO:HD2	1.80	0.64
1:D:78:PRO:HG2	1:D:249:THR:HB	1.80	0.63
1:B:94:GLU:HG3	2:B:272:HOH:O	1.98	0.63
1:C:115:ARG:HD3	1:C:207:GLY:O	1.97	0.63
1:B:150:ARG:NH2	1:B:152:MSE:HE2	2.14	0.62
1:A:89:LYS:HZ1	1:A:117:VAL:HG11	1.64	0.61
1:A:237:ALA:HB3	1:A:238:PRO:HD3	1.80	0.61
1:C:220:GLN:HA	1:C:220:GLN:HE21	1.65	0.61
1:A:16:ALA:HB1	1:A:17:PRO:CD	2.31	0.60
1:A:30:VAL:O	1:A:34:ARG:HA	2.00	0.60
1:C:93:LEU:HD12	1:C:132:TRP:CZ2	2.37	0.59
1:C:185:ALA:O	1:C:189:ILE:HG23	2.01	0.59
1:D:187:SER:O	1:D:191:SER:HB2	2.02	0.59
1:A:185:ALA:HB3	1:A:225:CYS:SG	2.42	0.59
1:B:129:ARG:HB2	1:B:129:ARG:HH21	1.66	0.59
1:C:9:THR:CG2	1:C:12:GLN:H	2.13	0.59
1:B:9:THR:OG1	1:B:10:LYS:N	2.36	0.58
1:B:117:VAL:O	1:B:117:VAL:HG12	2.03	0.58
1:D:3:ARG:HD3	1:D:141:GLU:HA	1.84	0.58
1:D:190:VAL:HA	1:D:193:LEU:HD12	1.86	0.58
1:B:87:LEU:HD23	1:B:112:GLN:HE21	1.68	0.58
1:B:97:ILE:HD12	1:B:108:PHE:CG	2.38	0.57
1:D:79:ILE:HD13	1:D:193:LEU:HD13	1.86	0.57
1:A:26:VAL:HG21	1:A:61:ASP:HA	1.87	0.57
1:D:93:LEU:HD23	1:D:132:TRP:CZ2	2.40	0.57
1:B:187:SER:O	1:B:191:SER:HB2	2.05	0.57
1:B:3:ARG:NH1	1:B:50:GLU:OE1	2.37	0.56
1:B:94:GLU:HG2	1:B:135:ILE:CD1	2.36	0.56
1:B:129:ARG:HG3	1:B:130:GLU:N	2.21	0.55
1:C:150:ARG:NH2	1:C:152:MSE:HE3	2.22	0.55
1:D:77:LEU:HD21	1:D:246:SER:HB2	1.89	0.55
1:B:161:LEU:HD22	1:B:220:GLN:HG3	1.89	0.55
1:A:35:MSE:CE	1:A:39:ASP:HB3	2.37	0.55
1:B:8:LEU:HD22	1:B:8:LEU:H	1.71	0.55
1:C:211:GLU:O	1:C:215:GLU:HG3	2.08	0.54
1:A:204:GLY:O	1:A:234:THR:HG22	2.08	0.54
1:B:87:LEU:HG	1:B:118:VAL:HG11	1.88	0.54
1:A:185:ALA:O	1:A:189:ILE:HG23	2.09	0.53
1:B:220:GLN:O	1:B:221:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ALA:HB1	1:C:154:VAL:CG2	2.38	0.53
1:D:104:GLY:O	1:D:105:ALA:C	2.51	0.53
1:A:59:SER:OG	1:A:60:LYS:N	2.41	0.53
1:A:220:GLN:O	1:A:221:ASP:HB2	2.09	0.53
1:A:240:TYR:HA	1:B:243:SER:OG	2.09	0.53
1:C:210:THR:O	1:C:214:VAL:HG23	2.09	0.52
1:A:210:THR:CG2	1:A:213:GLU:H	2.20	0.52
1:D:109:ILE:HG12	1:D:152:MSE:SE	2.59	0.52
1:A:3:ARG:HD3	1:A:141:GLU:HA	1.91	0.51
1:C:220:GLN:O	1:C:221:ASP:HB2	2.10	0.51
1:D:161:LEU:HD11	1:D:216:ARG:HD2	1.90	0.51
1:C:220:GLN:HA	1:C:220:GLN:NE2	2.24	0.51
1:B:93:LEU:HD23	1:B:132:TRP:CZ2	2.45	0.51
1:A:205:PRO:HA	1:A:234:THR:HG21	1.93	0.51
1:C:152:MSE:HE1	1:C:163:ARG:NH2	2.26	0.51
1:D:161:LEU:O	1:D:165:GLN:NE2	2.44	0.50
1:C:156:SER:OG	1:C:159:GLN:HG3	2.12	0.50
1:D:195:LYS:N	1:D:195:LYS:HD3	2.27	0.50
1:C:169:LYS:HD2	1:C:193:LEU:HD21	1.95	0.49
1:D:237:ALA:HB3	1:D:238:PRO:HD3	1.94	0.49
1:B:152:MSE:SE	1:B:163:ARG:NH2	2.96	0.49
1:B:210:THR:CG2	1:B:213:GLU:H	2.18	0.49
1:A:216:ARG:NH2	1:A:219:GLU:OE2	2.45	0.49
1:B:109:ILE:HG12	1:B:152:MSE:SE	2.63	0.49
1:C:120:LEU:O	1:C:120:LEU:HD23	2.12	0.49
1:C:248:GLN:HB2	1:D:247:TYR:CE2	2.47	0.49
1:C:50:GLU:OE1	1:C:75:ARG:NH1	2.46	0.48
1:C:218:THR:HA	1:C:222:GLY:O	2.12	0.48
1:C:168:ASP:OD1	1:C:197:SER:HB2	2.13	0.48
1:C:237:ALA:HB3	1:C:238:PRO:HD3	1.96	0.48
1:B:112:GLN:NE2	1:B:118:VAL:HG12	2.28	0.48
1:A:248:GLN:NE2	1:B:247:TYR:OH	2.46	0.48
1:B:3:ARG:HD2	1:B:144:TYR:CD1	2.48	0.48
1:A:8:LEU:O	1:A:46:GLN:HG3	2.13	0.48
1:A:52:LYS:HB2	1:A:52:LYS:HE2	1.63	0.48
1:B:164:MSE:SE	1:B:217:LEU:HD23	2.64	0.48
1:C:150:ARG:CZ	1:C:152:MSE:HE3	2.44	0.48
1:A:89:LYS:HB3	1:A:89:LYS:HZ2	1.78	0.47
1:A:101:THR:HG23	1:A:149:PRO:CG	2.44	0.47
1:C:125:ALA:HB1	1:C:154:VAL:HG21	1.95	0.47
1:B:247:TYR:HD1	1:B:251:LEU:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ALA:HB2	1:B:70:TRP:CE3	2.50	0.47
1:C:238:PRO:O	1:C:242:LEU:HD22	2.15	0.47
1:A:248:GLN:O	1:A:253:ARG:HG3	2.15	0.47
1:B:246:SER:O	1:B:250:GLU:HB2	2.15	0.47
1:C:158:GLN:O	1:C:162:GLN:HG3	2.15	0.47
1:A:86:GLY:O	1:A:87:LEU:C	2.59	0.46
1:C:235:GLU:HG2	1:D:99:LYS:HE3	1.97	0.46
1:A:152:MSE:HE1	1:A:163:ARG:CZ	2.45	0.46
1:D:6:ILE:O	1:D:46:GLN:HG3	2.15	0.46
1:C:80:LYS:HZ2	1:C:106:HIS:CE1	2.33	0.46
1:D:147:GLU:HG2	1:D:148:VAL:N	2.30	0.46
1:B:174:TYR:CE1	1:B:176:GLU:HG2	2.50	0.46
1:D:92:LYS:HE3	1:D:206:GLU:OE1	2.17	0.45
1:C:193:LEU:HA	1:C:194:PRO:HD3	1.77	0.45
1:C:23:GLY:O	1:C:26:VAL:HG13	2.17	0.45
1:C:186:PHE:O	1:C:190:VAL:HG23	2.17	0.45
1:B:220:GLN:HE21	1:B:220:GLN:HA	1.81	0.45
1:A:89:LYS:NZ	1:A:117:VAL:HG21	2.31	0.45
1:C:143:SER:O	1:C:144:TYR:HB2	2.17	0.45
1:A:171:VAL:CG2	1:A:201:ILE:HG23	2.47	0.44
1:C:163:ARG:O	1:C:164:MSE:C	2.59	0.44
1:C:146:ASN:O	1:C:147:GLU:HG3	2.18	0.44
1:A:129:ARG:HA	1:A:132:TRP:CE3	2.52	0.44
1:B:111:PHE:CD2	1:B:160:LEU:HD22	2.53	0.44
1:B:3:ARG:HA	1:B:42:ILE:O	2.18	0.44
1:A:10:LYS:HG3	1:A:70:TRP:CH2	2.53	0.43
1:B:129:ARG:HH12	1:B:151:VAL:HB	1.83	0.43
1:A:101:THR:O	1:A:102:GLU:C	2.61	0.43
1:C:6:ILE:HD12	1:C:21:ILE:HG12	2.01	0.43
1:B:174:TYR:CE1	1:B:214:VAL:HG21	2.54	0.43
1:A:89:LYS:HG2	1:A:206:GLU:OE2	2.18	0.43
1:D:147:GLU:HG2	1:D:148:VAL:H	1.84	0.43
1:C:71:THR:O	1:C:72:ASN:HB2	2.18	0.43
1:C:127:LYS:HG3	1:C:128:LYS:N	2.32	0.43
1:D:129:ARG:HH21	1:D:129:ARG:HG2	1.84	0.43
1:B:205:PRO:O	1:B:206:GLU:C	2.62	0.43
1:A:78:PRO:HG2	1:A:249:THR:CB	2.46	0.42
1:A:30:VAL:HG21	1:A:59:SER:O	2.18	0.42
1:A:189:ILE:HD11	1:A:199:LEU:HD13	2.01	0.42
1:A:210:THR:N	1:A:213:GLU:OE2	2.47	0.42
1:C:155:HIS:NE2	1:C:163:ARG:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:TYR:HD2	1:D:247:TYR:HD2	1.68	0.42
1:D:220:GLN:HG3	2:D:270:HOH:O	2.20	0.42
1:A:216:ARG:HD2	2:A:283:HOH:O	2.19	0.42
1:A:19:PHE:CZ	1:A:65:CYS:HB2	2.55	0.42
1:A:3:ARG:HG3	1:A:3:ARG:NH1	2.34	0.42
1:A:25:GLU:OE1	1:A:137:LYS:NZ	2.50	0.42
1:C:51:ALA:HB2	1:C:70:TRP:CE3	2.55	0.42
1:D:165:GLN:CD	1:D:165:GLN:H	2.28	0.42
1:A:16:ALA:HB1	1:A:17:PRO:HD2	2.00	0.41
1:B:7:GLU:O	1:B:46:GLN:NE2	2.53	0.41
1:C:129:ARG:HE	1:C:129:ARG:HB3	1.59	0.41
1:D:129:ARG:NH2	1:D:153:ASP:OD1	2.53	0.41
1:A:56:GLN:HE21	1:A:56:GLN:HB2	1.62	0.41
1:A:193:LEU:HA	1:A:194:PRO:HD3	1.79	0.41
1:C:99:LYS:HB2	1:C:239:LEU:HD11	2.03	0.41
1:A:194:PRO:O	1:A:195:LYS:C	2.63	0.41
1:C:56:GLN:HE21	1:C:56:GLN:HB2	1.62	0.41
1:C:231:ILE:HD13	1:C:231:ILE:HA	1.84	0.41
1:A:84:ALA:HA	1:A:109:ILE:O	2.21	0.41
1:A:75:ARG:HD3	1:B:229:PRO:O	2.20	0.41
1:C:2:GLN:NE2	2:C:278:HOH:O	2.53	0.41
1:C:204:GLY:HA3	1:C:209:LEU:HG	2.03	0.41
1:D:50:GLU:OE1	1:D:75:ARG:NH1	2.53	0.41
1:A:3:ARG:NH2	1:A:50:GLU:OE1	2.48	0.41
1:A:9:THR:HG23	1:A:47:ASP:CG	2.46	0.41
1:C:12:GLN:O	1:C:13:ILE:C	2.64	0.41
1:C:78:PRO:HD2	1:C:249:THR:CG2	2.51	0.41
1:C:11:GLN:O	1:C:12:GLN:C	2.63	0.41
1:A:99:LYS:NZ	1:A:102:GLU:OE2	2.50	0.40
1:A:212:ALA:O	1:A:216:ARG:HG2	2.21	0.40
1:B:101:THR:HG23	1:B:149:PRO:HG3	2.03	0.40
1:A:215:GLU:O	1:A:219:GLU:HG2	2.21	0.40
1:D:216:ARG:HE	1:D:216:ARG:HB2	1.74	0.40
1:A:210:THR:HG23	1:A:212:ALA:H	1.86	0.40
1:B:77:LEU:HD23	1:B:250:GLU:OE1	2.21	0.40
1:D:95:TRP:HE3	1:D:235:GLU:HG3	1.86	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	229/268 (85%)	217 (95%)	12 (5%)	0	100	100
1	B	170/268 (63%)	163 (96%)	7 (4%)	0	100	100
1	C	241/268 (90%)	228 (95%)	12 (5%)	1 (0%)	30	51
1	D	168/268 (63%)	160 (95%)	8 (5%)	0	100	100
All	All	808/1072 (75%)	768 (95%)	39 (5%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	61	ASP

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	196/227 (86%)	171 (87%)	25 (13%)	4	8
1	B	158/227 (70%)	140 (89%)	18 (11%)	5	11
1	C	210/227 (92%)	170 (81%)	40 (19%)	1	2
1	D	148/227 (65%)	136 (92%)	12 (8%)	11	24
All	All	712/908 (78%)	617 (87%)	95 (13%)	4	8

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	26	VAL
1	A	52	LYS
1	A	55	LEU
1	A	59	SER
1	A	62	LYS
1	A	67	VAL
1	A	81	VAL
1	A	87	LEU
1	A	93	LEU
1	A	95	TRP
1	A	99	LYS
1	A	117	VAL
1	A	154	VAL
1	A	161	LEU
1	A	163	ARG
1	A	164	MSE
1	A	171	VAL
1	A	189	ILE
1	A	202	VAL
1	A	210	THR
1	A	216	ARG
1	A	218	THR
1	A	232	LEU
1	A	242	LEU
1	B	3	ARG
1	B	6	ILE
1	B	9	THR
1	B	66	LEU
1	B	68	ILE
1	B	87	LEU
1	B	89	LYS
1	B	99	LYS
1	B	118	VAL
1	B	129	ARG
1	B	131	ARG
1	B	150	ARG
1	B	154	VAL
1	B	191	SER
1	B	198	SER
1	B	210	THR
1	B	227	LEU
1	B	232	LEU

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Mol	Chain	Res	Type
1	C	8	LEU
1	C	9	THR
1	C	15	GLU
1	C	26	VAL
1	C	36	ASN
1	C	47	ASP
1	C	52	LYS
1	C	55	LEU
1	C	56	GLN
1	C	59	SER
1	C	63	VAL
1	C	67	VAL
1	C	81	VAL
1	C	87	LEU
1	C	93	LEU
1	C	95	TRP
1	C	117	VAL
1	C	118	VAL
1	C	119	LYS
1	C	120	LEU
1	C	123	LYS
1	C	127	LYS
1	C	129	ARG
1	C	158	GLN
1	C	161	LEU
1	C	164	MSE
1	C	169	LYS
1	C	171	VAL
1	C	187	SER
1	C	189	ILE
1	C	192	SER
1	C	195	LYS
1	C	202	VAL
1	C	216	ARG
1	C	230	ARG
1	C	232	LEU
1	C	234	THR
1	C	239	LEU
1	C	242	LEU
1	C	249	THR
1	D	44	CYS
1	D	87	LEU

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Mol	Chain	Res	Type
1	D	89	LYS
1	D	117	VAL
1	D	154	VAL
1	D	165	GLN
1	D	189	ILE
1	D	191	SER
1	D	193	LEU
1	D	195	LYS
1	D	227	LEU
1	D	246	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	248	GLN
1	B	46	GLN
1	B	72	ASN
1	B	112	GLN
1	B	162	GLN
1	B	220	GLN
1	C	56	GLN
1	C	106	HIS
1	C	158	GLN
1	C	220	GLN
1	D	158	GLN
1	D	165	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	231/268 (86%)	0.39	14 (6%) 27 22	17, 40, 76, 92	0
1	B	194/268 (72%)	0.23	10 (5%) 33 27	17, 34, 71, 92	0
1	C	240/268 (89%)	0.30	4 (1%) 69 64	21, 41, 61, 70	1 (0%)
1	D	176/268 (65%)	0.59	21 (11%) 9 7	22, 45, 80, 91	0
All	All	841/1072 (78%)	0.37	49 (5%) 29 23	17, 40, 73, 92	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	LYS	4.7
1	A	128	LYS	4.2
1	A	129	ARG	4.1
1	D	6	ILE	3.9
1	B	65	CYS	3.9
1	D	43	CYS	3.7
1	D	128	LYS	3.7
1	B	66	LEU	3.6
1	A	95	TRP	3.5
1	B	43	CYS	3.5
1	D	51	ALA	3.5
1	A	118	VAL	3.4
1	B	9	THR	3.4
1	A	60	LYS	3.3
1	C	95	TRP	3.3
1	B	176	GLU	3.1
1	D	79	ILE	3.1
1	C	120	LEU	2.9
1	B	6	ILE	2.9
1	D	253	ARG	2.7
1	A	117	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	118	VAL	2.7
1	D	193	LEU	2.6
1	D	170	CYS	2.6
1	A	170	CYS	2.6
1	D	196	GLY	2.5
1	A	56	GLN	2.5
1	D	47	ASP	2.5
1	D	195	LYS	2.4
1	B	72	ASN	2.4
1	D	2	GLN	2.4
1	D	117	VAL	2.4
1	C	175	GLU	2.3
1	C	117	VAL	2.3
1	D	49	PHE	2.3
1	A	22	THR	2.2
1	D	138	GLU	2.2
1	A	23	GLY	2.2
1	D	45	SER	2.2
1	D	148	VAL	2.2
1	D	184	SER	2.1
1	D	144	TYR	2.1
1	A	21	ILE	2.1
1	A	61	ASP	2.1
1	D	3	ARG	2.1
1	A	12	GLN	2.1
1	D	74	ASN	2.1
1	A	24	GLU	2.0
1	B	8	LEU	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 ⓘ

There are no such residues in this entry.