



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:31 PM UTC

PDB ID : 1VHC / pdb_00001vhc
Title : Crystal structure of a putative KHG/KDPG aldolase
Authors : Structural GenomiX
Deposited on : 2003-12-01
Resolution : 1.89 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

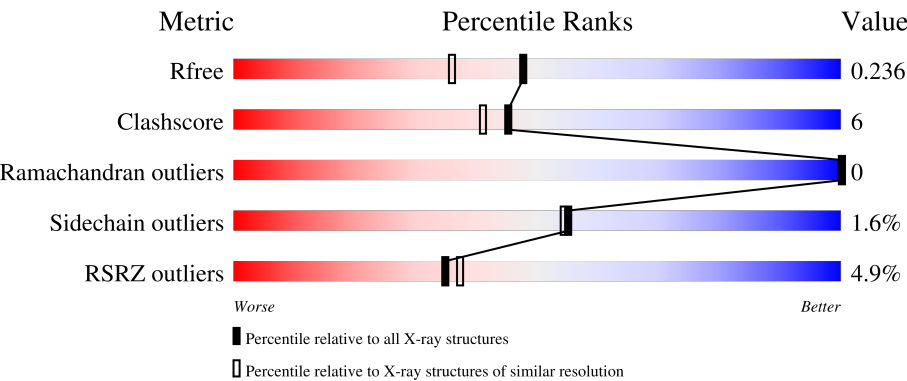
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	224	4% 82% 12% • 5%
1	B	224	8% 77% 15% • 5%
1	C	224	2% 78% 16% • 5%
1	D	224	4% 78% 15% • 5%
1	E	224	7% 81% 12% • 5%

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Mol	Chain	Length	Quality of chain
1	F	224	% 83% 11% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10319 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 KHG/KDPG aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	Se	0	2	0
			1600	1029	268	295	2	6			
1	B	212	Total	C	N	O	S	Se	0	2	0
			1576	1013	262	293	2	6			
1	C	212	Total	C	N	O	S	Se	0	2	0
			1600	1029	268	295	2	6			
1	D	212	Total	C	N	O	S	Se	0	2	0
			1596	1028	268	292	2	6			
1	E	212	Total	C	N	O	S	Se	0	2	0
			1594	1025	268	293	2	6			
1	F	213	Total	C	N	O	S	Se	0	2	0
			1609	1035	270	296	2	6			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP P44480
A	0	SER	-	cloning artifact	UNP P44480
A	1	LEU	-	cloning artifact	UNP P44480
A	119	MSE	MET	modified residue	UNP P44480
A	127	MSE	MET	modified residue	UNP P44480
A	145	MSE	MET	modified residue	UNP P44480
A	159	MSE	MET	modified residue	UNP P44480
A	213	GLU	-	cloning artifact	UNP P44480
A	214	GLY	-	cloning artifact	UNP P44480
A	215	GLY	-	cloning artifact	UNP P44480
A	216	SER	-	cloning artifact	UNP P44480
A	217	HIS	-	cloning artifact	UNP P44480
A	218	HIS	-	cloning artifact	UNP P44480
A	219	HIS	-	cloning artifact	UNP P44480
A	220	HIS	-	cloning artifact	UNP P44480
A	221	HIS	-	cloning artifact	UNP P44480
A	222	HIS	-	cloning artifact	UNP P44480

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MSE	-	cloning artifact	UNP P44480
B	0	SER	-	cloning artifact	UNP P44480
B	1	LEU	-	cloning artifact	UNP P44480
B	119	MSE	MET	modified residue	UNP P44480
B	127	MSE	MET	modified residue	UNP P44480
B	145	MSE	MET	modified residue	UNP P44480
B	159	MSE	MET	modified residue	UNP P44480
B	213	GLU	-	cloning artifact	UNP P44480
B	214	GLY	-	cloning artifact	UNP P44480
B	215	GLY	-	cloning artifact	UNP P44480
B	216	SER	-	cloning artifact	UNP P44480
B	217	HIS	-	cloning artifact	UNP P44480
B	218	HIS	-	cloning artifact	UNP P44480
B	219	HIS	-	cloning artifact	UNP P44480
B	220	HIS	-	cloning artifact	UNP P44480
B	221	HIS	-	cloning artifact	UNP P44480
B	222	HIS	-	cloning artifact	UNP P44480
C	-1	MSE	-	cloning artifact	UNP P44480
C	0	SER	-	cloning artifact	UNP P44480
C	1	LEU	-	cloning artifact	UNP P44480
C	119	MSE	MET	modified residue	UNP P44480
C	127	MSE	MET	modified residue	UNP P44480
C	145	MSE	MET	modified residue	UNP P44480
C	159	MSE	MET	modified residue	UNP P44480
C	213	GLU	-	cloning artifact	UNP P44480
C	214	GLY	-	cloning artifact	UNP P44480
C	215	GLY	-	cloning artifact	UNP P44480
C	216	SER	-	cloning artifact	UNP P44480
C	217	HIS	-	cloning artifact	UNP P44480
C	218	HIS	-	cloning artifact	UNP P44480
C	219	HIS	-	cloning artifact	UNP P44480
C	220	HIS	-	cloning artifact	UNP P44480
C	221	HIS	-	cloning artifact	UNP P44480
C	222	HIS	-	cloning artifact	UNP P44480
D	-1	MSE	-	cloning artifact	UNP P44480
D	0	SER	-	cloning artifact	UNP P44480
D	1	LEU	-	cloning artifact	UNP P44480
D	119	MSE	MET	modified residue	UNP P44480
D	127	MSE	MET	modified residue	UNP P44480
D	145	MSE	MET	modified residue	UNP P44480
D	159	MSE	MET	modified residue	UNP P44480
D	213	GLU	-	cloning artifact	UNP P44480

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Chain	Residue	Modelled	Actual	Comment	Reference
D	214	GLY	-	cloning artifact	UNP P44480
D	215	GLY	-	cloning artifact	UNP P44480
D	216	SER	-	cloning artifact	UNP P44480
D	217	HIS	-	cloning artifact	UNP P44480
D	218	HIS	-	cloning artifact	UNP P44480
D	219	HIS	-	cloning artifact	UNP P44480
D	220	HIS	-	cloning artifact	UNP P44480
D	221	HIS	-	cloning artifact	UNP P44480
D	222	HIS	-	cloning artifact	UNP P44480
E	-1	MSE	-	cloning artifact	UNP P44480
E	0	SER	-	cloning artifact	UNP P44480
E	1	LEU	-	cloning artifact	UNP P44480
E	119	MSE	MET	modified residue	UNP P44480
E	127	MSE	MET	modified residue	UNP P44480
E	145	MSE	MET	modified residue	UNP P44480
E	159	MSE	MET	modified residue	UNP P44480
E	213	GLU	-	cloning artifact	UNP P44480
E	214	GLY	-	cloning artifact	UNP P44480
E	215	GLY	-	cloning artifact	UNP P44480
E	216	SER	-	cloning artifact	UNP P44480
E	217	HIS	-	cloning artifact	UNP P44480
E	218	HIS	-	cloning artifact	UNP P44480
E	219	HIS	-	cloning artifact	UNP P44480
E	220	HIS	-	cloning artifact	UNP P44480
E	221	HIS	-	cloning artifact	UNP P44480
E	222	HIS	-	cloning artifact	UNP P44480
F	-1	MSE	-	cloning artifact	UNP P44480
F	0	SER	-	cloning artifact	UNP P44480
F	1	LEU	-	cloning artifact	UNP P44480
F	119	MSE	MET	modified residue	UNP P44480
F	127	MSE	MET	modified residue	UNP P44480
F	145	MSE	MET	modified residue	UNP P44480
F	159	MSE	MET	modified residue	UNP P44480
F	213	GLU	-	cloning artifact	UNP P44480
F	214	GLY	-	cloning artifact	UNP P44480
F	215	GLY	-	cloning artifact	UNP P44480
F	216	SER	-	cloning artifact	UNP P44480
F	217	HIS	-	cloning artifact	UNP P44480
F	218	HIS	-	cloning artifact	UNP P44480
F	219	HIS	-	cloning artifact	UNP P44480
F	220	HIS	-	cloning artifact	UNP P44480
F	221	HIS	-	cloning artifact	UNP P44480

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Chain	Residue	Modelled	Actual	Comment	Reference
F	222	HIS	-	cloning artifact	UNP P44480

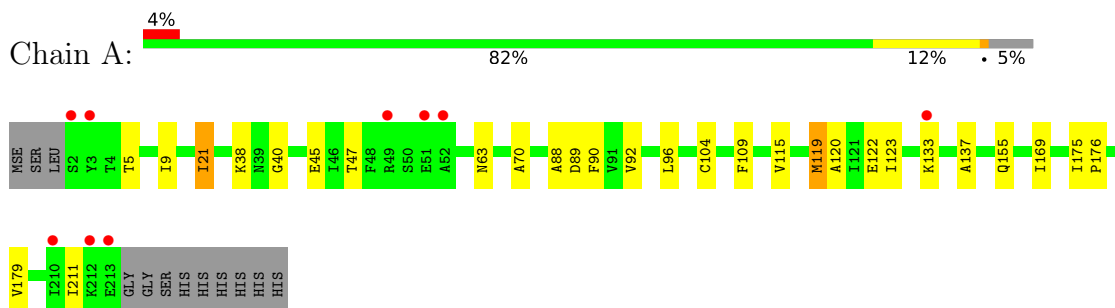
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	121	Total 121	O 121	0	0
2	B	98	Total 98	O 98	0	0
2	C	113	Total 113	O 113	0	0
2	D	122	Total 122	O 122	0	0
2	E	94	Total 94	O 94	0	0
2	F	196	Total 196	O 196	0	0

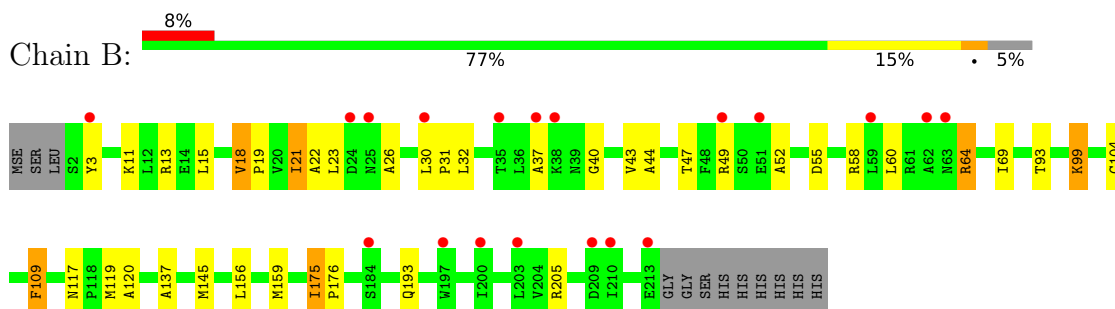
3 Residue-property plots [i](#)

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.

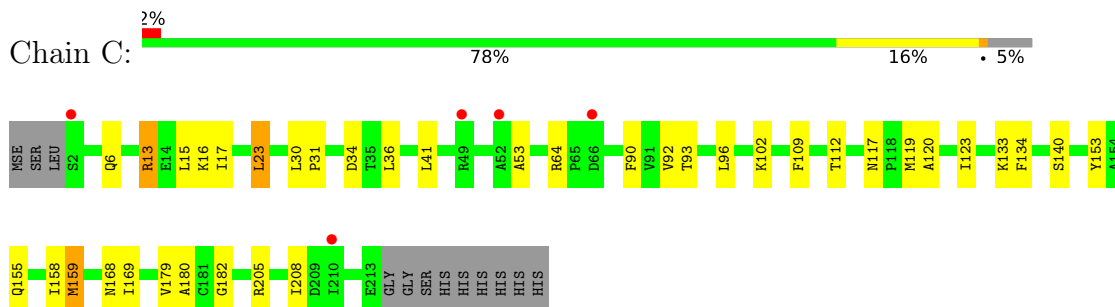
- Molecule 1: Putative KHG/KDPG aldolase



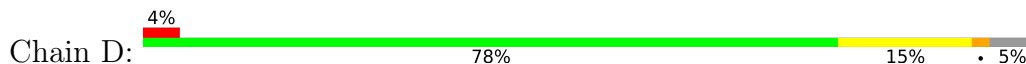
- Molecule 1: Putative KHG/KDPG aldolase

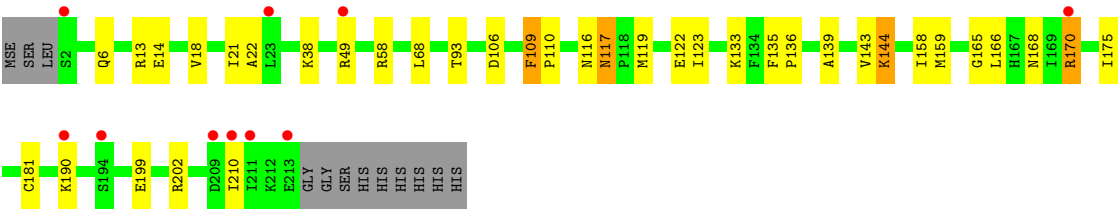


- Molecule 1: Putative KHG/KDPG aldolase

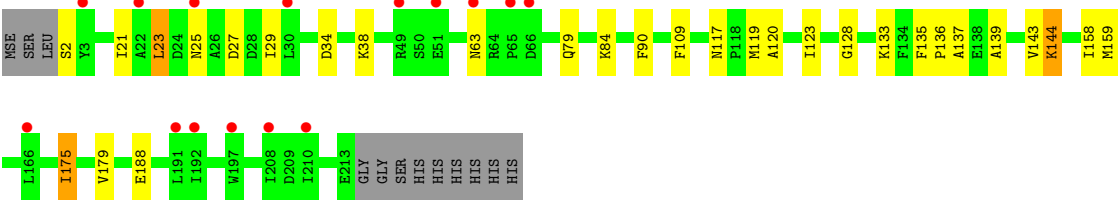
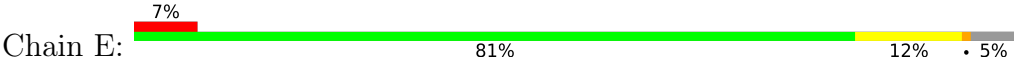


- Molecule 1: Putative KHG/KDPG aldolase

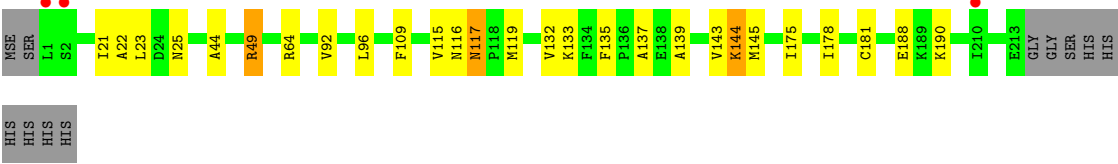
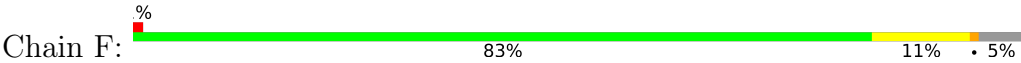




● Molecule 1: Putative KHG/KDPG aldolase



● Molecule 1: Putative KHG/KDPG aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.27Å 133.23Å 89.73Å 90.00° 105.82° 90.00°	Depositor
Resolution (Å)	30.40 – 1.89 30.40 – 1.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.40-1.89) 91.7 (30.40-1.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.89Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.219 , 0.256 0.202 , 0.236	Depositor DCC
R_{free} test set	6407 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10319	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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	1.05	2/1630 (0.1%)	1.51	10/2212 (0.5%)
1	B	1.02	3/1606 (0.2%)	1.50	14/2185 (0.6%)
1	C	1.11	0/1630	1.58	21/2212 (0.9%)
1	D	1.17	2/1626 (0.1%)	1.60	13/2206 (0.6%)
1	E	0.95	1/1624 (0.1%)	1.43	9/2204 (0.4%)
1	F	1.23	3/1639 (0.2%)	1.61	16/2223 (0.7%)
All	All	1.09	11/9755 (0.1%)	1.54	83/13242 (0.6%)

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	D	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	165	GLY	N-CA	7.07	1.52	1.45
1	B	145	MSE	SE-CE	-6.47	1.76	1.95
1	E	117	ASN	N-CA	5.94	1.51	1.46
1	A	119[A]	MSE	SE-CE	-5.92	1.77	1.95
1	A	119[B]	MSE	SE-CE	-5.92	1.77	1.95
1	F	135	PHE	CA-CB	5.28	1.61	1.53
1	B	159[A]	MSE	SE-CE	-5.20	1.79	1.95
1	B	159[B]	MSE	SE-CE	-5.20	1.79	1.95
1	F	92	VAL	C-O	5.16	1.29	1.24
1	D	68	LEU	N-CA	5.11	1.52	1.46
1	F	145	MSE	SE-CE	-5.09	1.80	1.95

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ARG	CD-NE-CZ	10.31	138.83	124.40
1	F	49	ARG	CD-NE-CZ	9.87	138.22	124.40
1	F	115	VAL	CA-C-O	-7.80	113.90	121.63
1	C	102	LYS	O-C-N	-7.68	114.16	122.07
1	D	181	CYS	CA-C-N	7.29	129.43	122.36
1	D	181	CYS	C-N-CA	7.29	129.43	122.36
1	D	158	ILE	N-CA-C	7.29	118.97	108.48
1	C	6	GLN	OE1-CD-NE2	-7.16	115.44	122.60
1	C	168	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	B	18	VAL	CA-C-O	6.96	125.97	119.98
1	B	205	ARG	CA-C-N	6.76	129.34	120.28
1	B	205	ARG	C-N-CA	6.76	129.34	120.28
1	F	178	ILE	O-C-N	-6.72	115.31	122.83
1	B	21	ILE	N-CA-C	6.70	117.55	108.17
1	A	90	PHE	CA-CB-CG	6.63	120.43	113.80
1	E	90	PHE	CA-CB-CG	6.57	120.37	113.80
1	C	180	ALA	CA-C-O	-6.54	114.23	121.23
1	D	18	VAL	N-CA-C	6.49	114.97	107.89
1	D	117	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	C	109	PHE	CA-CB-CG	6.32	120.12	113.80
1	F	64	ARG	NE-CZ-NH1	6.24	127.74	121.50
1	A	21	ILE	N-CA-C	6.19	116.78	107.80
1	D	109	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	40	GLY	N-CA-C	6.03	124.36	115.08
1	B	137	ALA	N-CA-C	6.02	118.36	111.02
1	F	109	PHE	CA-CB-CG	5.99	119.78	113.80
1	D	122	GLU	CA-CB-CG	-5.92	102.26	114.10
1	D	21	ILE	N-CA-C	5.90	116.43	108.17
1	A	122	GLU	CA-CB-CG	-5.89	102.32	114.10
1	D	117	ASN	O-C-N	-5.88	116.55	121.54
1	C	153	TYR	N-CA-CB	-5.82	103.66	110.35
1	C	117	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	89	ASP	CA-CB-CG	-5.80	106.80	112.60
1	C	158	ILE	N-CA-C	5.75	116.87	108.53
1	C	134	PHE	CA-CB-CG	5.75	119.55	113.80
1	F	25	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	D	170	ARG	CD-NE-CZ	5.73	132.42	124.40
1	F	137	ALA	N-CA-C	5.68	117.16	110.97
1	C	53	ALA	N-CA-C	5.68	117.94	111.02
1	B	109	PHE	CA-CB-CG	5.64	119.44	113.80
1	C	205	ARG	CD-NE-CZ	5.62	132.26	124.40
1	D	116	ASN	CA-CB-CG	5.61	118.20	112.60
1	E	21	ILE	N-CA-C	5.60	116.01	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	GLN	CB-CG-CD	5.58	122.09	112.60
1	A	137	ALA	N-CA-C	5.50	117.72	111.02
1	F	22	ALA	CA-C-N	-5.46	113.37	122.21
1	F	22	ALA	C-N-CA	-5.46	113.37	122.21
1	E	175	ILE	CA-C-N	5.39	125.03	119.05
1	E	175	ILE	C-N-CA	5.39	125.03	119.05
1	E	137	ALA	N-CA-C	5.37	116.83	110.97
1	B	175	ILE	CA-C-N	5.35	124.99	119.05
1	B	175	ILE	C-N-CA	5.35	124.99	119.05
1	F	178	ILE	CA-C-O	5.35	127.06	120.74
1	F	116	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	F	132	VAL	N-CA-C	5.33	117.07	108.85
1	C	90	PHE	CA-CB-CG	5.30	119.11	113.80
1	A	115	VAL	CA-C-O	-5.30	116.11	121.67
1	A	179	VAL	N-CA-C	5.27	115.94	110.82
1	B	117	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	C	140	SER	CA-C-N	-5.21	115.28	122.63
1	C	140	SER	C-N-CA	-5.21	115.28	122.63
1	C	13	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	B	32	LEU	O-C-N	-5.20	116.48	122.09
1	F	117	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	F	181	CYS	CA-C-N	-5.17	117.59	122.66
1	F	181	CYS	C-N-CA	-5.17	117.59	122.66
1	E	128	GLY	O-C-N	-5.17	116.23	122.38
1	E	158	ILE	N-CA-C	5.16	116.15	108.46
1	B	40	GLY	N-CA-C	5.16	122.55	115.27
1	A	88	ALA	CA-C-O	-5.15	115.90	121.87
1	E	109	PHE	CA-CB-CG	5.14	118.94	113.80
1	B	156	LEU	CA-C-O	-5.11	115.57	121.19
1	D	6	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	C	159[A]	MSE	CA-C-N	5.10	124.86	119.76
1	C	159[A]	MSE	C-N-CA	5.10	124.86	119.76
1	C	159[B]	MSE	CA-C-N	5.10	124.86	119.76
1	C	159[B]	MSE	C-N-CA	5.10	124.86	119.76
1	A	63	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	64	ARG	CA-C-N	5.08	124.80	119.82
1	B	64	ARG	C-N-CA	5.08	124.80	119.82
1	C	182	GLY	CA-C-O	-5.04	115.79	121.23
1	E	79	GLN	CA-C-O	-5.04	115.53	120.82
1	F	49	ARG	N-CA-C	-5.01	106.00	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	168	ASN	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	1600	0	1653	20	0
1	B	1576	0	1589	29	0
1	C	1600	0	1653	25	0
1	D	1596	0	1654	28	0
1	E	1594	0	1642	26	0
1	F	1609	0	1669	21	0
2	A	121	0	0	3	0
2	B	98	0	0	4	0
2	C	113	0	0	0	0
2	D	122	0	0	3	0
2	E	94	0	0	1	0
2	F	196	0	0	5	0
All	All	10319	0	9860	114	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 6.

All (114) 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:119[B]:MSE:HE1	1:B:119[B]:MSE:HG2	1.20	1.08
1:E:119[B]:MSE:SE	1:F:119[B]:MSE:SE	2.79	0.99
1:A:119[B]:MSE:SE	1:B:119[B]:MSE:SE	2.91	0.87
1:D:119[B]:MSE:SE	1:E:119[B]:MSE:HE2	2.28	0.83
1:D:144:LYS:HE2	1:E:139:ALA:HA	1.61	0.82
1:E:25:ASN:HD21	1:E:27:ASP:HB2	1.47	0.80
1:A:119[B]:MSE:HE3	1:B:120:ALA:HB2	1.66	0.76
1:B:119[B]:MSE:SE	1:C:119[B]:MSE:SE	3.05	0.74
1:B:119[B]:MSE:SE	1:C:119[B]:MSE:HG2	2.38	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119[B]:MSE:HE1	1:B:119[B]:MSE:CG	2.11	0.72
1:D:93:THR:HB	2:F:342:HOH:O	1.88	0.71
2:A:308:HOH:O	1:E:84:LYS:HE2	1.91	0.69
1:D:133:LYS:HE3	2:D:318:HOH:O	1.93	0.68
1:B:26:ALA:HB2	1:B:52:ALA:HB1	1.76	0.67
1:F:143:VAL:HG13	1:F:175:ILE:HD11	1.77	0.66
1:D:119[B]:MSE:HE1	1:E:120:ALA:HA	1.76	0.66
1:A:119[B]:MSE:CE	1:B:119[B]:MSE:HG2	2.12	0.64
1:E:119[B]:MSE:SE	1:F:119[B]:MSE:CG	2.95	0.64
2:A:338:HOH:O	1:B:93:THR:HB	1.98	0.62
1:C:23:LEU:H	1:C:23:LEU:HD12	1.64	0.62
1:F:188:GLU:HG2	2:F:378:HOH:O	2.00	0.61
1:E:119[B]:MSE:SE	1:F:119[B]:MSE:HG2	2.50	0.60
1:B:22:ALA:HB2	1:B:49:ARG:HH21	1.67	0.60
1:C:23:LEU:HD12	1:C:23:LEU:N	2.16	0.59
1:E:144:LYS:HE2	1:F:139:ALA:HA	1.84	0.59
1:C:112:THR:HG21	1:C:159[B]:MSE:HE1	1.84	0.59
1:B:99:LYS:HE2	1:D:106:ASP:OD2	2.02	0.58
1:D:119[B]:MSE:HG2	1:F:119[B]:MSE:HE1	1.86	0.58
1:C:112:THR:HG21	1:C:159[B]:MSE:CE	2.34	0.57
1:D:119[B]:MSE:SE	1:F:119[B]:MSE:SE	3.23	0.57
1:D:170:ARG:NH1	1:D:210:ILE:O	2.38	0.56
1:D:119[B]:MSE:HE1	1:E:123:ILE:HD12	1.87	0.56
1:D:143:VAL:HG13	1:D:175:ILE:HD11	1.88	0.56
1:B:3:TYR:CZ	1:B:11:LYS:HE3	2.41	0.55
1:D:123:ILE:HD12	1:F:119[A]:MSE:HE1	1.89	0.55
1:C:15:LEU:O	1:C:16:LYS:HB2	2.06	0.54
1:B:119[B]:MSE:SE	1:C:119[B]:MSE:CG	3.05	0.54
1:E:144:LYS:HB3	1:E:144:LYS:NZ	2.23	0.54
1:C:17:ILE:HD13	1:C:169:ILE:CD1	2.38	0.53
1:D:119[B]:MSE:SE	1:E:119[B]:MSE:CE	3.03	0.53
1:B:15:LEU:HD13	1:B:43:VAL:HG11	1.92	0.52
1:C:133:LYS:HZ2	1:C:159[B]:MSE:HE2	1.75	0.52
1:B:22:ALA:HA	1:B:47:THR:HG22	1.92	0.52
1:A:5:THR:O	1:A:9:ILE:HG12	2.10	0.51
1:A:92:VAL:HG13	1:A:133:LYS:HG3	1.91	0.51
1:A:119[A]:MSE:HE1	1:B:120:ALA:HA	1.93	0.51
1:F:188:GLU:OE1	1:F:190:LYS:HB3	2.12	0.50
1:A:96:LEU:C	1:A:96:LEU:HD23	2.37	0.50
1:B:55:ASP:OD1	1:B:58:ARG:NH2	2.42	0.50
1:D:117:ASN:ND2	2:D:342:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:HD12	1:B:44:ALA:HB1	1.93	0.49
1:B:37:ALA:HA	2:B:295:HOH:O	2.11	0.49
1:D:139:ALA:HA	1:F:144:LYS:HE2	1.94	0.49
1:C:34:ASP:OD1	1:C:64:ARG:NH1	2.45	0.49
1:D:199:GLU:CD	1:D:202:ARG:HH21	2.20	0.49
1:D:139:ALA:CB	1:F:144:LYS:HE2	2.43	0.48
2:B:265:HOH:O	1:C:93:THR:HB	2.13	0.48
1:D:119[B]:MSE:SE	1:E:119[B]:MSE:SE	3.32	0.48
1:A:169:ILE:CD1	1:A:211:ILE:HD11	2.44	0.48
1:D:22:ALA:HB2	1:D:49:ARG:HH21	1.78	0.48
1:E:25:ASN:ND2	1:E:27:ASP:HB2	2.22	0.48
1:E:23:LEU:HD12	1:E:23:LEU:H	1.78	0.48
1:E:119[B]:MSE:CE	1:F:119[B]:MSE:SE	3.12	0.47
1:A:120:ALA:HA	1:C:119[B]:MSE:HE1	1.97	0.47
1:C:13:ARG:HB2	1:C:179:VAL:HG13	1.97	0.47
1:C:92:VAL:HG13	1:C:133:LYS:HG3	1.97	0.47
1:A:38:LYS:HB3	1:A:38:LYS:NZ	2.29	0.47
1:B:60:LEU:HG	1:B:69:ILE:HD11	1.97	0.47
1:D:13:ARG:HH11	1:D:13:ARG:HG3	1.79	0.47
1:C:36:LEU:HB3	1:C:41:LEU:O	2.16	0.46
1:A:123:ILE:HD12	1:C:119[B]:MSE:HE1	1.97	0.46
1:E:159[B]:MSE:SE	1:E:179:VAL:HB	2.66	0.46
1:D:119[B]:MSE:CE	1:E:120:ALA:HA	2.43	0.45
1:A:45:GLU:HA	1:A:70:ALA:HB3	1.96	0.45
1:A:119[B]:MSE:HE3	1:B:120:ALA:CB	2.43	0.45
1:F:21:ILE:HD12	1:F:44:ALA:HB1	1.98	0.45
1:B:119[B]:MSE:HE1	1:C:123:ILE:HD12	1.99	0.45
1:C:30:LEU:HB2	1:C:31:PRO:CD	2.47	0.45
1:F:133:LYS:HG3	2:F:280:HOH:O	2.16	0.45
1:A:155:GLN:NE2	2:A:304:HOH:O	2.51	0.44
1:C:96:LEU:C	1:C:96:LEU:HD23	2.42	0.44
1:A:21:ILE:O	1:A:47:THR:HG22	2.17	0.44
1:E:143:VAL:HG13	1:E:175:ILE:HD11	1.99	0.44
1:D:135:PHE:CD1	1:D:136:PRO:HA	2.53	0.44
1:F:49:ARG:NH2	2:F:366:HOH:O	2.51	0.44
1:B:193:GLN:HG2	2:B:250:HOH:O	2.18	0.43
1:E:133:LYS:HE3	2:E:251:HOH:O	2.17	0.43
1:E:144:LYS:HE2	1:F:139:ALA:CB	2.49	0.43
1:E:144:LYS:CE	1:F:139:ALA:HA	2.48	0.43
1:C:17:ILE:HD13	1:C:169:ILE:HD12	2.01	0.43
1:F:96:LEU:C	1:F:96:LEU:HD23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ILE:HD12	1:F:119[B]:MSE:CE	2.49	0.42
1:B:104:CYS:HB3	1:B:109:PHE:O	2.19	0.42
1:B:18:VAL:HA	1:B:19:PRO:HD3	1.83	0.41
1:B:175:ILE:HA	1:B:176:PRO:HD3	1.86	0.41
1:C:155:GLN:NE2	1:C:155:GLN:HA	2.35	0.41
1:A:92:VAL:HG11	1:A:133:LYS:HE2	2.02	0.41
1:A:104:CYS:HB3	1:A:109:PHE:O	2.21	0.41
1:A:175:ILE:HA	1:A:176:PRO:HD3	1.90	0.41
1:C:133:LYS:NZ	1:C:159[B]:MSE:HE2	2.35	0.41
1:F:117:ASN:ND2	2:F:369:HOH:O	2.53	0.41
1:C:41:LEU:HG	1:C:208:ILE:HD11	2.02	0.41
1:D:13:ARG:HG3	1:D:13:ARG:NH1	2.34	0.41
1:E:135:PHE:CD2	1:E:136:PRO:HA	2.55	0.41
1:E:34:ASP:OD2	1:E:38:LYS:NZ	2.54	0.41
1:B:119[B]:MSE:HE1	1:C:120:ALA:HA	2.03	0.41
1:D:133:LYS:HE3	2:D:294:HOH:O	2.20	0.41
1:D:133:LYS:HD3	1:D:159[A]:MSE:HB2	2.03	0.41
1:E:29:ILE:HD12	1:E:29:ILE:HA	1.95	0.40
1:B:13:ARG:HD3	2:B:300:HOH:O	2.21	0.40
1:B:30:LEU:N	1:B:31:PRO:HD2	2.37	0.40
1:D:109:PHE:HA	1:D:110:PRO:HD3	1.97	0.40
1:D:133:LYS:HD3	1:D:159[B]:MSE:HB2	2.04	0.40
1:E:23:LEU:HD12	1:E:23:LEU:N	2.37	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	212/224 (95%)	205 (97%)	7 (3%)	0	100	100
1	B	212/224 (95%)	204 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	212/224 (95%)	207 (98%)	5 (2%)	0	100	100
1	D	212/224 (95%)	205 (97%)	7 (3%)	0	100	100
1	E	212/224 (95%)	205 (97%)	7 (3%)	0	100	100
1	F	213/224 (95%)	206 (97%)	7 (3%)	0	100	100
All	All	1273/1344 (95%)	1232 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	171/178 (96%)	171 (100%)	0	100	100
1	B	163/178 (92%)	160 (98%)	3 (2%)	51	50
1	C	171/178 (96%)	170 (99%)	1 (1%)	78	81
1	D	170/178 (96%)	165 (97%)	5 (3%)	37	31
1	E	169/178 (95%)	164 (97%)	5 (3%)	36	30
1	F	172/178 (97%)	170 (99%)	2 (1%)	63	63
All	All	1016/1068 (95%)	1000 (98%)	16 (2%)	55	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	LEU
1	B	64	ARG
1	B	99	LYS
1	C	23	LEU
1	D	14	GLU
1	D	38	LYS
1	D	144	LYS
1	D	166	LEU
1	D	190	LYS

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Mol	Chain	Res	Type
1	E	2	SER
1	E	23	LEU
1	E	63	ASN
1	E	144	LYS
1	E	188	GLU
1	F	23	LEU
1	F	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	105	GLN
1	A	157	GLN
1	A	193	GLN
1	A	195	ASN
1	B	6	GLN
1	B	7	GLN
1	B	116	ASN
1	B	157	GLN
1	B	195	ASN
1	B	196	ASN
1	C	155	GLN
1	D	6	GLN
1	D	25	ASN
1	D	63	ASN
1	D	155	GLN
1	D	157	GLN
1	E	25	ASN
1	F	6	GLN
1	F	157	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	208/224 (92%)	0.11	9 (4%)	40 42	23, 32, 46, 60	0
1	B	208/224 (92%)	0.61	19 (9%)	15 15	23, 36, 58, 71	0
1	C	208/224 (92%)	0.20	5 (2%)	59 63	22, 32, 49, 60	0
1	D	208/224 (92%)	0.23	10 (4%)	35 38	21, 31, 55, 67	0
1	E	208/224 (92%)	0.50	15 (7%)	21 23	23, 37, 56, 63	0
1	F	209/224 (93%)	-0.12	3 (1%)	73 76	20, 27, 42, 59	0
All	All	1249/1344 (92%)	0.25	61 (4%)	35 37	20, 32, 54, 71	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	LEU	5.5
1	D	210	ILE	4.0
1	E	210	ILE	3.9
1	E	197	TRP	3.8
1	A	49	ARG	3.8
1	B	210	ILE	3.8
1	D	190	LYS	3.7
1	E	191	LEU	3.7
1	B	49	ARG	3.6
1	F	2	SER	3.6
1	E	3	TYR	3.5
1	B	30	LEU	3.4
1	F	210	ILE	3.4
1	E	25	ASN	3.3
1	B	38	LYS	3.1
1	B	197	TRP	3.1
1	C	49	ARG	3.1
1	A	213	GLU	3.0
1	B	59	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	23	LEU	2.9
1	B	3	TYR	2.9
1	B	63	ASN	2.9
1	E	66	ASP	2.9
1	A	210	ILE	2.8
1	D	213	GLU	2.8
1	B	62	ALA	2.8
1	A	3	TYR	2.7
1	B	213	GLU	2.6
1	D	209	ASP	2.5
1	A	133	LYS	2.5
1	C	52	ALA	2.4
1	E	51	GLU	2.4
1	B	184	SER	2.4
1	B	24	ASP	2.4
1	C	210	ILE	2.4
1	B	25	ASN	2.4
1	D	194	SER	2.4
1	B	209	ASP	2.3
1	E	65	PRO	2.3
1	C	66	ASP	2.3
1	E	166	LEU	2.3
1	B	51	GLU	2.3
1	B	200	ILE	2.3
1	D	211	ILE	2.2
1	E	192	ILE	2.2
1	A	212	LYS	2.2
1	A	51	GLU	2.2
1	B	203	LEU	2.2
1	D	170	ARG	2.2
1	B	37	ALA	2.1
1	D	49	ARG	2.1
1	E	49	ARG	2.1
1	E	30	LEU	2.1
1	E	208	ILE	2.1
1	A	2	SER	2.1
1	E	63	ASN	2.1
1	E	22	ALA	2.1
1	C	2	SER	2.0
1	D	2	SER	2.0
1	B	35	THR	2.0
1	A	52	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 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.