



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 08:03 am GMT

PDB ID : 1VHC
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

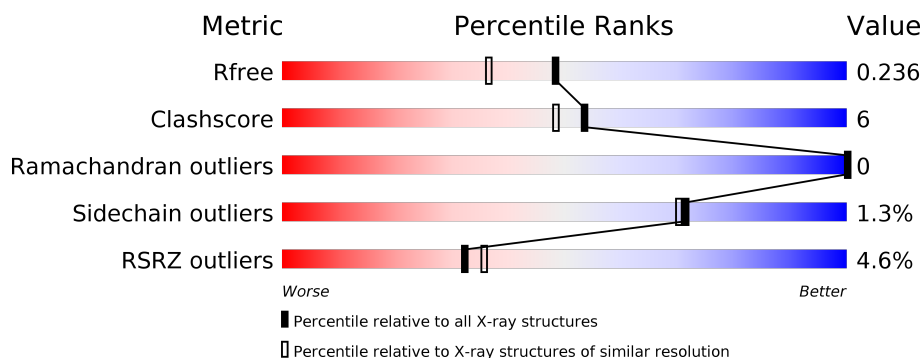
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	224	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	C	224	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	D	224	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	E	224	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	F	224	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

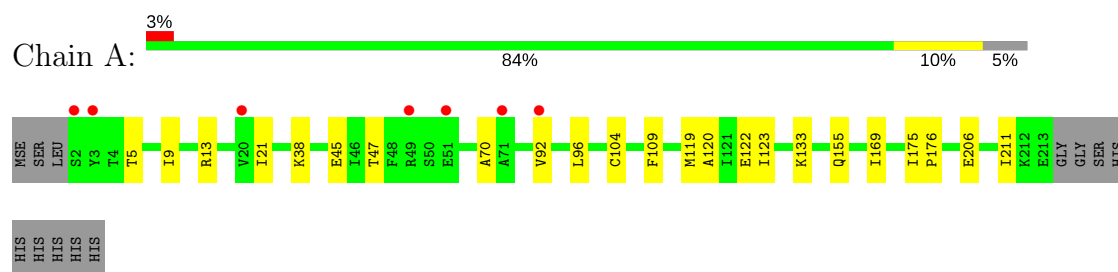
- Molecule 2 is water.

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

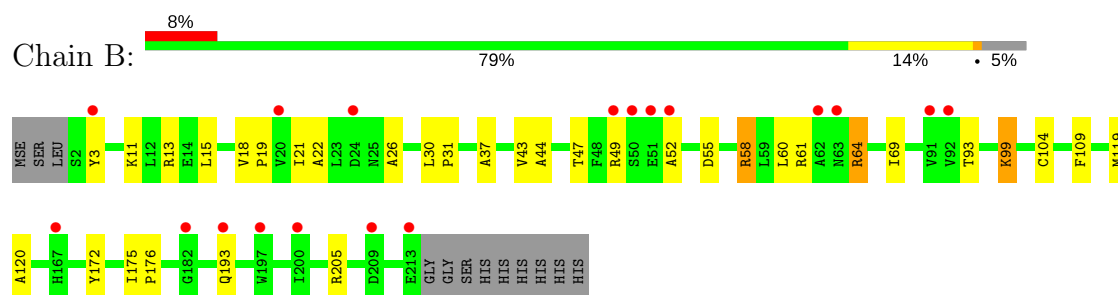
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

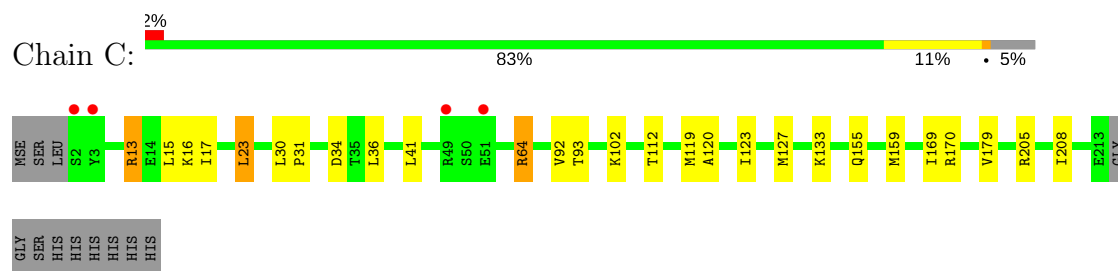
• Molecule 1: Putative KHG/KDPG aldolase



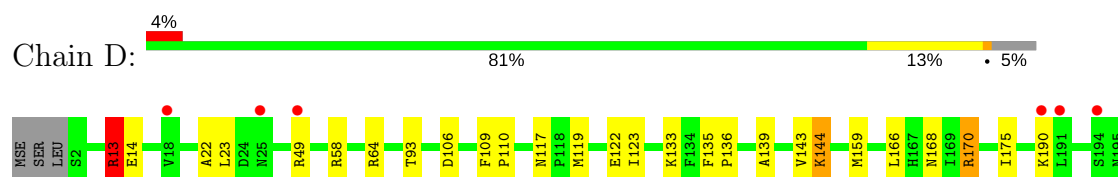
• Molecule 1: Putative KHG/KDPG aldolase



• Molecule 1: Putative KHG/KDPG aldolase

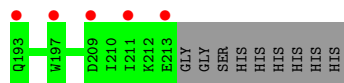
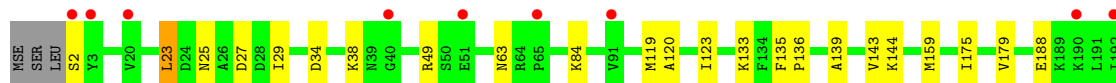
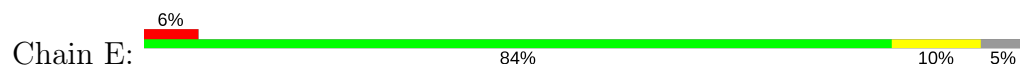


• Molecule 1: Putative KHG/KDPG aldolase

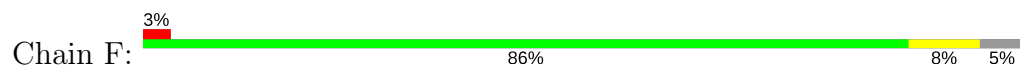




- Molecule 1: Putative KHG/KDPG aldolase



- 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) 91.2 (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)	0.37 , 59.0	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	0.78	0/1630	1.13	4/2212 (0.2%)
1	B	0.76	0/1606	1.17	7/2185 (0.3%)
1	C	0.81	0/1630	1.22	9/2212 (0.4%)
1	D	0.87	0/1626	1.29	10/2206 (0.5%)
1	E	0.71	0/1624	1.08	2/2204 (0.1%)
1	F	0.93	0/1639	1.31	9/2223 (0.4%)
All	All	0.81	0/9755	1.20	41/13242 (0.3%)

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

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	64	ARG	NE-CZ-NH1	14.88	127.74	120.30
1	D	170	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	D	58	ARG	CD-NE-CZ	10.88	138.83	123.60
1	F	49	ARG	CD-NE-CZ	10.45	138.22	123.60
1	D	64	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	B	58	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	C	13	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	C	64	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	C	64	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	E	49	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	D	205	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	172	TYR	CB-CG-CD1	7.23	125.34	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	C	170	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	58	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	F	13	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	122	GLU	OE1-CD-OE2	6.69	131.33	123.30
1	A	13	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	F	41	LEU	CA-CB-CG	6.45	130.14	115.30
1	D	170	ARG	CD-NE-CZ	6.30	132.42	123.60
1	C	205	ARG	CD-NE-CZ	6.19	132.26	123.60
1	F	49	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	172	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	C	127	MSE	CA-CB-CG	5.96	123.43	113.30
1	F	106	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	61	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	D	13	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	F	70	ALA	CB-CA-C	-5.52	101.83	110.10
1	B	205	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	B	64	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	102	LYS	O-C-N	-5.33	114.16	122.70
1	C	64	ARG	CD-NE-CZ	5.30	131.02	123.60
1	C	170	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	206	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	E	49	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	23	LEU	CB-CA-C	-5.21	100.31	110.20
1	D	64	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	F	170	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	122	GLU	CA-CB-CG	-5.07	102.26	113.40
1	F	24	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	122	GLU	CA-CB-CG	-5.04	102.32	113.40

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 [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	1600	0	1653	20	0
1	B	1576	0	1589	29	0
1	C	1600	0	1653	24	0
1	D	1596	0	1654	28	0
1	E	1594	0	1642	26	0
1	F	1609	0	1669	20	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	112	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 (112) 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
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:HD12	1:C:23:LEU:H	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:23:LEU:HD12	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:C:133:LYS:HZ2	1:C:159[B]:MSE:HE2	1.75	0.52
1:B:15:LEU:HD13	1:B:43:VAL:HG11	1.92	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: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
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: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:H	1:E:23:LEU:HD12	1.78	0.48
1:E:119[B]:MSE:CE	1:F:119[B]:MSE:SE	3.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ALA:HA	1:C:119[B]:MSE:HE1	1.97	0.47
1:C:92:VAL:HG13	1:C:133:LYS:HG3	1.97	0.47
1:C:13:ARG:HB2	1:C:179:VAL:HG13	1.97	0.47
1:A:38:LYS:NZ	1:A:38:LYS:HB3	2.29	0.47
1:B:60:LEU:HG	1:B:69:ILE:HD11	1.97	0.47
1:D:13:ARG:HG3	1:D:13:ARG:HH11	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:96:LEU:HD23	1:A:96:LEU:C	2.37	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:A:21:ILE:O	1:A:47:THR:HG22	2.17	0.44
1:D:199:GLU:CD	1:D:202:ARG:HH21	2.20	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: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:175:ILE:HA	1:B:176:PRO:HD3	1.86	0.41
1:B:18:VAL:HA	1:B:19:PRO:HD3	1.83	0.41
1:C:155:GLN:NE2	1:C:155:GLN:HA	2.35	0.41
1:A:104:CYS:HB3	1:A:109:PHE:O	2.21	0.41
1:A:92:VAL:HG11	1:A:133:LYS:HE2	2.02	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:NH1	1:D:13:ARG:HG3	2.34	0.41
1:E:135:PHE:CD2	1:E:136:PRO:HA	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:D:159[A]:MSE:HB2	2.03	0.41
1:D:133:LYS:HE3	2:D:294:HOH:O	2.20	0.41
1:E:29:ILE:HA	1:E:29:ILE:HD12	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:N	1:E:23:LEU:HD12	2.37	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	212/224 (95%)	205 (97%)	7 (3%)	0	100	100
1	B	212/224 (95%)	204 (96%)	8 (4%)	0	100	100
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%)	161 (99%)	2 (1%)	74	73
1	C	171/178 (96%)	170 (99%)	1 (1%)	87	88
1	D	170/178 (96%)	165 (97%)	5 (3%)	45	37
1	E	169/178 (95%)	165 (98%)	4 (2%)	52	45
1	F	172/178 (97%)	171 (99%)	1 (1%)	87	88
All	All	1016/1068 (95%)	1003 (99%)	13 (1%)	71	70

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	64	ARG
1	B	99	LYS
1	C	23	LEU
1	D	13	ARG
1	D	14	GLU
1	D	144	LYS
1	D	166	LEU
1	D	190	LYS
1	E	2	SER
1	E	23	LEU
1	E	63	ASN
1	E	188	GLU
1	F	23	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	B	7	GLN
1	B	195	ASN
1	C	155	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	155	GLN
1	D	195	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 carbohydrates 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%)	0.03	7 (3%) 45 49	23, 32, 46, 60	0
1	B	208/224 (92%)	0.46	18 (8%) 10 12	23, 36, 58, 71	0
1	C	208/224 (92%)	0.05	4 (1%) 66 70	22, 32, 49, 60	0
1	D	208/224 (92%)	0.07	8 (3%) 40 44	21, 31, 55, 67	0
1	E	208/224 (92%)	0.31	14 (6%) 18 20	23, 37, 56, 63	0
1	F	209/224 (93%)	-0.11	7 (3%) 46 50	20, 27, 42, 59	0
All	All	1249/1344 (92%)	0.13	58 (4%) 32 36	20, 32, 54, 71	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	SER	6.4
1	D	190	LYS	5.6
1	B	24	ASP	4.6
1	E	3	TYR	4.5
1	B	3	TYR	4.2
1	A	2	SER	4.2
1	E	192	ILE	4.0
1	D	194	SER	3.9
1	B	63	ASN	3.9
1	B	62	ALA	3.9
1	C	2	SER	3.9
1	B	51	GLU	3.7
1	E	197	TRP	3.4
1	A	49	ARG	3.3
1	C	51	GLU	3.2
1	E	65	PRO	3.1
1	F	1	LEU	3.0
1	E	190	LYS	3.0
1	B	209	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	51	GLU	2.8
1	E	193	GLN	2.8
1	D	49	ARG	2.7
1	B	92	VAL	2.7
1	F	213	GLU	2.7
1	B	197	TRP	2.7
1	B	50	SER	2.7
1	E	209	ASP	2.6
1	A	3	TYR	2.6
1	F	18	VAL	2.6
1	A	92	VAL	2.5
1	B	52	ALA	2.5
1	C	49	ARG	2.5
1	D	18	VAL	2.5
1	D	198	ASP	2.5
1	E	211	ILE	2.4
1	B	91	VAL	2.4
1	A	71	ALA	2.4
1	B	49	ARG	2.4
1	D	191	LEU	2.3
1	A	51	GLU	2.3
1	D	196	ASN	2.3
1	B	20	VAL	2.2
1	E	20	VAL	2.2
1	E	213	GLU	2.2
1	D	25	ASN	2.2
1	E	40	GLY	2.2
1	B	193	GLN	2.2
1	C	3	TYR	2.2
1	F	19	PRO	2.1
1	B	167	HIS	2.1
1	B	200	ILE	2.1
1	E	91	VAL	2.1
1	F	20	VAL	2.1
1	F	44	ALA	2.1
1	B	213	GLU	2.0
1	A	20	VAL	2.0
1	B	182	GLY	2.0
1	F	68	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 carbohydrates 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.