



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:48 AM UTC

PDB ID : 3Q7K / pdb_00003q7k
Title : Formate Channel FocA from Salmonella typhimurium
Authors : Lue, W.; Du, J.; Wacker, T.; Gerbig-Smentek, E.; Andrade, S.L.A.; Einsle, O.
Deposited on : 2011-01-05
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

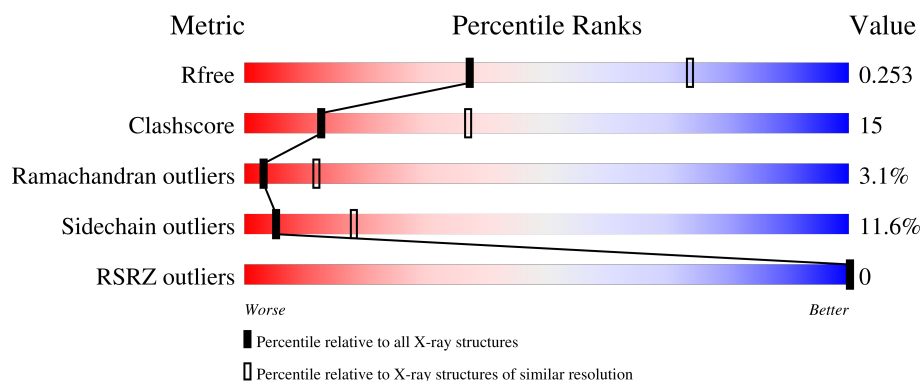
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	293	
1	B	293	
1	C	293	
1	D	293	
1	E	293	

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Mol	Chain	Length	Quality of chain
1	G	293	60%15%•23%
1	H	293	65%18%7%•9%
1	I	293	65%15%••15%
1	J	293	66%16%9%•8%
1	K	293	61%17%5%•16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19151 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 Probable formate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1979	1309	310	340	20			
1	B	248	Total	C	N	O	S	0	0	0
			1870	1239	290	321	20			
1	C	269	Total	C	N	O	S	0	0	0
			2043	1357	318	348	20			
1	D	254	Total	C	N	O	S	0	0	0
			1923	1273	301	329	20			
1	E	232	Total	C	N	O	S	0	0	0
			1758	1166	273	300	19			
1	G	226	Total	C	N	O	S	0	0	0
			1716	1139	264	294	19			
1	H	266	Total	C	N	O	S	0	0	0
			2016	1337	315	344	20			
1	I	248	Total	C	N	O	S	0	0	0
			1872	1239	291	322	20			
1	J	271	Total	C	N	O	S	0	0	0
			2059	1369	320	350	20			
1	K	247	Total	C	N	O	S	0	0	0
			1864	1233	290	321	20			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LEU	-	expression tag	UNP Q8XF76
A	287	GLU	-	expression tag	UNP Q8XF76
A	288	HIS	-	expression tag	UNP Q8XF76
A	289	HIS	-	expression tag	UNP Q8XF76
A	290	HIS	-	expression tag	UNP Q8XF76
A	291	HIS	-	expression tag	UNP Q8XF76
A	292	HIS	-	expression tag	UNP Q8XF76
A	293	HIS	-	expression tag	UNP Q8XF76
B	286	LEU	-	expression tag	UNP Q8XF76

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Chain	Residue	Modelled	Actual	Comment	Reference
B	287	GLU	-	expression tag	UNP Q8XF76
B	288	HIS	-	expression tag	UNP Q8XF76
B	289	HIS	-	expression tag	UNP Q8XF76
B	290	HIS	-	expression tag	UNP Q8XF76
B	291	HIS	-	expression tag	UNP Q8XF76
B	292	HIS	-	expression tag	UNP Q8XF76
B	293	HIS	-	expression tag	UNP Q8XF76
C	286	LEU	-	expression tag	UNP Q8XF76
C	287	GLU	-	expression tag	UNP Q8XF76
C	288	HIS	-	expression tag	UNP Q8XF76
C	289	HIS	-	expression tag	UNP Q8XF76
C	290	HIS	-	expression tag	UNP Q8XF76
C	291	HIS	-	expression tag	UNP Q8XF76
C	292	HIS	-	expression tag	UNP Q8XF76
C	293	HIS	-	expression tag	UNP Q8XF76
D	286	LEU	-	expression tag	UNP Q8XF76
D	287	GLU	-	expression tag	UNP Q8XF76
D	288	HIS	-	expression tag	UNP Q8XF76
D	289	HIS	-	expression tag	UNP Q8XF76
D	290	HIS	-	expression tag	UNP Q8XF76
D	291	HIS	-	expression tag	UNP Q8XF76
D	292	HIS	-	expression tag	UNP Q8XF76
D	293	HIS	-	expression tag	UNP Q8XF76
E	286	LEU	-	expression tag	UNP Q8XF76
E	287	GLU	-	expression tag	UNP Q8XF76
E	288	HIS	-	expression tag	UNP Q8XF76
E	289	HIS	-	expression tag	UNP Q8XF76
E	290	HIS	-	expression tag	UNP Q8XF76
E	291	HIS	-	expression tag	UNP Q8XF76
E	292	HIS	-	expression tag	UNP Q8XF76
E	293	HIS	-	expression tag	UNP Q8XF76
G	286	LEU	-	expression tag	UNP Q8XF76
G	287	GLU	-	expression tag	UNP Q8XF76
G	288	HIS	-	expression tag	UNP Q8XF76
G	289	HIS	-	expression tag	UNP Q8XF76
G	290	HIS	-	expression tag	UNP Q8XF76
G	291	HIS	-	expression tag	UNP Q8XF76
G	292	HIS	-	expression tag	UNP Q8XF76
G	293	HIS	-	expression tag	UNP Q8XF76
H	286	LEU	-	expression tag	UNP Q8XF76
H	287	GLU	-	expression tag	UNP Q8XF76
H	288	HIS	-	expression tag	UNP Q8XF76

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Chain	Residue	Modelled	Actual	Comment	Reference
H	289	HIS	-	expression tag	UNP Q8XF76
H	290	HIS	-	expression tag	UNP Q8XF76
H	291	HIS	-	expression tag	UNP Q8XF76
H	292	HIS	-	expression tag	UNP Q8XF76
H	293	HIS	-	expression tag	UNP Q8XF76
I	286	LEU	-	expression tag	UNP Q8XF76
I	287	GLU	-	expression tag	UNP Q8XF76
I	288	HIS	-	expression tag	UNP Q8XF76
I	289	HIS	-	expression tag	UNP Q8XF76
I	290	HIS	-	expression tag	UNP Q8XF76
I	291	HIS	-	expression tag	UNP Q8XF76
I	292	HIS	-	expression tag	UNP Q8XF76
I	293	HIS	-	expression tag	UNP Q8XF76
J	286	LEU	-	expression tag	UNP Q8XF76
J	287	GLU	-	expression tag	UNP Q8XF76
J	288	HIS	-	expression tag	UNP Q8XF76
J	289	HIS	-	expression tag	UNP Q8XF76
J	290	HIS	-	expression tag	UNP Q8XF76
J	291	HIS	-	expression tag	UNP Q8XF76
J	292	HIS	-	expression tag	UNP Q8XF76
J	293	HIS	-	expression tag	UNP Q8XF76
K	286	LEU	-	expression tag	UNP Q8XF76
K	287	GLU	-	expression tag	UNP Q8XF76
K	288	HIS	-	expression tag	UNP Q8XF76
K	289	HIS	-	expression tag	UNP Q8XF76
K	290	HIS	-	expression tag	UNP Q8XF76
K	291	HIS	-	expression tag	UNP Q8XF76
K	292	HIS	-	expression tag	UNP Q8XF76
K	293	HIS	-	expression tag	UNP Q8XF76

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		
2	C	1	Total	C	O	0	0
			3	1	2		
2	C	1	Total	C	O	0	0
			3	1	2		
2	D	1	Total	C	O	0	0
			3	1	2		
2	H	1	Total	C	O	0	0
			3	1	2		
2	H	1	Total	C	O	0	0
			3	1	2		
2	H	1	Total	C	O	0	0
			3	1	2		
2	I	1	Total	C	O	0	0
			3	1	2		
2	J	1	Total	C	O	0	0
			3	1	2		
2	K	1	Total	C	O	0	0
			3	1	2		
2	K	1	Total	C	O	0	0
			3	1	2		

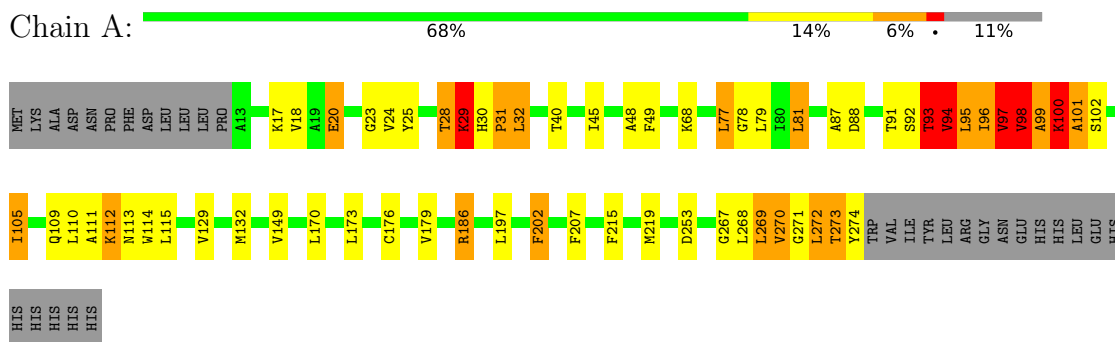
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	3	Total 3	O 3	0	0
3	C	1	Total 1	O 1	0	0
3	D	1	Total 1	O 1	0	0
3	H	2	Total 2	O 2	0	0
3	I	1	Total 1	O 1	0	0
3	K	2	Total 2	O 2	0	0

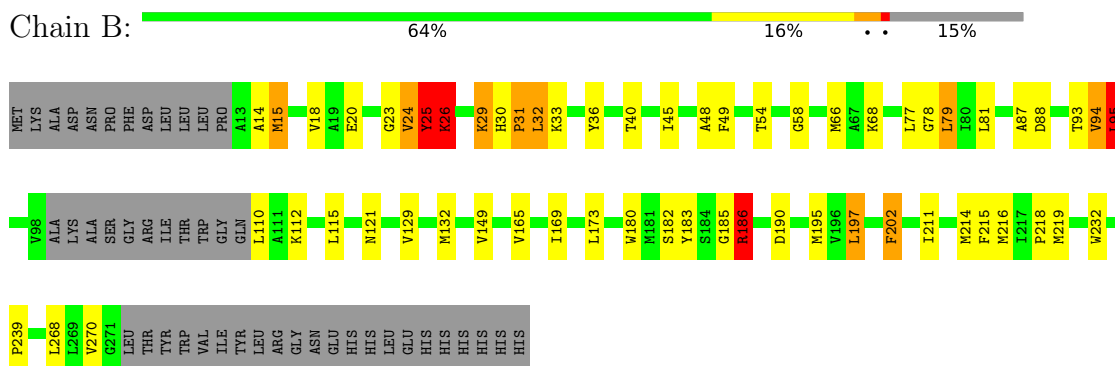
3 Residue-property plots [i](#)

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.

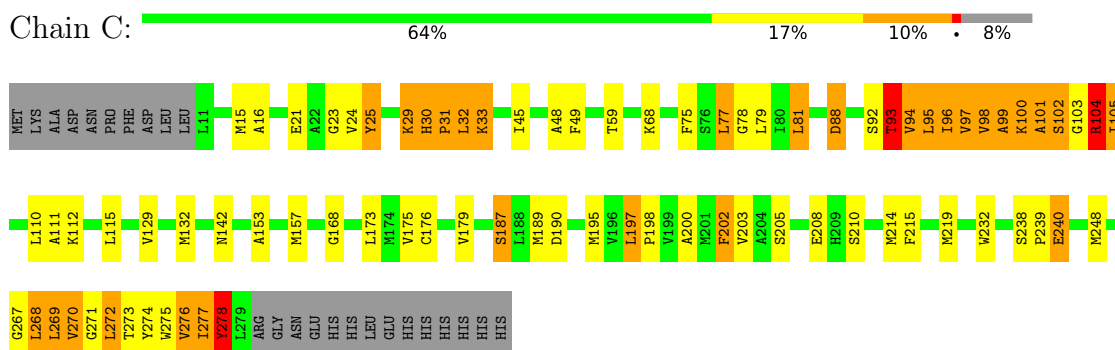
• Molecule 1: Probable formate transporter



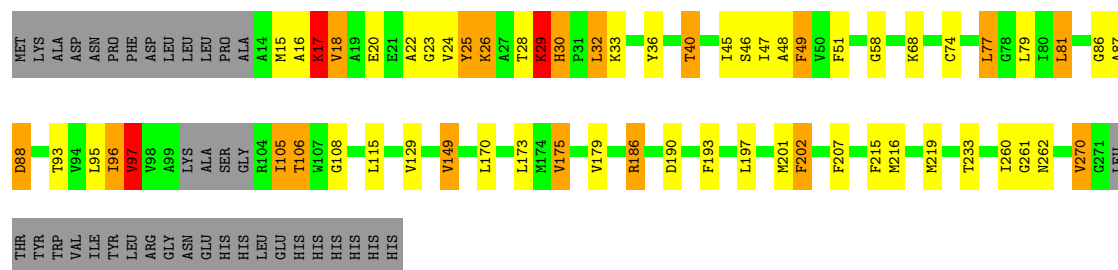
• Molecule 1: Probable formate transporter



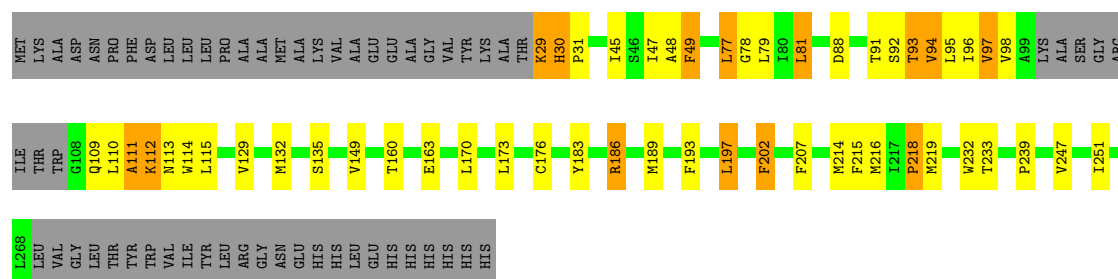
• Molecule 1: Probable formate transporter



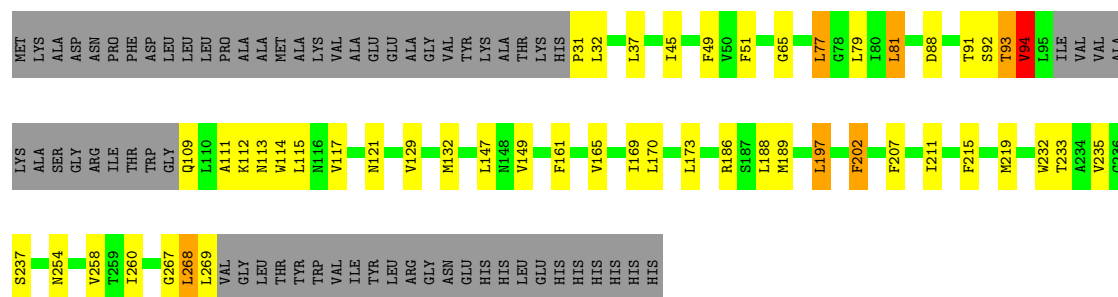
Chain D: 66% 14% 6% • 13%



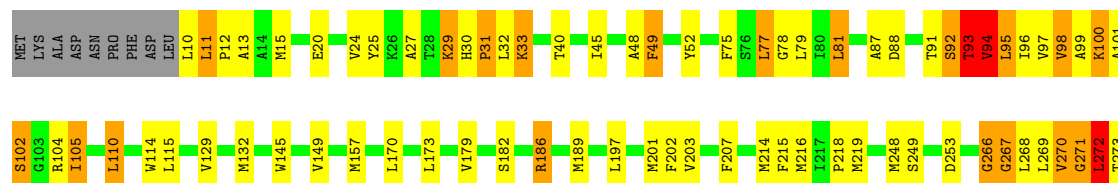
Chain E: 61% 13% 5% 21%

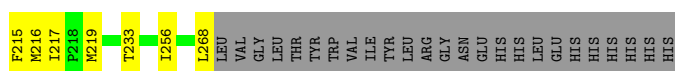


Chain G: 60% 15% • 23%



Chain H: 65% 18% 7% • 9%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.95Å 205.72Å 106.05Å 90.00° 115.49° 90.00°	Depositor
Resolution (Å)	43.64 – 2.80 43.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (43.64-2.80) 92.0 (43.64-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.219 , 0.254 0.220 , 0.253	Depositor DCC
R_{free} test set	4664 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.439 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19151	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT

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	0.96	1/2028 (0.0%)	1.14	10/2758 (0.4%)
1	B	1.09	0/1915	1.20	8/2603 (0.3%)
1	C	1.07	4/2096 (0.2%)	1.21	10/2854 (0.4%)
1	D	1.10	5/1970 (0.3%)	1.22	17/2678 (0.6%)
1	E	1.08	0/1802	1.17	8/2450 (0.3%)
1	G	1.07	1/1759 (0.1%)	1.15	3/2391 (0.1%)
1	H	1.07	2/2068 (0.1%)	1.28	11/2815 (0.4%)
1	I	1.09	2/1918 (0.1%)	1.20	8/2606 (0.3%)
1	J	1.06	2/2112 (0.1%)	1.23	11/2876 (0.4%)
1	K	1.10	3/1909 (0.2%)	1.24	8/2594 (0.3%)
All	All	1.07	20/19577 (0.1%)	1.21	94/26625 (0.4%)

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	5
1	C	0	3
1	D	0	3
1	E	0	1
1	G	0	2
1	H	0	2
1	I	0	1
1	J	0	4
1	K	0	5
All	All	0	26

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	VAL	CA-CB	8.32	1.65	1.54
1	K	256	ILE	CA-CB	6.60	1.57	1.54
1	J	94	VAL	CA-CB	6.41	1.63	1.54
1	C	277	ILE	CA-CB	6.09	1.60	1.55
1	I	196	VAL	CA-CB	6.00	1.61	1.54

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	LEU	N-CA-C	-12.25	97.08	112.88
1	A	186	ARG	CD-NE-CZ	10.01	138.41	124.40
1	A	94	VAL	CB-CA-C	9.71	127.22	111.29
1	D	29	LYS	N-CA-C	9.45	125.02	109.24
1	B	25	TYR	N-CA-C	9.10	122.90	109.07

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LYS	Peptide
1	A	101	ALA	Peptide
1	A	28	THR	Peptide
1	A	93	THR	Peptide
1	A	94	VAL	Peptide

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	1979	0	2027	84	2
1	B	1870	0	1916	46	0
1	C	2043	0	2094	93	2
1	D	1923	0	1968	52	0
1	E	1758	0	1795	47	0
1	G	1716	0	1750	27	0
1	H	2016	0	2066	85	2
1	I	1872	0	1914	40	0
1	J	2059	0	2117	85	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1864	0	1904	51	0
2	A	3	0	1	0	0
2	B	6	0	2	1	0
2	C	6	0	2	0	0
2	D	3	0	1	1	0
2	H	9	0	3	0	0
2	I	3	0	1	0	0
2	J	3	0	1	0	0
2	K	6	0	2	1	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	H	2	0	0	0	0
3	I	1	0	0	0	0
3	K	2	0	0	0	0
All	All	19151	0	19564	590	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 590 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:E:96:ILE:HG12	1:E:183:TYR:CE1	1.21	1.64
1:E:96:ILE:CG1	1:E:183:TYR:HE1	1.21	1.49
1:K:96:ILE:HD11	1:K:183:TYR:CE1	1.69	1.28
1:J:99:ALA:HB1	1:J:270:VAL:HG11	1.21	1.15
1:I:25:TYR:CB	1:I:26:LYS:HB2	1.76	1.14

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:CB	1:J:240:GLU:OE2[2_455]	1.37	0.83
1:C:240:GLU:OE2	1:H:253:ASP:CB[2_556]	1.38	0.82
1:C:240:GLU:OE2	1:H:253:ASP:CG[2_556]	1.79	0.41
1:A:253:ASP:CG	1:J:240:GLU:OE2[2_455]	1.89	0.31

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	260/293 (89%)	239 (92%)	11 (4%)	10 (4%)	2	9
1	B	244/293 (83%)	224 (92%)	13 (5%)	7 (3%)	3	13
1	C	267/293 (91%)	239 (90%)	17 (6%)	11 (4%)	2	8
1	D	250/293 (85%)	230 (92%)	13 (5%)	7 (3%)	4	14
1	E	228/293 (78%)	212 (93%)	12 (5%)	4 (2%)	6	23
1	G	222/293 (76%)	212 (96%)	8 (4%)	2 (1%)	14	41
1	H	264/293 (90%)	243 (92%)	14 (5%)	7 (3%)	4	15
1	I	244/293 (83%)	228 (93%)	5 (2%)	11 (4%)	2	7
1	J	269/293 (92%)	232 (86%)	27 (10%)	10 (4%)	2	9
1	K	243/293 (83%)	222 (91%)	14 (6%)	7 (3%)	3	13
All	All	2491/2930 (85%)	2281 (92%)	134 (5%)	76 (3%)	3	12

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	31	PRO
1	A	96	ILE
1	A	97	VAL
1	A	100	LYS

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	208/237 (88%)	180 (86%)	28 (14%)	4	13
1	B	198/237 (84%)	176 (89%)	22 (11%)	6	20
1	C	215/237 (91%)	187 (87%)	28 (13%)	4	14
1	D	203/237 (86%)	182 (90%)	21 (10%)	7	23
1	E	188/237 (79%)	172 (92%)	16 (8%)	10	31
1	G	184/237 (78%)	166 (90%)	18 (10%)	7	25
1	H	212/237 (90%)	187 (88%)	25 (12%)	5	17
1	I	198/237 (84%)	174 (88%)	24 (12%)	5	16
1	J	217/237 (92%)	185 (85%)	32 (15%)	3	10
1	K	197/237 (83%)	176 (89%)	21 (11%)	6	21
All	All	2020/2370 (85%)	1785 (88%)	235 (12%)	5	18

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	32	LEU
1	K	81	LEU
1	H	93	THR
1	K	77	LEU
1	J	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	158	HIS
1	J	142	ASN
1	K	30	HIS
1	E	142	ASN
1	D	151	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](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMT	H	294	-	2,2,2	0.65	0	1,1,1	0.00	0
2	FMT	C	294	-	2,2,2	0.57	0	1,1,1	0.12	0
2	FMT	B	294	-	2,2,2	0.76	0	1,1,1	0.27	0
2	FMT	B	295	-	2,2,2	0.59	0	1,1,1	0.03	0
2	FMT	J	294	-	2,2,2	0.69	0	1,1,1	0.10	0
2	FMT	K	294	-	2,2,2	0.69	0	1,1,1	0.16	0
2	FMT	H	296	-	2,2,2	0.58	0	1,1,1	0.16	0
2	FMT	D	294	-	2,2,2	0.66	0	1,1,1	0.12	0
2	FMT	H	295	-	2,2,2	0.78	0	1,1,1	0.35	0
2	FMT	I	294	-	2,2,2	0.74	0	1,1,1	0.13	0
2	FMT	C	295	-	2,2,2	0.65	0	1,1,1	0.17	0
2	FMT	K	295	-	2,2,2	0.58	0	1,1,1	0.25	0
2	FMT	A	294	-	2,2,2	0.72	0	1,1,1	0.23	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	295	FMT	1	0
2	K	294	FMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	294	FMT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	262/293 (89%)	-1.30	0 100 100	31, 43, 76, 93	0
1	B	248/293 (84%)	-1.28	0 100 100	26, 43, 76, 89	1 (0%)
1	C	269/293 (91%)	-1.33	0 100 100	26, 44, 81, 92	1 (0%)
1	D	254/293 (86%)	-1.30	0 100 100	26, 43, 84, 110	1 (0%)
1	E	232/293 (79%)	-1.32	0 100 100	26, 42, 72, 87	1 (0%)
1	G	226/293 (77%)	-1.34	0 100 100	26, 42, 66, 87	1 (0%)
1	H	266/293 (90%)	-1.38	0 100 100	26, 43, 81, 100	1 (0%)
1	I	248/293 (84%)	-1.29	0 100 100	26, 43, 77, 92	1 (0%)
1	J	271/293 (92%)	-1.30	0 100 100	26, 44, 83, 96	1 (0%)
1	K	247/293 (84%)	-1.29	0 100 100	26, 42, 75, 89	1 (0%)
All	All	2523/2930 (86%)	-1.31	0 100 100	26, 43, 79, 110	9 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMT	H	294	3/3	0.97	0.10	64,64,65,65	0
2	FMT	B	294	3/3	0.98	0.08	64,64,65,65	0
2	FMT	C	294	3/3	0.98	0.10	53,53,53,54	0
2	FMT	A	294	3/3	0.98	0.04	53,53,53,54	0
2	FMT	J	294	3/3	0.98	0.07	57,57,58,59	0
2	FMT	K	295	3/3	0.98	0.05	50,50,51,51	0
2	FMT	B	295	3/3	0.99	0.06	59,59,60,60	0
2	FMT	H	295	3/3	0.99	0.05	61,61,62,63	0
2	FMT	H	296	3/3	0.99	0.08	68,68,69,69	0
2	FMT	I	294	3/3	0.99	0.07	50,50,50,50	0
2	FMT	C	295	3/3	0.99	0.06	63,63,63,63	0
2	FMT	K	294	3/3	0.99	0.05	57,57,57,57	0
2	FMT	D	294	3/3	0.99	0.05	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.