Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:52 AM GMT

PDB ID	:	3Q7K
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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

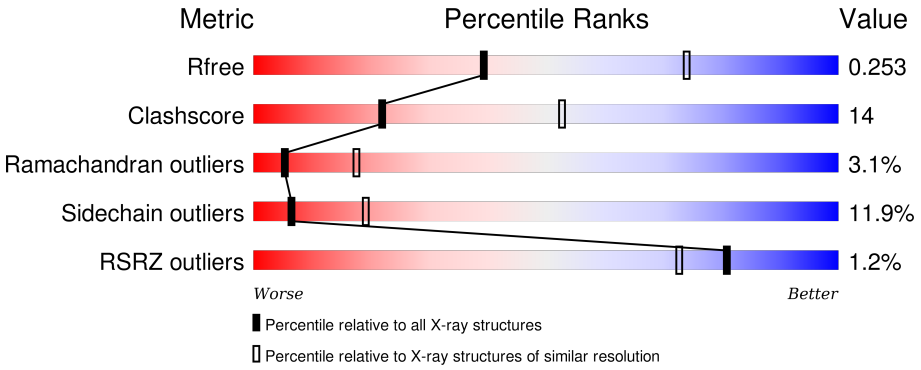
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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 <=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	68% 14% 6% 11%
1	B	293	65% 16% 15%
1	C	293	66% 18% 7% 8%
1	D	293	68% 14% 13%
1	E	293	61% 14% 21%

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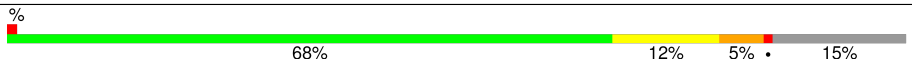
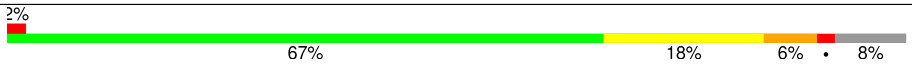
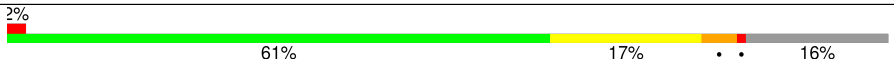
Mol	Chain	Length	Quality of chain
1	G	293	
1	H	293	
1	I	293	
1	J	293	
1	K	293	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMT	A	294	-	-	-	X
2	FMT	C	294	-	-	-	X
2	FMT	H	294	-	-	-	X
2	FMT	H	295	-	-	-	X

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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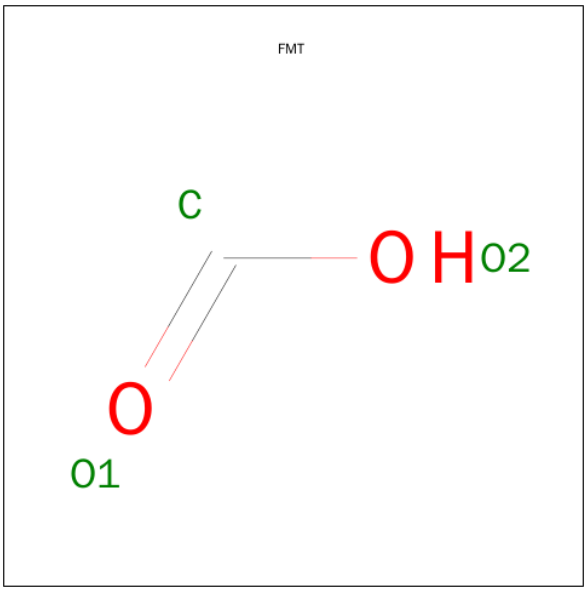
Chain	Residue	Modelled	Actual	Comment	Reference
H	289	HIS	-	EXPRESSION TAG	UNP Q8XF76
H	290	HIS	-	EXPRESSION TAG	UNP Q8XF76
H	291	HIS	-	EXPRESSION TAG	UNP Q8XF76
H	292	HIS	-	EXPRESSION TAG	UNP Q8XF76
H	293	HIS	-	EXPRESSION TAG	UNP Q8XF76
I	286	LEU	-	EXPRESSION TAG	UNP Q8XF76
I	287	GLU	-	EXPRESSION TAG	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 (three-letter code: FMT) (formula: CH_2O_2).



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.

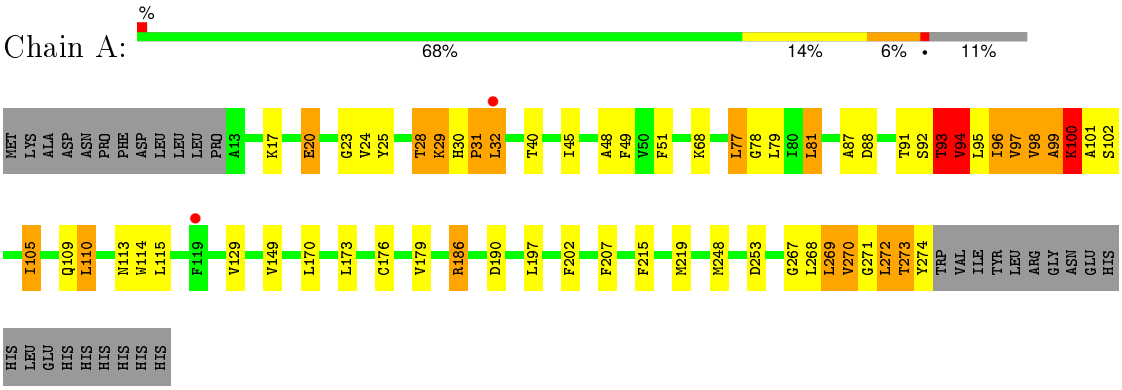
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	3	Total O 3 3	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	H	2	Total O 2 2	0	0
3	I	1	Total O 1 1	0	0
3	K	2	Total O 2 2	0	0

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 errors 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.

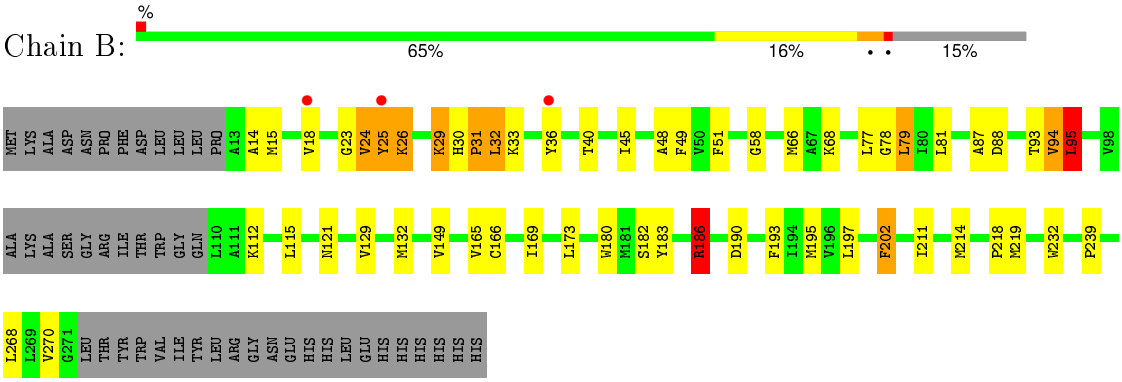
- Molecule 1: Probable formate transporter

Chain A:



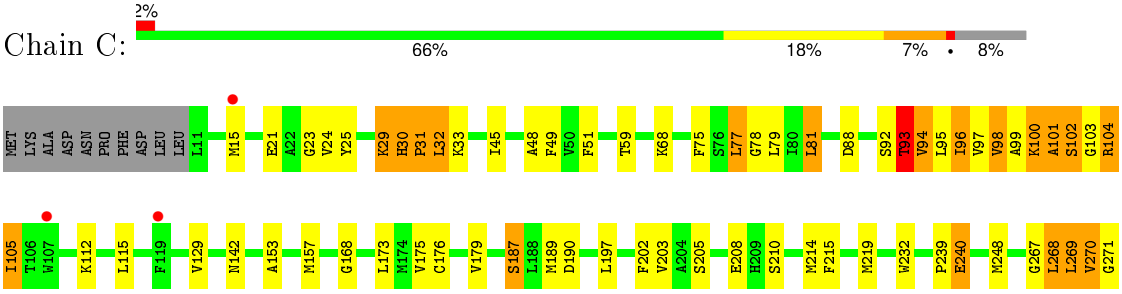
- Molecule 1: Probable formate transporter

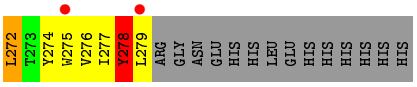
Chain B:



- Molecule 1: Probable formate transporter

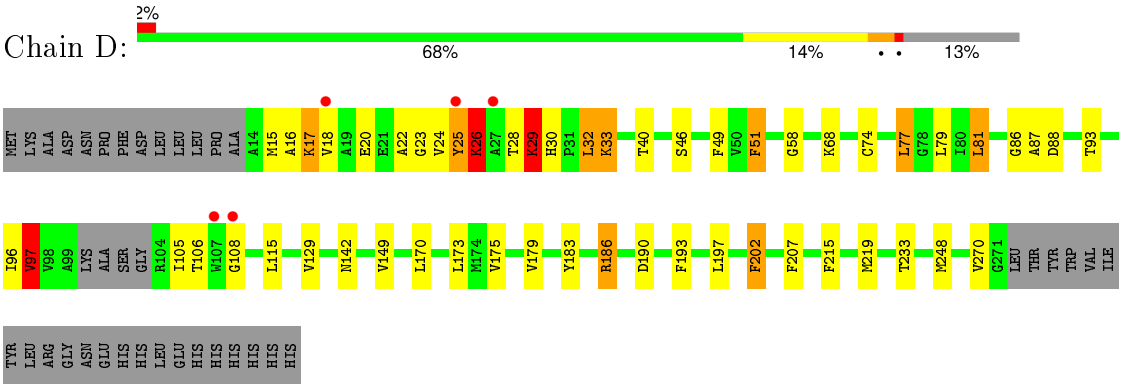
Chain C:





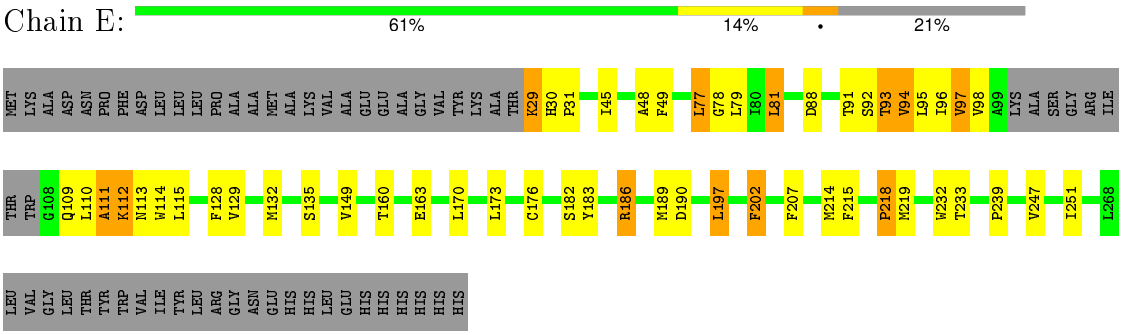
• Molecule 1: Probable formate transporter

Chain D:



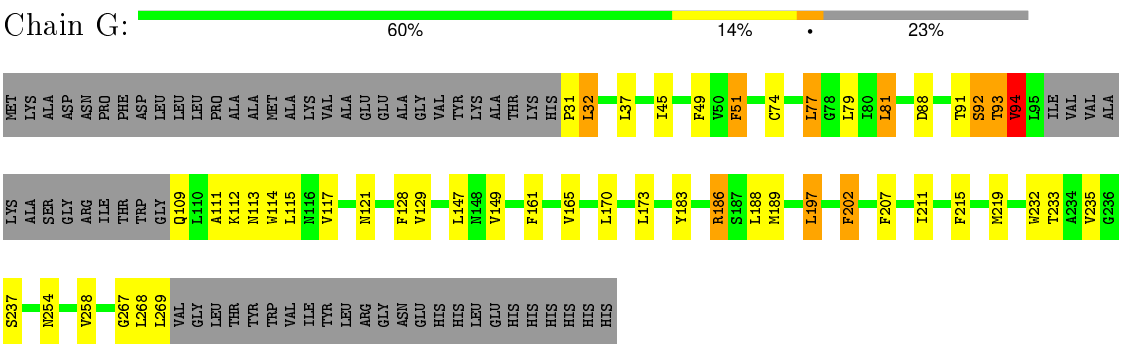
• Molecule 1: Probable formate transporter

Chain E:



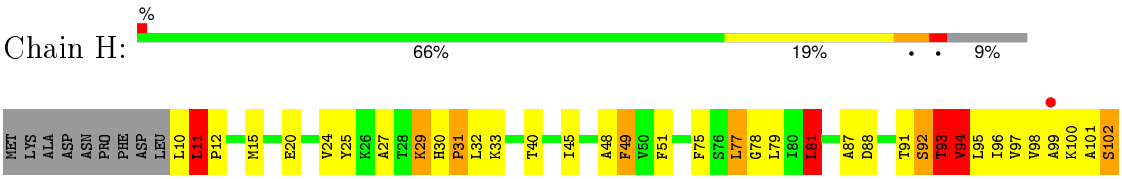
• Molecule 1: Probable formate transporter

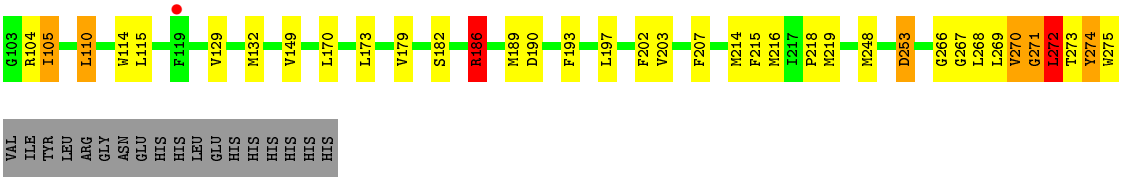
Chain G:



• Molecule 1: Probable formate transporter

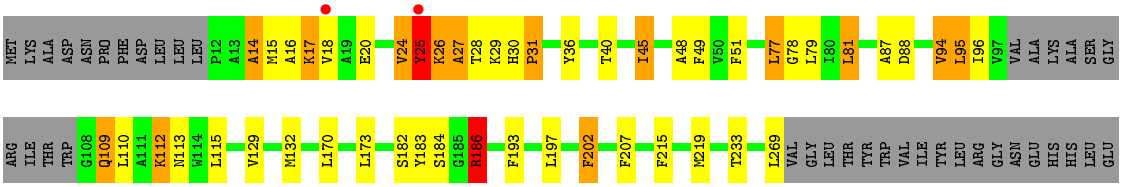
Chain H:





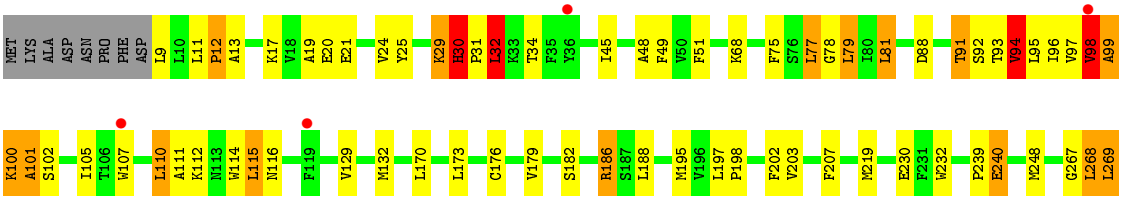
• Molecule 1: Probable formate transporter

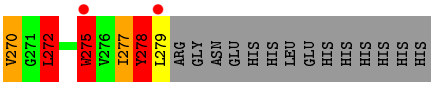
Chain I:



• Molecule 1: Probable formate transporter

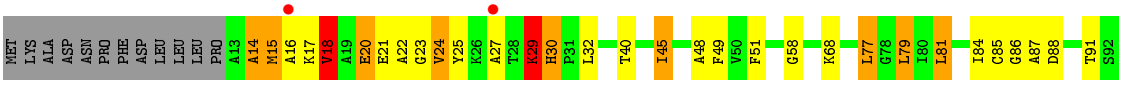
Chain J:





• Molecule 1: Probable formate transporter

Chain K:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.30%)	DCC
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 , 23.6	EDS
Estimated twinning fraction	0.439 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 92737 reflections	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.78	1/2028 (0.0%)	0.92	7/2758 (0.3%)
1	B	0.88	2/1915 (0.1%)	0.88	4/2603 (0.2%)
1	C	0.90	0/2096	0.87	4/2854 (0.1%)
1	D	0.91	2/1970 (0.1%)	0.91	5/2678 (0.2%)
1	E	0.86	0/1802	0.87	6/2450 (0.2%)
1	G	0.88	2/1759 (0.1%)	0.85	3/2391 (0.1%)
1	H	0.85	1/2068 (0.0%)	0.92	8/2815 (0.3%)
1	I	0.88	1/1918 (0.1%)	0.85	6/2606 (0.2%)
1	J	0.88	1/2112 (0.0%)	0.91	6/2876 (0.2%)
1	K	0.91	3/1909 (0.2%)	0.90	6/2594 (0.2%)
All	All	0.87	13/19577 (0.1%)	0.89	55/26625 (0.2%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	CYS	CB-SG	-6.31	1.71	1.82
1	D	193	PHE	CE1-CZ	5.94	1.48	1.37
1	K	21	GLU	CG-CD	5.66	1.60	1.51
1	K	193	PHE	CE1-CZ	5.62	1.48	1.37
1	D	186	ARG	CB-CG	5.40	1.67	1.52
1	G	183	TYR	CE2-CZ	5.32	1.45	1.38
1	H	193	PHE	CE1-CZ	5.26	1.47	1.37
1	A	94	VAL	CA-CB	5.25	1.65	1.54
1	I	193	PHE	CE1-CZ	5.14	1.47	1.37
1	K	166	CYS	CB-SG	-5.13	1.73	1.81
1	J	230	GLU	CG-CD	5.10	1.59	1.51
1	B	193	PHE	CE1-CZ	5.06	1.47	1.37
1	G	74	CYS	CB-SG	-5.03	1.73	1.81

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ARG	NE-CZ-NH1	16.03	128.31	120.30
1	A	186	ARG	NE-CZ-NH2	-14.70	112.95	120.30
1	D	186	ARG	NE-CZ-NH1	-12.86	113.87	120.30
1	D	186	ARG	NE-CZ-NH2	10.69	125.64	120.30
1	A	186	ARG	CD-NE-CZ	10.58	138.41	123.60
1	E	186	ARG	NE-CZ-NH1	-9.57	115.51	120.30
1	J	186	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	K	186	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	94	VAL	CB-CA-C	8.33	127.22	111.40
1	I	186	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	186	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	E	186	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	J	186	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	A	186	ARG	CG-CD-NE	7.39	127.31	111.80
1	D	186	ARG	CD-NE-CZ	7.35	133.89	123.60
1	H	186	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	H	94	VAL	CB-CA-C	6.77	124.27	111.40
1	G	32	LEU	CA-CB-CG	6.73	130.78	115.30
1	E	186	ARG	CD-NE-CZ	6.72	133.00	123.60
1	J	186	ARG	CD-NE-CZ	6.38	132.54	123.60
1	A	110	LEU	CA-CB-CG	6.38	129.97	115.30
1	G	186	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	190	ASP	CB-CG-OD1	6.12	123.81	118.30
1	E	45	ILE	CG1-CB-CG2	-5.98	98.25	111.40
1	H	11	LEU	CA-CB-CG	5.93	128.94	115.30
1	J	279	LEU	CA-CB-CG	5.93	128.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	190	ASP	CB-CG-OD1	5.75	123.47	118.30
1	H	81	LEU	CA-CB-CG	5.70	128.41	115.30
1	K	186	ARG	CG-CD-NE	5.63	123.62	111.80
1	H	102	SER	N-CA-C	-5.58	95.93	111.00
1	H	186	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	H	190	ASP	CB-CG-OD2	5.57	123.31	118.30
1	J	275	TRP	CA-CB-CG	5.53	124.21	113.70
1	C	279	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	186	ARG	CG-CD-NE	5.47	123.28	111.80
1	J	94	VAL	CB-CA-C	5.38	121.63	111.40
1	D	186	ARG	CG-CD-NE	-5.34	100.58	111.80
1	I	25	TYR	C-N-CA	5.31	134.98	121.70
1	C	101	ALA	N-CA-C	-5.29	96.70	111.00
1	K	186	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	G	92	SER	N-CA-CB	5.23	118.34	110.50
1	E	186	ARG	CG-CD-NE	-5.21	100.85	111.80
1	I	186	ARG	CD-NE-CZ	5.21	130.90	123.60
1	K	268	LEU	CA-CB-CG	5.20	127.27	115.30
1	D	29	LYS	N-CA-C	5.19	125.02	111.00
1	I	77	LEU	CB-CG-CD2	5.19	119.83	111.00
1	B	186	ARG	CD-NE-CZ	5.19	130.86	123.60
1	C	93	THR	N-CA-C	-5.18	97.02	111.00
1	H	253	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	95	LEU	N-CA-C	-5.16	97.08	111.00
1	I	81	LEU	CA-CB-CG	5.14	127.11	115.30
1	C	102	SER	N-CA-C	-5.12	97.17	111.00
1	K	197	LEU	CB-CG-CD1	5.11	119.68	111.00
1	K	186	ARG	CD-NE-CZ	5.08	130.71	123.60
1	I	186	ARG	CG-CD-NE	5.03	122.37	111.80

There are no chirality outliers.

All (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
1	C	101	ALA	Peptide
1	C	103	GLY	Peptide
1	C	93	THR	Peptide

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Mol	Chain	Res	Type	Group
1	D	17	LYS	Peptide
1	D	29	LYS	Peptide
1	D	97	VAL	Peptide
1	E	91	THR	Peptide
1	G	31	PRO	Peptide
1	G	91	THR	Peptide
1	H	93	THR	Peptide
1	H	94	VAL	Peptide
1	I	29	LYS	Peptide
1	J	30	HIS	Peptide
1	J	91	THR	Peptide
1	J	94	VAL	Peptide
1	J	98	VAL	Peptide
1	K	14	ALA	Peptide
1	K	17	LYS	Peptide
1	K	18	VAL	Peptide
1	K	24	VAL	Peptide
1	K	29	LYS	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	79	2
1	B	1870	0	1916	41	0
1	C	2043	0	2094	85	2
1	D	1923	0	1968	45	0
1	E	1758	0	1795	40	0
1	G	1716	0	1750	26	0
1	H	2016	0	2066	82	2
1	I	1872	0	1914	36	0
1	J	2059	0	2117	75	2
1	K	1864	0	1904	47	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	538	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 14.

All (538) 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
1:I:25:TYR:HB2	1:I:26:LYS:HB2	1.16	1.14
1:D:16:ALA:O	1:D:18:VAL:N	1.82	1.10
1:C:95:LEU:HD22	1:C:270:VAL:HG22	1.33	1.09
1:B:14:ALA:O	1:B:18:VAL:HG23	1.53	1.07
1:K:96:ILE:HD11	1:K:183:TYR:HE1	0.89	1.05
1:A:272:LEU:O	1:A:273:THR:HG22	1.59	1.02
1:A:96:ILE:HG22	1:A:97:VAL:H	1.19	1.02
1:H:99:ALA:HB2	1:H:270:VAL:HB	1.39	1.01
1:J:93:THR:HG23	1:J:95:LEU:HB3	1.37	1.00
1:J:91:THR:HA	1:J:94:VAL:HG22	1.44	0.99
1:I:25:TYR:HB2	1:I:26:LYS:CB	1.93	0.98
1:B:23:GLY:O	1:B:24:VAL:HG23	1.62	0.98
1:D:24:VAL:HG12	1:D:25:TYR:H	1.25	0.96
1:C:98:VAL:HG13	1:C:99:ALA:H	1.27	0.96
1:A:20:GLU:HG3	1:A:100:LYS:HB3	1.44	0.96
1:C:104:ARG:HH11	1:C:104:ARG:HG2	1.31	0.96
1:A:23:GLY:HA2	1:A:96:ILE:CG2	1.95	0.95
1:A:98:VAL:HG22	1:A:114:TRP:HZ2	1.25	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:THR:HA	1:D:96:ILE:HD13	1.46	0.94
1:K:96:ILE:CD1	1:K:183:TYR:HE1	1.78	0.94
1:B:24:VAL:HG12	1:B:25:TYR:H	1.31	0.94
1:C:274:TYR:HA	1:C:277:ILE:HG22	1.50	0.94
1:H:101:ALA:H	1:H:105:ILE:HG21	1.34	0.93
1:E:129:VAL:HA	1:E:219:MET:HE1	1.51	0.92
1:H:93:THR:HB	1:H:179:VAL:CG1	1.99	0.92
1:H:94:VAL:HG21	1:H:114:TRP:HE1	1.33	0.92
1:A:96:ILE:HG22	1:A:97:VAL:N	1.80	0.91
1:K:129:VAL:HA	1:K:219:MET:HE1	1.50	0.91
1:K:96:ILE:CD1	1:K:183:TYR:CE1	2.52	0.90
1:G:129:VAL:HA	1:G:219:MET:HE1	1.52	0.90
1:H:98:VAL:HG22	1:H:99:ALA:H	1.36	0.89
1:J:92:SER:HB2	1:J:176:CYS:SG	2.13	0.89
1:J:98:VAL:HG13	1:J:99:ALA:N	1.86	0.89
1:A:98:VAL:HG22	1:A:114:TRP:CZ2	2.08	0.89
1:H:93:THR:HB	1:H:179:VAL:HG11	1.52	0.89
1:E:109:GLN:O	1:E:112:LYS:HG2	1.73	0.88
1:H:92:SER:OG	1:H:93:THR:HA	1.72	0.88
1:A:94:VAL:HG21	1:A:114:TRP:HE1	1.40	0.86
1:A:99:ALA:O	1:A:100:LYS:HB2	1.72	0.86
1:K:15:MET:HG3	1:K:15:MET:O	1.74	0.86
1:G:92:SER:HA	1:G:93:THR:O	1.75	0.86
1:E:96:ILE:CG1	1:E:183:TYR:CE1	2.13	0.86
1:C:99:ALA:HB3	1:C:100:LYS:NZ	1.91	0.86
1:I:24:VAL:HG12	1:I:25:TYR:H	1.37	0.85
1:H:95:LEU:HD22	1:H:270:VAL:HG12	1.58	0.85
1:J:92:SER:HA	1:J:94:VAL:H	1.42	0.85
1:I:25:TYR:OH	1:I:183:TYR:HE2	1.59	0.84
1:B:95:LEU:HD23	1:B:180:TRP:HE3	1.42	0.84
1:B:24:VAL:CG1	1:B:25:TYR:H	1.89	0.84
1:D:129:VAL:HA	1:D:219:MET:HE1	1.60	0.84
1:A:91:THR:HA	1:A:94:VAL:HG22	1.60	0.84
1:A:93:THR:HB	1:A:179:VAL:CG1	2.08	0.83
1:D:24:VAL:HG13	1:D:86:GLY:HA3	1.58	0.83
1:C:93:THR:OG1	1:C:176:CYS:HA	1.78	0.83
1:H:267:GLY:O	1:H:270:VAL:HG22	1.78	0.82
1:J:129:VAL:HA	1:J:219:MET:HE1	1.60	0.82
1:J:99:ALA:HB1	1:J:270:VAL:CG1	2.07	0.82
1:C:93:THR:O	1:C:94:VAL:HG13	1.78	0.82
1:H:98:VAL:CG2	1:H:99:ALA:H	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:THR:HG23	1:H:95:LEU:HB3	1.61	0.81
1:C:129:VAL:HA	1:C:219:MET:HE1	1.62	0.81
1:D:96:ILE:H	1:D:96:ILE:HD12	1.46	0.81
1:A:30:HIS:HB3	1:A:31:PRO:HD2	1.63	0.80
1:I:25:TYR:HH	1:I:183:TYR:HE2	0.81	0.80
1:B:94:VAL:O	1:B:94:VAL:HG12	1.81	0.80
1:H:101:ALA:H	1:H:105:ILE:CG2	1.94	0.80
1:B:129:VAL:HA	1:B:219:MET:HE1	1.62	0.80
1:C:99:ALA:CB	1:C:100:LYS:NZ	2.45	0.79
1:J:98:VAL:HG13	1:J:99:ALA:H	1.45	0.79
1:A:93:THR:HG23	1:A:95:LEU:HB3	1.64	0.79
1:A:272:LEU:HD22	1:B:36:TYR:CE2	2.17	0.79
1:C:98:VAL:HG13	1:C:99:ALA:N	1.98	0.79
1:A:129:VAL:HA	1:A:219:MET:HE1	1.63	0.79
1:A:23:GLY:HA2	1:A:96:ILE:HG23	1.64	0.78
1:C:99:ALA:HB3	1:C:100:LYS:HZ1	1.49	0.78
1:B:31:PRO:O	1:B:33:LYS:N	2.16	0.78
1:C:98:VAL:CG1	1:C:99:ALA:H	1.96	0.77
1:A:93:THR:HB	1:A:179:VAL:HG11	1.65	0.77
1:J:99:ALA:HB2	1:J:270:VAL:HG21	1.67	0.77
1:C:270:VAL:O	1:C:272:LEU:N	2.14	0.76
1:A:23:GLY:CA	1:A:96:ILE:HG23	2.16	0.76
1:D:15:MET:O	1:D:15:MET:CG	2.30	0.76
1:D:15:MET:O	1:D:15:MET:HG3	1.84	0.76
1:D:24:VAL:O	1:D:25:TYR:HB2	1.84	0.75
1:H:98:VAL:HG22	1:H:99:ALA:N	2.02	0.75
1:A:20:GLU:HG3	1:A:100:LYS:CB	2.17	0.75
1:K:95:LEU:C	1:K:96:ILE:HD12	2.07	0.75
1:A:98:VAL:CG2	1:A:114:TRP:HZ2	2.00	0.74
1:D:29:LYS:H	1:D:29:LYS:HD3	1.51	0.74
1:A:92:SER:HA	1:A:94:VAL:N	2.03	0.74
1:H:11:LEU:HB3	1:H:12:PRO:HD2	1.69	0.74
1:H:99:ALA:HB3	1:H:100:LYS:HG2	1.68	0.74
1:A:95:LEU:O	1:A:99:ALA:HB3	1.88	0.73
1:H:93:THR:HG23	1:H:95:LEU:CB	2.17	0.73
1:B:24:VAL:HG12	1:B:25:TYR:N	2.02	0.73
1:D:24:VAL:HG12	1:D:25:TYR:N	2.02	0.73
1:J:92:SER:HA	1:J:94:VAL:N	2.04	0.73
1:C:99:ALA:O	1:C:100:LYS:HG2	1.87	0.73
1:C:95:LEU:CD2	1:C:270:VAL:HG22	2.16	0.73
1:H:270:VAL:CG2	1:H:271:GLY:H	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:16:ALA:O	1:K:18:VAL:HG12	1.89	0.73
1:D:29:LYS:N	1:D:29:LYS:HD3	2.02	0.73
1:C:95:LEU:HD11	1:C:269:LEU:HD13	1.69	0.72
1:G:92:SER:HA	1:G:93:THR:C	2.09	0.72
1:H:11:LEU:HB3	1:H:12:PRO:CD	2.18	0.72
1:H:92:SER:HA	1:H:94:VAL:N	2.05	0.71
1:J:92:SER:OG	1:J:93:THR:HA	1.89	0.71
1:J:272:LEU:HA	1:J:275:TRP:CD1	2.26	0.71
1:D:93:THR:CA	1:D:96:ILE:HD13	2.19	0.71
1:A:272:LEU:O	1:A:273:THR:CG2	2.37	0.70
1:C:95:LEU:HD22	1:C:270:VAL:CG2	2.17	0.70
1:A:99:ALA:O	1:A:100:LYS:CB	2.40	0.70
1:I:14:ALA:O	1:I:18:VAL:HG23	1.90	0.70
1:A:94:VAL:HB	1:A:97:VAL:HG13	1.73	0.69
1:I:129:VAL:HA	1:I:219:MET:HE1	1.73	0.69
1:G:129:VAL:HA	1:G:219:MET:CE	2.22	0.69
1:H:20:GLU:HG3	1:H:100:LYS:HB3	1.75	0.69
1:A:94:VAL:HG23	1:A:98:VAL:HG23	1.75	0.69
1:E:214:MET:O	1:E:218:PRO:HG2	1.92	0.69
1:J:92:SER:CB	1:J:176:CYS:SG	2.81	0.68
1:K:77:LEU:HD22	1:K:81:LEU:HD22	1.74	0.68
1:B:93:THR:O	1:B:94:VAL:HG23	1.93	0.68
1:I:186:ARG:HH11	1:I:186:ARG:HB2	1.58	0.68
1:J:77:LEU:HD22	1:J:81:LEU:HD22	1.75	0.68
1:C:99:ALA:O	1:C:100:LYS:CG	2.42	0.67
1:E:129:VAL:HA	1:E:219:MET:CE	2.23	0.67
1:A:99:ALA:O	1:A:100:LYS:HD2	1.93	0.67
1:A:93:THR:HG23	1:A:95:LEU:CB	2.25	0.67
1:E:77:LEU:HD22	1:E:81:LEU:HD22	1.77	0.67
1:I:24:VAL:HG12	1:I:25:TYR:N	2.09	0.66
1:J:100:LYS:HD2	1:J:100:LYS:N	2.10	0.66
1:A:270:VAL:O	1:A:272:LEU:O	2.14	0.66
1:D:24:VAL:HG13	1:D:86:GLY:CA	2.25	0.66
1:C:99:ALA:HB1	1:C:100:LYS:HZ3	1.60	0.66
1:I:25:TYR:HB3	1:I:26:LYS:HB2	1.72	0.66
1:C:270:VAL:C	1:C:272:LEU:H	1.98	0.66
1:A:95:LEU:HD23	1:A:269:LEU:HB3	1.76	0.66
1:H:92:SER:HA	1:H:94:VAL:H	1.61	0.66
1:H:104:ARG:O	1:H:105:ILE:HB	1.96	0.66
1:C:278:TYR:O	1:C:278:TYR:HD1	1.79	0.66
1:A:23:GLY:HA2	1:A:96:ILE:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:CG2	1:A:97:VAL:N	2.54	0.65
1:H:129:VAL:HA	1:H:219:MET:HE1	1.78	0.65
1:K:129:VAL:HA	1:K:219:MET:CE	2.23	0.65
1:C:100:LYS:N	1:C:100:LYS:HD3	2.11	0.65
1:J:129:VAL:HA	1:J:219:MET:CE	2.27	0.65
1:A:93:THR:HG23	1:A:95:LEU:H	1.62	0.64
1:A:92:SER:HA	1:A:94:VAL:H	1.62	0.64
1:I:40:THR:HG22	1:I:87:ALA:HB2	1.79	0.64
1:I:95:LEU:O	1:I:96:ILE:HD13	1.98	0.64
1:J:20:GLU:O	1:J:24:VAL:HG23	1.98	0.64
1:H:266:GLY:O	1:H:270:VAL:HG13	1.96	0.64
1:C:104:ARG:HH11	1:C:104:ARG:CG	2.08	0.64
1:A:129:VAL:HA	1:A:219:MET:CE	2.28	0.64
1:K:29:LYS:N	1:K:29:LYS:HD3	2.13	0.63
1:H:269:LEU:O	1:H:273:THR:HG23	1.99	0.63
1:C:129:VAL:HA	1:C:219:MET:CE	2.27	0.63
1:B:94:VAL:O	1:B:94:VAL:CG1	2.46	0.63
1:B:24:VAL:CG1	1:B:25:TYR:N	2.57	0.62
1:H:270:VAL:CG2	1:H:271:GLY:N	2.61	0.62
1:H:91:THR:O	1:H:92:SER:HB2	1.99	0.62
1:D:25:TYR:O	1:D:26:LYS:HB2	1.99	0.62
1:C:268:LEU:O	1:C:272:LEU:HB2	2.00	0.62
1:J:270:VAL:C	1:J:272:LEU:N	2.53	0.61
1:G:111:ALA:HA	1:G:114:TRP:HB2	1.82	0.61
1:C:21:GLU:O	1:C:24:VAL:HG22	2.01	0.61
1:J:232:TRP:CE2	1:J:239:PRO:HD3	2.35	0.61
1:E:96:ILE:HG12	1:E:183:TYR:CZ	2.18	0.61
1:D:22:ALA:O	1:D:24:VAL:O	2.18	0.61
1:I:129:VAL:HA	1:I:219:MET:CE	2.30	0.61
1:I:186:ARG:HH11	1:I:186:ARG:CB	2.14	0.61
1:H:98:VAL:C	1:H:100:LYS:H	2.04	0.60
1:B:129:VAL:HA	1:B:219:MET:CE	2.31	0.60
1:I:14:ALA:C	1:I:18:VAL:HG23	2.22	0.60
1:D:96:ILE:H	1:D:96:ILE:CD1	2.12	0.60
1:A:94:VAL:HG21	1:A:114:TRP:NE1	2.14	0.60
1:H:93:THR:C	1:H:95:LEU:H	2.04	0.60
1:J:272:LEU:HD22	1:J:275:TRP:HE1	1.67	0.60
1:C:276:VAL:HG13	1:D:33:LYS:HG2	1.84	0.60
1:C:93:THR:OG1	1:C:179:VAL:HB	2.01	0.60
1:C:104:ARG:NH1	1:C:104:ARG:HG2	2.11	0.59
1:D:129:VAL:HA	1:D:219:MET:CE	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:C	1:B:25:TYR:CD1	2.76	0.59
1:C:270:VAL:C	1:C:272:LEU:N	2.53	0.59
1:H:101:ALA:N	1:H:105:ILE:HG21	2.12	0.59
1:J:95:LEU:HD13	1:J:269:LEU:HD12	1.83	0.59
1:H:270:VAL:HG23	1:H:271:GLY:N	2.17	0.59
1:I:16:ALA:O	1:I:20:GLU:HG2	2.03	0.59
1:D:24:VAL:O	1:D:25:TYR:CB	2.50	0.59
1:B:95:LEU:HD23	1:B:180:TRP:CE3	2.30	0.59
1:H:272:LEU:HG	1:I:36:TYR:HE2	1.67	0.58
1:G:113:ASN:O	1:G:117:VAL:HG23	2.03	0.58
1:C:32:LEU:HD13	1:C:32:LEU:N	2.18	0.58
1:J:99:ALA:CB	1:J:270:VAL:HG11	2.14	0.58
1:H:274:TYR:O	1:H:275:TRP:HB2	2.03	0.58
1:J:98:VAL:HG22	1:J:99:ALA:H	1.68	0.58
1:A:30:HIS:HB3	1:A:31:PRO:CD	2.32	0.58
1:J:268:LEU:O	1:J:272:LEU:HB2	2.03	0.58
1:J:95:LEU:CD1	1:J:269:LEU:HD12	2.33	0.58
1:C:278:TYR:OH	1:D:32:LEU:CD1	2.51	0.58
1:E:96:ILE:CG2	1:E:183:TYR:CE1	2.87	0.58
1:K:95:LEU:O	1:K:96:ILE:HD12	2.03	0.58
1:H:149:VAL:HG11	1:H:219:MET:HG3	1.84	0.58
1:C:99:ALA:HB3	1:C:100:LYS:CE	2.32	0.58
1:C:99:ALA:CB	1:C:100:LYS:HZ1	2.11	0.57
1:A:20:GLU:HA	1:A:100:LYS:HB3	1.86	0.57
1:H:98:VAL:CG2	1:H:99:ALA:N	2.61	0.57
1:C:99:ALA:CB	1:C:100:LYS:HZ3	2.13	0.57
1:G:77:LEU:HD22	1:G:81:LEU:HD22	1.85	0.57
1:A:272:LEU:HD22	1:B:36:TYR:HE2	1.68	0.57
1:J:98:VAL:HG13	1:J:99:ALA:CB	2.33	0.57
1:C:99:ALA:HB1	1:C:100:LYS:NZ	2.18	0.57
1:A:91:THR:O	1:A:92:SER:HB2	2.05	0.57
1:J:29:LYS:O	1:J:30:HIS:O	2.23	0.57
1:A:267:GLY:O	1:A:270:VAL:N	2.36	0.57
1:A:92:SER:CA	1:A:94:VAL:H	2.17	0.57
1:J:270:VAL:C	1:J:272:LEU:H	2.07	0.56
1:D:93:THR:O	1:D:96:ILE:HB	2.04	0.56
1:E:96:ILE:HG21	1:E:183:TYR:CE1	2.40	0.56
1:J:19:ALA:HB1	1:J:100:LYS:HG3	1.87	0.56
1:J:95:LEU:CD1	1:J:269:LEU:CD1	2.83	0.56
1:B:95:LEU:CD2	1:B:180:TRP:HA	2.35	0.56
1:C:93:THR:CB	1:C:179:VAL:HB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:SER:H	1:C:190:ASP:HB2	1.70	0.56
1:A:24:VAL:HA	1:A:105:ILE:HD11	1.86	0.56
1:H:27:ALA:HB2	1:H:97:VAL:HG13	1.88	0.56
1:E:96:ILE:HD12	1:E:96:ILE:N	2.20	0.56
1:H:270:VAL:HG22	1:H:271:GLY:H	1.71	0.56
1:J:91:THR:O	1:J:92:SER:HB2	2.06	0.56
1:C:93:THR:HB	1:C:179:VAL:CG1	2.36	0.56
1:G:93:THR:OG1	1:G:94:VAL:N	2.39	0.55
1:I:202:PHE:CD1	1:I:202:PHE:C	2.79	0.55
1:H:129:VAL:HA	1:H:219:MET:CE	2.37	0.55
1:K:109:GLN:O	1:K:110:LEU:HB2	2.06	0.55
1:J:99:ALA:CB	1:J:270:VAL:HG21	2.36	0.55
1:E:95:LEU:HD12	1:E:176:CYS:HB3	1.87	0.55
1:B:48:ALA:HB2	1:B:78:GLY:HA3	1.89	0.55
1:E:96:ILE:CB	1:E:183:TYR:HE1	2.10	0.55
1:J:98:VAL:CG1	1:J:99:ALA:N	2.56	0.54
1:A:273:THR:HG23	1:A:274:TYR:CD2	2.41	0.54
1:H:77:LEU:HD22	1:H:81:LEU:HD22	1.87	0.54
1:A:77:LEU:HD22	1:A:81:LEU:HD22	1.88	0.54
1:J:101:ALA:O	1:J:105:ILE:HG22	2.07	0.54
1:B:23:GLY:O	1:B:24:VAL:CG2	2.46	0.54
1:J:92:SER:OG	1:J:93:THR:CA	2.55	0.54
1:I:17:LYS:HD2	1:I:17:LYS:C	2.28	0.54
1:B:214:MET:O	1:B:218:PRO:HG2	2.08	0.54
1:I:24:VAL:C	1:I:25:TYR:CD2	2.81	0.53
1:C:98:VAL:CG1	1:C:99:ALA:N	2.61	0.53
1:K:16:ALA:C	1:K:18:VAL:HG12	2.28	0.53
1:C:31:PRO:HB2	1:C:32:LEU:HD13	1.90	0.53
1:K:22:ALA:C	1:K:24:VAL:H	2.11	0.53
1:K:24:VAL:HG13	1:K:86:GLY:HA3	1.90	0.53
1:C:232:TRP:CE2	1:C:239:PRO:HD3	2.43	0.53
1:H:99:ALA:HB2	1:H:270:VAL:CB	2.26	0.53
1:C:274:TYR:C	1:C:276:VAL:H	2.11	0.53
1:B:190:ASP:OD1	1:C:189:MET:HB2	2.08	0.53
1:J:20:GLU:HG3	1:J:100:LYS:CB	2.39	0.53
1:D:24:VAL:CG1	1:D:25:TYR:H	2.10	0.53
1:E:92:SER:HA	1:E:93:THR:C	2.29	0.53
1:C:268:LEU:HD22	1:C:272:LEU:HD12	1.91	0.53
1:H:266:GLY:O	1:H:270:VAL:CG1	2.57	0.53
1:C:278:TYR:O	1:C:278:TYR:CD1	2.61	0.53
1:K:22:ALA:O	1:K:24:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HD22	1:C:81:LEU:HD22	1.89	0.53
1:A:92:SER:HB2	1:A:176:CYS:SG	2.49	0.52
1:C:95:LEU:HB3	1:C:270:VAL:CG1	2.39	0.52
1:A:95:LEU:CD2	1:A:269:LEU:HB3	2.39	0.52
1:J:269:LEU:HD13	1:J:269:LEU:O	2.08	0.52
1:C:274:TYR:C	1:C:276:VAL:N	2.63	0.52
1:C:29:LYS:O	1:C:30:HIS:O	2.27	0.52
1:J:101:ALA:O	1:J:105:ILE:CG2	2.57	0.52
1:E:110:LEU:O	1:E:112:LYS:N	2.43	0.52
1:C:48:ALA:HB2	1:C:78:GLY:HA3	1.90	0.52
1:E:96:ILE:C	1:E:98:VAL:H	2.13	0.52
1:A:99:ALA:C	1:A:100:LYS:HD2	2.30	0.52
1:A:272:LEU:HA	1:B:36:TYR:HE2	1.74	0.52
1:A:29:LYS:HG3	1:A:30:HIS:N	2.24	0.52
1:C:278:TYR:OH	1:D:32:LEU:HD12	2.10	0.52
1:D:40:THR:HG22	1:D:87:ALA:CB	2.40	0.52
1:D:30:HIS:NE2	1:D:32:LEU:HG	2.25	0.51
1:J:111:ALA:O	1:J:115:LEU:HB2	2.10	0.51
1:H:93:THR:O	1:H:93:THR:CG2	2.58	0.51
1:E:215:PHE:CZ	1:E:219:MET:HE3	2.45	0.51
1:E:109:GLN:HB3	1:E:112:LYS:HE2	1.92	0.51
1:H:11:LEU:CB	1:H:12:PRO:CD	2.87	0.51
1:H:186:ARG:HB2	1:H:186:ARG:HH11	1.76	0.51
1:D:18:VAL:HG12	1:D:18:VAL:O	2.11	0.51
1:C:95:LEU:HD13	1:C:270:VAL:HG13	1.93	0.51
1:K:170:LEU:HD13	1:K:207:PHE:CE1	2.46	0.51
1:J:267:GLY:O	1:J:270:VAL:HG23	2.11	0.51
1:H:93:THR:C	1:H:95:LEU:N	2.62	0.51
1:I:215:PHE:CZ	1:I:219:MET:HE3	2.45	0.51
1:H:11:LEU:CB	1:H:12:PRO:HD2	2.41	0.51
1:H:215:PHE:CZ	1:H:219:MET:HE3	2.46	0.50
1:K:24:VAL:HG13	1:K:86:GLY:CA	2.41	0.50
1:J:98:VAL:CG1	1:J:99:ALA:H	2.13	0.50
1:C:99:ALA:O	1:C:100:LYS:CB	2.58	0.50
1:C:95:LEU:O	1:C:96:ILE:C	2.49	0.50
1:C:98:VAL:C	1:C:99:ALA:O	2.42	0.50
1:K:58:GLY:H	2:K:294:FMT:H	1.77	0.50
1:J:97:VAL:O	1:J:101:ALA:HB3	2.12	0.50
1:A:93:THR:CG2	1:A:95:LEU:HB3	2.38	0.50
1:B:93:THR:O	1:B:94:VAL:CG2	2.59	0.50
1:D:40:THR:HG22	1:D:87:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:ILE:O	1:J:278:TYR:HB2	2.10	0.50
1:J:98:VAL:O	1:J:100:LYS:O	2.29	0.50
1:J:105:ILE:HG23	1:J:105:ILE:O	2.11	0.50
1:B:232:TRP:CE2	1:B:239:PRO:HD3	2.47	0.50
1:H:15:MET:SD	1:I:18:VAL:HG11	2.51	0.50
1:K:170:LEU:HB3	1:K:207:PHE:CD2	2.47	0.50
1:D:175:VAL:O	1:D:179:VAL:HG23	2.11	0.50
1:B:79:LEU:HD13	1:B:195:MET:SD	2.51	0.50
1:G:267:GLY:C	1:G:268:LEU:HD12	2.32	0.50
1:A:20:GLU:O	1:A:24:VAL:HG23	2.12	0.50
1:K:185:GLY:O	1:K:191:LYS:HE3	2.12	0.50
1:B:66:MET:HE2	1:C:59:THR:HG21	1.94	0.49
1:H:20:GLU:CG	1:H:100:LYS:HB3	2.42	0.49
1:J:93:THR:HB	1:J:179:VAL:HG11	1.93	0.49
1:K:215:PHE:CZ	1:K:219:MET:HE3	2.48	0.49
1:J:12:PRO:O	1:J:13:ALA:HB3	2.13	0.49
1:C:99:ALA:HB3	1:C:100:LYS:HE2	1.93	0.49
1:H:30:HIS:HB3	1:H:31:PRO:HD2	1.93	0.49
1:C:93:THR:HB	1:C:179:VAL:HB	1.94	0.49
1:K:30:HIS:CE1	1:K:32:LEU:HB3	2.48	0.49
1:G:129:VAL:CA	1:G:219:MET:HE1	2.36	0.49
1:C:93:THR:HA	1:C:176:CYS:SG	2.53	0.49
1:A:149:VAL:HG11	1:A:219:MET:HG3	1.94	0.49
1:B:165:VAL:O	1:B:169:ILE:HG13	2.12	0.49
1:I:25:TYR:HE1	1:I:183:TYR:OH	1.96	0.48
1:H:93:THR:O	1:H:93:THR:HG22	2.13	0.48
1:B:132:MET:HB2	1:B:219:MET:CE	2.43	0.48
1:J:48:ALA:HB2	1:J:78:GLY:HA3	1.94	0.48
1:H:272:LEU:HD23	1:H:273:THR:N	2.29	0.48
1:C:215:PHE:CZ	1:C:219:MET:HE3	2.48	0.48
1:H:105:ILE:HG23	1:H:105:ILE:O	2.14	0.48
1:D:58:GLY:H	2:D:294:FMT:H	1.78	0.48
1:I:215:PHE:CE1	1:I:219:MET:CE	2.96	0.48
1:D:149:VAL:HG11	1:D:219:MET:HG3	1.96	0.48
1:E:96:ILE:CB	1:E:183:TYR:CE1	2.93	0.48
1:J:112:LYS:O	1:J:116:ASN:HB2	2.13	0.48
1:C:267:GLY:O	1:C:270:VAL:HG23	2.13	0.48
1:H:270:VAL:HG23	1:H:271:GLY:H	1.72	0.48
1:G:197:LEU:HB3	1:H:77:LEU:HG	1.94	0.47
1:D:46:SER:OG	1:D:215:PHE:HB2	2.14	0.47
1:H:40:THR:HG22	1:H:87:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:THR:HG22	1:K:87:ALA:HB2	1.97	0.47
1:J:100:LYS:O	1:J:102:SER:N	2.48	0.47
1:A:92:SER:OG	1:A:93:THR:HA	2.15	0.47
1:A:93:THR:HB	1:A:179:VAL:HG12	1.94	0.47
1:J:75:PHE:CD2	1:J:203:VAL:HG21	2.49	0.47
1:I:26:LYS:NZ	1:I:113:ASN:OD1	2.47	0.47
1:A:96:ILE:O	1:A:97:VAL:C	2.53	0.47
1:C:23:GLY:HA2	1:C:96:ILE:HG23	1.96	0.47
1:A:272:LEU:O	1:A:273:THR:CB	2.63	0.47
1:D:24:VAL:CG1	1:D:86:GLY:CA	2.91	0.47
1:I:48:ALA:HB2	1:I:78:GLY:HA3	1.97	0.47
1:J:95:LEU:O	1:J:95:LEU:HD23	2.14	0.47
1:H:170:LEU:HB3	1:H:207:PHE:CD2	2.50	0.47
1:C:24:VAL:HG12	1:C:105:ILE:HD12	1.96	0.47
1:E:48:ALA:HB2	1:E:78:GLY:HA3	1.96	0.47
1:B:24:VAL:HA	1:B:25:TYR:CE1	2.49	0.46
1:B:93:THR:O	1:B:94:VAL:CB	2.63	0.46
1:K:18:VAL:H	1:K:20:GLU:H	1.63	0.46
1:C:96:ILE:HA	1:C:100:LYS:CG	2.46	0.46
1:K:68:LYS:HA	1:K:68:LYS:HD3	1.63	0.46
1:G:188:LEU:HD13	1:K:184:SER:HB2	1.97	0.46
1:D:215:PHE:CZ	1:D:219:MET:HE3	2.51	0.46
1:D:24:VAL:CG1	1:D:86:GLY:HA3	2.36	0.46
1:J:92:SER:CA	1:J:94:VAL:H	2.19	0.46
1:I:40:THR:HG22	1:I:87:ALA:CB	2.45	0.46
1:B:79:LEU:CD1	1:B:195:MET:SD	3.04	0.46
1:E:170:LEU:HD13	1:E:207:PHE:CE1	2.51	0.46
1:C:93:THR:HB	1:C:179:VAL:HG11	1.97	0.46
1:I:26:LYS:O	1:I:27:ALA:CB	2.63	0.46
1:A:92:SER:HA	1:A:93:THR:HA	1.45	0.46
1:K:14:ALA:O	1:K:15:MET:HB3	2.15	0.46
1:C:92:SER:HB3	1:C:175:VAL:HG11	1.98	0.46
1:B:40:THR:HG22	1:B:87:ALA:HB2	1.98	0.46
1:G:254:ASN:O	1:G:258:VAL:HG23	2.15	0.46
1:A:24:VAL:O	1:A:28:THR:HG22	2.15	0.46
1:J:94:VAL:HG23	1:J:114:TRP:HE1	1.80	0.46
1:A:29:LYS:HG3	1:A:30:HIS:H	1.81	0.46
1:A:272:LEU:HD13	1:A:273:THR:H	1.80	0.45
1:H:268:LEU:O	1:H:272:LEU:CB	2.64	0.45
1:A:48:ALA:HB2	1:A:78:GLY:HA3	1.98	0.45
1:J:179:VAL:O	1:J:182:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:MET:CG	1:K:15:MET:O	2.50	0.45
1:K:22:ALA:C	1:K:24:VAL:N	2.69	0.45
1:D:77:LEU:HD22	1:D:81:LEU:HD22	1.97	0.45
1:B:186:ARG:HB2	1:B:186:ARG:HH11	1.81	0.45
1:A:40:THR:HG22	1:A:87:ALA:HB2	1.98	0.45
1:A:23:GLY:CA	1:A:96:ILE:CG2	2.75	0.45
1:H:94:VAL:HG21	1:H:114:TRP:NE1	2.16	0.45
1:A:77:LEU:HG	1:E:197:LEU:HB3	1.98	0.45
1:J:20:GLU:HG3	1:J:100:LYS:HB3	1.99	0.45
1:J:93:THR:HB	1:J:179:VAL:CG1	2.47	0.45
1:H:268:LEU:O	1:H:272:LEU:HB3	2.16	0.45
1:D:29:LYS:CD	1:D:29:LYS:N	2.77	0.45
1:E:93:THR:OG1	1:E:94:VAL:N	2.49	0.45
1:B:29:LYS:HA	1:B:30:HIS:C	2.36	0.45
1:E:96:ILE:HG21	1:E:183:TYR:CZ	2.52	0.45
1:A:94:VAL:HG23	1:A:98:VAL:CG2	2.44	0.45
1:G:92:SER:OG	1:G:93:THR:HA	2.17	0.45
1:J:25:TYR:O	1:J:29:LYS:HB2	2.16	0.45
1:J:29:LYS:HB3	1:J:30:HIS:H	1.61	0.45
1:E:29:LYS:HE2	1:E:113:ASN:ND2	2.31	0.45
1:G:215:PHE:CZ	1:G:219:MET:HE3	2.52	0.45
1:J:105:ILE:HD13	1:J:110:LEU:HD23	1.99	0.45
1:E:160:THR:OG1	1:E:163:GLU:HG3	2.17	0.45
1:H:75:PHE:CG	1:H:203:VAL:HG21	2.51	0.45
1:H:214:MET:O	1:H:218:PRO:HG2	2.17	0.45
1:E:215:PHE:CE1	1:E:219:MET:CE	3.00	0.44
1:K:121:ASN:CB	1:K:211:ILE:HD12	2.47	0.44
1:D:25:TYR:HB3	1:D:26:LYS:H	1.70	0.44
1:G:149:VAL:HG11	1:G:219:MET:HG3	1.99	0.44
1:H:93:THR:HG23	1:H:95:LEU:H	1.82	0.44
1:J:272:LEU:HA	1:J:275:TRP:HD1	1.77	0.44
1:H:92:SER:OG	1:H:93:THR:CA	2.55	0.44
1:E:132:MET:HB2	1:E:219:MET:CE	2.47	0.44
1:E:97:VAL:HG12	1:E:97:VAL:O	2.17	0.44
1:C:95:LEU:HB3	1:C:270:VAL:HG11	2.00	0.44
1:C:95:LEU:HB3	1:C:270:VAL:HG13	1.99	0.44
1:J:79:LEU:HD13	1:J:195:MET:SD	2.58	0.43
1:C:274:TYR:O	1:C:276:VAL:N	2.51	0.43
1:G:129:VAL:HG22	1:G:219:MET:HE2	2.00	0.43
1:I:170:LEU:HB3	1:I:207:PHE:CD2	2.53	0.43
1:H:25:TYR:O	1:H:29:LYS:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:ILE:CG2	1:K:212:ALA:HA	2.48	0.43
1:J:98:VAL:HG22	1:J:99:ALA:N	2.33	0.43
1:J:95:LEU:CD1	1:J:269:LEU:HD13	2.48	0.43
1:H:132:MET:HB2	1:H:219:MET:HE1	2.00	0.43
1:B:202:PHE:CD1	1:B:202:PHE:C	2.90	0.43
1:D:170:LEU:HB3	1:D:207:PHE:CD2	2.54	0.43
1:J:100:LYS:O	1:J:101:ALA:C	2.57	0.43
1:J:170:LEU:HB3	1:J:207:PHE:CD2	2.54	0.43
1:A:267:GLY:C	1:A:269:LEU:N	2.72	0.43
1:E:247:VAL:O	1:E:251:ILE:HD12	2.18	0.43
1:E:30:HIS:HA	1:E:31:PRO:HD2	1.74	0.43
1:J:95:LEU:HD11	1:J:269:LEU:HD13	2.00	0.43
1:G:93:THR:O	1:G:94:VAL:HG13	2.18	0.43
1:K:84:ILE:HD12	1:K:188:LEU:HD12	2.01	0.43
1:H:48:ALA:HB2	1:H:78:GLY:HA3	2.01	0.43
1:C:269:LEU:O	1:C:269:LEU:HD22	2.19	0.43
1:K:81:LEU:O	1:K:85:CYS:HB2	2.18	0.43
1:D:97:VAL:CG1	1:D:97:VAL:O	2.67	0.43
1:E:129:VAL:HG22	1:E:219:MET:HE2	2.01	0.43
1:K:215:PHE:CE1	1:K:219:MET:CE	3.02	0.43
1:J:132:MET:HB2	1:J:219:MET:CE	2.48	0.43
1:B:132:MET:HB2	1:B:219:MET:HE1	2.00	0.43
1:K:91:THR:O	1:K:94:VAL:HG23	2.19	0.43
1:G:189:MET:HB2	1:K:190:ASP:OD1	2.19	0.42
1:A:25:TYR:O	1:A:29:LYS:HB2	2.18	0.42
1:H:110:LEU:C	1:H:110:LEU:HD13	2.39	0.42
1:C:219:MET:HB2	1:C:219:MET:HE2	1.89	0.42
1:D:29:LYS:CD	1:D:29:LYS:H	2.26	0.42
1:K:24:VAL:CG1	1:K:86:GLY:CA	2.97	0.42
1:H:186:ARG:CG	1:H:186:ARG:HH11	2.33	0.42
1:H:95:LEU:HD21	1:H:269:LEU:HD22	2.01	0.42
1:H:98:VAL:C	1:H:100:LYS:N	2.72	0.42
1:H:105:ILE:CG2	1:H:105:ILE:O	2.68	0.42
1:H:29:LYS:NZ	1:H:30:HIS:HB2	2.35	0.42
1:K:79:LEU:HD13	1:K:195:MET:SD	2.59	0.42
1:H:274:TYR:O	1:H:275:TRP:CB	2.67	0.42
1:H:110:LEU:HD13	1:H:110:LEU:O	2.19	0.42
1:D:51:PHE:CG	1:D:74:CYS:HB3	2.55	0.42
1:C:96:ILE:HA	1:C:100:LYS:HG3	2.02	0.42
1:H:269:LEU:O	1:H:269:LEU:HD23	2.20	0.42
1:I:132:MET:HB2	1:I:219:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:MET:O	1:J:198:PRO:HD2	2.20	0.42
1:A:93:THR:HG23	1:A:95:LEU:N	2.33	0.42
1:A:98:VAL:HB	1:A:99:ALA:H	1.58	0.42
1:J:93:THR:C	1:J:95:LEU:H	2.23	0.42
1:K:24:VAL:CG1	1:K:86:GLY:HA2	2.49	0.42
1:G:202:PHE:C	1:G:202:PHE:CD1	2.93	0.42
1:J:31:PRO:HB2	1:J:32:LEU:HG	2.02	0.42
1:I:17:LYS:C	1:I:17:LYS:CD	2.88	0.41
1:K:79:LEU:CD1	1:K:195:MET:SD	3.08	0.41
1:A:272:LEU:CD2	1:B:36:TYR:CE2	2.97	0.41
1:I:215:PHE:CE1	1:I:219:MET:HE2	2.55	0.41
1:C:32:LEU:CD1	1:C:32:LEU:N	2.83	0.41
1:C:142:ASN:HA	1:C:142:ASN:HD22	1.71	0.41
1:E:202:PHE:C	1:E:202:PHE:CD1	2.94	0.41
1:C:153:ALA:O	1:C:157:MET:HG2	2.20	0.41
1:C:100:LYS:N	1:C:100:LYS:CD	2.82	0.41
1:A:92:SER:CA	1:A:94:VAL:N	2.77	0.41
1:C:24:VAL:HA	1:C:105:ILE:CD1	2.51	0.41
1:J:32:LEU:C	1:J:34:THR:N	2.74	0.41
1:A:170:LEU:HB3	1:A:207:PHE:CD2	2.55	0.41
1:K:121:ASN:HB3	1:K:211:ILE:HD12	2.02	0.41
1:G:147:LEU:HD22	1:G:235:VAL:HB	2.02	0.41
1:H:24:VAL:HG22	1:H:104:ARG:O	2.20	0.41
1:A:31:PRO:HB2	1:A:32:LEU:HG	2.03	0.41
1:I:184:SER:HB2	1:J:188:LEU:HD13	2.02	0.41
1:A:272:LEU:HD13	1:A:273:THR:N	2.35	0.41
1:H:25:TYR:O	1:H:29:LYS:HB2	2.21	0.41
1:C:97:VAL:N	1:C:100:LYS:HG2	2.36	0.41
1:A:24:VAL:HG22	1:A:105:ILE:HD11	2.03	0.41
1:C:93:THR:HB	1:C:179:VAL:CB	2.51	0.41
1:B:149:VAL:HG11	1:B:219:MET:HG3	2.03	0.41
1:E:96:ILE:HD12	1:E:96:ILE:H	1.85	0.41
1:A:105:ILE:HA	1:A:109:GLN:OE1	2.21	0.41
1:H:104:ARG:O	1:H:105:ILE:CB	2.66	0.41
1:A:215:PHE:CZ	1:A:219:MET:HE3	2.55	0.41
1:H:29:LYS:HB3	1:H:30:HIS:H	1.53	0.41
1:G:232:TRP:HB3	1:G:237:SER:O	2.21	0.41
1:C:210:SER:O	1:C:214:MET:HG3	2.20	0.41
1:H:98:VAL:O	1:H:100:LYS:HG2	2.21	0.41
1:E:215:PHE:CZ	1:E:219:MET:CE	3.04	0.41
1:K:93:THR:O	1:K:94:VAL:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLY:HA2	1:C:208:GLU:O	2.21	0.41
1:G:161:PHE:O	1:G:165:VAL:HG23	2.21	0.41
1:K:149:VAL:HG11	1:K:219:MET:HG3	2.03	0.40
1:C:93:THR:H	1:C:179:VAL:HG21	1.86	0.40
1:I:30:HIS:HA	1:I:31:PRO:HD3	1.84	0.40
1:D:202:PHE:C	1:D:202:PHE:CD1	2.94	0.40
1:D:190:ASP:OD1	1:E:189:MET:HB2	2.21	0.40
1:A:270:VAL:HB	1:A:271:GLY:H	1.76	0.40
1:D:97:VAL:HG13	1:D:97:VAL:O	2.21	0.40
1:H:49:PHE:CG	1:H:216:MET:HE2	2.57	0.40
1:B:58:GLY:H	2:B:295:FMT:H	1.86	0.40
1:B:121:ASN:HB3	1:B:211:ILE:HD12	2.03	0.40
1:C:98:VAL:O	1:C:99:ALA:C	2.60	0.40
1:I:45:ILE:HA	1:I:45:ILE:HD12	1.84	0.40
1:G:121:ASN:HB3	1:G:211:ILE:HG23	2.03	0.40
1:G:51:PHE:CE1	1:K:201:MET:HA	2.56	0.40
1:E:232:TRP:CE2	1:E:239:PRO:HD3	2.57	0.40
1:E:111:ALA:HA	1:E:114:TRP:HB2	2.04	0.40
1:E:149:VAL:HG11	1:E:219:MET:HG3	2.03	0.40
1:J:195:MET:C	1:J:198:PRO:HD2	2.42	0.40
1:K:45:ILE:O	1:K:48:ALA:HB3	2.21	0.40
1:C:75:PHE:CD2	1:C:203:VAL:HG21	2.56	0.40
1:G:170:LEU:HB3	1:G:207:PHE:CD2	2.57	0.40

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%)	4 13
1	B	244/293 (83%)	224 (92%)	13 (5%)	7 (3%)	6 19
1	C	267/293 (91%)	239 (90%)	17 (6%)	11 (4%)	3 11
1	D	250/293 (85%)	230 (92%)	13 (5%)	7 (3%)	6 21
1	E	228/293 (78%)	212 (93%)	12 (5%)	4 (2%)	11 34
1	G	222/293 (76%)	212 (96%)	8 (4%)	2 (1%)	21 55
1	H	264/293 (90%)	243 (92%)	14 (5%)	7 (3%)	6 21
1	I	244/293 (83%)	228 (93%)	5 (2%)	11 (4%)	3 10
1	J	269/293 (92%)	232 (86%)	27 (10%)	10 (4%)	4 14
1	K	243/293 (83%)	222 (91%)	14 (6%)	7 (3%)	6 19
All	All	2491/2930 (85%)	2281 (92%)	134 (5%)	76 (3%)	5 17

All (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
1	A	270	VAL
1	B	24	VAL
1	B	32	LEU
1	B	94	VAL
1	C	15	MET
1	C	31	PRO
1	C	96	ILE
1	C	102	SER
1	C	278	TYR
1	D	17	LYS
1	D	25	TYR
1	D	26	LYS
1	D	28	THR
1	D	105	ILE
1	E	97	VAL
1	E	111	ALA
1	G	94	VAL

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Mol	Chain	Res	Type
1	H	11	LEU
1	H	31	PRO
1	H	102	SER
1	H	105	ILE
1	I	15	MET
1	I	24	VAL
1	J	30	HIS
1	J	32	LEU
1	J	98	VAL
1	J	99	ALA
1	J	101	ALA
1	J	278	TYR
1	K	15	MET
1	K	18	VAL
1	K	110	LEU
1	A	98	VAL
1	B	26	LYS
1	B	31	PRO
1	B	270	VAL
1	C	30	HIS
1	C	98	VAL
1	E	112	LYS
1	H	272	LEU
1	I	27	ALA
1	I	28	THR
1	I	94	VAL
1	J	12	PRO
1	K	23	GLY
1	K	27	ALA
1	A	105	ILE
1	A	268	LEU
1	B	29	LYS
1	C	29	LYS
1	E	94	VAL
1	H	29	LYS
1	I	109	GLN
1	A	99	ALA
1	C	271	GLY
1	C	272	LEU
1	G	93	THR
1	I	14	ALA
1	I	26	LYS

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Mol	Chain	Res	Type
1	K	95	LEU
1	C	275	TRP
1	H	271	GLY
1	I	110	LEU
1	I	112	LYS
1	J	272	LEU
1	J	107	TRP
1	D	23	GLY
1	K	96	ILE
1	D	108	GLY
1	I	31	PRO
1	J	94	VAL

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%)	182 (88%)	26 (12%)	6	17
1	B	198/237 (84%)	176 (89%)	22 (11%)	8	23
1	C	215/237 (91%)	186 (86%)	29 (14%)	5	14
1	D	203/237 (86%)	179 (88%)	24 (12%)	6	19
1	E	188/237 (79%)	171 (91%)	17 (9%)	12	34
1	G	184/237 (78%)	164 (89%)	20 (11%)	8	23
1	H	212/237 (90%)	186 (88%)	26 (12%)	6	18
1	I	198/237 (84%)	177 (89%)	21 (11%)	8	24
1	J	217/237 (92%)	185 (85%)	32 (15%)	4	11
1	K	197/237 (83%)	174 (88%)	23 (12%)	7	20
All	All	2020/2370 (85%)	1780 (88%)	240 (12%)	6	19

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS

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Mol	Chain	Res	Type
1	A	20	GLU
1	A	32	LEU
1	A	45	ILE
1	A	49	PHE
1	A	51	PHE
1	A	68	LYS
1	A	77	LEU
1	A	79	LEU
1	A	81	LEU
1	A	88	ASP
1	A	93	THR
1	A	94	VAL
1	A	100	LYS
1	A	102	SER
1	A	110	LEU
1	A	113	ASN
1	A	115	LEU
1	A	173	LEU
1	A	186	ARG
1	A	197	LEU
1	A	202	PHE
1	A	248	MET
1	A	269	LEU
1	A	272	LEU
1	A	273	THR
1	B	15	MET
1	B	25	TYR
1	B	26	LYS
1	B	32	LEU
1	B	45	ILE
1	B	49	PHE
1	B	51	PHE
1	B	68	LYS
1	B	77	LEU
1	B	79	LEU
1	B	81	LEU
1	B	88	ASP
1	B	95	LEU
1	B	112	LYS
1	B	115	LEU
1	B	173	LEU
1	B	182	SER

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Mol	Chain	Res	Type
1	B	183	TYR
1	B	186	ARG
1	B	197	LEU
1	B	202	PHE
1	B	268	LEU
1	C	25	TYR
1	C	32	LEU
1	C	33	LYS
1	C	45	ILE
1	C	49	PHE
1	C	51	PHE
1	C	68	LYS
1	C	77	LEU
1	C	79	LEU
1	C	81	LEU
1	C	88	ASP
1	C	93	THR
1	C	94	VAL
1	C	100	LYS
1	C	104	ARG
1	C	105	ILE
1	C	112	LYS
1	C	115	LEU
1	C	173	LEU
1	C	187	SER
1	C	197	LEU
1	C	202	PHE
1	C	205	SER
1	C	240	GLU
1	C	248	MET
1	C	268	LEU
1	C	269	LEU
1	C	270	VAL
1	C	278	TYR
1	D	20	GLU
1	D	26	LYS
1	D	29	LYS
1	D	32	LEU
1	D	33	LYS
1	D	49	PHE
1	D	51	PHE
1	D	68	LYS

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Mol	Chain	Res	Type
1	D	77	LEU
1	D	79	LEU
1	D	81	LEU
1	D	88	ASP
1	D	97	VAL
1	D	106	THR
1	D	115	LEU
1	D	142	ASN
1	D	173	LEU
1	D	183	TYR
1	D	186	ARG
1	D	197	LEU
1	D	202	PHE
1	D	233	THR
1	D	248	MET
1	D	270	VAL
1	E	29	LYS
1	E	49	PHE
1	E	77	LEU
1	E	79	LEU
1	E	81	LEU
1	E	88	ASP
1	E	93	THR
1	E	115	LEU
1	E	128	PHE
1	E	135	SER
1	E	173	LEU
1	E	182	SER
1	E	186	ARG
1	E	197	LEU
1	E	202	PHE
1	E	218	PRO
1	E	233	THR
1	G	32	LEU
1	G	37	LEU
1	G	45	ILE
1	G	49	PHE
1	G	51	PHE
1	G	77	LEU
1	G	79	LEU
1	G	81	LEU
1	G	88	ASP

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Mol	Chain	Res	Type
1	G	94	VAL
1	G	109	GLN
1	G	112	LYS
1	G	115	LEU
1	G	128	PHE
1	G	173	LEU
1	G	186	ARG
1	G	197	LEU
1	G	202	PHE
1	G	233	THR
1	G	269	LEU
1	H	10	LEU
1	H	32	LEU
1	H	33	LYS
1	H	45	ILE
1	H	49	PHE
1	H	51	PHE
1	H	77	LEU
1	H	79	LEU
1	H	81	LEU
1	H	88	ASP
1	H	92	SER
1	H	93	THR
1	H	94	VAL
1	H	96	ILE
1	H	110	LEU
1	H	115	LEU
1	H	173	LEU
1	H	182	SER
1	H	186	ARG
1	H	189	MET
1	H	197	LEU
1	H	202	PHE
1	H	248	MET
1	H	270	VAL
1	H	272	LEU
1	H	274	TYR
1	I	17	LYS
1	I	25	TYR
1	I	45	ILE
1	I	49	PHE
1	I	51	PHE

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Mol	Chain	Res	Type
1	I	77	LEU
1	I	79	LEU
1	I	81	LEU
1	I	88	ASP
1	I	94	VAL
1	I	95	LEU
1	I	109	GLN
1	I	112	LYS
1	I	115	LEU
1	I	173	LEU
1	I	182	SER
1	I	186	ARG
1	I	197	LEU
1	I	202	PHE
1	I	233	THR
1	I	269	LEU
1	J	9	LEU
1	J	11	LEU
1	J	17	LYS
1	J	21	GLU
1	J	29	LYS
1	J	32	LEU
1	J	45	ILE
1	J	49	PHE
1	J	51	PHE
1	J	68	LYS
1	J	77	LEU
1	J	79	LEU
1	J	81	LEU
1	J	88	ASP
1	J	94	VAL
1	J	96	ILE
1	J	100	LYS
1	J	110	LEU
1	J	115	LEU
1	J	173	LEU
1	J	186	ARG
1	J	197	LEU
1	J	202	PHE
1	J	240	GLU
1	J	248	MET
1	J	268	LEU

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Mol	Chain	Res	Type
1	J	269	LEU
1	J	270	VAL
1	J	272	LEU
1	J	275	TRP
1	J	277	ILE
1	J	278	TYR
1	K	20	GLU
1	K	25	TYR
1	K	29	LYS
1	K	30	HIS
1	K	45	ILE
1	K	49	PHE
1	K	51	PHE
1	K	77	LEU
1	K	79	LEU
1	K	81	LEU
1	K	88	ASP
1	K	95	LEU
1	K	97	VAL
1	K	98	VAL
1	K	110	LEU
1	K	112	LYS
1	K	115	LEU
1	K	142	ASN
1	K	173	LEU
1	K	186	ARG
1	K	197	LEU
1	K	202	PHE
1	K	233	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	151	GLN
1	B	142	ASN
1	B	151	GLN
1	B	158	HIS
1	C	142	ASN
1	C	151	GLN
1	C	158	HIS
1	D	142	ASN

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Mol	Chain	Res	Type
1	D	151	GLN
1	E	142	ASN
1	E	151	GLN
1	E	158	HIS
1	G	109	GLN
1	G	142	ASN
1	G	151	GLN
1	H	30	HIS
1	H	142	ASN
1	H	151	GLN
1	I	142	ASN
1	I	151	GLN
1	I	158	HIS
1	J	142	ASN
1	J	151	GLN
1	J	158	HIS
1	K	142	ASN
1	K	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	B	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	B	295	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	295	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	D	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	H	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	H	295	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	H	296	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	I	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	J	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	K	294	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	K	295	-	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMT	A	294	-	-	0/0/0/0	0/0/0/0
2	FMT	B	294	-	-	0/0/0/0	0/0/0/0
2	FMT	B	295	-	-	0/0/0/0	0/0/0/0
2	FMT	C	294	-	-	0/0/0/0	0/0/0/0
2	FMT	C	295	-	-	0/0/0/0	0/0/0/0
2	FMT	D	294	-	-	0/0/0/0	0/0/0/0
2	FMT	H	294	-	-	0/0/0/0	0/0/0/0
2	FMT	H	295	-	-	0/0/0/0	0/0/0/0
2	FMT	H	296	-	-	0/0/0/0	0/0/0/0
2	FMT	I	294	-	-	0/0/0/0	0/0/0/0
2	FMT	J	294	-	-	0/0/0/0	0/0/0/0
2	FMT	K	294	-	-	0/0/0/0	0/0/0/0
2	FMT	K	295	-	-	0/0/0/0	0/0/0/0

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	D	294	FMT	1	0
2	K	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

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, 95^{th} 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%)	-0.33	2 (0%) 87 81	31, 43, 76, 93	0
1	B	248/293 (84%)	-0.33	3 (1%) 81 73	31, 43, 77, 89	1 (0%)
1	C	269/293 (91%)	-0.28	5 (1%) 70 59	31, 44, 81, 92	1 (0%)
1	D	254/293 (86%)	-0.33	5 (1%) 68 58	31, 43, 84, 110	1 (0%)
1	E	232/293 (79%)	-0.46	0 100 100	31, 42, 72, 87	1 (0%)
1	G	226/293 (77%)	-0.46	0 100 100	31, 42, 66, 87	1 (0%)
1	H	266/293 (90%)	-0.35	2 (0%) 87 81	31, 44, 81, 100	1 (0%)
1	I	248/293 (84%)	-0.36	2 (0%) 87 81	31, 43, 77, 92	1 (0%)
1	J	271/293 (92%)	-0.23	6 (2%) 65 54	31, 44, 83, 96	1 (0%)
1	K	247/293 (84%)	-0.33	5 (2%) 68 58	31, 43, 75, 89	1 (0%)
All	All	2523/2930 (86%)	-0.34	30 (1%) 81 73	31, 43, 79, 110	9 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	107	TRP	5.6
1	H	99	ALA	4.8
1	J	36	TYR	4.7
1	B	25	TYR	4.4
1	K	16	ALA	3.9
1	J	275	TRP	3.8
1	C	275	TRP	3.6
1	K	112	LYS	3.3
1	C	107	TRP	3.3
1	J	107	TRP	3.3
1	C	119	PHE	3.1
1	I	18	VAL	3.0
1	J	119	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	25	TYR	2.7
1	J	279	LEU	2.7
1	H	119	PHE	2.6
1	D	108	GLY	2.6
1	J	98	VAL	2.5
1	A	32	LEU	2.5
1	C	279	LEU	2.4
1	D	18	VAL	2.4
1	C	15	MET	2.3
1	K	113	ASN	2.3
1	A	119	PHE	2.3
1	B	18	VAL	2.2
1	D	27	ALA	2.2
1	I	25	TYR	2.1
1	K	27	ALA	2.1
1	B	36	TYR	2.0
1	K	110	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	FMT	H	295	3/3	0.87	0.27	4.68	61,61,62,63	0
2	FMT	C	294	3/3	0.97	0.18	3.44	53,53,53,54	0
2	FMT	A	294	3/3	0.93	0.24	2.54	53,53,53,54	0
2	FMT	H	294	3/3	0.90	0.21	2.44	64,64,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FMT	K	294	3/3	0.92	0.21	1.99	57,57,57,57	0
2	FMT	B	295	3/3	0.92	0.17	1.63	59,59,60,60	0
2	FMT	C	295	3/3	0.88	0.17	1.53	63,63,63,63	0
2	FMT	B	294	3/3	0.86	0.17	1.46	64,64,65,65	0
2	FMT	J	294	3/3	0.86	0.16	0.47	57,57,58,59	0
2	FMT	D	294	3/3	0.94	0.13	-0.64	62,62,62,62	0
2	FMT	K	295	3/3	0.95	0.13	-1.03	50,50,51,51	0
2	FMT	I	294	3/3	0.94	0.12	-1.65	50,50,50,50	0
2	FMT	H	296	3/3	0.85	0.16	-	68,68,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.