wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 03:17 AM EDT

PDB ID	:	3Q6C
Title	:	X-ray crystal structure of duf2500 (pf10694) from klebsiella pneumoniae, northeast structural genomics consortium target kpr96
Authors	:	Seetharaman, J.; Su, M.; Wang, D.; Ciccosanti, C.; Sahdev, S.; Nair, R.; Rost, B.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-12-31
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

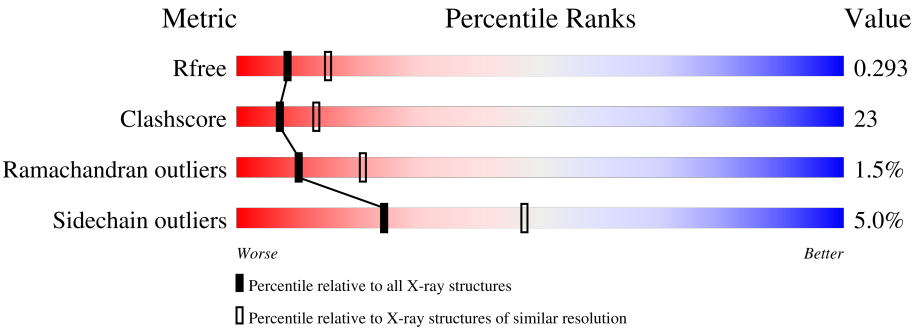
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	83	46% 31% • 20%
1	B	83	51% 27% • 19%
1	C	83	52% 25% • 19%
1	D	83	42% 37% • 19%
1	E	83	45% 29% • 23%
1	F	83	48% 31% • 19%

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Mol	Chain	Length	Quality of chain
1	G	83	48% 30% 19%
1	H	83	39% 40% 19%
1	I	83	45% 35% 6% 14%
1	J	83	41% 30% 6% 23%
1	K	83	42% 35% 22%
1	L	83	55% 20% 5% 19%
1	M	83	46% 33% 19%
1	N	83	41% 37% 20%
1	O	83	46% 35% 16%
1	P	83	37% 40% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8847 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 receptor YhhM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	Se	0	0	0
			527	336	94	95	2			
1	B	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	C	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	D	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	E	64	Total	C	N	O	Se	0	0	0
			515	330	91	92	2			
1	F	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	G	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	H	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	I	71	Total	C	N	O	Se	0	0	0
			576	363	106	105	2			
1	J	64	Total	C	N	O	Se	0	0	0
			510	327	91	90	2			
1	K	65	Total	C	N	O	Se	0	0	0
			519	332	92	93	2			
1	L	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	M	67	Total	C	N	O	Se	0	0	0
			531	338	95	96	2			
1	N	66	Total	C	N	O	Se	0	0	0
			526	335	94	95	2			
1	O	70	Total	C	N	O	Se	0	0	0
			558	352	102	102	2			
1	P	65	Total	C	N	O	Se	0	0	0
			485	310	85	88	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	LEU	-	EXPRESSION TAG	UNP D3RD65
B	120	LEU	-	EXPRESSION TAG	UNP D3RD65
C	120	LEU	-	EXPRESSION TAG	UNP D3RD65
D	120	LEU	-	EXPRESSION TAG	UNP D3RD65
E	120	LEU	-	EXPRESSION TAG	UNP D3RD65
F	120	LEU	-	EXPRESSION TAG	UNP D3RD65
G	120	LEU	-	EXPRESSION TAG	UNP D3RD65
H	120	LEU	-	EXPRESSION TAG	UNP D3RD65
I	120	LEU	-	EXPRESSION TAG	UNP D3RD65
J	120	LEU	-	EXPRESSION TAG	UNP D3RD65
K	120	LEU	-	EXPRESSION TAG	UNP D3RD65
L	120	LEU	-	EXPRESSION TAG	UNP D3RD65
M	120	LEU	-	EXPRESSION TAG	UNP D3RD65
N	120	LEU	-	EXPRESSION TAG	UNP D3RD65
O	120	LEU	-	EXPRESSION TAG	UNP D3RD65
P	120	LEU	-	EXPRESSION TAG	UNP D3RD65

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	27	Total O 27 27	0	0
2	C	19	Total O 19 19	0	0
2	D	23	Total O 23 23	0	0
2	E	22	Total O 22 22	0	0
2	F	21	Total O 21 21	0	0
2	G	19	Total O 19 19	0	0
2	H	23	Total O 23 23	0	0
2	I	29	Total O 29 29	0	0
2	J	28	Total O 28 28	0	0
2	K	25	Total O 25 25	0	0

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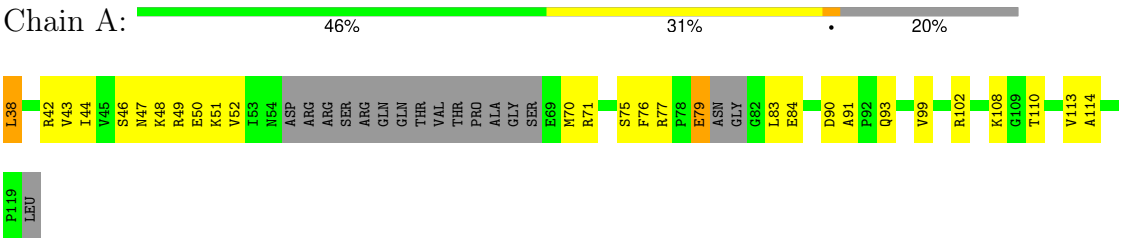
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	24	Total O 24 24	0	0
2	M	22	Total O 22 22	0	0
2	N	27	Total O 27 27	0	0
2	O	32	Total O 32 32	0	0
2	P	13	Total O 13 13	0	0

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. 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. 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.

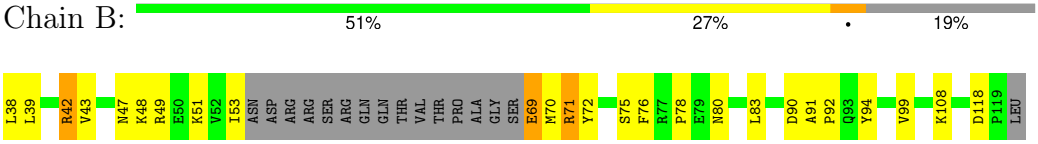
- Molecule 1: probable receptor YhhM

Chain A:



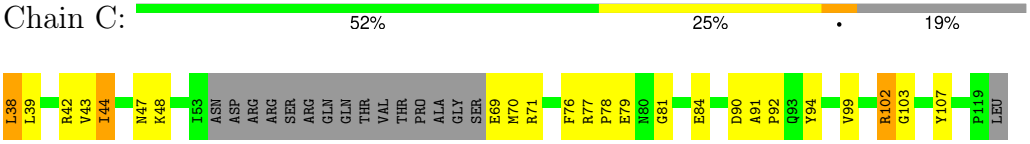
- Molecule 1: probable receptor YhhM

Chain B:



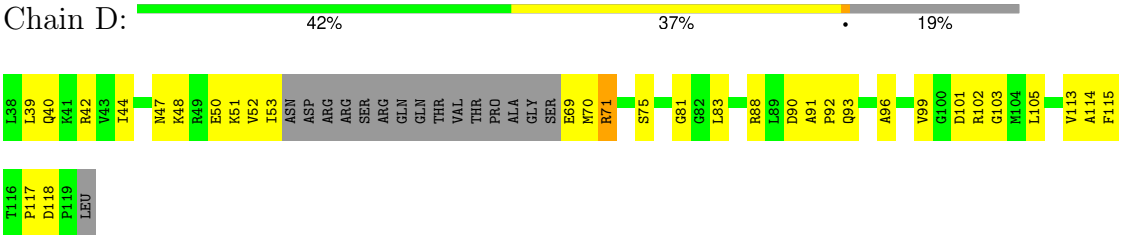
- Molecule 1: probable receptor YhhM

Chain C:



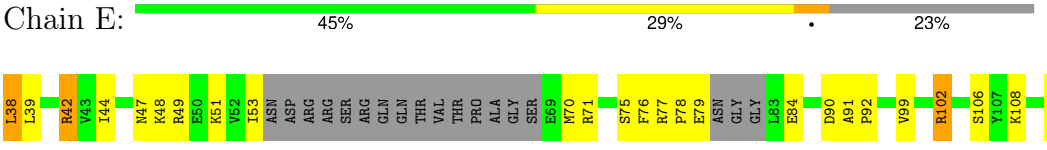
- Molecule 1: probable receptor YhhM

Chain D:



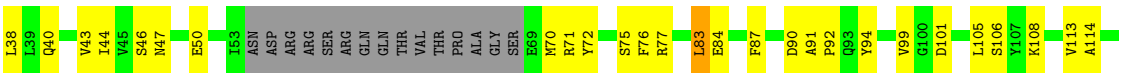
- Molecule 1: probable receptor YhhM

Chain E:



• Molecule 1: probable receptor YhhM

Chain F:

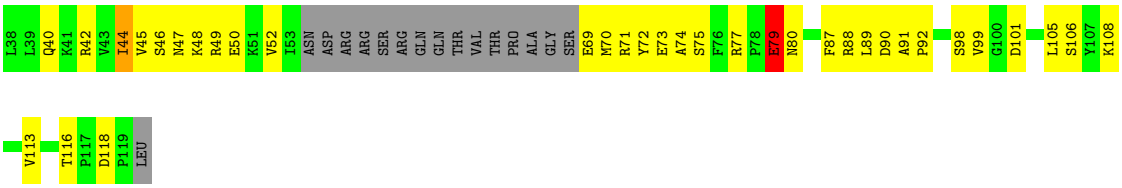


• Molecule 1: probable receptor YhhM

Chain G:

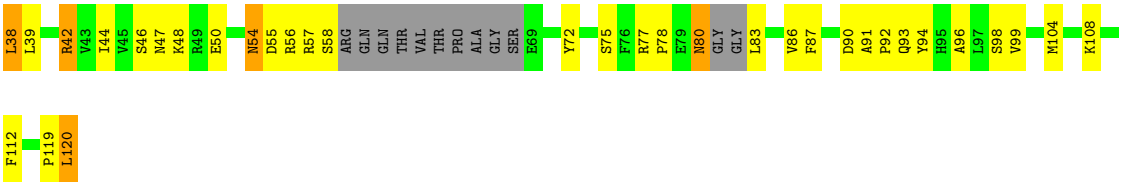
• Molecule 1: probable receptor YhhM

Chain H:



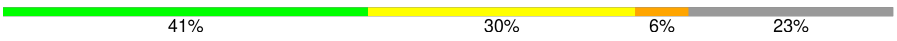
• Molecule 1: probable receptor YhhM

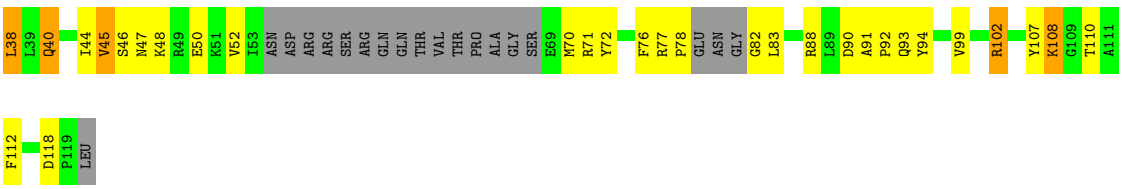
Chain I:



• Molecule 1: probable receptor YhhM

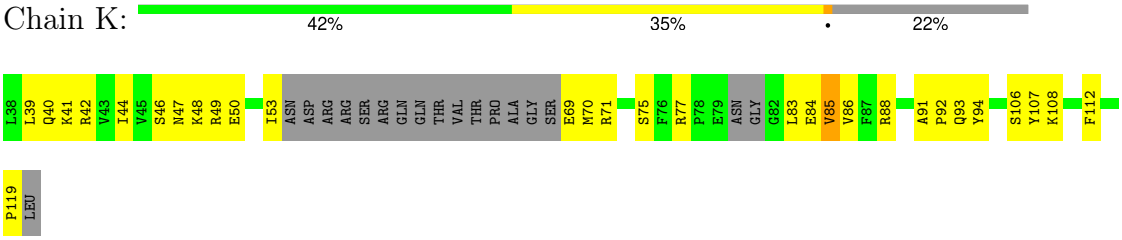
Chain J:





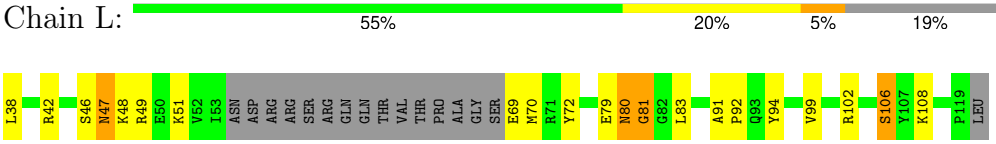
• Molecule 1: probable receptor YhhM

Chain K:



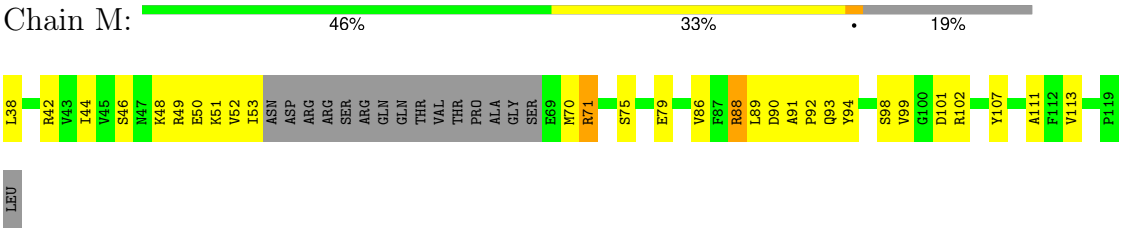
• Molecule 1: probable receptor YhhM

Chain L:



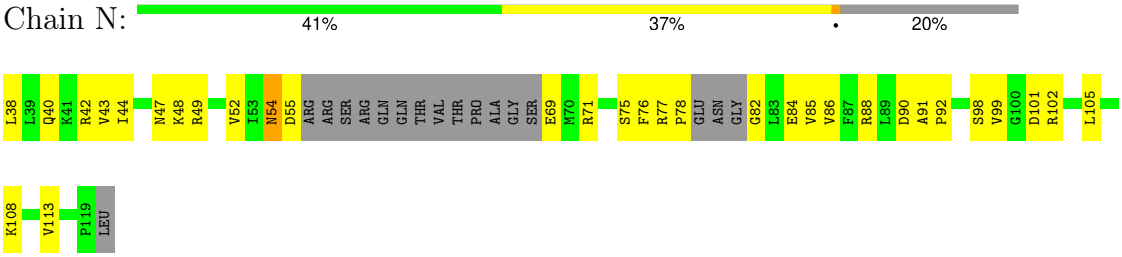
• Molecule 1: probable receptor YhhM

Chain M:



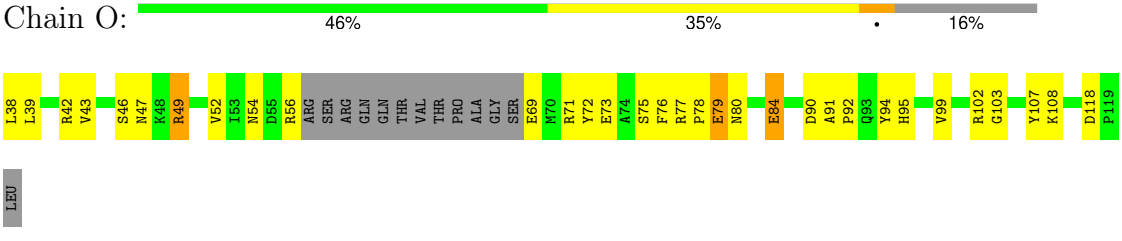
• Molecule 1: probable receptor YhhM

Chain N:



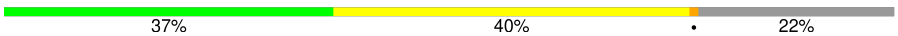
• Molecule 1: probable receptor YhhM

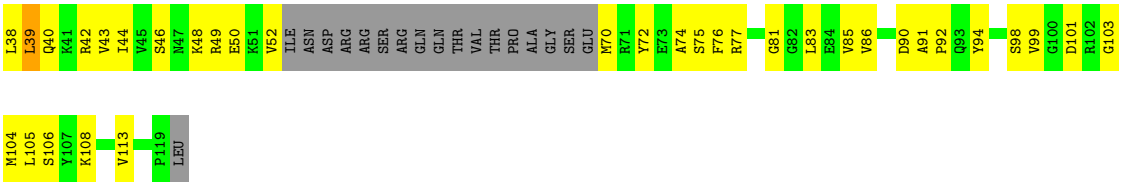
Chain O:



• Molecule 1: probable receptor YhhM

Chain P:




L38
L39
Q40
K41
R42
V43
I44
V45
S46
N47
K48
R49
E50
K51
V52
ILE
ASN
ASP
ARG
ARG
SER
ARG
GLN
GLN
THR
VAL
THR
PRO
ALA
GLY
SER
GLU
M70
R71
Y72
E73
A74
S75
F76
R77
G81
G82
L83
E84
V85
V86
D90
A91
P92
Q93
Y94
S98
V99
G100
D101
R102
G103
M104
L105
S106
Y107
K108
V113
P119
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.71Å 93.61Å 137.34Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	49.45 – 2.60 49.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	83.9 (49.45-2.60) 96.6 (49.45-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.284 0.287 , 0.293	Depositor DCC
R_{free} test set	3651 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	8847	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.61% 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, 0.333 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	0.41	0/534	0.65	0/712
1	B	0.40	0/539	0.66	0/720
1	C	0.38	0/539	0.65	0/720
1	D	0.40	0/539	0.66	0/720
1	E	0.39	0/522	0.64	0/696
1	F	0.40	0/539	0.66	0/720
1	G	0.39	0/539	0.62	0/720
1	H	0.37	0/539	0.60	0/720
1	I	0.41	0/583	0.66	0/776
1	J	0.42	0/517	0.64	0/689
1	K	0.38	0/526	0.66	0/701
1	L	0.39	0/539	0.66	0/720
1	M	0.39	0/539	0.65	0/720
1	N	0.39	0/533	0.63	0/711
1	O	0.39	0/566	0.64	0/756
1	P	0.33	0/493	0.55	0/664
All	All	0.39	0/8586	0.64	0/11465

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	527	0	525	31	0
1	B	531	0	529	23	0
1	C	531	0	529	25	0
1	D	531	0	529	33	0
1	E	515	0	516	21	0
1	F	531	0	529	25	0
1	G	531	0	529	23	0
1	H	531	0	529	35	1
1	I	576	0	574	37	0
1	J	510	0	513	35	0
1	K	519	0	519	28	0
1	L	531	0	529	20	0
1	M	531	0	529	31	0
1	N	526	0	523	30	1
1	O	558	0	552	21	0
1	P	485	0	465	25	0
2	A	29	0	0	0	0
2	B	27	0	0	2	0
2	C	19	0	0	1	0
2	D	23	0	0	4	0
2	E	22	0	0	0	0
2	F	21	0	0	1	0
2	G	19	0	0	1	0
2	H	23	0	0	2	0
2	I	29	0	0	2	0
2	J	28	0	0	2	0
2	K	25	0	0	3	0
2	L	24	0	0	2	0
2	M	22	0	0	0	0
2	N	27	0	0	1	0
2	O	32	0	0	3	0
2	P	13	0	0	1	0
All	All	8847	0	8419	383	1

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 23.

The worst 5 of 383 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:MSE:HE1	1:F:99:VAL:HB	1.32	1.10
1:I:42:ARG:HH11	1:I:42:ARG:HB3	1.18	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:51:LYS:HE3	1:M:71:ARG:NH1	1.82	0.93
1:K:50:GLU:HG2	1:N:99:VAL:HG21	1.52	0.92
1:D:99:VAL:HB	1:G:70:MSE:HE1	1.53	0.91

All (1) 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:H:116:THR:OG1	1:N:113:VAL:O[2_647]	1.98	0.22

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	60/83 (72%)	55 (92%)	4 (7%)	1 (2%)	9 18
1	B	63/83 (76%)	59 (94%)	3 (5%)	1 (2%)	9 19
1	C	63/83 (76%)	61 (97%)	2 (3%)	0	100 100
1	D	63/83 (76%)	58 (92%)	4 (6%)	1 (2%)	9 19
1	E	58/83 (70%)	56 (97%)	1 (2%)	1 (2%)	9 18
1	F	63/83 (76%)	57 (90%)	5 (8%)	1 (2%)	9 19
1	G	63/83 (76%)	57 (90%)	5 (8%)	1 (2%)	9 19
1	H	63/83 (76%)	59 (94%)	3 (5%)	1 (2%)	9 19
1	I	65/83 (78%)	59 (91%)	6 (9%)	0	100 100
1	J	58/83 (70%)	54 (93%)	2 (3%)	2 (3%)	3 5
1	K	59/83 (71%)	54 (92%)	4 (7%)	1 (2%)	9 18
1	L	63/83 (76%)	58 (92%)	3 (5%)	2 (3%)	4 6
1	M	63/83 (76%)	61 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	60/83 (72%)	56 (93%)	4 (7%)	0	100 100
1	O	66/83 (80%)	60 (91%)	5 (8%)	1 (2%)	10 21
1	P	61/83 (74%)	52 (85%)	7 (12%)	2 (3%)	4 6
All	All	991/1328 (75%)	916 (92%)	60 (6%)	15 (2%)	10 21

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	B	83	LEU
1	F	83	LEU
1	G	83	LEU
1	K	83	LEU

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	56/69 (81%)	53 (95%)	3 (5%)	22 44
1	B	56/69 (81%)	53 (95%)	3 (5%)	22 44
1	C	56/69 (81%)	53 (95%)	3 (5%)	22 44
1	D	56/69 (81%)	55 (98%)	1 (2%)	59 80
1	E	55/69 (80%)	51 (93%)	4 (7%)	14 28
1	F	56/69 (81%)	56 (100%)	0	100 100
1	G	56/69 (81%)	53 (95%)	3 (5%)	22 44
1	H	56/69 (81%)	54 (96%)	2 (4%)	35 61
1	I	62/69 (90%)	56 (90%)	6 (10%)	8 15
1	J	54/69 (78%)	50 (93%)	4 (7%)	13 28
1	K	55/69 (80%)	53 (96%)	2 (4%)	35 61
1	L	56/69 (81%)	53 (95%)	3 (5%)	22 44
1	M	56/69 (81%)	52 (93%)	4 (7%)	14 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	56/69 (81%)	54 (96%)	2 (4%)	35 61
1	O	59/69 (86%)	55 (93%)	4 (7%)	16 32
1	P	48/69 (70%)	47 (98%)	1 (2%)	53 77
All	All	893/1104 (81%)	848 (95%)	45 (5%)	24 47

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	102	ARG
1	M	71	ARG
1	K	85	VAL
1	L	80	ASN
1	M	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	40	GLN
1	K	40	GLN
1	N	54	ASN
1	L	47	ASN
1	N	40	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.