



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:37 PM GMT

PDB ID : 4P5H
Title : Structure of Clostridium perfringens Enterotoxin with a peptide derived from a modified version of ECL-2 of Claudin 2
Authors : Naylor, C.E.; Yelland, T.S.; Basak, A.K.
Deposited on : 2014-03-17
Resolution : 3.38 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

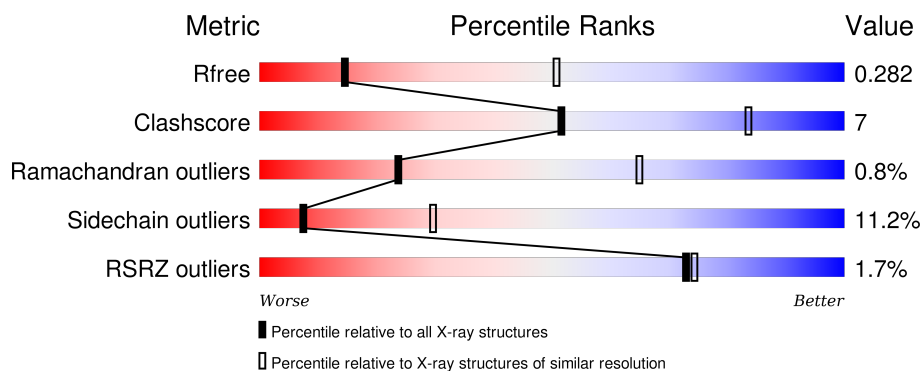
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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.















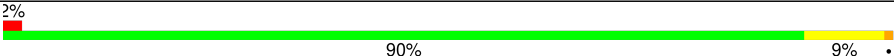
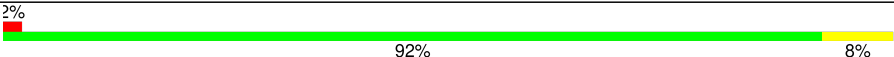
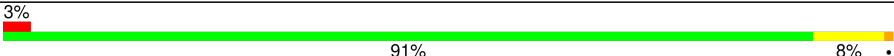

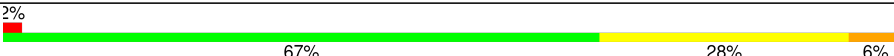
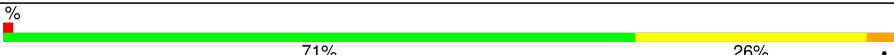
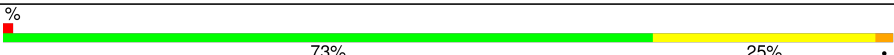
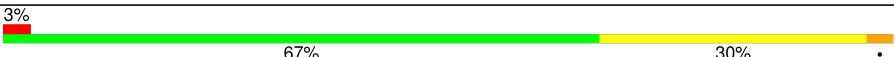
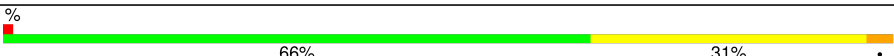



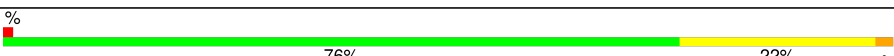
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	20	
1	2	20	
1	3	20	
1	4	20	
1	P	20	

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Mol	Chain	Length	Quality of chain
1	Q	20	
1	R	20	
1	S	20	
1	T	20	
1	U	20	
1	V	20	
1	W	20	
1	X	20	
1	Y	20	
1	Z	20	
2	A	286	
2	B	286	
2	C	286	
2	D	286	
2	E	286	
2	F	286	
2	G	286	
2	H	286	
2	I	286	
2	J	286	
2	K	286	
2	L	286	
2	M	286	
2	N	286	
2	O	286	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34251 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 Claudin-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	1	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	2	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	3	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	4	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	P	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	Q	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	R	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	S	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	T	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	U	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	V	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	W	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	X	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	Y	9	Total	C	N	O	0	0	0
			60	38	10	12			
1	Z	9	Total	C	N	O	0	0	0
			60	38	10	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	149	ASN	SER	engineered mutation	UNP O88552
1	155	ALA	SER	engineered mutation	UNP O88552
2	149	ASN	SER	engineered mutation	UNP O88552
2	155	ALA	SER	engineered mutation	UNP O88552
3	149	ASN	SER	engineered mutation	UNP O88552
3	155	ALA	SER	engineered mutation	UNP O88552
4	149	ASN	SER	engineered mutation	UNP O88552
4	155	ALA	SER	engineered mutation	UNP O88552
P	149	ASN	SER	engineered mutation	UNP O88552
P	155	ALA	SER	engineered mutation	UNP O88552
Q	149	ASN	SER	engineered mutation	UNP O88552
Q	155	ALA	SER	engineered mutation	UNP O88552
R	149	ASN	SER	engineered mutation	UNP O88552
R	155	ALA	SER	engineered mutation	UNP O88552
S	149	ASN	SER	engineered mutation	UNP O88552
S	155	ALA	SER	engineered mutation	UNP O88552
T	149	ASN	SER	engineered mutation	UNP O88552
T	155	ALA	SER	engineered mutation	UNP O88552
U	149	ASN	SER	engineered mutation	UNP O88552
U	155	ALA	SER	engineered mutation	UNP O88552
V	149	ASN	SER	engineered mutation	UNP O88552
V	155	ALA	SER	engineered mutation	UNP O88552
W	149	ASN	SER	engineered mutation	UNP O88552
W	155	ALA	SER	engineered mutation	UNP O88552
X	149	ASN	SER	engineered mutation	UNP O88552
X	155	ALA	SER	engineered mutation	UNP O88552
Y	149	ASN	SER	engineered mutation	UNP O88552
Y	155	ALA	SER	engineered mutation	UNP O88552
Z	149	ASN	SER	engineered mutation	UNP O88552
Z	155	ALA	SER	engineered mutation	UNP O88552

- Molecule 2 is a protein called Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	B	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	C	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	D	286	Total	C	N	O	S	0	4	0
			2229	1413	360	452	4			
2	E	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	G	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	H	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	I	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	J	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	K	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	L	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	M	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	N	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			
2	O	286	Total	C	N	O	S	0	4	0
			2223	1410	357	452	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP P01558
A	35	ALA	-	expression tag	UNP P01558
A	36	MET	-	expression tag	UNP P01558
A	37	GLY	-	expression tag	UNP P01558
B	34	GLY	-	expression tag	UNP P01558
B	35	ALA	-	expression tag	UNP P01558
B	36	MET	-	expression tag	UNP P01558
B	37	GLY	-	expression tag	UNP P01558
C	34	GLY	-	expression tag	UNP P01558
C	35	ALA	-	expression tag	UNP P01558
C	36	MET	-	expression tag	UNP P01558
C	37	GLY	-	expression tag	UNP P01558
D	34	GLY	-	expression tag	UNP P01558
D	35	ALA	-	expression tag	UNP P01558
D	36	MET	-	expression tag	UNP P01558
D	37	GLY	-	expression tag	UNP P01558
E	34	GLY	-	expression tag	UNP P01558
E	35	ALA	-	expression tag	UNP P01558
E	36	MET	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
E	37	GLY	-	expression tag	UNP P01558
F	34	GLY	-	expression tag	UNP P01558
F	35	ALA	-	expression tag	UNP P01558
F	36	MET	-	expression tag	UNP P01558
F	37	GLY	-	expression tag	UNP P01558
G	34	GLY	-	expression tag	UNP P01558
G	35	ALA	-	expression tag	UNP P01558
G	36	MET	-	expression tag	UNP P01558
G	37	GLY	-	expression tag	UNP P01558
H	34	GLY	-	expression tag	UNP P01558
H	35	ALA	-	expression tag	UNP P01558
H	36	MET	-	expression tag	UNP P01558
H	37	GLY	-	expression tag	UNP P01558
I	34	GLY	-	expression tag	UNP P01558
I	35	ALA	-	expression tag	UNP P01558
I	36	MET	-	expression tag	UNP P01558
I	37	GLY	-	expression tag	UNP P01558
J	34	GLY	-	expression tag	UNP P01558
J	35	ALA	-	expression tag	UNP P01558
J	36	MET	-	expression tag	UNP P01558
J	37	GLY	-	expression tag	UNP P01558
K	34	GLY	-	expression tag	UNP P01558
K	35	ALA	-	expression tag	UNP P01558
K	36	MET	-	expression tag	UNP P01558
K	37	GLY	-	expression tag	UNP P01558
L	34	GLY	-	expression tag	UNP P01558
L	35	ALA	-	expression tag	UNP P01558
L	36	MET	-	expression tag	UNP P01558
L	37	GLY	-	expression tag	UNP P01558
M	34	GLY	-	expression tag	UNP P01558
M	35	ALA	-	expression tag	UNP P01558
M	36	MET	-	expression tag	UNP P01558
M	37	GLY	-	expression tag	UNP P01558
N	34	GLY	-	expression tag	UNP P01558
N	35	ALA	-	expression tag	UNP P01558
N	36	MET	-	expression tag	UNP P01558
N	37	GLY	-	expression tag	UNP P01558
O	34	GLY	-	expression tag	UNP P01558
O	35	ALA	-	expression tag	UNP P01558
O	36	MET	-	expression tag	UNP P01558
O	37	GLY	-	expression tag	UNP P01558

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: Claudin-2

Chain 1: 




- Molecule 1: Claudin-2

Chain 2: 




- Molecule 1: Claudin-2

Chain 3: 



- Molecule 1: Claudin-2

Chain 4: 




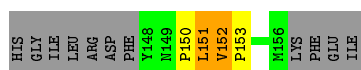
- Molecule 1: Claudin-2

Chain P: 

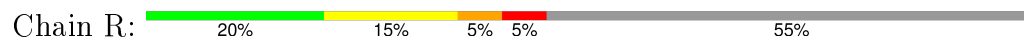


- Molecule 1: Claudin-2

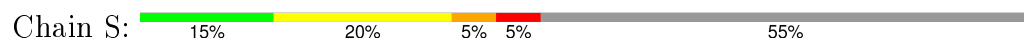
Chain Q: 



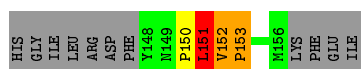
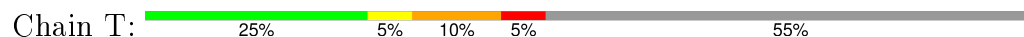
● Molecule 1: Claudin-2



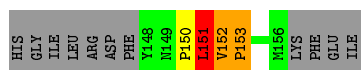
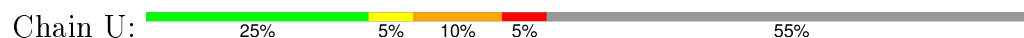
● Molecule 1: Claudin-2



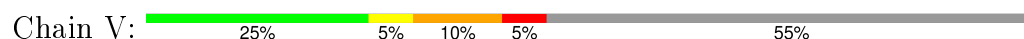
● Molecule 1: Claudin-2



● Molecule 1: Claudin-2



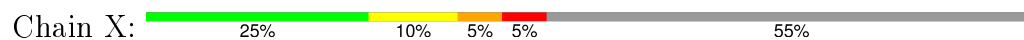
● Molecule 1: Claudin-2




● Molecule 1: Claudin-2

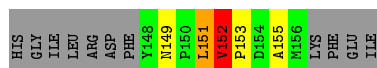


● Molecule 1: Claudin-2




● Molecule 1: Claudin-2

Chain Y: 

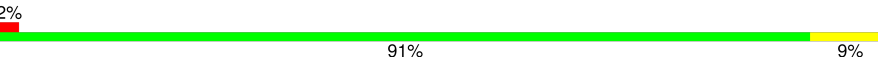


- Molecule 1: Claudin-2

Chain Z: 




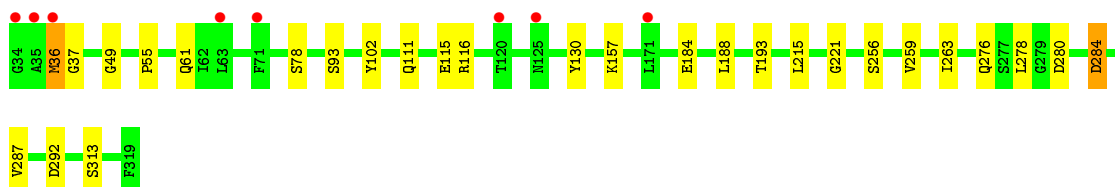
- Molecule 2: Heat-labile enterotoxin B chain

Chain A: 




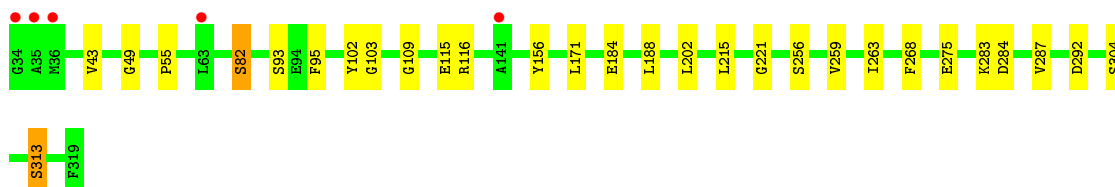
- Molecule 2: Heat-labile enterotoxin B chain

Chain B: 



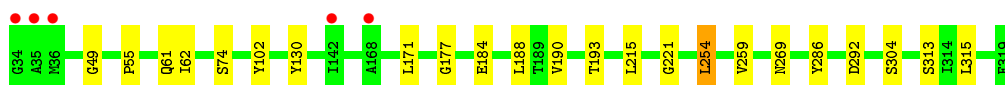
- Molecule 2: Heat-labile enterotoxin B chain

Chain C: 



- Molecule 2: Heat-labile enterotoxin B chain

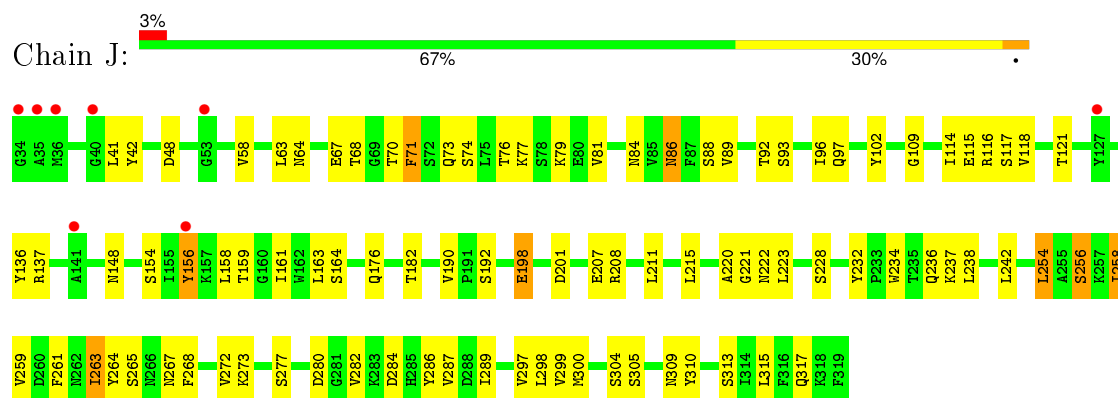
Chain D: 



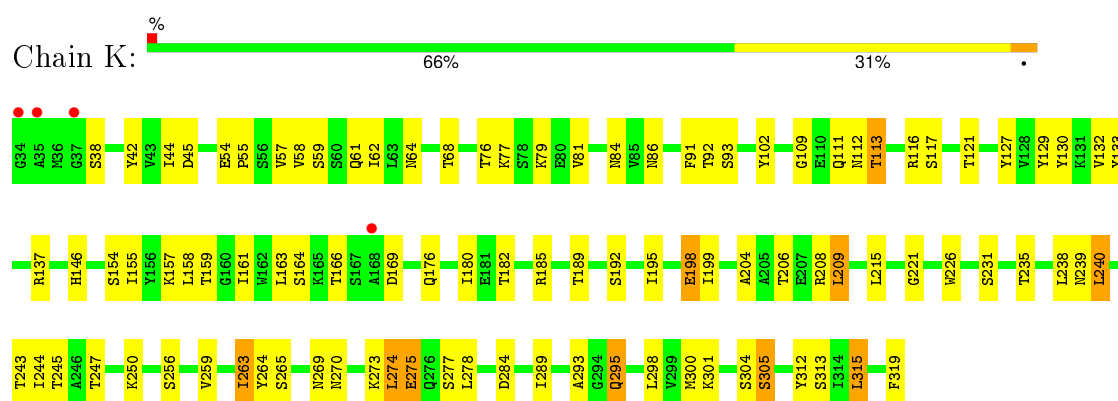
- Molecule 2: Heat-labile enterotoxin B chain

Chain E: 

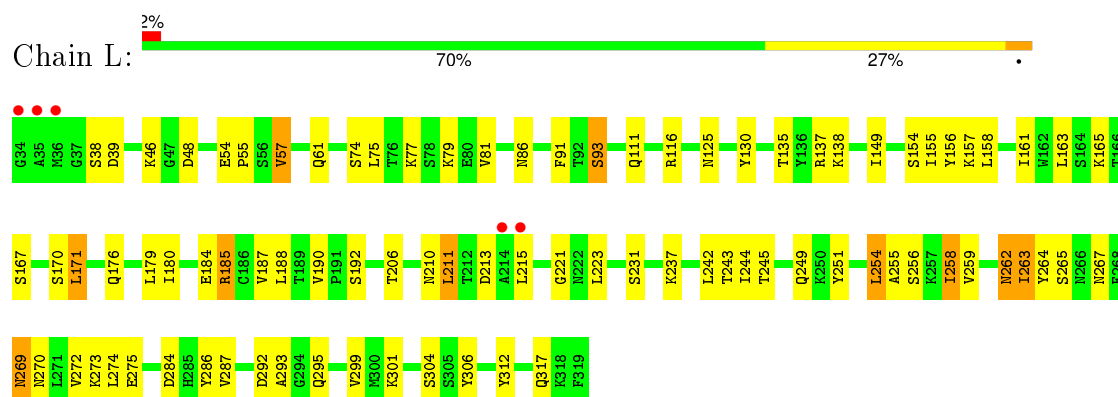
- Molecule 2: Heat-labile enterotoxin B chain



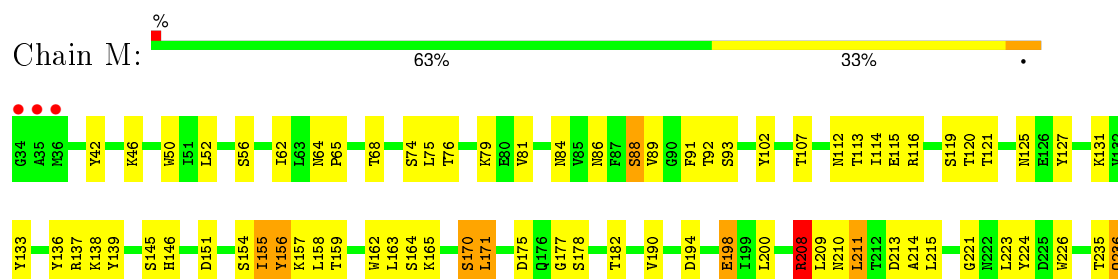
- Molecule 2: Heat-labile enterotoxin B chain

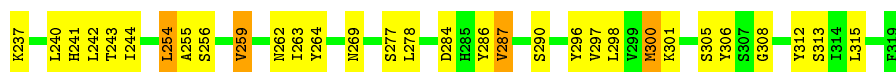


- Molecule 2: Heat-labile enterotoxin B chain



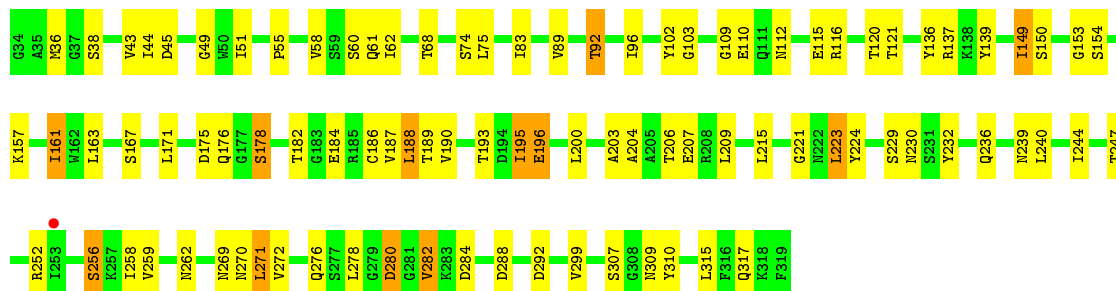
- Molecule 2: Heat-labile enterotoxin B chain





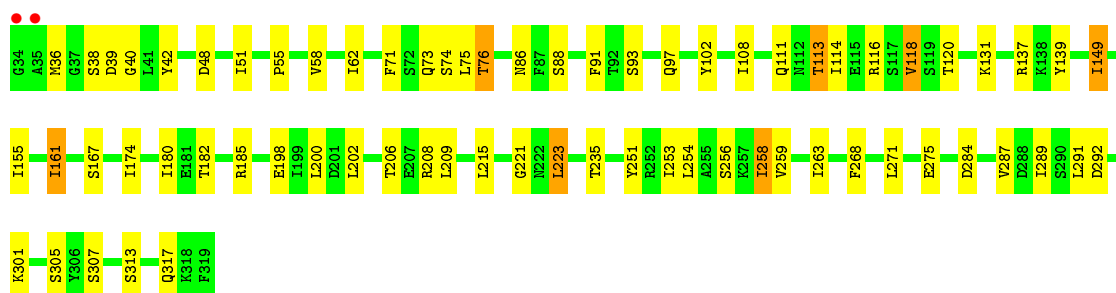
• Molecule 2: Heat-labile enterotoxin B chain

Chain N: 67% 28% .



• Molecule 2: Heat-labile enterotoxin B chain

Chain O: 76% 22% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	369.60 Å 100.26 Å 265.36 Å 90.00° 119.74° 90.00°	Depositor
Resolution (Å)	48.98 – 3.38 48.98 – 3.37	Depositor EDS
% Data completeness (in resolution range)	80.8 (48.98-3.38) 81.2 (48.98-3.37)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.40 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.204 , 0.240 0.244 , 0.282	Depositor DCC
R_{free} test set	4848 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	1.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 101.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 96759 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	34251	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1	0.98	0/61	1.53	2/85 (2.4%)
1	2	1.13	0/61	1.61	2/85 (2.4%)
1	3	1.02	0/61	1.54	2/85 (2.4%)
1	4	1.11	0/61	1.59	2/85 (2.4%)
1	P	0.91	0/61	1.48	2/85 (2.4%)
1	Q	1.21	0/61	1.76	2/85 (2.4%)
1	R	1.14	0/61	1.56	3/85 (3.5%)
1	S	1.29	0/61	1.63	2/85 (2.4%)
1	T	1.05	0/61	1.41	2/85 (2.4%)
1	U	1.08	0/61	1.60	2/85 (2.4%)
1	V	0.97	0/61	1.65	2/85 (2.4%)
1	W	1.17	0/61	1.45	0/85
1	X	1.12	0/61	2.06	4/85 (4.7%)
1	Y	1.16	0/61	1.51	2/85 (2.4%)
1	Z	1.06	0/61	1.50	1/85 (1.2%)
2	A	0.46	0/2276	0.71	0/3094
2	B	0.47	0/2276	0.71	0/3094
2	C	0.48	0/2276	0.75	1/3094 (0.0%)
2	D	0.49	0/2282	0.72	0/3101
2	E	0.44	0/2276	0.71	0/3094
2	F	0.46	0/2276	0.72	0/3094
2	G	0.52	0/2276	0.85	1/3094 (0.0%)
2	H	0.54	0/2276	0.86	0/3094
2	I	0.51	0/2276	0.82	1/3094 (0.0%)
2	J	0.51	0/2276	0.81	0/3094
2	K	0.53	0/2276	0.84	0/3094
2	L	0.52	0/2276	0.84	0/3094
2	M	0.53	0/2276	0.85	1/3094 (0.0%)
2	N	0.54	0/2276	0.84	1/3094 (0.0%)
2	O	0.55	0/2276	0.84	3/3094 (0.1%)
All	All	0.53	0/35061	0.83	38/47692 (0.1%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	150	PRO	C-N-CA	7.56	140.60	121.70
1	X	151	LEU	N-CA-C	7.19	130.40	111.00
2	N	190	VAL	N-CA-CB	6.89	126.66	111.50
1	Q	151	LEU	N-CA-C	6.57	128.74	111.00
1	X	150	PRO	CB-CA-C	6.52	128.31	112.00
1	3	151	LEU	N-CA-C	6.42	128.32	111.00
1	U	151	LEU	N-CA-C	6.09	127.44	111.00
1	P	151	LEU	N-CA-C	5.83	126.74	111.00
2	O	42	TYR	CA-CB-CG	5.80	124.42	113.40
2	G	92	THR	CB-CA-C	-5.77	96.02	111.60
1	1	152	VAL	N-CA-C	5.76	126.54	111.00
1	V	152	VAL	N-CA-C	5.73	126.48	111.00
1	4	151	LEU	N-CA-C	5.72	126.45	111.00
2	O	287	VAL	N-CA-CB	5.68	124.01	111.50
1	U	152	VAL	N-CA-C	5.68	126.34	111.00
2	C	283	LYS	CB-CA-C	-5.65	99.10	110.40
1	3	152	VAL	N-CA-C	5.60	126.12	111.00
1	P	152	VAL	N-CA-C	5.60	126.12	111.00
1	V	151	LEU	N-CA-C	5.60	126.11	111.00
1	1	151	LEU	N-CA-C	5.53	125.93	111.00
1	Y	152	VAL	N-CA-C	5.44	125.69	111.00
1	S	151	LEU	C-N-CA	5.42	135.25	121.70
1	Z	151	LEU	N-CA-C	5.38	125.53	111.00
1	4	152	VAL	N-CA-C	5.33	125.41	111.00
2	M	208	ARG	CB-CA-C	5.33	121.06	110.40
1	R	151	LEU	N-CA-C	5.30	125.31	111.00
2	I	64	ASN	CB-CA-C	5.28	120.96	110.40
1	Q	152	VAL	N-CA-C	5.23	125.12	111.00
2	O	42	TYR	CB-CA-C	-5.22	99.96	110.40
1	X	150	PRO	CA-N-CD	-5.21	104.21	111.50
1	T	151	LEU	N-CA-C	5.16	124.94	111.00
1	S	151	LEU	N-CA-C	5.15	124.91	111.00
1	R	152	VAL	N-CA-C	5.14	124.87	111.00
1	2	151	LEU	C-N-CA	5.09	134.43	121.70
1	Y	151	LEU	N-CA-C	5.06	124.67	111.00
1	R	151	LEU	C-N-CA	5.03	134.26	121.70
1	2	151	LEU	N-CA-C	5.02	124.56	111.00
1	T	152	VAL	N-CA-C	5.01	124.52	111.00

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	1	60	0	52	5	0
1	2	60	0	52	6	0
1	3	60	0	52	1	0
1	4	60	0	52	3	0
1	P	60	0	52	4	0
1	Q	60	0	52	3	0
1	R	60	0	52	4	0
1	S	60	0	52	5	0
1	T	60	0	52	7	0
1	U	60	0	52	5	0
1	V	60	0	52	4	0
1	W	60	0	52	5	0
1	X	60	0	52	2	0
1	Y	60	0	52	2	0
1	Z	60	0	52	4	0
2	A	2223	0	2147	21	0
2	B	2223	0	2147	19	0
2	C	2223	0	2147	21	0
2	D	2229	0	2158	15	0
2	E	2223	0	2147	15	0
2	F	2223	0	2147	16	0
2	G	2223	0	2147	46	0
2	H	2223	0	2147	37	0
2	I	2223	0	2147	34	0
2	J	2223	0	2147	46	0
2	K	2223	0	2147	53	0
2	L	2223	0	2147	45	0
2	M	2223	0	2147	55	0
2	N	2223	0	2147	50	0
2	O	2223	0	2147	34	0
All	All	34251	0	32996	455	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (455) 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)
2:G:111:GLN:HE22	2:I:109:GLY:HA2	1.19	1.07
2:A:259:VAL:HG21	1:P:152:VAL:HG21	1.46	0.97
2:M:254:LEU:HG	2:M:286:TYR:HB3	1.50	0.94
2:B:259:VAL:HG21	1:Q:152:VAL:HG21	1.51	0.93
2:E:259:VAL:HG21	1:T:152:VAL:HG21	1.52	0.91
2:L:54:GLU:O	2:L:57:VAL:HG22	1.78	0.84
2:B:263:ILE:HD11	2:B:287:VAL:HG21	1.60	0.83
2:K:81:VAL:HG21	2:K:93:SER:HB3	1.62	0.81
2:G:46:LYS:HD2	2:G:194:ASP:OD2	1.83	0.80
2:G:111:GLN:NE2	2:I:109:GLY:HA2	1.98	0.79
2:D:254:LEU:HD12	2:D:286:TYR:HB3	1.65	0.78
2:D:259:VAL:HG21	1:S:152:VAL:HG21	1.66	0.77
2:G:54:GLU:O	2:G:57:VAL:HG23	1.84	0.77
2:L:86:ASN:ND2	2:L:91:PHE:HB3	1.99	0.77
2:G:57:VAL:HG22	2:G:133:TYR:CE2	2.19	0.77
2:K:263:ILE:HD12	2:K:274:LEU:HB2	1.67	0.77
2:H:259:VAL:HG21	1:W:152:VAL:HG21	1.67	0.76
2:L:171:LEU:H	2:L:171:LEU:HD12	1.52	0.74
2:N:276:GLN:HE21	2:N:278:LEU:HD11	1.53	0.73
2:M:262:ASN:HB3	2:M:264:TYR:HE1	1.52	0.73
1:4:152:VAL:HG21	2:O:259:VAL:HG21	1.69	0.73
2:F:263:ILE:HD11	2:F:287:VAL:HG21	1.71	0.72
1:4:152:VAL:H	2:O:256:SER:HB3	1.54	0.72
2:A:258:ILE:HD11	1:P:153:PRO:HG3	1.72	0.72
2:F:259:VAL:HG21	1:U:152:VAL:HG21	1.72	0.72
1:S:150:PRO:O	1:S:151:LEU:HD12	1.90	0.72
2:F:313:SER:H	1:U:152:VAL:HG22	1.53	0.72
2:K:68:THR:OG1	2:K:121:THR:HG23	1.88	0.71
2:E:61:GLN:HB3	2:E:130:TYR:CE2	2.25	0.71
2:K:259:VAL:HG21	1:Z:152:VAL:HG21	1.72	0.71
2:C:259:VAL:HG21	1:R:152:VAL:HG21	1.72	0.71
2:I:212:THR:HG21	2:I:246:ALA:H	1.56	0.71
2:G:71:PHE:HB3	2:G:118:VAL:HG23	1.74	0.70
2:I:130:TYR:HB2	2:I:163:LEU:HD21	1.73	0.70
2:L:264:TYR:CE2	2:L:273:LYS:HG3	2.27	0.70
2:C:313:SER:H	1:R:152:VAL:HG22	1.56	0.70
2:E:258:ILE:HD11	1:T:153:PRO:HG3	1.73	0.70
1:1:152:VAL:HG21	2:L:259:VAL:HG21	1.73	0.70
2:D:304:SER:HB3	2:L:116:ARG:HD3	1.74	0.69
2:D:61:GLN:HB3	2:D:130:TYR:CE2	2.28	0.69
2:H:265:SER:HB3	2:H:274:LEU:HD21	1.76	0.67
2:A:111:GLN:HE22	2:C:109:GLY:HA2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:304:SER:HB3	2:I:116:ARG:HD3	1.75	0.67
2:I:166:THR:HG23	2:I:174:ILE:HD12	1.76	0.67
2:K:137:ARG:HB2	2:K:159:THR:HG21	1.75	0.67
2:N:137:ARG:HG3	2:N:139:TYR:CE2	2.29	0.67
2:K:116:ARG:HG3	2:K:161:ILE:HG12	1.77	0.67
2:N:109:GLY:HA2	2:O:111:GLN:HE22	1.59	0.67
2:H:134:ALA:HB1	2:H:158:LEU:HD11	1.77	0.66
2:G:79:LYS:HD2	2:G:155:ILE:HD11	1.77	0.66
2:B:313:SER:H	1:Q:152:VAL:HG22	1.60	0.66
1:1:153:PRO:HD3	2:L:258:ILE:HD11	1.78	0.66
2:J:267:ASN:HA	2:K:176:GLN:HE22	1.61	0.66
2:B:116:ARG:HD3	2:J:304:SER:HB3	1.78	0.65
2:K:265:SER:HB3	2:K:274:LEU:HD21	1.78	0.65
2:M:102:TYR:CE1	2:N:55:PRO:HA	2.32	0.65
2:K:130:TYR:HB2	2:K:163:LEU:HD11	1.78	0.65
2:B:61:GLN:HB3	2:B:130:TYR:CE2	2.32	0.64
1:2:151:LEU:HD12	2:M:255:ALA:HA	1.80	0.64
2:J:263:ILE:HD11	2:J:287:VAL:HG21	1.80	0.64
1:2:152:VAL:HG21	2:M:259:VAL:HG21	1.80	0.63
2:I:130:TYR:HB2	2:I:163:LEU:CD2	2.27	0.63
2:I:200:LEU:HD21	2:I:297:VAL:HG11	1.81	0.63
2:O:258:ILE:HD13	2:O:258:ILE:H	1.64	0.63
2:N:186:CYS:SG	2:N:188:LEU:HB2	2.39	0.62
2:M:50:TRP:CD1	2:M:138:LYS:HB3	2.34	0.62
1:2:150:PRO:O	1:2:151:LEU:HG	1.99	0.62
2:L:254:LEU:HD12	2:L:286:TYR:HB3	1.80	0.62
2:N:92:THR:O	2:N:96:ILE:HG13	1.99	0.62
2:C:263:ILE:HD11	2:C:287:VAL:HG21	1.81	0.62
2:H:77:LYS:HB2	2:H:158:LEU:HD13	1.80	0.62
2:A:129:TYR:CZ	2:C:268:PHE:HD1	2.17	0.62
2:N:149:ILE:HD12	2:N:149:ILE:H	1.64	0.62
2:H:139:TYR:HB2	2:H:155:ILE:HG23	1.82	0.62
2:G:204:ALA:HB2	2:G:237:LYS:HD2	1.81	0.62
2:H:211:LEU:HD22	2:H:244:ILE:HG12	1.81	0.62
2:K:42:TYR:CE2	2:K:198:GLU:HB2	2.35	0.61
2:D:55:PRO:HA	2:F:102:TYR:CE1	2.35	0.61
2:H:130:TYR:HB2	2:H:163:LEU:HD21	1.83	0.61
2:C:256:SER:HB2	1:R:152:VAL:H	1.66	0.61
2:H:223:LEU:HD12	2:H:317:GLN:HG3	1.83	0.60
2:L:258:ILE:HD13	2:L:258:ILE:H	1.66	0.60
2:H:137:ARG:HB2	2:H:159:THR:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:109:GLY:HA2	2:O:111:GLN:NE2	2.17	0.60
2:N:102:TYR:CE1	2:O:55:PRO:HA	2.36	0.60
2:M:236:GLN:HA	2:M:236:GLN:HE21	1.67	0.60
2:I:46:LYS:HG3	2:I:138:LYS:HE2	1.83	0.60
2:N:252:ARG:HG3	2:N:288:ASP:OD1	2.01	0.60
2:N:112:ASN:HB2	2:N:157:LYS:HE2	1.84	0.59
2:E:95:PHE:HE2	2:E:203:ALA:HB2	1.67	0.59
2:L:86:ASN:HD22	2:L:91:PHE:HB3	1.68	0.59
2:N:149:ILE:H	2:N:149:ILE:CD1	2.15	0.59
2:J:261:PHE:HD2	2:J:298:LEU:HD11	1.66	0.59
2:E:284:ASP:OD2	1:T:150:PRO:HA	2.02	0.59
2:G:109:GLY:HA2	2:H:111:GLN:HE22	1.67	0.59
2:H:62:ILE:H	2:H:62:ILE:HD12	1.67	0.59
2:N:200:LEU:HG	2:N:271:LEU:HD13	1.85	0.59
2:A:116:ARG:HD3	2:L:304:SER:HB3	1.84	0.59
2:N:171:LEU:H	2:N:171:LEU:HD12	1.67	0.59
2:F:61:GLN:HB3	2:F:130:TYR:CE2	2.38	0.59
1:3:152:VAL:HG23	2:N:256:SER:HB2	1.85	0.59
2:B:263:ILE:CD1	2:B:287:VAL:HG21	2.30	0.59
2:N:276:GLN:NE2	2:N:278:LEU:HD11	2.18	0.59
2:N:44:ILE:HG13	2:N:196:GLU:HB2	1.85	0.59
2:K:256:SER:HB2	1:Z:152:VAL:H	1.68	0.58
2:I:138:LYS:HG3	2:I:156:TYR:CE2	2.38	0.58
2:H:305:SER:O	2:O:116:ARG:NH2	2.36	0.58
2:H:304:SER:HB3	2:O:116:ARG:HD3	1.85	0.58
2:F:171:LEU:H	2:F:171:LEU:HD23	1.68	0.58
2:K:313:SER:H	1:Z:152:VAL:HG22	1.68	0.57
2:H:170:SER:HB3	2:H:173:ASN:HD22	1.69	0.57
2:M:209:LEU:HD11	2:M:214:ALA:HB2	1.86	0.57
2:H:51:ILE:HD11	2:H:185:ARG:HG3	1.86	0.57
2:E:102:TYR:CE1	2:F:55:PRO:HA	2.39	0.57
2:N:68:THR:OG1	2:N:121:THR:HG23	2.04	0.57
2:D:254:LEU:HD23	1:S:151:LEU:HD11	1.87	0.57
2:J:81:VAL:HG11	2:J:93:SER:HA	1.87	0.57
2:I:259:VAL:HG21	1:X:152:VAL:HG21	1.87	0.57
2:M:50:TRP:CE2	2:M:138:LYS:HD3	2.40	0.56
2:G:256:SER:HB3	1:V:152:VAL:H	1.69	0.56
2:I:164:SER:OG	2:I:179:LEU:HD22	2.02	0.56
2:G:209:LEU:HD11	2:G:214:ALA:HB2	1.87	0.56
2:N:116:ARG:HB3	2:N:161:ILE:HD11	1.88	0.55
2:H:313:SER:H	1:W:152:VAL:HG22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:237:LYS:HE2	2:L:299:VAL:HG13	1.88	0.55
2:O:235:THR:HA	2:O:301:LYS:NZ	2.21	0.55
2:I:237:LYS:HD3	2:I:299:VAL:HG13	1.88	0.55
2:D:62:ILE:HD11	2:F:268:PHE:CD2	2.42	0.55
2:G:102:TYR:CE1	2:H:55:PRO:HA	2.42	0.55
2:M:162:TRP:CZ3	2:M:164:SER:HB2	2.41	0.55
2:N:262:ASN:ND2	2:N:276:GLN:OE1	2.39	0.55
2:M:208:ARG:HB2	2:M:241:HIS:HB2	1.88	0.55
2:K:81:VAL:CG1	2:K:155:ILE:HD12	2.37	0.54
2:O:114:ILE:HD12	2:O:116:ARG:HG2	1.89	0.54
2:M:114:ILE:HD13	2:M:116:ARG:HG3	1.88	0.54
2:K:244:ILE:HG22	2:K:293:ALA:HA	1.89	0.54
2:B:102:TYR:CE1	2:C:55:PRO:HA	2.43	0.54
2:G:46:LYS:HG3	2:G:138:LYS:HG2	1.89	0.54
2:B:284:ASP:OD2	1:Q:150:PRO:HA	2.07	0.54
2:O:149:ILE:H	2:O:149:ILE:HD12	1.72	0.54
2:O:223:LEU:HD11	2:O:317:GLN:HG2	1.90	0.54
2:C:115:GLU:H	2:K:305:SER:HB3	1.72	0.54
2:K:295:GLN:CG	2:L:176:GLN:HB2	2.37	0.54
2:K:226:TRP:HH2	2:K:238:LEU:HD21	1.71	0.54
2:H:140:GLN:HG3	2:H:154:SER:OG	2.08	0.53
2:G:51:ILE:HD12	2:G:53:GLY:H	1.74	0.53
2:M:262:ASN:HB3	2:M:264:TYR:CE1	2.40	0.53
2:N:96:ILE:HD13	2:N:153:GLY:HA3	1.91	0.53
2:F:263:ILE:CD1	2:F:287:VAL:HG21	2.37	0.53
2:O:223:LEU:CD1	2:O:317:GLN:HG2	2.38	0.53
2:K:102:TYR:HE2	2:K:199:ILE:HB	1.72	0.53
2:H:45:ASP:HB3	2:H:195:ILE:HB	1.90	0.53
2:M:156:TYR:N	2:M:156:TYR:CD1	2.76	0.53
1:W:150:PRO:O	1:W:151:LEU:HD12	2.09	0.53
1:U:150:PRO:O	1:U:151:LEU:HG	2.09	0.53
2:I:41:LEU:HD23	2:I:201:ASP:HA	1.91	0.53
2:L:46:LYS:HG3	2:L:138:LYS:HE3	1.90	0.53
1:2:151:LEU:HB2	2:M:256:SER:HB2	1.90	0.52
2:J:298:LEU:HD23	2:J:300:MET:CE	2.39	0.52
2:G:208:ARG:NH1	2:H:180:ILE:O	2.43	0.52
2:M:131:LYS:HD3	2:M:133:TYR:OH	2.10	0.52
2:A:102:TYR:CE1	2:B:55:PRO:HA	2.45	0.52
2:H:112:ASN:HB2	2:H:157:LYS:HE2	1.92	0.52
2:K:263:ILE:HD11	2:K:275:GLU:HB2	1.90	0.52
1:V:150:PRO:O	1:V:151:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:46:LYS:HG3	2:M:138:LYS:HE2	1.92	0.52
2:J:136:TYR:HB3	2:J:156:TYR:HB3	1.91	0.52
2:A:313:SER:H	1:P:152:VAL:HG22	1.75	0.52
2:D:55:PRO:HA	2:F:102:TYR:HE1	1.75	0.51
2:M:244:ILE:HD12	2:M:296:TYR:CD2	2.45	0.51
2:N:280:ASP:OD2	2:N:282:VAL:HG23	2.09	0.51
2:J:109:GLY:HA2	2:K:111:GLN:HE22	1.75	0.51
2:J:92:THR:O	2:J:96:ILE:HG13	2.09	0.51
2:O:71:PHE:HB3	2:O:118:VAL:HG23	1.93	0.51
2:I:249:GLN:HB3	2:I:318:LYS:NZ	2.26	0.51
2:I:247:THR:O	2:I:249:GLN:NE2	2.36	0.51
2:G:200:LEU:HD23	2:G:239:ASN:ND2	2.24	0.51
2:I:68:THR:OG1	2:I:121:THR:HG23	2.11	0.51
2:L:48:ASP:OD2	2:L:137:ARG:HD3	2.10	0.51
2:K:240:LEU:HD23	2:K:298:LEU:HB3	1.92	0.51
2:M:211:LEU:HB2	2:M:242:LEU:HD22	1.92	0.51
2:I:249:GLN:HB2	2:I:251:TYR:CZ	2.46	0.51
2:J:71:PHE:C	2:J:71:PHE:CD1	2.85	0.51
2:H:166:THR:HB	2:H:179:LEU:HD21	1.92	0.51
2:L:211:LEU:HD12	2:L:242:LEU:HD22	1.92	0.51
2:E:256:SER:HB3	1:T:152:VAL:H	1.76	0.51
2:J:71:PHE:CE1	2:J:73:GLN:HG2	2.46	0.50
2:I:249:GLN:HB3	2:I:318:LYS:HZ3	1.75	0.50
2:K:300:MET:HG3	2:K:312:TYR:CD2	2.46	0.50
2:N:252:ARG:HB3	2:N:317:GLN:HB2	1.93	0.50
2:J:261:PHE:CE1	2:J:277:SER:HB3	2.46	0.50
2:I:256:SER:HB3	1:X:152:VAL:H	1.77	0.50
2:M:263:ILE:HG22	2:M:298:LEU:HD13	1.93	0.50
2:B:276:GLN:NE2	2:B:278:LEU:HD21	2.27	0.50
2:J:42:TYR:CE2	2:J:198:GLU:HB2	2.47	0.50
2:M:300:MET:HG3	2:M:312:TYR:CD1	2.47	0.50
2:N:223:LEU:HG	2:N:317:GLN:HG2	1.93	0.50
1:I:152:VAL:H	2:L:256:SER:HB2	1.77	0.49
2:D:61:GLN:HB3	2:D:130:TYR:HE2	1.72	0.49
2:G:259:VAL:HG21	1:V:152:VAL:HG21	1.94	0.49
2:N:206:THR:HG22	2:O:182:THR:HG22	1.93	0.49
2:B:102:TYR:HE1	2:C:55:PRO:HA	1.77	0.49
2:G:226:TRP:CZ3	2:G:314:ILE:HD11	2.47	0.49
2:G:101:GLU:OE1	2:H:78:SER:HB2	2.12	0.49
2:M:224:TYR:CE1	2:M:226:TRP:HB2	2.47	0.49
2:G:49:GLY:O	2:G:187:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:264:TYR:CE2	2:I:273:LYS:HG3	2.47	0.49
2:K:45:ASP:HB3	2:K:195:ILE:HB	1.93	0.49
2:M:306:TYR:HE1	2:M:308:GLY:O	1.95	0.49
1:L:153:PRO:CD	2:L:258:ILE:HD11	2.41	0.49
2:L:263:ILE:HD11	2:L:287:VAL:HG21	1.93	0.49
2:K:102:TYR:CE1	2:L:55:PRO:HA	2.48	0.49
2:H:214:ALA:HB1	2:H:224:TYR:CD2	2.48	0.49
2:M:210:ASN:HA	2:M:243:THR:HB	1.94	0.49
2:A:256:SER:HB2	1:P:152:VAL:H	1.77	0.49
2:C:49:GLY:HA3	2:C:188:LEU:HG	1.94	0.49
2:D:313:SER:H	1:S:152:VAL:HG22	1.78	0.48
2:I:41:LEU:HG	2:I:199:ILE:HG13	1.94	0.48
2:J:64:ASN:O	2:J:67:GLU:HB2	2.13	0.48
2:J:77:LYS:HB2	2:J:158:LEU:HD22	1.95	0.48
2:M:52:LEU:HG	2:M:56:SER:OG	2.12	0.48
2:M:127:TYR:HD2	2:M:170:SER:HA	1.79	0.48
2:C:116:ARG:HD3	2:K:304:SER:HB3	1.95	0.48
2:B:78:SER:HA	2:B:111:GLN:HG3	1.95	0.48
2:G:99:SER:HA	2:G:202:LEU:HD11	1.95	0.48
2:M:64:ASN:HA	2:M:127:TYR:CD1	2.49	0.48
2:J:309:ASN:O	2:J:310:TYR:HD2	1.96	0.48
2:M:81:VAL:HG11	2:M:93:SER:HB2	1.94	0.48
2:M:286:TYR:C	2:M:286:TYR:CD2	2.87	0.48
2:K:295:GLN:HG3	2:L:176:GLN:HB2	1.95	0.48
2:G:262:ASN:HB3	2:G:264:TYR:CE1	2.48	0.48
1:T:150:PRO:O	1:T:151:LEU:HB2	2.14	0.48
1:2:152:VAL:HG21	2:M:259:VAL:CG2	2.43	0.48
2:I:252:ARG:HB3	2:I:317:GLN:HB2	1.96	0.48
2:G:211:LEU:HB2	2:G:242:LEU:HD22	1.96	0.48
2:J:77:LYS:HA	2:J:77:LYS:HD3	1.71	0.47
2:L:265:SER:OG	2:L:272:VAL:HB	2.14	0.47
2:K:264:TYR:CE2	2:K:273:LYS:HE2	2.49	0.47
2:N:112:ASN:HB2	2:N:157:LYS:CE	2.43	0.47
2:G:259:VAL:CG2	1:V:152:VAL:HG21	2.45	0.47
2:O:139:TYR:HB2	2:O:155:ILE:HG23	1.96	0.47
2:N:175:ASP:O	2:N:178:SER:OG	2.31	0.47
2:B:115:GLU:HB2	2:J:305:SER:HB3	1.96	0.47
2:L:149:ILE:O	2:L:149:ILE:HD12	2.14	0.47
2:J:234:TRP:CD2	2:J:305:SER:HA	2.49	0.47
2:G:146:HIS:HA	2:G:278:LEU:HD22	1.95	0.47
2:O:251:TYR:CD1	2:O:291:LEU:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:GLY:HA3	2:A:188:LEU:HG	1.96	0.47
2:J:211:LEU:HB2	2:J:242:LEU:HD22	1.97	0.47
2:B:36[A]:MET:HB2	2:B:37:GLY:H	1.53	0.47
2:B:280:ASP:O	2:H:118:VAL:HA	2.15	0.47
2:C:263:ILE:CD1	2:C:287:VAL:HG21	2.44	0.47
2:K:81:VAL:HG13	2:K:155:ILE:HD12	1.96	0.47
2:G:262:ASN:O	2:G:298:LEU:HD12	2.14	0.47
2:M:42:TYR:CE2	2:M:198:GLU:HB2	2.50	0.47
2:J:256:SER:HB3	1:Y:152:VAL:HG23	1.96	0.47
2:N:43:VAL:HG21	2:N:103:GLY:HA3	1.95	0.47
2:G:86:ASN:ND2	2:G:88:SER:O	2.48	0.47
1:R:150:PRO:O	1:R:151:LEU:HB2	2.14	0.47
2:J:264:TYR:CD1	2:J:273:LYS:HA	2.50	0.47
2:E:61:GLN:HB3	2:E:130:TYR:HE2	1.74	0.46
2:I:282:VAL:HG11	2:M:163:LEU:HD23	1.96	0.46
2:D:315:LEU:HB2	1:S:151:LEU:HD21	1.97	0.46
2:K:77:LYS:HB2	2:K:158:LEU:HD22	1.98	0.46
2:I:254:LEU:HG	2:I:286:TYR:HB3	1.96	0.46
2:J:298:LEU:HD23	2:J:300:MET:HE2	1.98	0.46
2:J:63:LEU:HD22	2:J:67:GLU:HB3	1.96	0.46
2:O:102:TYR:HD2	2:O:202:LEU:HD11	1.81	0.46
2:F:110:GLU:HG3	2:F:111:GLN:HG3	1.96	0.46
2:G:77:LYS:HA	2:G:77:LYS:HD2	1.67	0.46
2:M:139:TYR:HB2	2:M:155:ILE:HG23	1.98	0.46
2:J:41:LEU:HD22	2:J:201:ASP:HA	1.97	0.46
2:K:146:HIS:HA	2:K:278:LEU:HD21	1.98	0.46
2:A:62:ILE:HD11	2:C:268:PHE:CD1	2.51	0.46
2:G:263:ILE:HD11	2:G:287:VAL:HG21	1.98	0.46
2:H:260:ASP:HB3	2:H:278:LEU:HD23	1.97	0.45
2:G:81:VAL:HG11	2:G:93:SER:HA	1.98	0.45
2:M:137:ARG:HB2	2:M:159:THR:HG21	1.97	0.45
2:A:244:ILE:HD13	2:A:251:TYR:HE1	1.81	0.45
2:K:86:ASN:HD22	2:K:91:PHE:HB3	1.81	0.45
2:H:249:GLN:HB2	2:H:251:TYR:CZ	2.51	0.45
2:J:137:ARG:HB2	2:J:159:THR:HG21	1.97	0.45
2:M:102:TYR:HE1	2:N:55:PRO:HA	1.80	0.45
2:L:263:ILE:CD1	2:L:275:GLU:HB3	2.47	0.45
2:G:71:PHE:HB3	2:G:118:VAL:CG2	2.42	0.45
2:H:255:ALA:HA	1:W:151:LEU:HD22	1.98	0.45
2:G:276:GLN:NE2	2:G:278:LEU:HD11	2.32	0.45
2:B:49:GLY:HA3	2:B:188:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:315:LEU:HD21	2:N:317:GLN:HE21	1.81	0.45
2:N:171:LEU:N	2:N:171:LEU:HD12	2.31	0.45
2:D:215:LEU:O	2:D:221:GLY:HA2	2.17	0.45
2:N:207:GLU:OE2	2:N:229:SER:N	2.49	0.45
2:I:49:GLY:O	2:I:187:VAL:HG22	2.17	0.45
2:N:171:LEU:H	2:N:171:LEU:CD1	2.30	0.44
2:K:76:THR:OG1	2:K:113:THR:HG23	2.17	0.44
2:H:263:ILE:HG23	2:H:298:LEU:CD1	2.47	0.44
2:E:304:SER:HB3	2:J:116:ARG:HD2	1.99	0.44
2:H:112:ASN:HD22	2:H:157:LYS:HD3	1.82	0.44
2:M:127:TYR:CD2	2:M:170:SER:HA	2.53	0.44
2:N:204:ALA:HB3	2:N:239:ASN:ND2	2.31	0.44
2:G:137:ARG:HB2	2:G:159:THR:HG21	1.99	0.44
2:G:207:GLU:OE2	2:G:228:SER:HB2	2.17	0.44
2:J:71:PHE:HD1	2:J:71:PHE:C	2.21	0.44
2:K:315:LEU:HB2	1:Z:151:LEU:HD21	1.98	0.44
2:H:68:THR:OG1	2:H:121:THR:HG23	2.17	0.44
2:M:88:SER:HB2	2:M:151:ASP:OD1	2.18	0.44
2:L:263:ILE:HD12	2:L:275:GLU:HB3	1.98	0.44
2:N:49:GLY:O	2:N:187:VAL:HG22	2.17	0.44
2:L:185:ARG:NH2	2:L:187:VAL:HG12	2.33	0.44
2:L:75:LEU:HD23	2:L:158:LEU:HD21	1.98	0.44
2:E:254:LEU:HD23	1:T:151:LEU:CD2	2.48	0.44
2:E:280:ASP:O	2:J:118:VAL:HA	2.17	0.44
2:A:305:SER:O	2:G:116:ARG:NH2	2.51	0.44
2:A:263:ILE:HD11	2:A:287:VAL:HG21	2.00	0.44
2:G:215:LEU:O	2:G:221:GLY:HA2	2.18	0.44
2:H:215:LEU:O	2:H:221:GLY:HA2	2.18	0.44
1:2:152:VAL:HG22	2:M:313:SER:H	1.82	0.44
2:G:252:ARG:HB3	2:G:317:GLN:HB2	2.00	0.44
2:O:200:LEU:HG	2:O:271:LEU:HD22	1.99	0.44
2:N:230:ASN:HB3	2:N:232:TYR:CZ	2.53	0.43
2:I:83:ILE:HG12	2:I:96:ILE:HD11	2.00	0.43
2:J:68:THR:OG1	2:J:121:THR:HG23	2.18	0.43
2:O:131:LYS:NZ	2:O:180:ILE:HD13	2.34	0.43
2:B:215:LEU:O	2:B:221:GLY:HA2	2.18	0.43
2:K:54:GLU:O	2:K:57:VAL:HG23	2.18	0.43
2:O:48:ASP:OD2	2:O:137:ARG:HD3	2.18	0.43
2:J:220:ALA:HB1	2:J:222:ASN:OD1	2.19	0.43
2:M:200:LEU:HD21	2:M:297:VAL:HG11	2.00	0.43
2:K:235:THR:O	2:K:301:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:254:LEU:HG	2:J:286:TYR:HB3	2.01	0.43
2:M:240:LEU:HD23	2:M:298:LEU:HD23	2.00	0.43
2:K:64:ASN:HD22	2:K:127:TYR:HE1	1.66	0.43
2:L:81:VAL:HG22	2:L:155:ILE:HD12	1.99	0.43
2:M:75:LEU:HD23	2:M:158:LEU:HD21	2.00	0.43
2:G:304:SER:HB3	2:N:116:ARG:HD3	2.00	0.43
2:J:268:PHE:HB3	2:K:129:TYR:CE1	2.53	0.43
2:A:215:LEU:O	2:A:221:GLY:HA2	2.18	0.43
2:I:52:LEU:HD23	2:I:184[B]:GLU:HG3	2.01	0.43
2:J:280:ASP:OD2	2:J:282:VAL:HG22	2.18	0.43
2:N:223:LEU:HD23	2:N:224:TYR:N	2.33	0.43
2:K:209:LEU:HD13	2:K:226:TRP:CD1	2.54	0.43
2:L:81:VAL:HG11	2:L:93:SER:HA	2.01	0.43
2:M:175:ASP:OD2	2:M:178:SER:HB3	2.19	0.43
2:D:49:GLY:HA3	2:D:188:LEU:HG	1.99	0.43
1:4:152:VAL:HG22	2:O:313:SER:H	1.83	0.43
2:M:146:HIS:HA	2:M:278:LEU:HD13	2.01	0.43
2:A:102:TYR:HE1	2:B:55:PRO:HA	1.83	0.43
2:A:251:TYR:HD1	2:A:291:LEU:HD12	1.83	0.43
2:O:215:LEU:O	2:O:221:GLY:HA2	2.19	0.43
2:J:215:LEU:O	2:J:221:GLY:HA2	2.19	0.43
2:A:43:VAL:HG21	2:A:103:GLY:HA3	2.01	0.43
2:G:171:LEU:H	2:G:171:LEU:HG	1.37	0.43
2:N:307:SER:O	2:N:310:TYR:HE1	2.02	0.43
2:L:61:GLN:HB3	2:L:130:TYR:CE2	2.53	0.43
2:O:76:THR:OG1	2:O:113:THR:HG23	2.19	0.43
2:B:263:ILE:HD11	2:B:287:VAL:CG2	2.40	0.42
2:G:276:GLN:HE21	2:G:278:LEU:HD11	1.84	0.42
2:I:215:LEU:O	2:I:221:GLY:HA2	2.19	0.42
2:K:215:LEU:O	2:K:221:GLY:HA2	2.18	0.42
2:E:215:LEU:O	2:E:221:GLY:HA2	2.19	0.42
1:W:150:PRO:C	1:W:151:LEU:HD12	2.40	0.42
2:C:215:LEU:O	2:C:221:GLY:HA2	2.18	0.42
2:D:102:TYR:CE1	2:E:55:PRO:HA	2.54	0.42
2:M:277:SER:OG	2:M:287:VAL:HG13	2.19	0.42
2:K:58:VAL:HG22	2:K:132:VAL:O	2.20	0.42
2:I:253:ILE:HD12	2:I:287:VAL:HG23	2.00	0.42
2:I:174:ILE:HA	2:I:174:ILE:HD13	1.96	0.42
2:F:258:ILE:HD11	1:U:153:PRO:HG3	2.01	0.42
2:J:261:PHE:CD2	2:J:298:LEU:HD11	2.52	0.42
2:M:209:LEU:HD23	2:M:242:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:239:ASN:OD1	2:N:299:VAL:HG22	2.19	0.42
2:J:232:TYR:HE2	2:J:238:LEU:HD22	1.85	0.42
2:M:171:LEU:H	2:M:171:LEU:HG	1.46	0.42
2:K:57:VAL:HG22	2:K:133:TYR:CE2	2.55	0.42
2:J:268:PHE:HA	2:K:129:TYR:OH	2.19	0.42
2:G:265:SER:HB3	2:G:274:LEU:HD21	2.02	0.42
2:K:112:ASN:HB2	2:K:157:LYS:HD3	2.02	0.42
2:K:112:ASN:CB	2:K:157:LYS:HD3	2.50	0.42
2:N:209:LEU:HB2	2:N:240:LEU:HD11	2.01	0.42
2:J:182:THR:HG22	2:L:206:THR:HG22	2.02	0.42
2:M:215:LEU:O	2:M:221:GLY:HA2	2.19	0.42
2:N:102:TYR:HE1	2:O:55:PRO:HA	1.82	0.42
1:U:150:PRO:C	1:U:151:LEU:HG	2.40	0.42
2:J:102:TYR:CE1	2:K:55:PRO:HA	2.55	0.42
2:G:253:ILE:HG12	2:G:316:PHE:HD1	1.85	0.42
2:L:215:LEU:O	2:L:221:GLY:HA2	2.19	0.42
2:F:215:LEU:O	2:F:221:GLY:HA2	2.19	0.42
1:1:153:PRO:HB2	1:1:154:ASP:H	1.75	0.42
2:L:265:SER:HB3	2:L:274:LEU:HD21	2.02	0.42
2:A:305:SER:O	2:G:116:ARG:CZ	2.67	0.42
2:M:86:ASN:HD22	2:M:91:PHE:HB3	1.85	0.42
2:H:226:TRP:HB3	2:H:316:PHE:HE2	1.85	0.42
2:E:313:SER:H	1:T:152:VAL:HG22	1.85	0.42
2:N:203:ALA:O	2:N:236:GLN:NE2	2.52	0.42
2:N:45:ASP:HB3	2:N:195:ILE:HD13	2.01	0.42
2:K:264:TYR:HA	2:K:274:LEU:HG	2.02	0.41
2:F:127:TYR:CD1	2:F:170:SER:HA	2.55	0.41
2:K:250:LYS:HB3	2:K:319:PHE:HD2	1.84	0.41
2:D:177:GLY:O	2:F:208:ARG:NH1	2.53	0.41
2:K:102:TYR:CE2	2:K:199:ILE:HB	2.55	0.41
2:L:130:TYR:HB2	2:L:163:LEU:HD21	2.01	0.41
2:K:109:GLY:HA2	2:L:111:GLN:HE22	1.84	0.41
2:J:86:ASN:ND2	2:J:88:SER:O	2.54	0.41
2:N:58:VAL:HG11	2:N:75:LEU:HD21	2.01	0.41
2:A:129:TYR:CE1	2:C:268:PHE:CD1	3.09	0.41
2:J:208:ARG:NH1	2:K:180:ILE:O	2.53	0.41
2:H:102:TYR:CE1	2:I:55:PRO:HA	2.55	0.41
2:M:235:THR:HA	2:M:301:LYS:NZ	2.35	0.41
2:N:215:LEU:O	2:N:221:GLY:HA2	2.19	0.41
2:L:262:ASN:HB2	2:L:264:TYR:CE1	2.55	0.41
2:O:40:GLY:HA3	2:O:198:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:TYR:CD2	2:E:273:LYS:HA	2.55	0.41
2:I:305:SER:HB3	2:M:115:GLU:H	1.86	0.41
2:C:95:PHE:CE2	2:C:202:LEU:HB2	2.56	0.41
2:L:86:ASN:HD21	2:L:91:PHE:HB3	1.80	0.41
2:L:301:LYS:HA	2:L:312:TYR:OH	2.21	0.41
2:H:112:ASN:ND2	2:H:157:LYS:HD3	2.35	0.41
2:C:82:SER:OG	2:C:156:TYR:HE2	2.03	0.41
2:G:282:VAL:HG11	2:N:163:LEU:HD23	2.01	0.41
2:L:254:LEU:HG	2:L:255:ALA:N	2.36	0.41
2:G:305:SER:HB3	2:N:115:GLU:HB2	2.01	0.41
2:M:81:VAL:HG11	2:M:93:SER:CB	2.50	0.41
2:O:131:LYS:HZ1	2:O:180:ILE:HD13	1.85	0.41
2:L:237:LYS:HG3	2:L:301:LYS:HB2	2.02	0.41
2:M:65:PRO:HD3	2:M:127:TYR:CD1	2.56	0.41
2:F:43:VAL:HG21	2:F:103:GLY:HA3	2.01	0.41
2:L:306:TYR:CD1	2:L:306:TYR:C	2.94	0.41
2:K:263:ILE:HG23	2:K:298:LEU:CD1	2.50	0.41
2:J:207:GLU:OE2	2:J:228:SER:HB2	2.20	0.41
2:L:244:ILE:HG22	2:L:293:ALA:HA	2.02	0.41
2:H:134:ALA:HB1	2:H:158:LEU:CD1	2.49	0.40
2:O:116:ARG:HB3	2:O:161:ILE:HD11	2.03	0.40
2:H:263:ILE:HG23	2:H:298:LEU:HD13	2.01	0.40
2:N:51:ILE:HG12	2:N:187:VAL:HG13	2.02	0.40
2:G:254:LEU:HD11	2:G:284:ASP:HB2	2.02	0.40
2:A:129:TYR:CE1	2:C:268:PHE:HD1	2.39	0.40
2:K:204:ALA:HB3	2:K:239:ASN:ND2	2.36	0.40
2:M:136:TYR:HB3	2:M:156:TYR:HB3	2.03	0.40
2:M:237:LYS:HA	2:M:301:LYS:HB2	2.04	0.40
2:O:86:ASN:ND2	2:O:88:SER:O	2.54	0.40
2:J:258:ILE:HG13	2:J:304:SER:HB2	2.03	0.40
2:K:238:LEU:HD12	2:K:239:ASN:N	2.37	0.40
2:N:75:LEU:HA	2:N:75:LEU:HD12	1.98	0.40
2:O:86:ASN:HD22	2:O:91:PHE:HB3	1.86	0.40
2:I:47:GLY:C	2:I:137:ARG:HD2	2.42	0.40
2:J:259:VAL:HG21	1:Y:152:VAL:HG21	2.04	0.40
2:O:86:ASN:ND2	2:O:91:PHE:HB3	2.37	0.40
2:C:43:VAL:HG21	2:C:103:GLY:HA3	2.02	0.40
2:J:176:GLN:HB2	2:L:295:GLN:HB2	2.04	0.40
2:L:269:ASN:HA	2:L:269:ASN:HD22	1.78	0.40
2:O:268:PHE:N	2:O:268:PHE:CD1	2.89	0.40
2:A:55:PRO:HA	2:C:102:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:116:ARG:HG3	2:L:161:ILE:HG12	2.02	0.40
2:M:177:GLY:O	2:O:208:ARG:NH1	2.55	0.40
2:O:58:VAL:HG11	2:O:75:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	2	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	3	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	4	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	P	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	Q	7/20 (35%)	1 (14%)	4 (57%)	2 (29%)	0	0
1	R	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	S	7/20 (35%)	2 (29%)	1 (14%)	4 (57%)	0	0
1	T	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	U	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	V	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	W	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
1	X	7/20 (35%)	1 (14%)	3 (43%)	3 (43%)	0	0
1	Y	7/20 (35%)	2 (29%)	1 (14%)	4 (57%)	0	0
1	Z	7/20 (35%)	2 (29%)	3 (43%)	2 (29%)	0	0
2	A	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	B	287/286 (100%)	283 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	D	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	E	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	F	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	G	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	H	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	I	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	J	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	K	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	L	287/286 (100%)	282 (98%)	5 (2%)	0	100	100
2	M	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	N	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
2	O	287/286 (100%)	283 (99%)	4 (1%)	0	100	100
All	All	4410/4590 (96%)	4272 (97%)	103 (2%)	35 (1%)	24	65

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	151	LEU
1	1	153	PRO
1	2	151	LEU
1	2	153	PRO
1	3	151	LEU
1	3	153	PRO
1	4	151	LEU
1	4	153	PRO
1	P	151	LEU
1	P	153	PRO
1	Q	151	LEU
1	Q	153	PRO
1	R	151	LEU
1	R	153	PRO
1	S	151	LEU
1	S	153	PRO
1	T	151	LEU
1	T	153	PRO
1	U	151	LEU

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Mol	Chain	Res	Type
1	U	153	PRO
1	V	151	LEU
1	V	153	PRO
1	W	151	LEU
1	W	153	PRO
1	X	150	PRO
1	X	151	LEU
1	X	153	PRO
1	Y	151	LEU
1	Y	153	PRO
1	Z	151	LEU
1	Z	153	PRO
1	S	152	VAL
1	S	155	ALA
1	Y	155	ALA
1	Y	152	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	6/18 (33%)	6 (100%)	0	100	100
1	2	6/18 (33%)	6 (100%)	0	100	100
1	3	6/18 (33%)	4 (67%)	2 (33%)	0	1
1	4	6/18 (33%)	6 (100%)	0	100	100
1	P	6/18 (33%)	6 (100%)	0	100	100
1	Q	6/18 (33%)	6 (100%)	0	100	100
1	R	6/18 (33%)	5 (83%)	1 (17%)	3	13
1	S	6/18 (33%)	5 (83%)	1 (17%)	3	13
1	T	6/18 (33%)	5 (83%)	1 (17%)	3	13
1	U	6/18 (33%)	6 (100%)	0	100	100
1	V	6/18 (33%)	5 (83%)	1 (17%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	6/18 (33%)	5 (83%)	1 (17%)	3	13
1	X	6/18 (33%)	5 (83%)	1 (17%)	3	13
1	Y	6/18 (33%)	5 (83%)	1 (17%)	3	13
1	Z	6/18 (33%)	6 (100%)	0	100	100
2	A	245/247 (99%)	239 (98%)	6 (2%)	57	84
2	B	245/247 (99%)	234 (96%)	11 (4%)	34	72
2	C	245/247 (99%)	236 (96%)	9 (4%)	41	76
2	D	246/247 (100%)	236 (96%)	10 (4%)	37	74
2	E	245/247 (99%)	234 (96%)	11 (4%)	34	72
2	F	245/247 (99%)	233 (95%)	12 (5%)	31	69
2	G	245/247 (99%)	199 (81%)	46 (19%)	2	8
2	H	245/247 (99%)	201 (82%)	44 (18%)	2	10
2	I	245/247 (99%)	209 (85%)	36 (15%)	4	18
2	J	245/247 (99%)	206 (84%)	39 (16%)	3	15
2	K	245/247 (99%)	207 (84%)	38 (16%)	3	16
2	L	245/247 (99%)	202 (82%)	43 (18%)	2	10
2	M	245/247 (99%)	203 (83%)	42 (17%)	2	12
2	N	245/247 (99%)	201 (82%)	44 (18%)	2	10
2	O	245/247 (99%)	212 (86%)	33 (14%)	5	21
All	All	3766/3975 (95%)	3333 (88%)	433 (12%)	7	28

All (433) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	149	ASN
1	3	150	PRO
2	A	171	LEU
2	A	197	LYS
2	A	269	ASN
2	A	284	ASP
2	A	292	ASP
2	A	305	SER
2	B	36[A]	MET
2	B	36[B]	MET
2	B	93	SER

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Mol	Chain	Res	Type
2	B	157	LYS
2	B	184[A]	GLU
2	B	184[B]	GLU
2	B	193[A]	THR
2	B	193[B]	THR
2	B	256	SER
2	B	284	ASP
2	B	292	ASP
2	C	82	SER
2	C	93	SER
2	C	171	LEU
2	C	184[A]	GLU
2	C	184[B]	GLU
2	C	275	GLU
2	C	284	ASP
2	C	292	ASP
2	C	313	SER
2	D	74	SER
2	D	171	LEU
2	D	184[A]	GLU
2	D	184[B]	GLU
2	D	190	VAL
2	D	193[A]	THR
2	D	193[B]	THR
2	D	254	LEU
2	D	269	ASN
2	D	292	ASP
2	E	117	SER
2	E	125	ASN
2	E	184[A]	GLU
2	E	184[B]	GLU
2	E	256	SER
2	E	269	ASN
2	E	284	ASP
2	E	292	ASP
2	E	305	SER
2	E	313	SER
2	E	318	LYS
2	F	111	GLN
2	F	125	ASN
2	F	171	LEU
2	F	190	VAL

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Mol	Chain	Res	Type
2	F	193[A]	THR
2	F	193[B]	THR
2	F	247	THR
2	F	256	SER
2	F	258	ILE
2	F	284	ASP
2	F	292	ASP
2	F	318	LYS
2	G	36[A]	MET
2	G	36[B]	MET
2	G	44	ILE
2	G	59	SER
2	G	61	GLN
2	G	75	LEU
2	G	76	THR
2	G	77	LYS
2	G	79	LYS
2	G	82	SER
2	G	89	VAL
2	G	92	THR
2	G	93	SER
2	G	94	GLU
2	G	113	THR
2	G	116	ARG
2	G	117	SER
2	G	118	VAL
2	G	127	TYR
2	G	130	TYR
2	G	143	ARG
2	G	149	ILE
2	G	163	LEU
2	G	166	THR
2	G	171	LEU
2	G	178	SER
2	G	182	THR
2	G	185	ARG
2	G	192	SER
2	G	196	GLU
2	G	200	LEU
2	G	206	THR
2	G	235	THR
2	G	237	LYS

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Mol	Chain	Res	Type
2	G	254	LEU
2	G	256	SER
2	G	259	VAL
2	G	263	ILE
2	G	272	VAL
2	G	273	LYS
2	G	278	LEU
2	G	284	ASP
2	G	309	ASN
2	G	311	PRO
2	G	313	SER
2	G	314	ILE
2	H	36[A]	MET
2	H	36[B]	MET
2	H	38	SER
2	H	52	LEU
2	H	59	SER
2	H	61	GLN
2	H	62	ILE
2	H	68	THR
2	H	72	SER
2	H	78	SER
2	H	84	ASN
2	H	86	ASN
2	H	92	THR
2	H	93	SER
2	H	106	ILE
2	H	107	THR
2	H	116	ARG
2	H	121	THR
2	H	145	SER
2	H	154	SER
2	H	165	LYS
2	H	166	THR
2	H	170	SER
2	H	171	LEU
2	H	182	THR
2	H	184[A]	GLU
2	H	184[B]	GLU
2	H	189	THR
2	H	194	ASP
2	H	208	ARG

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Mol	Chain	Res	Type
2	H	209	LEU
2	H	211	LEU
2	H	242	LEU
2	H	243	THR
2	H	245	THR
2	H	247	THR
2	H	263	ILE
2	H	269	ASN
2	H	274	LEU
2	H	277	SER
2	H	292	ASP
2	H	297	VAL
2	H	315	LEU
2	H	317	GLN
2	I	38	SER
2	I	60	SER
2	I	61	GLN
2	I	62	ILE
2	I	67	GLU
2	I	68	THR
2	I	76	THR
2	I	79	LYS
2	I	80	GLU
2	I	84	ASN
2	I	107	THR
2	I	113	THR
2	I	120	THR
2	I	125	ASN
2	I	135	THR
2	I	142[A]	ILE
2	I	149	ILE
2	I	163	LEU
2	I	167	SER
2	I	171	LEU
2	I	184[A]	GLU
2	I	184[B]	GLU
2	I	185	ARG
2	I	189	THR
2	I	209	LEU
2	I	222	ASN
2	I	223	LEU
2	I	254	LEU

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Mol	Chain	Res	Type
2	I	265	SER
2	I	267	ASN
2	I	272	VAL
2	I	305	SER
2	I	313	SER
2	I	315	LEU
2	I	317	GLN
2	I	318	LYS
2	J	48	ASP
2	J	58	VAL
2	J	70	THR
2	J	71	PHE
2	J	74	SER
2	J	76	THR
2	J	79	LYS
2	J	84	ASN
2	J	86	ASN
2	J	89	VAL
2	J	97	GLN
2	J	114	ILE
2	J	115	GLU
2	J	117	SER
2	J	148	ASN
2	J	154	SER
2	J	156	TYR
2	J	161	ILE
2	J	163	LEU
2	J	164	SER
2	J	190	VAL
2	J	192	SER
2	J	198	GLU
2	J	223	LEU
2	J	236	GLN
2	J	237	LYS
2	J	254	LEU
2	J	256	SER
2	J	258	ILE
2	J	263	ILE
2	J	265	SER
2	J	272	VAL
2	J	284	ASP
2	J	289	ILE

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Mol	Chain	Res	Type
2	J	297	VAL
2	J	299	VAL
2	J	313	SER
2	J	315	LEU
2	J	317	GLN
2	K	38	SER
2	K	44	ILE
2	K	59	SER
2	K	61	GLN
2	K	62	ILE
2	K	79	LYS
2	K	84	ASN
2	K	92	THR
2	K	113	THR
2	K	117	SER
2	K	154	SER
2	K	164	SER
2	K	166	THR
2	K	169	ASP
2	K	182	THR
2	K	185	ARG
2	K	189	THR
2	K	192	SER
2	K	198	GLU
2	K	206	THR
2	K	208	ARG
2	K	209	LEU
2	K	231	SER
2	K	240	LEU
2	K	243	THR
2	K	245	THR
2	K	247	THR
2	K	263	ILE
2	K	269	ASN
2	K	270	ASN
2	K	274	LEU
2	K	275	GLU
2	K	277	SER
2	K	284	ASP
2	K	289	ILE
2	K	295	GLN
2	K	305	SER

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Mol	Chain	Res	Type
2	K	315	LEU
2	L	38	SER
2	L	39	ASP
2	L	57	VAL
2	L	74	SER
2	L	77	LYS
2	L	79	LYS
2	L	93	SER
2	L	125	ASN
2	L	135	THR
2	L	154	SER
2	L	156	TYR
2	L	157	LYS
2	L	165	LYS
2	L	167	SER
2	L	170	SER
2	L	171	LEU
2	L	179	LEU
2	L	180	ILE
2	L	184[A]	GLU
2	L	184[B]	GLU
2	L	185	ARG
2	L	188	LEU
2	L	190	VAL
2	L	192	SER
2	L	210	ASN
2	L	211	LEU
2	L	213	ASP
2	L	223	LEU
2	L	231	SER
2	L	243	THR
2	L	245	THR
2	L	249	GLN
2	L	251	TYR
2	L	254	LEU
2	L	258	ILE
2	L	262	ASN
2	L	263	ILE
2	L	267	ASN
2	L	269	ASN
2	L	270	ASN
2	L	284	ASP

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Mol	Chain	Res	Type
2	L	292	ASP
2	L	317	GLN
2	M	62	ILE
2	M	68	THR
2	M	74	SER
2	M	76	THR
2	M	79	LYS
2	M	84	ASN
2	M	88	SER
2	M	89	VAL
2	M	92	THR
2	M	107	THR
2	M	112	ASN
2	M	113	THR
2	M	119	SER
2	M	120	THR
2	M	121	THR
2	M	125	ASN
2	M	145	SER
2	M	154	SER
2	M	155	ILE
2	M	156	TYR
2	M	157	LYS
2	M	165	LYS
2	M	170	SER
2	M	171	LEU
2	M	182	THR
2	M	190	VAL
2	M	194	ASP
2	M	198	GLU
2	M	208	ARG
2	M	211	LEU
2	M	213	ASP
2	M	223	LEU
2	M	236	GLN
2	M	254	LEU
2	M	259	VAL
2	M	269	ASN
2	M	284	ASP
2	M	287	VAL
2	M	290	SER
2	M	300	MET

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Mol	Chain	Res	Type
2	M	305	SER
2	M	315	LEU
2	N	36[A]	MET
2	N	36[B]	MET
2	N	38	SER
2	N	60	SER
2	N	61	GLN
2	N	62	ILE
2	N	74	SER
2	N	83	ILE
2	N	89	VAL
2	N	92	THR
2	N	110	GLU
2	N	120	THR
2	N	136	TYR
2	N	149	ILE
2	N	150	SER
2	N	154	SER
2	N	161	ILE
2	N	167	SER
2	N	176	GLN
2	N	178	SER
2	N	182	THR
2	N	184[A]	GLU
2	N	184[B]	GLU
2	N	188	LEU
2	N	189	THR
2	N	193[A]	THR
2	N	193[B]	THR
2	N	195	ILE
2	N	196	GLU
2	N	223	LEU
2	N	244	ILE
2	N	247	THR
2	N	256	SER
2	N	258	ILE
2	N	259	VAL
2	N	269	ASN
2	N	270	ASN
2	N	271	LEU
2	N	272	VAL
2	N	280	ASP

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Mol	Chain	Res	Type
2	N	282	VAL
2	N	284	ASP
2	N	292	ASP
2	N	309	ASN
2	O	36[A]	MET
2	O	36[B]	MET
2	O	38	SER
2	O	39	ASP
2	O	51	ILE
2	O	62	ILE
2	O	73	GLN
2	O	74	SER
2	O	76	THR
2	O	93	SER
2	O	97	GLN
2	O	108	ILE
2	O	113	THR
2	O	118	VAL
2	O	120	THR
2	O	149	ILE
2	O	161	ILE
2	O	167	SER
2	O	174	ILE
2	O	185	ARG
2	O	206	THR
2	O	209	LEU
2	O	223	LEU
2	O	253	ILE
2	O	254	LEU
2	O	258	ILE
2	O	263	ILE
2	O	275	GLU
2	O	284	ASP
2	O	289	ILE
2	O	292	ASP
2	O	305	SER
2	O	307	SER
1	R	149	ASN
1	S	149	ASN
1	T	151	LEU
1	V	150	PRO
1	W	149	ASN

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Mol	Chain	Res	Type
1	X	150	PRO
1	Y	149	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	149	ASN
2	A	111	GLN
2	A	241	HIS
2	B	241	HIS
2	C	64	ASN
2	D	86	ASN
2	F	66	ASN
2	G	66	ASN
2	G	86	ASN
2	G	111	GLN
2	G	173	ASN
2	G	317	GLN
2	H	66	ASN
2	H	84	ASN
2	H	111	GLN
2	H	173	ASN
2	H	269	ASN
2	I	173	ASN
2	I	317	GLN
2	J	86	ASN
2	J	266	ASN
2	K	64	ASN
2	K	86	ASN
2	K	111	GLN
2	K	173	ASN
2	L	86	ASN
2	L	111	GLN
2	L	173	ASN
2	L	236	GLN
2	L	269	ASN
2	M	66	ASN
2	M	73	GLN
2	M	86	ASN
2	M	111	GLN
2	M	112	ASN
2	M	148	ASN

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Mol	Chain	Res	Type
2	M	236	GLN
2	N	216	ASN
2	N	262	ASN
2	N	269	ASN
2	N	276	GLN
2	N	317	GLN
2	O	73	GLN
2	O	86	ASN
2	O	111	GLN
2	O	173	ASN
1	W	149	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	9/20 (45%)	-0.70	0 100 100	133, 141, 145, 158	0
1	2	9/20 (45%)	-0.42	0 100 100	120, 130, 150, 156	0
1	3	9/20 (45%)	-0.59	0 100 100	123, 129, 138, 144	0
1	4	9/20 (45%)	-0.20	0 100 100	108, 117, 143, 145	0
1	P	9/20 (45%)	-0.49	0 100 100	125, 137, 144, 155	0
1	Q	9/20 (45%)	-0.54	0 100 100	103, 113, 129, 169	0
1	R	9/20 (45%)	-0.32	0 100 100	103, 111, 128, 147	0
1	S	9/20 (45%)	-0.33	0 100 100	84, 93, 127, 141	0
1	T	9/20 (45%)	-0.27	0 100 100	140, 148, 156, 157	0
1	U	9/20 (45%)	-0.32	0 100 100	114, 128, 150, 168	0
1	V	9/20 (45%)	-0.42	0 100 100	117, 123, 150, 176	0
1	W	9/20 (45%)	-0.41	0 100 100	116, 127, 138, 142	0
1	X	9/20 (45%)	-0.63	0 100 100	126, 138, 147, 152	0
1	Y	9/20 (45%)	-0.33	0 100 100	115, 123, 137, 137	0
1	Z	9/20 (45%)	-0.79	0 100 100	111, 121, 144, 145	0
2	A	286/286 (100%)	0.11	7 (2%) 62 63	86, 119, 163, 203	1 (0%)
2	B	286/286 (100%)	0.05	8 (2%) 56 58	75, 113, 184, 198	1 (0%)
2	C	286/286 (100%)	0.04	5 (1%) 73 74	71, 104, 161, 207	1 (0%)
2	D	286/286 (100%)	-0.04	5 (1%) 73 74	72, 103, 144, 187	1 (0%)
2	E	286/286 (100%)	0.15	9 (3%) 52 55	81, 123, 167, 195	1 (0%)
2	F	286/286 (100%)	-0.00	5 (1%) 73 74	82, 118, 165, 206	1 (0%)
2	G	286/286 (100%)	0.04	6 (2%) 67 68	75, 113, 165, 210	1 (0%)
2	H	286/286 (100%)	-0.03	4 (1%) 78 80	79, 111, 154, 190	1 (0%)
2	I	286/286 (100%)	0.03	4 (1%) 78 80	84, 117, 160, 184	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	J	286/286 (100%)	0.06	8 (2%)	56	58	80, 123, 168, 222	1 (0%)
2	K	286/286 (100%)	0.00	4 (1%)	78	80	84, 112, 155, 199	1 (0%)
2	L	286/286 (100%)	0.03	5 (1%)	73	74	79, 120, 159, 180	1 (0%)
2	M	286/286 (100%)	0.00	3 (1%)	84	86	69, 114, 152, 189	1 (0%)
2	N	286/286 (100%)	-0.06	1 (0%)	94	95	71, 110, 154, 186	1 (0%)
2	O	286/286 (100%)	-0.04	2 (0%)	89	90	72, 111, 153, 184	1 (0%)
All	All	4425/4590 (96%)	0.01	76 (1%)	73	74	69, 115, 161, 222	15 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	34	GLY	7.6
2	F	34	GLY	7.3
2	C	35	ALA	6.1
2	M	34	GLY	5.2
2	C	34	GLY	5.2
2	A	34	GLY	4.9
2	J	35	ALA	4.6
2	D	34	GLY	4.6
2	L	34	GLY	4.5
2	I	35	ALA	4.3
2	D	35	ALA	4.0
2	O	35	ALA	3.9
2	B	35	ALA	3.9
2	B	34	GLY	3.7
2	E	319	PHE	3.5
2	G	34	GLY	3.5
2	A	291	LEU	3.5
2	B	36[A]	MET	3.4
2	G	313	SER	3.4
2	F	35	ALA	3.4
2	C	36[A]	MET	3.2
2	E	34	GLY	3.2
2	B	71	PHE	3.1
2	J	141	ALA	3.1
2	H	34	GLY	3.1
2	E	35	ALA	3.1
2	E	253	ILE	3.1
2	A	36[A]	MET	3.1
2	B	125	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	251	TYR	3.0
2	L	214	ALA	3.0
2	O	34	GLY	2.9
2	A	211	LEU	2.9
2	H	35	ALA	2.9
2	A	289	ILE	2.9
2	B	171	LEU	2.8
2	B	63	LEU	2.8
2	H	125	ASN	2.8
2	J	127	TYR	2.8
2	F	316	PHE	2.8
2	E	36[A]	MET	2.8
2	A	171	LEU	2.7
2	I	34	GLY	2.6
2	E	37	GLY	2.6
2	K	35	ALA	2.6
2	L	36[A]	MET	2.6
2	J	40	GLY	2.5
2	D	36[A]	MET	2.5
2	B	120	THR	2.5
2	F	171	LEU	2.5
2	D	168	ALA	2.5
2	H	128	VAL	2.4
2	E	289	ILE	2.4
2	A	35	ALA	2.4
2	M	36[A]	MET	2.3
2	F	36[A]	MET	2.3
2	J	36[A]	MET	2.3
2	M	35	ALA	2.3
2	C	141	ALA	2.2
2	G	36[A]	MET	2.2
2	I	36[A]	MET	2.2
2	G	35	ALA	2.2
2	G	319	PHE	2.2
2	J	53	GLY	2.2
2	G	168	ALA	2.2
2	I	255	ALA	2.1
2	D	142[A]	ILE	2.1
2	L	35	ALA	2.1
2	E	281	GLY	2.1
2	K	34	GLY	2.1
2	K	168	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	63	LEU	2.1
2	N	253	ILE	2.0
2	J	156	TYR	2.0
2	K	37	GLY	2.0
2	L	215	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.