



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2019 – 07:53 PM EDT

PDB ID : 6QWP
Title : Crystal structure of T7 bacteriophage portal protein, 13mer, closed valve
Authors : Fabrega-Ferrer, M.; Cuervo, A.; Machon, C.; Fernandez, F.J.; Perez-Luque, R.; Pous, J.; Vega, M.C.; Carrascosa, J.L.; Coll, M.
Deposited on : 2019-03-06
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

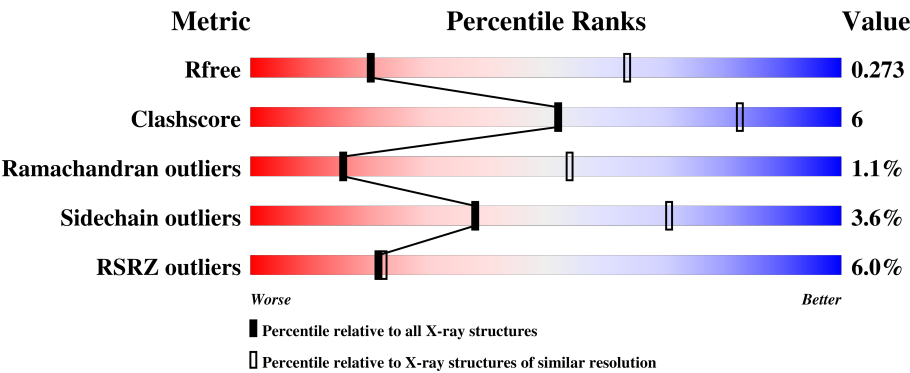
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 3.40 Å.

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




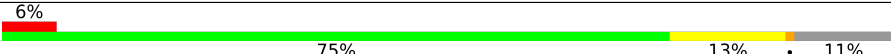
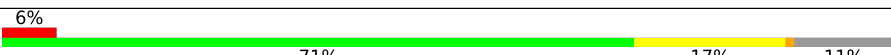
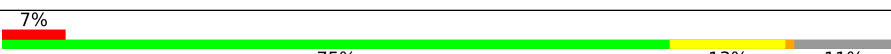
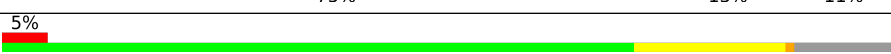
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	111664	1928 (3.50-3.30)
Clashscore	122126	2051 (3.50-3.30)
Ramachandran outliers	120053	2006 (3.50-3.30)
Sidechain outliers	120020	2006 (3.50-3.30)
RSRZ outliers	108989	1827 (3.50-3.30)

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	A	547	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>74%14%•11%</div></div>
1	B	547	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>73%16%•11%</div></div>
1	C	547	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>74%15%•11%</div></div>
1	D	547	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>75%13%•11%</div></div>
1	E	547	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>72%17%•11%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 49530 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 Portal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	B	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	C	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	D	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	E	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	F	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	G	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	H	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	I	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	J	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	K	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	L	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			
1	M	486	Total	C	N	O	S	0	0	0
			3810	2397	646	749	18			

There are 143 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	ALA	-	expression tag	UNP P03728
A	538	ALA	-	expression tag	UNP P03728
A	539	ALA	-	expression tag	UNP P03728

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Chain	Residue	Modelled	Actual	Comment	Reference
A	540	LEU	-	expression tag	UNP P03728
A	541	GLU	-	expression tag	UNP P03728
A	542	HIS	-	expression tag	UNP P03728
A	543	HIS	-	expression tag	UNP P03728
A	544	HIS	-	expression tag	UNP P03728
A	545	HIS	-	expression tag	UNP P03728
A	546	HIS	-	expression tag	UNP P03728
A	547	HIS	-	expression tag	UNP P03728
B	537	ALA	-	expression tag	UNP P03728
B	538	ALA	-	expression tag	UNP P03728
B	539	ALA	-	expression tag	UNP P03728
B	540	LEU	-	expression tag	UNP P03728
B	541	GLU	-	expression tag	UNP P03728
B	542	HIS	-	expression tag	UNP P03728
B	543	HIS	-	expression tag	UNP P03728
B	544	HIS	-	expression tag	UNP P03728
B	545	HIS	-	expression tag	UNP P03728
B	546	HIS	-	expression tag	UNP P03728
B	547	HIS	-	expression tag	UNP P03728
C	537	ALA	-	expression tag	UNP P03728
C	538	ALA	-	expression tag	UNP P03728
C	539	ALA	-	expression tag	UNP P03728
C	540	LEU	-	expression tag	UNP P03728
C	541	GLU	-	expression tag	UNP P03728
C	542	HIS	-	expression tag	UNP P03728
C	543	HIS	-	expression tag	UNP P03728
C	544	HIS	-	expression tag	UNP P03728
C	545	HIS	-	expression tag	UNP P03728
C	546	HIS	-	expression tag	UNP P03728
C	547	HIS	-	expression tag	UNP P03728
D	537	ALA	-	expression tag	UNP P03728
D	538	ALA	-	expression tag	UNP P03728
D	539	ALA	-	expression tag	UNP P03728
D	540	LEU	-	expression tag	UNP P03728
D	541	GLU	-	expression tag	UNP P03728
D	542	HIS	-	expression tag	UNP P03728
D	543	HIS	-	expression tag	UNP P03728
D	544	HIS	-	expression tag	UNP P03728
D	545	HIS	-	expression tag	UNP P03728
D	546	HIS	-	expression tag	UNP P03728
D	547	HIS	-	expression tag	UNP P03728
E	537	ALA	-	expression tag	UNP P03728

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Chain	Residue	Modelled	Actual	Comment	Reference
E	538	ALA	-	expression tag	UNP P03728
E	539	ALA	-	expression tag	UNP P03728
E	540	LEU	-	expression tag	UNP P03728
E	541	GLU	-	expression tag	UNP P03728
E	542	HIS	-	expression tag	UNP P03728
E	543	HIS	-	expression tag	UNP P03728
E	544	HIS	-	expression tag	UNP P03728
E	545	HIS	-	expression tag	UNP P03728
E	546	HIS	-	expression tag	UNP P03728
E	547	HIS	-	expression tag	UNP P03728
F	537	ALA	-	expression tag	UNP P03728
F	538	ALA	-	expression tag	UNP P03728
F	539	ALA	-	expression tag	UNP P03728
F	540	LEU	-	expression tag	UNP P03728
F	541	GLU	-	expression tag	UNP P03728
F	542	HIS	-	expression tag	UNP P03728
F	543	HIS	-	expression tag	UNP P03728
F	544	HIS	-	expression tag	UNP P03728
F	545	HIS	-	expression tag	UNP P03728
F	546	HIS	-	expression tag	UNP P03728
F	547	HIS	-	expression tag	UNP P03728
G	537	ALA	-	expression tag	UNP P03728
G	538	ALA	-	expression tag	UNP P03728
G	539	ALA	-	expression tag	UNP P03728
G	540	LEU	-	expression tag	UNP P03728
G	541	GLU	-	expression tag	UNP P03728
G	542	HIS	-	expression tag	UNP P03728
G	543	HIS	-	expression tag	UNP P03728
G	544	HIS	-	expression tag	UNP P03728
G	545	HIS	-	expression tag	UNP P03728
G	546	HIS	-	expression tag	UNP P03728
G	547	HIS	-	expression tag	UNP P03728
H	537	ALA	-	expression tag	UNP P03728
H	538	ALA	-	expression tag	UNP P03728
H	539	ALA	-	expression tag	UNP P03728
H	540	LEU	-	expression tag	UNP P03728
H	541	GLU	-	expression tag	UNP P03728
H	542	HIS	-	expression tag	UNP P03728
H	543	HIS	-	expression tag	UNP P03728
H	544	HIS	-	expression tag	UNP P03728
H	545	HIS	-	expression tag	UNP P03728
H	546	HIS	-	expression tag	UNP P03728

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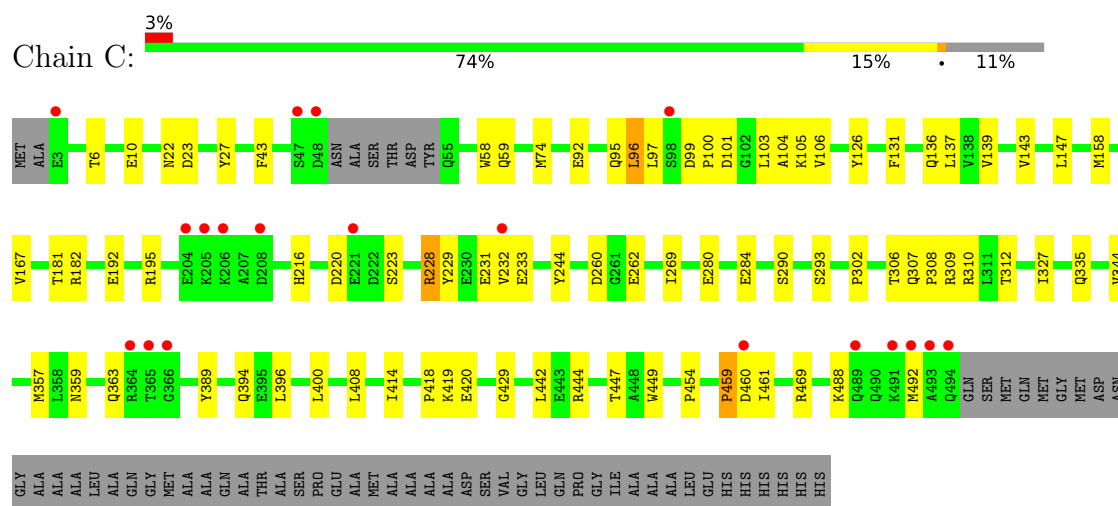
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Chain	Residue	Modelled	Actual	Comment	Reference
H	547	HIS	-	expression tag	UNP P03728
I	537	ALA	-	expression tag	UNP P03728
I	538	ALA	-	expression tag	UNP P03728
I	539	ALA	-	expression tag	UNP P03728
I	540	LEU	-	expression tag	UNP P03728
I	541	GLU	-	expression tag	UNP P03728
I	542	HIS	-	expression tag	UNP P03728
I	543	HIS	-	expression tag	UNP P03728
I	544	HIS	-	expression tag	UNP P03728
I	545	HIS	-	expression tag	UNP P03728
I	546	HIS	-	expression tag	UNP P03728
I	547	HIS	-	expression tag	UNP P03728
J	537	ALA	-	expression tag	UNP P03728
J	538	ALA	-	expression tag	UNP P03728
J	539	ALA	-	expression tag	UNP P03728
J	540	LEU	-	expression tag	UNP P03728
J	541	GLU	-	expression tag	UNP P03728
J	542	HIS	-	expression tag	UNP P03728
J	543	HIS	-	expression tag	UNP P03728
J	544	HIS	-	expression tag	UNP P03728
J	545	HIS	-	expression tag	UNP P03728
J	546	HIS	-	expression tag	UNP P03728
J	547	HIS	-	expression tag	UNP P03728
K	537	ALA	-	expression tag	UNP P03728
K	538	ALA	-	expression tag	UNP P03728
K	539	ALA	-	expression tag	UNP P03728
K	540	LEU	-	expression tag	UNP P03728
K	541	GLU	-	expression tag	UNP P03728
K	542	HIS	-	expression tag	UNP P03728
K	543	HIS	-	expression tag	UNP P03728
K	544	HIS	-	expression tag	UNP P03728
K	545	HIS	-	expression tag	UNP P03728
K	546	HIS	-	expression tag	UNP P03728
K	547	HIS	-	expression tag	UNP P03728
L	537	ALA	-	expression tag	UNP P03728
L	538	ALA	-	expression tag	UNP P03728
L	539	ALA	-	expression tag	UNP P03728
L	540	LEU	-	expression tag	UNP P03728
L	541	GLU	-	expression tag	UNP P03728
L	542	HIS	-	expression tag	UNP P03728
L	543	HIS	-	expression tag	UNP P03728
L	544	HIS	-	expression tag	UNP P03728

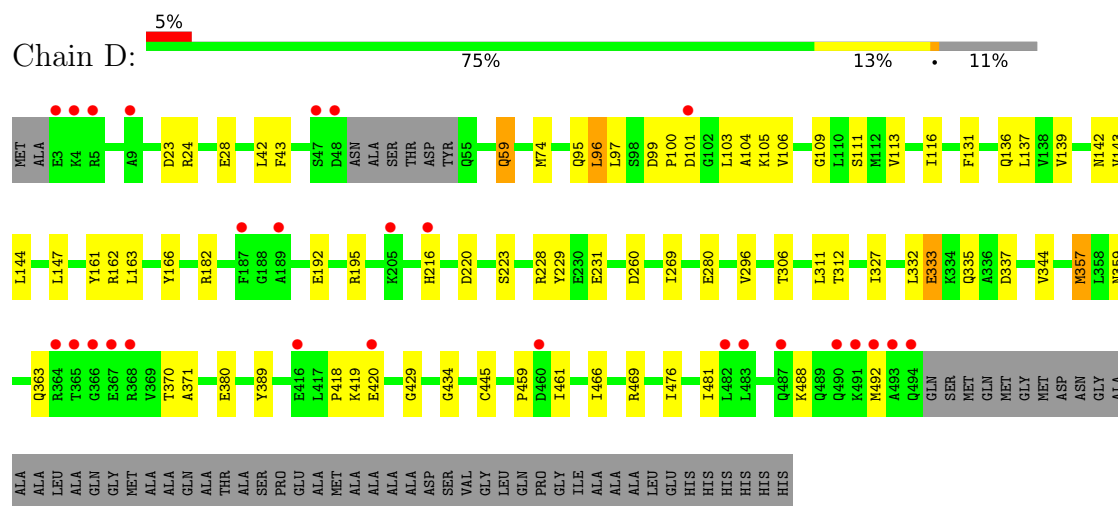
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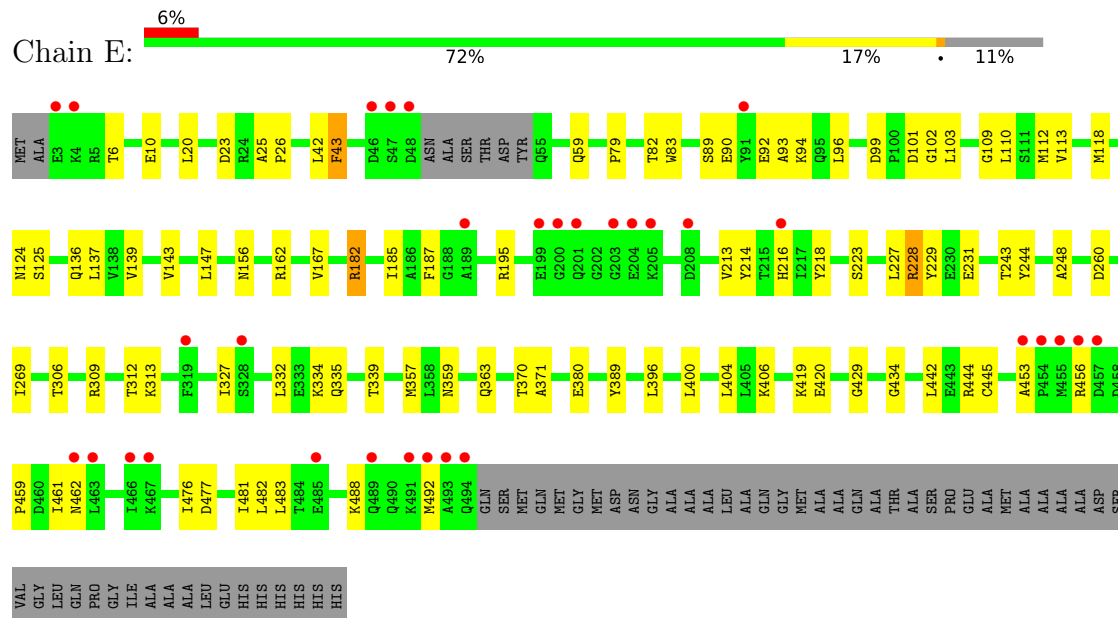
Chain	Residue	Modelled	Actual	Comment	Reference
L	545	HIS	-	expression tag	UNP P03728
L	546	HIS	-	expression tag	UNP P03728
L	547	HIS	-	expression tag	UNP P03728
M	537	ALA	-	expression tag	UNP P03728
M	538	ALA	-	expression tag	UNP P03728
M	539	ALA	-	expression tag	UNP P03728
M	540	LEU	-	expression tag	UNP P03728
M	541	GLU	-	expression tag	UNP P03728
M	542	HIS	-	expression tag	UNP P03728
M	543	HIS	-	expression tag	UNP P03728
M	544	HIS	-	expression tag	UNP P03728
M	545	HIS	-	expression tag	UNP P03728
M	546	HIS	-	expression tag	UNP P03728
M	547	HIS	-	expression tag	UNP P03728



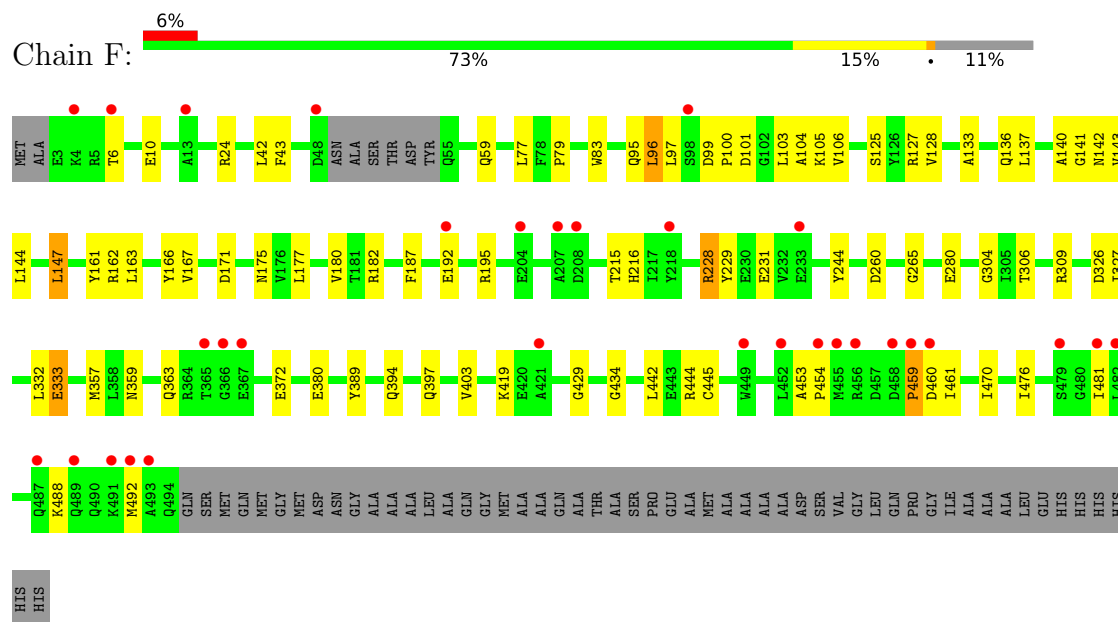
- Molecule 1: Portal protein



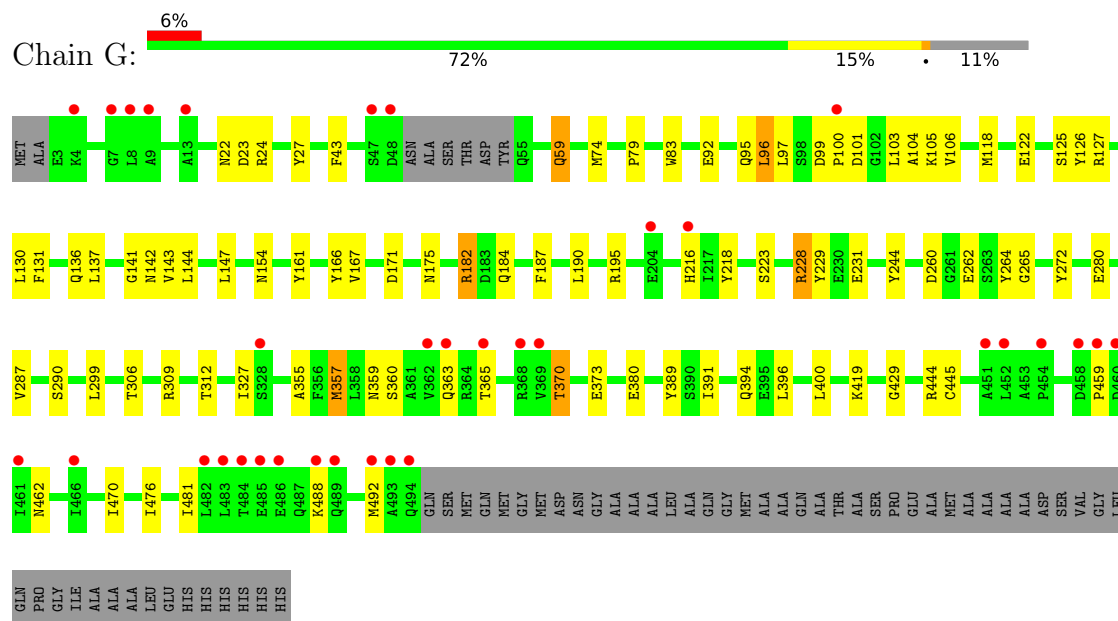
- Molecule 1: Portal protein



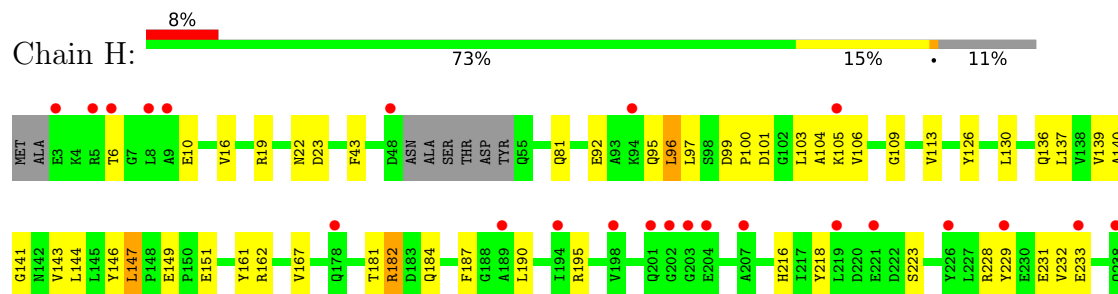
- Molecule 1: Portal protein

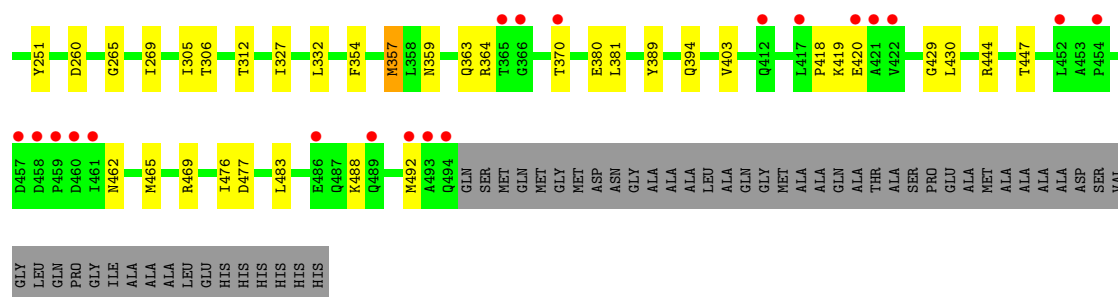


- Molecule 1: Portal protein

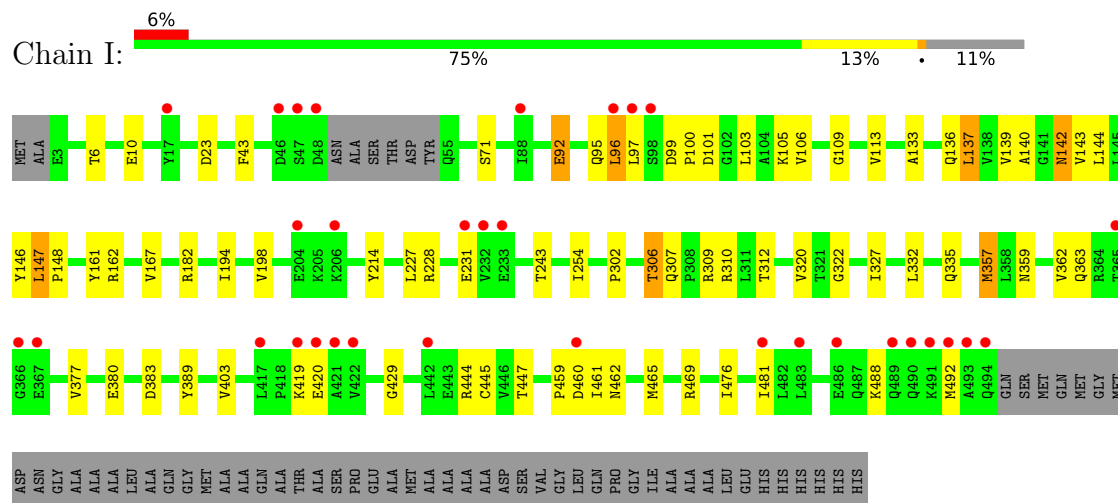


- Molecule 1: Portal protein

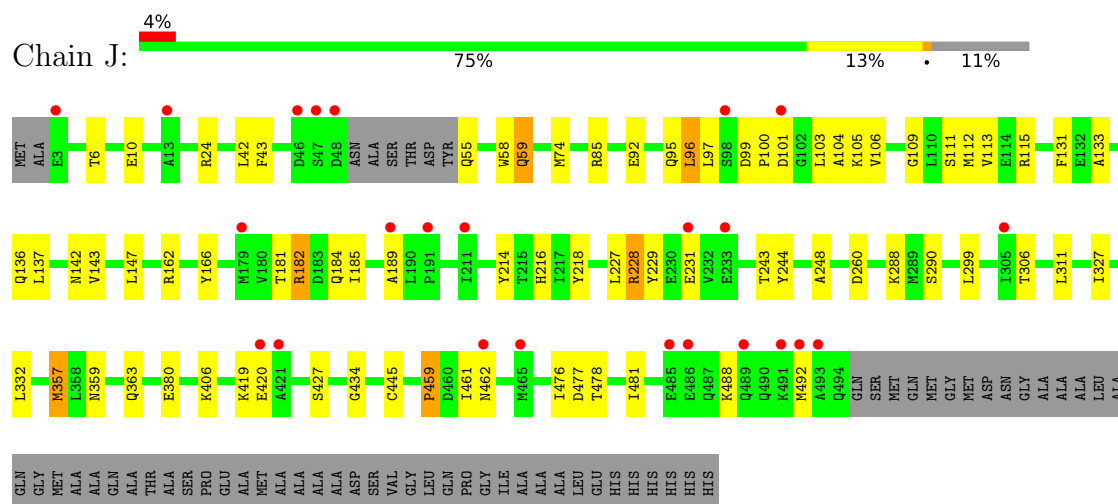




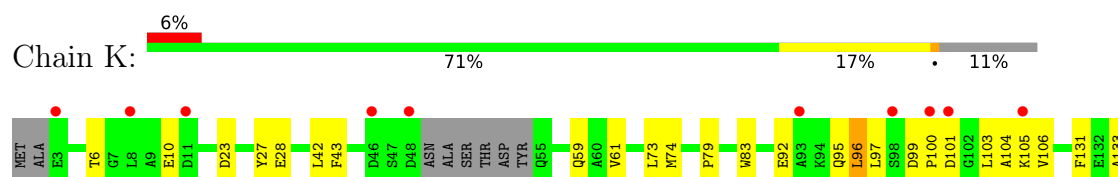
• Molecule 1: Portal protein

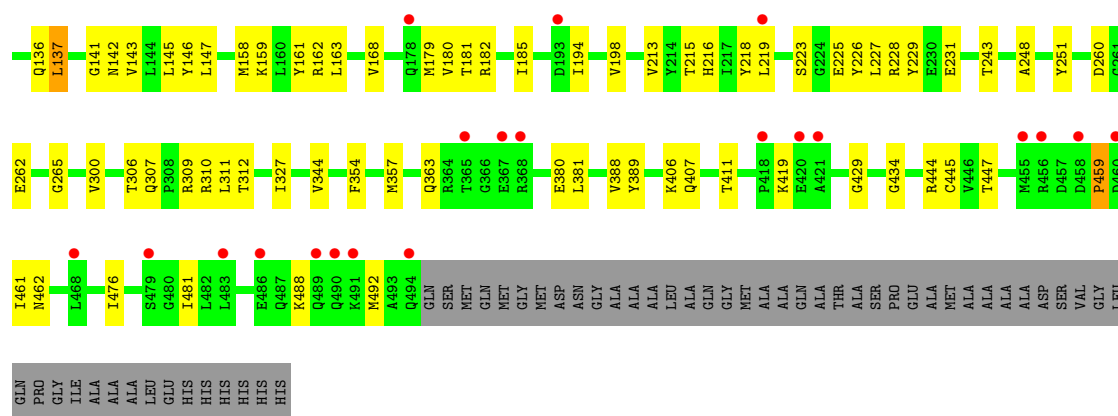


• Molecule 1: Portal protein

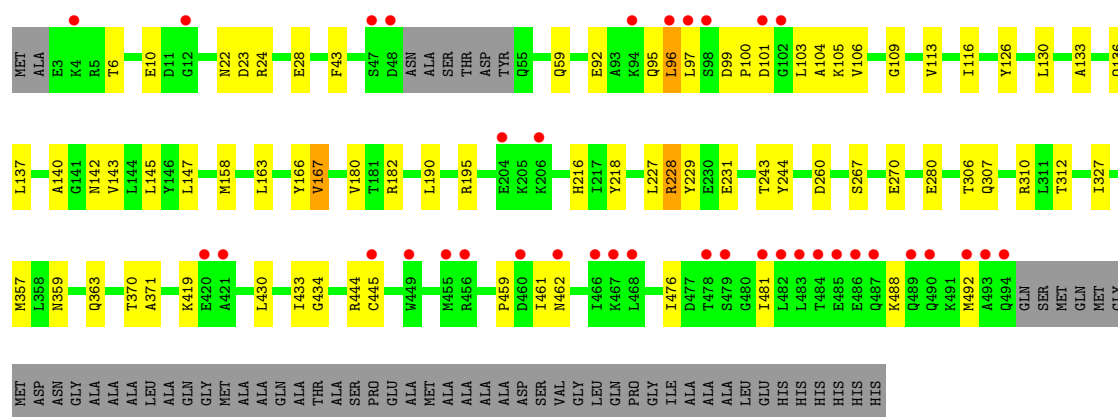
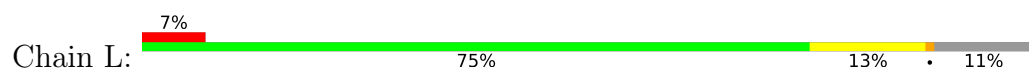


• Molecule 1: Portal protein

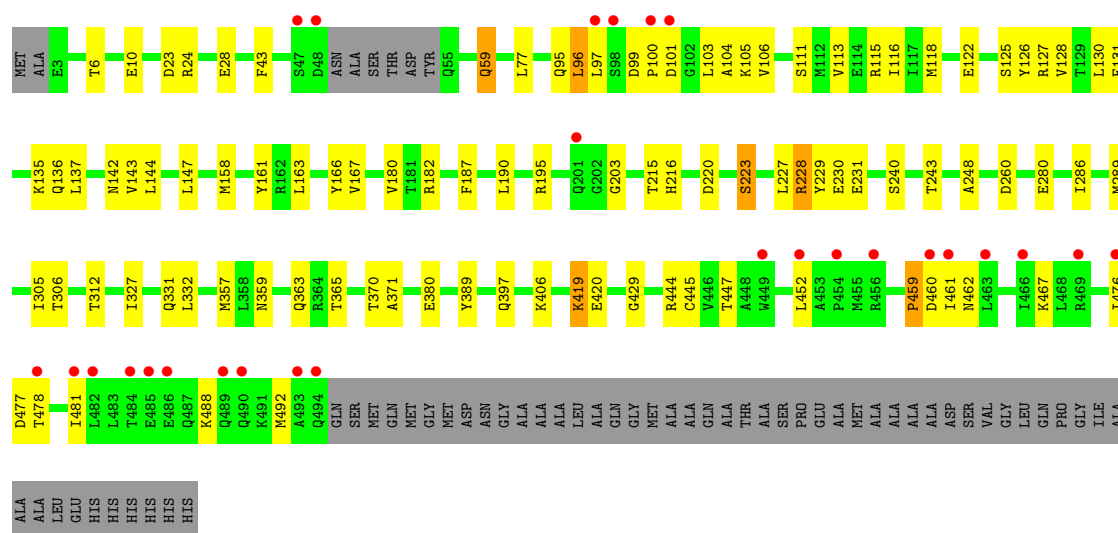
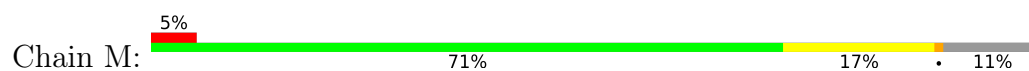




• Molecule 1: Portal protein



• Molecule 1: Portal protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	261.57Å 261.57Å 256.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.56 – 3.40 58.49 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (58.56-3.40) 95.8 (58.49-3.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.230 , 0.275 0.229 , 0.273	Depositor DCC
R_{free} test set	5822 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for -h,-l,-k 0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	49530	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/3868	0.61	0/5232
1	B	0.40	0/3868	0.63	0/5232
1	C	0.40	0/3868	0.62	0/5232
1	D	0.40	0/3868	0.62	0/5232
1	E	0.40	0/3868	0.62	0/5232
1	F	0.40	0/3868	0.61	0/5232
1	G	0.39	0/3868	0.62	0/5232
1	H	0.40	0/3868	0.62	0/5232
1	I	0.40	0/3868	0.63	0/5232
1	J	0.40	0/3868	0.63	0/5232
1	K	0.39	0/3868	0.61	0/5232
1	L	0.38	0/3868	0.61	0/5232
1	M	0.39	0/3868	0.61	0/5232
All	All	0.40	0/50284	0.62	0/68016

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	M	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	228	ARG	Sidechain

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	3810	0	3823	58	0
1	B	3810	0	3823	49	0
1	C	3810	0	3823	49	0
1	D	3810	0	3823	41	0
1	E	3810	0	3823	57	0
1	F	3810	0	3823	53	0
1	G	3810	0	3823	54	0
1	H	3810	0	3823	52	0
1	I	3810	0	3823	45	0
1	J	3810	0	3823	47	0
1	K	3810	0	3823	57	0
1	L	3810	0	3823	44	0
1	M	3810	0	3823	61	0
All	All	49530	0	49699	596	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD13	1:A:143:VAL:HG23	1.29	1.11
1:J:137:LEU:HD13	1:J:143:VAL:HG23	1.53	0.91
1:A:137:LEU:HD13	1:A:143:VAL:CG2	2.02	0.89
1:M:137:LEU:HD13	1:M:143:VAL:HG23	1.60	0.84
1:E:92:GLU:HG2	1:E:420:GLU:HA	1.63	0.80
1:B:478:THR:HA	1:B:481:ILE:HD12	1.64	0.79
1:C:137:LEU:HD13	1:C:143:VAL:HG23	1.66	0.77
1:J:311:LEU:HD11	1:J:327:ILE:HD11	1.66	0.76
1:L:306:THR:HG21	1:L:327:ILE:HD11	1.66	0.76
1:E:483:LEU:HB2	1:F:460:ASP:HA	1.67	0.76
1:I:137:LEU:HD13	1:I:143:VAL:HG23	1.69	0.74
1:I:142:ASN:HB3	1:I:254:ILE:O	1.86	0.74
1:K:311:LEU:HD11	1:K:327:ILE:HD11	1.69	0.73
1:D:137:LEU:HD13	1:D:143:VAL:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:THR:HG21	1:G:327:ILE:HD11	1.70	0.72
1:K:168:VAL:HG22	1:K:179:MET:HG2	1.71	0.72
1:E:137:LEU:HD13	1:E:143:VAL:HG23	1.70	0.72
1:I:306:THR:HG23	1:I:322:GLY:HA3	1.71	0.72
1:F:137:LEU:HD13	1:F:143:VAL:HG23	1.73	0.71
1:I:306:THR:HG21	1:I:327:ILE:HD11	1.73	0.70
1:A:389:TYR:OH	1:A:429:GLY:HA2	1.93	0.69
1:K:306:THR:HG21	1:K:327:ILE:HD11	1.73	0.69
1:G:24:ARG:NH1	1:G:166:TYR:O	2.22	0.69
1:M:478:THR:HA	1:M:481:ILE:HD12	1.74	0.69
1:K:137:LEU:HD13	1:K:143:VAL:HG23	1.76	0.67
1:L:137:LEU:HD13	1:L:143:VAL:HG23	1.75	0.67
1:B:103:LEU:O	1:B:106:VAL:N	2.26	0.66
1:H:190:LEU:O	1:H:195:ARG:NH1	2.29	0.66
1:E:89:SER:OG	1:E:92:GLU:HB2	1.97	0.65
1:H:136:GLN:OE1	1:H:162:ARG:NH1	2.30	0.65
1:A:103:LEU:O	1:A:106:VAL:N	2.27	0.65
1:B:306:THR:HG21	1:B:327:ILE:HD11	1.79	0.64
1:M:306:THR:HG21	1:M:327:ILE:HD11	1.79	0.64
1:G:389:TYR:OH	1:G:429:GLY:HA2	1.96	0.64
1:F:103:LEU:O	1:F:106:VAL:N	2.31	0.64
1:H:137:LEU:HD13	1:H:143:VAL:HG23	1.80	0.64
1:A:483:LEU:HD12	1:B:460:ASP:HA	1.80	0.64
1:G:103:LEU:O	1:G:106:VAL:N	2.30	0.64
1:G:59:GLN:HG3	1:G:280:GLU:OE1	1.97	0.64
1:D:306:THR:HG21	1:D:327:ILE:HD11	1.77	0.64
1:M:389:TYR:OH	1:M:429:GLY:HA2	1.98	0.64
1:C:290:SER:HB3	1:D:344:VAL:HG21	1.79	0.63
1:J:311:LEU:HD11	1:J:327:ILE:CD1	2.27	0.63
1:F:79:PRO:HD2	1:F:83:TRP:CD1	2.34	0.62
1:G:141:GLY:HA3	1:G:265:GLY:O	1.98	0.62
1:B:216:HIS:HB3	1:B:229:TYR:CE1	2.34	0.62
1:M:24:ARG:NH1	1:M:166:TYR:O	2.32	0.62
1:K:434:GLY:O	1:L:444:ARG:NH2	2.33	0.62
1:C:103:LEU:O	1:C:106:VAL:N	2.32	0.62
1:E:306:THR:HG21	1:E:327:ILE:HD11	1.81	0.62
1:A:144:LEU:HD12	1:A:253:PRO:HA	1.82	0.62
1:I:103:LEU:O	1:I:106:VAL:N	2.32	0.62
1:G:359:ASN:HB2	1:H:380:GLU:HB2	1.82	0.61
1:K:103:LEU:O	1:K:106:VAL:N	2.34	0.61
1:A:142:ASN:OD1	1:A:265:GLY:N	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:GLN:HE21	1:C:310:ARG:NH1	1.99	0.61
1:B:137:LEU:HD13	1:B:143:VAL:HG23	1.83	0.60
1:B:290:SER:HB3	1:C:344:VAL:HG21	1.83	0.60
1:A:144:LEU:HD13	1:A:253:PRO:HB3	1.84	0.60
1:F:434:GLY:O	1:G:444:ARG:NH2	2.34	0.59
1:L:103:LEU:O	1:L:106:VAL:N	2.33	0.59
1:D:24:ARG:NH1	1:D:166:TYR:O	2.34	0.59
1:A:354:PHE:HD1	1:A:381:LEU:HD21	1.66	0.59
1:M:190:LEU:O	1:M:195:ARG:NH1	2.35	0.59
1:M:103:LEU:O	1:M:106:VAL:N	2.35	0.58
1:J:103:LEU:O	1:J:106:VAL:N	2.33	0.57
1:K:311:LEU:HD11	1:K:327:ILE:CD1	2.34	0.57
1:L:190:LEU:O	1:L:195:ARG:NH1	2.38	0.57
1:J:216:HIS:HB3	1:J:229:TYR:CE1	2.39	0.57
1:F:187:PHE:CZ	1:F:195:ARG:HG3	2.39	0.57
1:G:228:ARG:HG2	1:G:244:TYR:CE2	2.39	0.57
1:H:103:LEU:O	1:H:106:VAL:N	2.32	0.57
1:B:488:LYS:O	1:B:492:MET:HG2	2.05	0.57
1:D:103:LEU:O	1:D:106:VAL:N	2.36	0.57
1:H:354:PHE:HD1	1:H:381:LEU:HD21	1.68	0.57
1:J:478:THR:HA	1:J:481:ILE:HD12	1.87	0.57
1:L:126:TYR:O	1:L:130:LEU:HD23	2.05	0.56
1:K:227:LEU:HD23	1:K:243:THR:HG22	1.88	0.56
1:K:59:GLN:OE1	1:K:61:VAL:N	2.38	0.56
1:A:144:LEU:HD12	1:A:253:PRO:CA	2.35	0.56
1:C:6:THR:HA	1:C:10:GLU:HA	1.86	0.56
1:K:6:THR:HA	1:K:10:GLU:HA	1.87	0.56
1:E:389:TYR:OH	1:E:429:GLY:HA2	2.06	0.56
1:H:182:ARG:NE	1:H:184:GLN:HE21	2.02	0.56
1:G:136:GLN:HB3	1:G:143:VAL:HG22	1.88	0.56
1:E:371:ALA:HB1	1:F:372:GLU:HG3	1.88	0.56
1:H:182:ARG:NH2	1:H:184:GLN:NE2	2.53	0.56
1:F:481:ILE:O	1:G:462:ASN:HB3	2.06	0.56
1:H:306:THR:HG21	1:H:327:ILE:HD11	1.88	0.56
1:E:42:LEU:O	1:E:162:ARG:NH1	2.39	0.56
1:F:128:VAL:HG23	1:G:391:ILE:HG23	1.88	0.56
1:A:109:GLY:O	1:A:113:VAL:HG23	2.06	0.55
1:K:389:TYR:OH	1:K:429:GLY:HA2	2.07	0.55
1:K:459:PRO:HD2	1:K:461:ILE:HD11	1.89	0.55
1:D:74:MET:SD	1:D:131:PHE:HB2	2.47	0.55
1:F:101:ASP:OD1	1:F:101:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:488:LYS:O	1:I:492:MET:HG2	2.07	0.54
1:D:488:LYS:O	1:D:492:MET:HG2	2.07	0.54
1:I:142:ASN:CB	1:I:254:ILE:O	2.54	0.54
1:H:182:ARG:NH2	1:H:184:GLN:HE21	2.05	0.54
1:K:159:LYS:HE3	1:K:161:TYR:CZ	2.43	0.54
1:B:136:GLN:HB3	1:B:143:VAL:HG22	1.90	0.54
1:C:216:HIS:HB3	1:C:229:TYR:CE1	2.43	0.54
1:D:389:TYR:OH	1:D:429:GLY:HA2	2.08	0.54
1:H:101:ASP:OD1	1:H:101:ASP:N	2.41	0.54
1:E:459:PRO:HD2	1:E:461:ILE:HD11	1.90	0.53
1:E:136:GLN:OE1	1:E:162:ARG:NH1	2.41	0.53
1:H:6:THR:HA	1:H:10:GLU:HA	1.89	0.53
1:H:216:HIS:CE1	1:H:218:TYR:HB3	2.42	0.53
1:M:101:ASP:N	1:M:101:ASP:OD1	2.41	0.53
1:A:302:PRO:HG3	1:M:305:ILE:HG21	1.91	0.53
1:A:380:GLU:HB2	1:M:359:ASN:HB2	1.91	0.53
1:A:359:ASN:HB2	1:B:380:GLU:HB2	1.90	0.53
1:K:488:LYS:O	1:K:492:MET:HG2	2.08	0.53
1:B:478:THR:CA	1:B:481:ILE:HD12	2.35	0.53
1:I:444:ARG:O	1:I:447:THR:HG22	2.08	0.53
1:B:109:GLY:O	1:B:113:VAL:HG23	2.08	0.53
1:C:101:ASP:OD1	1:C:101:ASP:N	2.41	0.53
1:A:327:ILE:HD12	1:B:299:LEU:HD11	1.91	0.53
1:H:109:GLY:O	1:H:113:VAL:HG23	2.09	0.53
1:D:101:ASP:OD1	1:D:101:ASP:N	2.42	0.53
1:E:371:ALA:CB	1:F:372:GLU:HG3	2.39	0.53
1:L:136:GLN:HB3	1:L:143:VAL:HG22	1.90	0.53
1:C:228:ARG:HG2	1:C:244:TYR:CE2	2.44	0.53
1:C:27:TYR:OH	1:C:262:GLU:HG2	2.09	0.52
1:D:59:GLN:HG3	1:D:280:GLU:OE1	2.09	0.52
1:A:394:GLN:OE1	1:M:125:SER:HA	2.08	0.52
1:E:89:SER:O	1:E:93:ALA:HB2	2.10	0.52
1:G:187:PHE:CZ	1:G:195:ARG:HG3	2.44	0.52
1:F:125:SER:HA	1:G:394:GLN:OE1	2.08	0.52
1:G:396:LEU:O	1:G:400:LEU:HB2	2.10	0.52
1:K:307:GLN:HE21	1:K:310:ARG:CZ	2.23	0.52
1:B:478:THR:HA	1:B:481:ILE:CD1	2.37	0.52
1:I:109:GLY:O	1:I:113:VAL:HG23	2.10	0.52
1:K:101:ASP:OD1	1:K:101:ASP:N	2.42	0.52
1:M:445:CYS:CB	1:M:476:ILE:HD11	2.39	0.52
1:C:103:LEU:O	1:C:105:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:ASP:N	1:J:101:ASP:OD1	2.43	0.52
1:A:299:LEU:HD11	1:M:327:ILE:HD12	1.92	0.52
1:D:296:VAL:HG22	1:E:334:LYS:HD3	1.92	0.52
1:L:145:LEU:HD22	1:L:158:MET:SD	2.50	0.52
1:A:101:ASP:OD1	1:A:101:ASP:N	2.43	0.52
1:A:103:LEU:O	1:A:105:LYS:N	2.42	0.52
1:H:182:ARG:HH21	1:H:184:GLN:NE2	2.07	0.52
1:L:6:THR:HA	1:L:10:GLU:HA	1.91	0.52
1:L:24:ARG:NH1	1:L:166:TYR:O	2.33	0.52
1:L:307:GLN:HE21	1:L:310:ARG:NH1	2.07	0.52
1:M:103:LEU:O	1:M:105:LYS:N	2.43	0.52
1:C:306:THR:HG21	1:C:327:ILE:HD11	1.91	0.52
1:F:306:THR:HG21	1:F:327:ILE:HD11	1.92	0.52
1:L:101:ASP:N	1:L:101:ASP:OD1	2.43	0.52
1:M:77:LEU:O	1:M:397:GLN:NE2	2.43	0.52
1:K:141:GLY:HA3	1:K:265:GLY:O	2.10	0.52
1:B:101:ASP:N	1:B:101:ASP:OD1	2.42	0.51
1:C:459:PRO:HD2	1:C:461:ILE:HD11	1.91	0.51
1:L:216:HIS:HB3	1:L:229:TYR:CE1	2.45	0.51
1:J:136:GLN:HB3	1:J:143:VAL:HG22	1.92	0.51
1:L:359:ASN:HB2	1:M:380:GLU:HB2	1.91	0.51
1:F:59:GLN:HG3	1:F:280:GLU:OE1	2.10	0.51
1:D:481:ILE:O	1:E:462:ASN:HB3	2.09	0.51
1:H:139:VAL:HA	1:H:269:ILE:HD12	1.92	0.51
1:F:24:ARG:NH1	1:F:166:TYR:O	2.34	0.51
1:H:182:ARG:CZ	1:H:184:GLN:HE21	2.23	0.51
1:E:481:ILE:O	1:F:461:ILE:O	2.29	0.51
1:B:59:GLN:HG3	1:B:280:GLU:OE1	2.11	0.51
1:I:307:GLN:HE21	1:I:310:ARG:NH1	2.09	0.51
1:L:133:ALA:O	1:L:137:LEU:HB2	2.10	0.51
1:A:135:LYS:O	1:A:139:VAL:HG12	2.12	0.50
1:A:248:ALA:HB2	1:A:406:LYS:CE	2.40	0.50
1:E:309:ARG:HG3	1:E:313:LYS:HE3	1.93	0.50
1:G:101:ASP:N	1:G:101:ASP:OD1	2.44	0.50
1:K:103:LEU:O	1:K:105:LYS:N	2.44	0.50
1:F:216:HIS:HB3	1:F:229:TYR:CE1	2.47	0.50
1:K:445:CYS:CB	1:K:476:ILE:HD11	2.41	0.50
1:D:136:GLN:HB3	1:D:143:VAL:HG22	1.93	0.50
1:I:227:LEU:HD23	1:I:243:THR:HG22	1.92	0.50
1:I:459:PRO:HD2	1:I:461:ILE:HD11	1.94	0.50
1:J:42:LEU:O	1:J:162:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:488:LYS:O	1:J:492:MET:HG2	2.11	0.50
1:I:389:TYR:OH	1:I:429:GLY:HA2	2.11	0.50
1:I:101:ASP:OD1	1:I:101:ASP:N	2.43	0.50
1:M:248:ALA:HB2	1:M:406:LYS:CE	2.42	0.50
1:K:136:GLN:HB3	1:K:143:VAL:HG22	1.93	0.50
1:F:187:PHE:CZ	1:F:195:ARG:CG	2.95	0.50
1:F:445:CYS:CB	1:F:476:ILE:HD11	2.41	0.50
1:J:227:LEU:HD23	1:J:243:THR:HG22	1.93	0.50
1:B:192:GLU:HA	1:B:195:ARG:NH1	2.26	0.50
1:K:306:THR:HG21	1:K:327:ILE:CD1	2.40	0.50
1:K:309:ARG:HB2	1:K:309:ARG:HH11	1.76	0.50
1:M:230:GLU:HG3	1:M:240:SER:HB2	1.94	0.50
1:C:307:GLN:NE2	1:C:310:ARG:CZ	2.75	0.49
1:D:332:LEU:O	1:D:333:GLU:C	2.51	0.49
1:G:481:ILE:O	1:H:462:ASN:HB3	2.12	0.49
1:M:127:ARG:HB2	1:M:127:ARG:NH1	2.27	0.49
1:E:185:ILE:HD12	1:E:213:VAL:HG21	1.92	0.49
1:K:216:HIS:HB3	1:K:229:TYR:CE1	2.47	0.49
1:E:216:HIS:HB3	1:E:229:TYR:CE1	2.46	0.49
1:J:459:PRO:HD2	1:J:461:ILE:HD11	1.94	0.49
1:F:103:LEU:O	1:F:105:LYS:N	2.45	0.49
1:J:434:GLY:O	1:K:444:ARG:NH2	2.46	0.49
1:D:42:LEU:O	1:D:162:ARG:NH1	2.45	0.49
1:D:445:CYS:HB3	1:D:476:ILE:HD11	1.95	0.49
1:L:445:CYS:CB	1:L:476:ILE:HD11	2.43	0.49
1:B:125:SER:O	1:B:128:VAL:HG12	2.13	0.48
1:D:220:ASP:O	1:D:223:SER:O	2.31	0.48
1:E:20:LEU:HB2	1:E:167:VAL:HG21	1.95	0.48
1:E:216:HIS:CE1	1:E:218:TYR:HB3	2.47	0.48
1:L:488:LYS:O	1:L:492:MET:HG2	2.13	0.48
1:A:96:LEU:HD12	1:A:103:LEU:HD23	1.95	0.48
1:L:59:GLN:HG3	1:L:280:GLU:OE1	2.14	0.48
1:K:145:LEU:HD22	1:K:158:MET:SD	2.53	0.48
1:C:139:VAL:HA	1:C:269:ILE:HD12	1.94	0.48
1:D:109:GLY:O	1:D:113:VAL:HG23	2.13	0.48
1:F:95:GLN:C	1:F:97:LEU:H	2.17	0.48
1:H:389:TYR:OH	1:H:429:GLY:HA2	2.13	0.48
1:L:227:LEU:HD23	1:L:243:THR:HG22	1.95	0.48
1:F:42:LEU:O	1:F:162:ARG:NH1	2.46	0.48
1:H:126:TYR:O	1:H:130:LEU:HD23	2.13	0.48
1:K:185:ILE:HD12	1:K:213:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:481:ILE:O	1:L:461:ILE:O	2.31	0.48
1:L:307:GLN:NE2	1:L:310:ARG:CZ	2.77	0.48
1:B:323:ARG:HB3	1:B:325:GLU:OE1	2.14	0.48
1:J:74:MET:SD	1:J:131:PHE:HB2	2.54	0.48
1:H:141:GLY:HA3	1:H:265:GLY:O	2.14	0.48
1:D:216:HIS:HB3	1:D:229:TYR:CE1	2.49	0.48
1:H:305:ILE:HG21	1:I:302:PRO:HG3	1.94	0.48
1:A:354:PHE:CD1	1:A:381:LEU:HD21	2.46	0.48
1:K:74:MET:SD	1:K:131:PHE:HB2	2.54	0.48
1:K:248:ALA:HB2	1:K:406:LYS:CE	2.44	0.48
1:K:445:CYS:HB3	1:K:476:ILE:HD11	1.96	0.48
1:H:359:ASN:HB2	1:I:380:GLU:HB2	1.95	0.47
1:I:362:VAL:HG22	1:I:377:VAL:CG2	2.43	0.47
1:L:307:GLN:HE21	1:L:310:ARG:CZ	2.27	0.47
1:G:216:HIS:CE1	1:G:218:TYR:HB3	2.49	0.47
1:G:24:ARG:HG3	1:G:264:TYR:CE1	2.49	0.47
1:K:307:GLN:NE2	1:K:310:ARG:CZ	2.77	0.47
1:L:103:LEU:O	1:L:105:LYS:N	2.48	0.47
1:L:228:ARG:HG2	1:L:244:TYR:CE2	2.49	0.47
1:A:128:VAL:HG23	1:B:391:ILE:HG23	1.97	0.47
1:A:420:GLU:CD	1:A:420:GLU:H	2.17	0.47
1:F:228:ARG:HG2	1:F:244:TYR:CE2	2.49	0.47
1:F:77:LEU:O	1:F:397:GLN:NE2	2.47	0.47
1:H:216:HIS:HE1	1:H:218:TYR:HB3	1.77	0.47
1:J:95:GLN:C	1:J:97:LEU:H	2.18	0.47
1:K:95:GLN:C	1:K:97:LEU:H	2.18	0.47
1:C:418:PRO:O	1:C:420:GLU:N	2.48	0.47
1:I:95:GLN:C	1:I:97:LEU:H	2.18	0.47
1:L:434:GLY:O	1:M:444:ARG:NH2	2.48	0.47
1:M:459:PRO:HD2	1:M:461:ILE:HD11	1.97	0.47
1:G:103:LEU:O	1:G:105:LYS:N	2.47	0.47
1:I:144:LEU:HB3	1:I:161:TYR:HB2	1.97	0.47
1:K:219:LEU:HG	1:K:226:TYR:CE1	2.50	0.47
1:L:95:GLN:C	1:L:97:LEU:H	2.17	0.47
1:M:96:LEU:HD12	1:M:103:LEU:HD23	1.96	0.47
1:C:420:GLU:CD	1:C:420:GLU:H	2.17	0.47
1:E:434:GLY:O	1:F:444:ARG:NH2	2.48	0.47
1:E:488:LYS:O	1:E:492:MET:HG2	2.15	0.47
1:F:127:ARG:NH1	1:F:127:ARG:HB2	2.30	0.47
1:H:16:VAL:HA	1:H:19:ARG:HH12	1.79	0.47
1:M:445:CYS:HB3	1:M:476:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:HD12	1:C:103:LEU:HD23	1.97	0.46
1:G:125:SER:HA	1:H:394:GLN:OE1	2.14	0.46
1:J:306:THR:HG21	1:J:327:ILE:HD11	1.97	0.46
1:M:28:GLU:HB3	1:M:163:LEU:HD12	1.96	0.46
1:F:6:THR:HA	1:F:10:GLU:HA	1.96	0.46
1:F:163:LEU:HA	1:F:166:TYR:CE2	2.51	0.46
1:F:442:LEU:HD23	1:G:470:ILE:HG13	1.97	0.46
1:C:359:ASN:HB2	1:D:380:GLU:HB2	1.97	0.46
1:F:136:GLN:HB3	1:F:143:VAL:HG22	1.97	0.46
1:G:370:THR:HG23	1:G:373:GLU:HG2	1.96	0.46
1:H:95:GLN:C	1:H:97:LEU:H	2.18	0.46
1:I:320:VAL:O	1:J:299:LEU:HA	2.15	0.46
1:K:27:TYR:OH	1:K:262:GLU:HG2	2.14	0.46
1:M:488:LYS:O	1:M:492:MET:HG2	2.15	0.46
1:A:306:THR:HG23	1:A:322:GLY:HA3	1.98	0.46
1:F:389:TYR:OH	1:F:429:GLY:HA2	2.14	0.46
1:F:96:LEU:HD12	1:F:103:LEU:HD23	1.96	0.46
1:F:137:LEU:O	1:F:140:ALA:O	2.34	0.46
1:G:187:PHE:CZ	1:G:195:ARG:CG	2.99	0.46
1:H:139:VAL:HG13	1:H:140:ALA:N	2.31	0.46
1:B:430:LEU:HD12	1:B:433:ILE:HD12	1.98	0.46
1:C:192:GLU:HA	1:C:195:ARG:NH1	2.30	0.46
1:A:74:MET:SD	1:A:131:PHE:HB2	2.55	0.46
1:B:136:GLN:OE1	1:B:162:ARG:NH1	2.49	0.46
1:D:139:VAL:HA	1:D:269:ILE:HD12	1.98	0.46
1:F:488:LYS:O	1:F:492:MET:HG2	2.15	0.46
1:I:362:VAL:HG22	1:I:377:VAL:HG23	1.98	0.46
1:I:481:ILE:O	1:J:462:ASN:HB3	2.15	0.46
1:L:137:LEU:O	1:L:140:ALA:O	2.33	0.46
1:B:95:GLN:C	1:B:97:LEU:H	2.18	0.46
1:C:95:GLN:C	1:C:97:LEU:H	2.19	0.46
1:G:136:GLN:HB3	1:G:143:VAL:CG2	2.46	0.46
1:I:133:ALA:O	1:I:137:LEU:HB2	2.15	0.46
1:G:389:TYR:CD1	1:G:389:TYR:C	2.89	0.46
1:K:444:ARG:O	1:K:447:THR:HG22	2.16	0.46
1:M:216:HIS:HB3	1:M:229:TYR:CE1	2.51	0.46
1:M:59:GLN:HG3	1:M:280:GLU:OE1	2.16	0.46
1:A:445:CYS:HB3	1:A:476:ILE:HD11	1.99	0.46
1:G:96:LEU:HD12	1:G:103:LEU:HD23	1.97	0.46
1:H:216:HIS:HB3	1:H:229:TYR:CE1	2.51	0.46
1:L:459:PRO:HD2	1:L:461:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:LEU:HD12	1:H:103:LEU:HD23	1.98	0.45
1:H:103:LEU:O	1:H:105:LYS:N	2.50	0.45
1:H:483:LEU:HD12	1:I:460:ASP:HA	1.98	0.45
1:K:300:VAL:HG23	1:K:300:VAL:O	2.16	0.45
1:L:109:GLY:O	1:L:113:VAL:HG23	2.16	0.45
1:H:97:LEU:HA	1:H:97:LEU:HD23	1.88	0.45
1:J:359:ASN:HB2	1:K:380:GLU:HB2	1.97	0.45
1:L:96:LEU:HD12	1:L:103:LEU:HD23	1.98	0.45
1:E:216:HIS:HE1	1:E:218:TYR:HB3	1.81	0.45
1:E:139:VAL:HA	1:E:269:ILE:HD12	1.97	0.45
1:E:335:GLN:O	1:E:339:THR:HG23	2.15	0.45
1:G:216:HIS:HE1	1:G:218:TYR:HB3	1.81	0.45
1:I:194:ILE:O	1:I:198:VAL:HG23	2.16	0.45
1:D:418:PRO:O	1:D:420:GLU:N	2.50	0.45
1:I:146:TYR:CE2	1:I:148:PRO:HG3	2.52	0.45
1:K:79:PRO:HD2	1:K:83:TRP:CD1	2.51	0.45
1:M:118:MET:O	1:M:122:GLU:HG2	2.17	0.45
1:A:149:GLU:O	1:A:151:GLU:HB2	2.16	0.45
1:A:333:GLU:O	1:M:331:GLN:NE2	2.50	0.45
1:B:96:LEU:HD12	1:B:103:LEU:HD23	1.98	0.45
1:G:365:THR:HG22	1:H:364:ARG:NH1	2.30	0.45
1:G:79:PRO:HD2	1:G:83:TRP:CD1	2.52	0.45
1:G:97:LEU:HD23	1:G:97:LEU:HA	1.87	0.45
1:M:113:VAL:HA	1:M:116:ILE:HD12	1.97	0.45
1:A:469:ARG:NH2	1:M:477:ASP:HB3	2.32	0.45
1:A:126:TYR:CE2	1:A:158:MET:HE3	2.51	0.45
1:F:180:VAL:HA	1:F:215:THR:O	2.17	0.45
1:G:118:MET:O	1:G:122:GLU:HG2	2.16	0.45
1:C:449:TRP:HZ3	1:D:466:ILE:HD13	1.82	0.45
1:L:267:SER:OG	1:L:270:GLU:HB2	2.17	0.45
1:B:362:VAL:HG22	1:B:377:VAL:CG2	2.47	0.45
1:A:118:MET:O	1:A:122:GLU:HG2	2.17	0.45
1:A:195:ARG:NH2	1:B:221:GLU:OE2	2.47	0.45
1:B:248:ALA:HB2	1:B:406:LYS:CE	2.47	0.45
1:D:95:GLN:C	1:D:97:LEU:H	2.20	0.45
1:J:109:GLY:O	1:J:113:VAL:HG23	2.16	0.45
1:M:136:GLN:HB3	1:M:143:VAL:HG22	1.99	0.45
1:B:85:ARG:HB3	1:B:427:SER:HB2	1.99	0.44
1:E:396:LEU:O	1:E:400:LEU:HB2	2.17	0.44
1:J:248:ALA:HB2	1:J:406:LYS:CE	2.46	0.44
1:B:228:ARG:HG2	1:B:244:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:GLN:OE1	1:I:162:ARG:NH1	2.51	0.44
1:M:220:ASP:O	1:M:223:SER:O	2.34	0.44
1:A:126:TYR:O	1:A:130:LEU:HD23	2.16	0.44
1:J:481:ILE:O	1:K:462:ASN:HB3	2.17	0.44
1:K:146:TYR:CE1	1:K:251:TYR:CZ	3.05	0.44
1:A:95:GLN:C	1:A:97:LEU:H	2.19	0.44
1:B:478:THR:HG22	1:B:481:ILE:HD12	1.99	0.44
1:C:103:LEU:C	1:C:105:LYS:N	2.71	0.44
1:I:6:THR:HA	1:I:10:GLU:HA	2.00	0.44
1:M:95:GLN:C	1:M:97:LEU:H	2.20	0.44
1:A:306:THR:HG21	1:A:327:ILE:HD11	1.98	0.44
1:D:96:LEU:HD12	1:D:103:LEU:HD23	2.00	0.44
1:E:187:PHE:CZ	1:E:195:ARG:HG3	2.52	0.44
1:G:445:CYS:CB	1:G:476:ILE:HD11	2.47	0.44
1:I:445:CYS:CB	1:I:476:ILE:HD11	2.48	0.44
1:J:185:ILE:HG22	1:J:189:ALA:HB3	1.99	0.44
1:J:92:GLU:HB3	1:J:420:GLU:HG3	1.98	0.44
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.87	0.44
1:B:28:GLU:HB3	1:B:163:LEU:HD12	2.00	0.44
1:B:259:LEU:O	1:B:262:GLU:HB3	2.18	0.44
1:J:24:ARG:NH1	1:J:166:TYR:O	2.42	0.44
1:A:302:PRO:CG	1:M:305:ILE:HG21	2.48	0.44
1:E:453:ALA:HA	1:E:456:ARG:HG3	2.00	0.44
1:H:444:ARG:O	1:H:447:THR:HG22	2.18	0.44
1:I:142:ASN:N	1:I:142:ASN:ND2	2.63	0.44
1:J:216:HIS:HE1	1:J:218:TYR:HB3	1.82	0.44
1:K:194:ILE:O	1:K:198:VAL:HG23	2.17	0.44
1:C:307:GLN:HE21	1:C:310:ARG:CZ	2.31	0.44
1:K:96:LEU:HD12	1:K:103:LEU:HD23	1.99	0.44
1:M:187:PHE:CZ	1:M:195:ARG:HG3	2.53	0.44
1:C:103:LEU:C	1:C:105:LYS:H	2.21	0.43
1:C:396:LEU:O	1:C:400:LEU:HB2	2.18	0.43
1:F:133:ALA:O	1:F:137:LEU:HB2	2.17	0.43
1:H:187:PHE:HA	1:H:190:LEU:HD12	2.00	0.43
1:J:96:LEU:HD12	1:J:103:LEU:HD23	1.98	0.43
1:M:127:ARG:HH11	1:M:127:ARG:HB2	1.82	0.43
1:A:190:LEU:O	1:A:195:ARG:NH1	2.51	0.43
1:B:389:TYR:OH	1:B:429:GLY:HA2	2.18	0.43
1:E:103:LEU:HD23	1:E:103:LEU:C	2.39	0.43
1:F:97:LEU:HD23	1:F:97:LEU:HA	1.87	0.43
1:I:359:ASN:HB2	1:J:380:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:407:GLN:O	1:K:411:THR:HG23	2.18	0.43
1:L:126:TYR:CE2	1:L:158:MET:HE3	2.53	0.43
1:A:445:CYS:CB	1:A:476:ILE:HD11	2.48	0.43
1:B:477:ASP:HB3	1:C:469:ARG:NH2	2.33	0.43
1:D:28:GLU:HB3	1:D:163:LEU:HD12	2.00	0.43
1:G:95:GLN:C	1:G:97:LEU:H	2.20	0.43
1:J:85:ARG:HB3	1:J:427:SER:HB2	2.01	0.43
1:A:113:VAL:HA	1:A:116:ILE:HD12	2.01	0.43
1:B:139:VAL:HA	1:B:269:ILE:HD12	2.00	0.43
1:C:408:LEU:HB3	1:C:414:ILE:HD11	2.00	0.43
1:C:444:ARG:HA	1:C:447:THR:HG22	1.99	0.43
1:C:58:TRP:CE2	1:C:284:GLU:HG3	2.54	0.43
1:H:465:MET:HE3	1:H:469:ARG:HG3	2.01	0.43
1:D:359:ASN:HB2	1:E:380:GLU:HB2	2.01	0.43
1:G:272:TYR:CE2	1:G:355:ALA:HB1	2.54	0.43
1:B:103:LEU:O	1:B:105:LYS:N	2.51	0.43
1:C:99:ASP:N	1:C:100:PRO:CD	2.82	0.43
1:E:136:GLN:HB3	1:E:143:VAL:HG22	1.99	0.43
1:E:227:LEU:HD23	1:E:243:THR:HG22	1.99	0.43
1:F:141:GLY:HA3	1:F:265:GLY:O	2.19	0.43
1:I:139:VAL:HG13	1:I:140:ALA:N	2.33	0.43
1:I:96:LEU:HD12	1:I:103:LEU:HD23	2.01	0.43
1:K:99:ASP:N	1:K:100:PRO:CD	2.81	0.43
1:M:103:LEU:HD23	1:M:103:LEU:HA	1.86	0.43
1:A:488:LYS:O	1:A:492:MET:HG2	2.19	0.43
1:D:116:ILE:CG1	1:E:90:GLU:HG2	2.48	0.43
1:F:144:LEU:HB3	1:F:161:TYR:HB2	2.00	0.43
1:H:144:LEU:HB3	1:H:161:TYR:HB2	2.00	0.43
1:L:97:LEU:HD23	1:L:97:LEU:HA	1.88	0.43
1:M:103:LEU:C	1:M:105:LYS:H	2.22	0.43
1:C:59:GLN:HG3	1:C:280:GLU:OE1	2.18	0.43
1:E:125:SER:HA	1:F:394:GLN:NE2	2.34	0.43
1:G:144:LEU:HB3	1:G:161:TYR:HB2	2.01	0.43
1:I:147:LEU:HD11	1:I:403:VAL:HG12	2.01	0.43
1:I:462:ASN:HD21	1:I:465:MET:HB2	1.84	0.43
1:K:103:LEU:C	1:K:105:LYS:H	2.22	0.43
1:E:25:ALA:HB3	1:E:26:PRO:HD3	1.99	0.43
1:F:459:PRO:HD2	1:F:461:ILE:HD11	1.99	0.43
1:G:287:VAL:O	1:G:290:SER:OG	2.25	0.43
1:H:477:ASP:HB3	1:I:469:ARG:NH2	2.34	0.43
1:J:214:TYR:N	1:J:214:TYR:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:CD1	1:A:253:PRO:CA	2.97	0.42
1:E:124:ASN:HB3	1:E:156:ASN:O	2.19	0.42
1:G:299:LEU:O	1:G:327:ILE:HA	2.19	0.42
1:G:74:MET:SD	1:G:131:PHE:HB2	2.58	0.42
1:J:216:HIS:CE1	1:J:218:TYR:HB3	2.54	0.42
1:J:311:LEU:CD1	1:J:327:ILE:CD1	2.96	0.42
1:A:364:ARG:NH1	1:M:365:THR:HG22	2.34	0.42
1:C:103:LEU:HD23	1:C:103:LEU:HA	1.84	0.42
1:C:389:TYR:OH	1:C:429:GLY:HA2	2.19	0.42
1:E:248:ALA:HB2	1:E:406:LYS:CE	2.49	0.42
1:E:79:PRO:HD2	1:E:83:TRP:CD1	2.54	0.42
1:F:332:LEU:O	1:F:333:GLU:C	2.57	0.42
1:G:190:LEU:O	1:G:195:ARG:NH1	2.51	0.42
1:H:476:ILE:HG22	1:H:477:ASP:N	2.34	0.42
1:A:103:LEU:C	1:A:105:LYS:H	2.23	0.42
1:B:389:TYR:CD1	1:B:389:TYR:C	2.92	0.42
1:C:136:GLN:HB3	1:C:143:VAL:HG22	2.00	0.42
1:E:476:ILE:HG22	1:E:477:ASP:N	2.34	0.42
1:I:307:GLN:NE2	1:I:310:ARG:CZ	2.82	0.42
1:J:111:SER:O	1:J:115:ARG:NH1	2.52	0.42
1:M:99:ASP:N	1:M:100:PRO:CD	2.82	0.42
1:D:459:PRO:HD2	1:D:461:ILE:HD11	2.02	0.42
1:I:99:ASP:N	1:I:100:PRO:CD	2.82	0.42
1:J:228:ARG:HG2	1:J:244:TYR:CE2	2.54	0.42
1:M:6:THR:HA	1:M:10:GLU:HA	2.00	0.42
1:B:305:ILE:HG21	1:C:302:PRO:HG3	2.02	0.42
1:H:488:LYS:O	1:H:492:MET:HG2	2.19	0.42
1:I:103:LEU:HA	1:I:103:LEU:HD23	1.84	0.42
1:I:103:LEU:O	1:I:105:LYS:N	2.52	0.42
1:J:55:GLN:O	1:J:55:GLN:CD	2.58	0.42
1:L:99:ASP:N	1:L:100:PRO:CD	2.83	0.42
1:A:99:ASP:N	1:A:100:PRO:CD	2.82	0.42
1:B:99:ASP:N	1:B:100:PRO:CD	2.83	0.42
1:B:197:ALA:HB1	1:B:235:MET:HE3	2.01	0.42
1:D:103:LEU:HA	1:D:103:LEU:HD23	1.86	0.42
1:E:103:LEU:O	1:E:103:LEU:HD23	2.20	0.42
1:H:149:GLU:O	1:H:151:GLU:HB2	2.19	0.42
1:J:290:SER:HB3	1:K:344:VAL:HG21	2.02	0.42
1:K:354:PHE:HD1	1:K:381:LEU:HD21	1.84	0.42
1:L:216:HIS:CE1	1:L:218:TYR:HB3	2.54	0.42
1:M:389:TYR:C	1:M:389:TYR:CD1	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:TYR:OH	1:C:262:GLU:CG	2.67	0.42
1:D:99:ASP:N	1:D:100:PRO:CD	2.83	0.42
1:E:6:THR:HA	1:E:10:GLU:HA	2.02	0.42
1:E:110:LEU:O	1:E:113:VAL:N	2.52	0.42
1:G:182:ARG:NE	1:G:184:GLN:HE21	2.17	0.42
1:H:232:VAL:O	1:H:233:GLU:C	2.58	0.42
1:H:389:TYR:C	1:H:389:TYR:CD1	2.93	0.42
1:H:99:ASP:N	1:H:100:PRO:CD	2.83	0.42
1:J:99:ASP:N	1:J:100:PRO:CD	2.83	0.42
1:K:133:ALA:O	1:K:137:LEU:HB2	2.19	0.42
1:K:481:ILE:O	1:L:462:ASN:HB3	2.18	0.42
1:M:370:THR:OG1	1:M:371:ALA:N	2.53	0.42
1:C:488:LYS:O	1:C:492:MET:HG2	2.20	0.42
1:E:228:ARG:HG2	1:E:244:TYR:CE2	2.54	0.42
1:E:442:LEU:HD23	1:F:470:ILE:HG13	2.02	0.42
1:G:187:PHE:CE1	1:G:195:ARG:HG3	2.55	0.42
1:H:146:TYR:CE1	1:H:251:TYR:CZ	3.08	0.42
1:J:112:MET:HA	1:J:115:ARG:NH2	2.35	0.42
1:K:103:LEU:C	1:K:105:LYS:N	2.73	0.42
1:K:28:GLU:HB3	1:K:163:LEU:HD12	2.01	0.42
1:M:126:TYR:CE2	1:M:158:MET:HE3	2.54	0.42
1:I:214:TYR:N	1:I:214:TYR:CD1	2.88	0.42
1:L:430:LEU:HD12	1:L:433:ILE:HD12	2.01	0.42
1:M:444:ARG:HA	1:M:447:THR:HG22	2.02	0.42
1:E:99:ASP:OD1	1:E:102:GLY:N	2.42	0.42
1:G:445:CYS:HB3	1:G:476:ILE:HD11	2.01	0.42
1:L:113:VAL:HA	1:L:116:ILE:HD12	2.01	0.42
1:M:180:VAL:HA	1:M:215:THR:O	2.20	0.42
1:B:5:ARG:HD3	1:B:218:TYR:OH	2.20	0.41
1:D:103:LEU:O	1:D:105:LYS:N	2.53	0.41
1:D:445:CYS:CB	1:D:476:ILE:HD11	2.49	0.41
1:G:365:THR:HG22	1:H:364:ARG:HH11	1.84	0.41
1:L:103:LEU:HD23	1:L:103:LEU:HA	1.84	0.41
1:F:192:GLU:HA	1:F:195:ARG:NH1	2.35	0.41
1:H:430:LEU:HA	1:H:430:LEU:HD12	1.92	0.41
1:I:97:LEU:HA	1:I:97:LEU:HD23	1.88	0.41
1:K:223:SER:HB3	1:K:225:GLU:CG	2.50	0.41
1:L:28:GLU:HB3	1:L:163:LEU:HD12	2.02	0.41
1:C:308:PRO:O	1:C:309:ARG:C	2.59	0.41
1:D:311:LEU:HD11	1:D:327:ILE:CD1	2.51	0.41
1:E:359:ASN:HB2	1:F:380:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:PHE:CZ	1:H:195:ARG:HG3	2.55	0.41
1:K:73:LEU:HD21	1:K:388:VAL:HG23	2.02	0.41
1:B:125:SER:HA	1:C:394:GLN:OE1	2.21	0.41
1:G:99:ASP:N	1:G:100:PRO:CD	2.83	0.41
1:H:418:PRO:O	1:H:420:GLU:N	2.53	0.41
1:K:180:VAL:HA	1:K:215:THR:O	2.21	0.41
1:M:131:PHE:CE2	1:M:135:LYS:HE2	2.55	0.41
1:M:286:ILE:O	1:M:289:MET:HB3	2.21	0.41
1:C:442:LEU:HD21	1:D:469:ARG:HB3	2.01	0.41
1:D:144:LEU:HB3	1:D:161:TYR:HB2	2.01	0.41
1:F:99:ASP:N	1:F:100:PRO:CD	2.83	0.41
1:L:370:THR:OG1	1:L:371:ALA:N	2.53	0.41
1:L:445:CYS:HB3	1:L:476:ILE:HD11	2.03	0.41
1:M:111:SER:O	1:M:115:ARG:NH1	2.53	0.41
1:M:126:TYR:O	1:M:130:LEU:HD23	2.19	0.41
1:M:452:LEU:HD11	1:M:467:LYS:HE3	2.03	0.41
1:A:103:LEU:C	1:A:105:LYS:N	2.73	0.41
1:A:133:ALA:O	1:A:137:LEU:HB2	2.21	0.41
1:E:109:GLY:O	1:E:112:MET:HB3	2.20	0.41
1:H:147:LEU:HD11	1:H:403:VAL:HG12	2.01	0.41
1:J:476:ILE:HG22	1:J:477:ASP:N	2.34	0.41
1:C:126:TYR:CD2	1:C:158:MET:HE3	2.56	0.41
1:D:370:THR:OG1	1:D:371:ALA:N	2.53	0.41
1:E:43:PHE:HD2	1:E:136:GLN:HE22	1.68	0.41
1:F:147:LEU:HD11	1:F:403:VAL:HG12	2.02	0.41
1:F:171:ASP:OD1	1:F:175:ASN:N	2.54	0.41
1:I:139:VAL:HG13	1:I:140:ALA:H	1.85	0.41
1:J:103:LEU:HD23	1:J:103:LEU:HA	1.83	0.41
1:J:133:ALA:O	1:J:137:LEU:HB2	2.20	0.41
1:M:227:LEU:HD23	1:M:243:THR:HG22	2.02	0.41
1:A:364:ARG:HH11	1:M:365:THR:HG22	1.86	0.41
1:A:305:ILE:HG21	1:B:302:PRO:HG3	2.02	0.41
1:C:293:SER:O	1:D:337:ASP:HB3	2.20	0.41
1:G:126:TYR:O	1:G:130:LEU:HD23	2.21	0.41
1:J:58:TRP:CZ2	1:J:288:LYS:HE3	2.56	0.41
1:M:419:LYS:O	1:M:420:GLU:C	2.59	0.41
1:B:483:LEU:HD12	1:C:460:ASP:HA	2.03	0.41
1:M:459:PRO:O	1:M:460:ASP:CG	2.58	0.41
1:A:171:ASP:OD1	1:A:174:GLY:N	2.53	0.41
1:A:430:LEU:HA	1:A:430:LEU:HD12	1.91	0.41
1:B:241:ASP:OD1	1:B:241:ASP:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:ARG:HG3	1:E:214:TYR:CE2	2.56	0.41
1:E:482:LEU:HD13	1:F:460:ASP:O	2.21	0.41
1:G:488:LYS:O	1:G:492:MET:HG2	2.21	0.41
1:I:444:ARG:HA	1:I:447:THR:HG22	2.02	0.41
1:J:445:CYS:CB	1:J:476:ILE:HD11	2.51	0.41
1:M:229:TYR:CD2	1:M:229:TYR:O	2.74	0.41
1:B:434:GLY:O	1:C:444:ARG:NH2	2.52	0.41
1:F:453:ALA:N	1:F:454:PRO:CD	2.84	0.41
1:G:103:LEU:C	1:G:105:LYS:N	2.74	0.41
1:G:24:ARG:HG3	1:G:264:TYR:CZ	2.54	0.41
1:H:136:GLN:HB3	1:H:143:VAL:HG22	2.02	0.41
1:I:92:GLU:HB3	1:I:420:GLU:HG3	2.02	0.41
1:L:167:VAL:HG12	1:L:180:VAL:HB	2.03	0.41
1:A:391:ILE:HG23	1:M:128:VAL:HG23	2.03	0.41
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.84	0.40
1:A:248:ALA:HB2	1:A:406:LYS:HD3	2.03	0.40
1:A:92:GLU:HB3	1:A:420:GLU:HG3	2.03	0.40
1:E:404:LEU:HD23	1:E:404:LEU:HA	1.97	0.40
1:J:103:LEU:O	1:J:105:LYS:N	2.54	0.40
1:M:103:LEU:C	1:M:105:LYS:N	2.74	0.40
1:A:131:PHE:CG	1:B:391:ILE:HD11	2.57	0.40
1:B:445:CYS:HB3	1:B:476:ILE:HD11	2.03	0.40
1:E:445:CYS:CB	1:E:476:ILE:HD11	2.51	0.40
1:K:216:HIS:CE1	1:K:218:TYR:HB3	2.56	0.40
1:K:42:LEU:O	1:K:162:ARG:NH1	2.54	0.40
1:C:220:ASP:O	1:C:223:SER:O	2.39	0.40
1:C:232:VAL:O	1:C:233:GLU:C	2.60	0.40
1:C:307:GLN:NE2	1:C:310:ARG:NH1	2.69	0.40
1:E:445:CYS:HB3	1:E:476:ILE:HD11	2.04	0.40
1:G:171:ASP:OD1	1:G:175:ASN:N	2.54	0.40
1:G:27:TYR:OH	1:G:262:GLU:HG2	2.21	0.40
1:J:182:ARG:NE	1:J:184:GLN:HE21	2.19	0.40
1:K:103:LEU:HA	1:K:103:LEU:HD23	1.85	0.40
1:M:144:LEU:HB3	1:M:161:TYR:HB2	2.04	0.40
1:B:25:ALA:O	1:B:26:PRO:C	2.60	0.40
1:C:74:MET:SD	1:C:131:PHE:HB2	2.61	0.40
1:D:434:GLY:O	1:E:444:ARG:NH2	2.55	0.40
1:E:93:ALA:O	1:E:94:LYS:C	2.60	0.40
1:F:309:ARG:HH11	1:F:309:ARG:HB2	1.87	0.40
1:F:359:ASN:HB2	1:G:380:GLU:HB2	2.03	0.40
1:J:59:GLN:OE1	1:J:59:GLN:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:481:ILE:O	1:M:462:ASN:HB3	2.21	0.40
1:D:116:ILE:HG12	1:E:90:GLU:HG2	2.04	0.40
1:D:192:GLU:HA	1:D:195:ARG:NH1	2.36	0.40
1:E:82:THR:HA	1:E:118:MET:SD	2.61	0.40
1:F:304:GLY:HA3	1:F:326:ASP:CG	2.42	0.40
1:G:127:ARG:NH1	1:G:127:ARG:HB2	2.37	0.40
1:G:216:HIS:HB3	1:G:229:TYR:CE1	2.56	0.40
1:J:6:THR:HA	1:J:10:GLU:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/547 (88%)	438 (91%)	38 (8%)	6 (1%)	14	51
1	B	482/547 (88%)	444 (92%)	31 (6%)	7 (2%)	11	46
1	C	482/547 (88%)	437 (91%)	39 (8%)	6 (1%)	14	51
1	D	482/547 (88%)	445 (92%)	31 (6%)	6 (1%)	14	51
1	E	482/547 (88%)	448 (93%)	32 (7%)	2 (0%)	36	73
1	F	482/547 (88%)	444 (92%)	32 (7%)	6 (1%)	14	51
1	G	482/547 (88%)	444 (92%)	32 (7%)	6 (1%)	14	51
1	H	482/547 (88%)	438 (91%)	38 (8%)	6 (1%)	14	51
1	I	482/547 (88%)	442 (92%)	36 (8%)	4 (1%)	21	60
1	J	482/547 (88%)	438 (91%)	38 (8%)	6 (1%)	14	51
1	K	482/547 (88%)	439 (91%)	38 (8%)	5 (1%)	17	56
1	L	482/547 (88%)	439 (91%)	39 (8%)	4 (1%)	21	60
1	M	482/547 (88%)	444 (92%)	32 (7%)	6 (1%)	14	51
All	All	6266/7111 (88%)	5740 (92%)	456 (7%)	70 (1%)	16	54

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	363	GLN
1	D	419	LYS
1	E	363	GLN
1	E	419	LYS
1	H	363	GLN
1	H	419	LYS
1	I	363	GLN
1	A	104	ALA
1	A	357	MET
1	A	363	GLN
1	B	363	GLN
1	B	419	LYS
1	C	363	GLN
1	C	419	LYS
1	F	363	GLN
1	F	419	LYS
1	G	357	MET
1	G	363	GLN
1	G	419	LYS
1	H	357	MET
1	J	363	GLN
1	K	363	GLN
1	K	419	LYS
1	L	363	GLN
1	M	363	GLN
1	M	419	LYS
1	A	419	LYS
1	B	104	ALA
1	C	104	ALA
1	F	104	ALA
1	G	104	ALA
1	I	419	LYS
1	K	104	ALA
1	L	419	LYS
1	M	104	ALA
1	B	96	LEU
1	B	357	MET
1	D	333	GLU
1	D	357	MET
1	F	96	LEU
1	F	333	GLU
1	H	81	GLN

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Mol	Chain	Res	Type
1	H	104	ALA
1	J	96	LEU
1	J	357	MET
1	J	419	LYS
1	L	104	ALA
1	A	96	LEU
1	C	96	LEU
1	D	96	LEU
1	D	104	ALA
1	G	96	LEU
1	H	96	LEU
1	I	96	LEU
1	I	357	MET
1	J	104	ALA
1	K	96	LEU
1	L	96	LEU
1	M	96	LEU
1	M	203	GLY
1	A	459	PRO
1	G	459	PRO
1	C	454	PRO
1	C	459	PRO
1	J	459	PRO
1	K	459	PRO
1	B	454	PRO
1	B	459	PRO
1	F	459	PRO
1	M	459	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/450 (92%)	390 (95%)	22 (5%)	25	60
1	B	412/450 (92%)	396 (96%)	16 (4%)	35	69
1	C	412/450 (92%)	398 (97%)	14 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	412/450 (92%)	399 (97%)	13 (3%)	42	74
1	E	412/450 (92%)	397 (96%)	15 (4%)	38	71
1	F	412/450 (92%)	402 (98%)	10 (2%)	52	80
1	G	412/450 (92%)	392 (95%)	20 (5%)	27	63
1	H	412/450 (92%)	396 (96%)	16 (4%)	35	69
1	I	412/450 (92%)	394 (96%)	18 (4%)	31	66
1	J	412/450 (92%)	401 (97%)	11 (3%)	48	77
1	K	412/450 (92%)	399 (97%)	13 (3%)	42	74
1	L	412/450 (92%)	399 (97%)	13 (3%)	42	74
1	M	412/450 (92%)	398 (97%)	14 (3%)	40	72
All	All	5356/5850 (92%)	5161 (96%)	195 (4%)	38	71

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	23	ASP
1	A	43	PHE
1	A	71	SER
1	A	92	GLU
1	A	137	LEU
1	A	139	VAL
1	A	142	ASN
1	A	143	VAL
1	A	147	LEU
1	A	154	ASN
1	A	181	THR
1	A	182	ARG
1	A	204	GLU
1	A	223	SER
1	A	228	ARG
1	A	231	GLU
1	A	312	THR
1	A	332	LEU
1	A	357	MET
1	A	360	SER
1	A	427	SER
1	B	22	ASN

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Mol	Chain	Res	Type
1	B	23	ASP
1	B	43	PHE
1	B	92	GLU
1	B	142	ASN
1	B	147	LEU
1	B	167	VAL
1	B	181	THR
1	B	182	ARG
1	B	228	ARG
1	B	231	GLU
1	B	260	ASP
1	B	332	LEU
1	B	357	MET
1	B	370	THR
1	B	383	ASP
1	C	22	ASN
1	C	23	ASP
1	C	43	PHE
1	C	92	GLU
1	C	147	LEU
1	C	167	VAL
1	C	181	THR
1	C	182	ARG
1	C	228	ARG
1	C	231	GLU
1	C	260	ASP
1	C	312	THR
1	C	335	GLN
1	C	357	MET
1	D	23	ASP
1	D	43	PHE
1	D	59	GLN
1	D	111	SER
1	D	142	ASN
1	D	147	LEU
1	D	182	ARG
1	D	228	ARG
1	D	231	GLU
1	D	260	ASP
1	D	312	THR
1	D	335	GLN
1	D	357	MET

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Mol	Chain	Res	Type
1	E	23	ASP
1	E	43	PHE
1	E	59	GLN
1	E	96	LEU
1	E	101	ASP
1	E	147	LEU
1	E	182	ARG
1	E	223	SER
1	E	228	ARG
1	E	231	GLU
1	E	260	ASP
1	E	312	THR
1	E	332	LEU
1	E	357	MET
1	E	370	THR
1	F	43	PHE
1	F	142	ASN
1	F	147	LEU
1	F	167	VAL
1	F	177	LEU
1	F	182	ARG
1	F	228	ARG
1	F	231	GLU
1	F	260	ASP
1	F	357	MET
1	G	22	ASN
1	G	23	ASP
1	G	43	PHE
1	G	59	GLN
1	G	92	GLU
1	G	137	LEU
1	G	142	ASN
1	G	147	LEU
1	G	154	ASN
1	G	167	VAL
1	G	182	ARG
1	G	223	SER
1	G	228	ARG
1	G	231	GLU
1	G	260	ASP
1	G	309	ARG
1	G	312	THR

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Mol	Chain	Res	Type
1	G	357	MET
1	G	360	SER
1	G	370	THR
1	H	22	ASN
1	H	23	ASP
1	H	43	PHE
1	H	92	GLU
1	H	147	LEU
1	H	167	VAL
1	H	181	THR
1	H	182	ARG
1	H	223	SER
1	H	228	ARG
1	H	231	GLU
1	H	260	ASP
1	H	312	THR
1	H	332	LEU
1	H	357	MET
1	H	370	THR
1	I	23	ASP
1	I	43	PHE
1	I	71	SER
1	I	92	GLU
1	I	137	LEU
1	I	142	ASN
1	I	147	LEU
1	I	167	VAL
1	I	182	ARG
1	I	228	ARG
1	I	231	GLU
1	I	306	THR
1	I	309	ARG
1	I	312	THR
1	I	332	LEU
1	I	335	GLN
1	I	357	MET
1	I	383	ASP
1	J	43	PHE
1	J	59	GLN
1	J	142	ASN
1	J	147	LEU
1	J	181	THR

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Mol	Chain	Res	Type
1	J	182	ARG
1	J	228	ARG
1	J	231	GLU
1	J	260	ASP
1	J	332	LEU
1	J	357	MET
1	K	23	ASP
1	K	43	PHE
1	K	92	GLU
1	K	137	LEU
1	K	142	ASN
1	K	147	LEU
1	K	181	THR
1	K	182	ARG
1	K	228	ARG
1	K	231	GLU
1	K	260	ASP
1	K	312	THR
1	K	357	MET
1	L	22	ASN
1	L	23	ASP
1	L	43	PHE
1	L	92	GLU
1	L	142	ASN
1	L	147	LEU
1	L	167	VAL
1	L	182	ARG
1	L	228	ARG
1	L	231	GLU
1	L	260	ASP
1	L	312	THR
1	L	357	MET
1	M	23	ASP
1	M	43	PHE
1	M	59	GLN
1	M	142	ASN
1	M	147	LEU
1	M	167	VAL
1	M	182	ARG
1	M	223	SER
1	M	228	ARG
1	M	231	GLU

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Mol	Chain	Res	Type
1	M	260	ASP
1	M	312	THR
1	M	332	LEU
1	M	357	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	B	156	ASN
1	C	32	GLN
1	C	156	ASN
1	C	307	GLN
1	C	335	GLN
1	D	124	ASN
1	D	156	ASN
1	D	216	HIS
1	D	307	GLN
1	D	335	GLN
1	F	216	HIS
1	F	394	GLN
1	G	184	GLN
1	H	156	ASN
1	H	184	GLN
1	H	307	GLN
1	H	487	GLN
1	I	156	ASN
1	I	307	GLN
1	I	335	GLN
1	I	462	ASN
1	J	184	GLN
1	J	307	GLN
1	K	184	GLN
1	K	307	GLN
1	L	184	GLN
1	L	307	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	486/547 (88%)	0.32	24 (4%)	29	29	33, 70, 153, 199	1 (0%)
1	B	486/547 (88%)	0.22	21 (4%)	35	34	31, 71, 141, 194	1 (0%)
1	C	486/547 (88%)	0.21	19 (3%)	39	37	30, 73, 139, 198	1 (0%)
1	D	486/547 (88%)	0.33	27 (5%)	24	24	35, 75, 146, 183	1 (0%)
1	E	486/547 (88%)	0.36	32 (6%)	18	19	36, 75, 132, 208	1 (0%)
1	F	486/547 (88%)	0.40	31 (6%)	19	20	37, 80, 143, 192	1 (0%)
1	G	486/547 (88%)	0.32	34 (6%)	16	18	37, 79, 144, 225	1 (0%)
1	H	486/547 (88%)	0.43	43 (8%)	10	11	38, 79, 149, 224	1 (0%)
1	I	486/547 (88%)	0.39	32 (6%)	18	19	38, 80, 155, 215	1 (0%)
1	J	486/547 (88%)	0.39	24 (4%)	29	29	39, 89, 150, 215	1 (0%)
1	K	486/547 (88%)	0.33	31 (6%)	19	20	38, 88, 156, 203	1 (0%)
1	L	486/547 (88%)	0.43	37 (7%)	14	15	37, 84, 151, 197	1 (0%)
1	M	486/547 (88%)	0.34	27 (5%)	24	24	37, 80, 150, 195	1 (0%)
All	All	6318/7111 (88%)	0.34	382 (6%)	22	22	30, 79, 148, 225	13 (0%)

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	48	ASP	10.0
1	M	47	SER	7.4
1	J	3	GLU	7.3
1	I	48	ASP	6.4
1	A	98	SER	6.3
1	I	493	ALA	6.2
1	I	494	GLN	6.1
1	A	421	ALA	6.0
1	J	48	ASP	5.7

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Mol	Chain	Res	Type	RSRZ
1	H	460	ASP	5.6
1	I	490	GLN	5.4
1	C	48	ASP	5.4
1	D	48	ASP	5.2
1	J	98	SER	5.2
1	B	98	SER	5.2
1	F	48	ASP	5.2
1	A	489	GLN	4.8
1	K	3	GLU	4.7
1	B	494	GLN	4.6
1	H	421	ALA	4.6
1	F	489	GLN	4.6
1	E	492	MET	4.6
1	D	365	THR	4.5
1	I	492	MET	4.5
1	I	491	LYS	4.5
1	L	98	SER	4.4
1	H	492	MET	4.4
1	A	96	LEU	4.3
1	C	494	GLN	4.3
1	J	47	SER	4.2
1	G	48	ASP	4.2
1	L	485	GLU	4.2
1	B	421	ALA	4.1
1	A	493	ALA	4.1
1	K	48	ASP	4.1
1	H	461	ILE	4.1
1	F	458	ASP	4.1
1	G	482	LEU	4.1
1	K	421	ALA	4.1
1	G	204	GLU	4.0
1	A	48	ASP	4.0
1	C	47	SER	4.0
1	H	457	ASP	4.0
1	L	486	GLU	4.0
1	L	483	LEU	4.0
1	M	98	SER	3.9
1	K	420	GLU	3.9
1	G	484	THR	3.9
1	M	484	THR	3.9
1	J	493	ALA	3.9
1	A	459	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	L	48	ASP	3.8
1	M	485	GLU	3.8
1	B	47	SER	3.8
1	L	482	LEU	3.8
1	L	420	GLU	3.7
1	E	48	ASP	3.7
1	H	459	PRO	3.7
1	E	204	GLU	3.6
1	F	460	ASP	3.6
1	M	460	ASP	3.6
1	B	493	ALA	3.6
1	G	47	SER	3.6
1	G	460	ASP	3.6
1	M	463	LEU	3.6
1	A	492	MET	3.5
1	G	486	GLU	3.5
1	D	494	GLN	3.5
1	K	100	PRO	3.5
1	I	96	LEU	3.5
1	I	421	ALA	3.5
1	D	47	SER	3.5
1	H	9	ALA	3.5
1	M	486	GLU	3.5
1	B	224	GLY	3.5
1	I	98	SER	3.5
1	M	494	GLN	3.5
1	I	47	SER	3.4
1	A	422	VAL	3.4
1	A	490	GLN	3.4
1	H	366	GLY	3.4
1	E	493	ALA	3.4
1	J	420	GLU	3.4
1	F	459	PRO	3.4
1	D	4	LYS	3.4
1	E	454	PRO	3.3
1	D	3	GLU	3.3
1	D	493	ALA	3.3
1	H	493	ALA	3.3
1	E	200	GLY	3.3
1	I	422	VAL	3.3
1	L	47	SER	3.3
1	J	492	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	233	GLU	3.3
1	H	365	THR	3.3
1	I	206	LYS	3.3
1	K	8	LEU	3.3
1	F	365	THR	3.2
1	E	199	GLU	3.2
1	J	489	GLN	3.2
1	L	97	LEU	3.2
1	K	458	ASP	3.2
1	K	98	SER	3.2
1	M	454	PRO	3.2
1	F	482	LEU	3.2
1	A	460	ASP	3.2
1	L	421	ALA	3.1
1	G	4	LYS	3.1
1	J	491	LYS	3.1
1	C	205	LYS	3.1
1	L	455	MET	3.1
1	H	207	ALA	3.1
1	H	202	GLY	3.1
1	J	101	ASP	3.1
1	B	365	THR	3.1
1	L	481	ILE	3.1
1	L	494	GLN	3.1
1	G	369	VAL	3.1
1	C	366	GLY	3.0
1	E	457	ASP	3.0
1	I	367	GLU	3.0
1	H	422	VAL	3.0
1	E	467	LYS	3.0
1	I	460	ASP	3.0
1	F	492	MET	3.0
1	M	461	ILE	3.0
1	L	484	THR	3.0
1	J	486	GLU	3.0
1	I	365	THR	3.0
1	L	456	ARG	3.0
1	E	205	LYS	3.0
1	K	490	GLN	3.0
1	E	203	GLY	3.0
1	L	102	GLY	3.0
1	F	366	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	2.9
1	A	485	GLU	2.9
1	E	47	SER	2.9
1	I	489	GLN	2.9
1	K	486	GLU	2.9
1	M	489	GLN	2.9
1	E	455	MET	2.9
1	H	417	LEU	2.9
1	B	485	GLU	2.9
1	C	492	MET	2.9
1	G	8	LEU	2.9
1	I	97	LEU	2.9
1	A	491	LYS	2.9
1	G	488	LYS	2.9
1	B	48	ASP	2.9
1	E	216	HIS	2.9
1	K	418	PRO	2.9
1	D	366	GLY	2.9
1	G	365	THR	2.9
1	F	493	ALA	2.9
1	C	491	LYS	2.9
1	A	419	LYS	2.8
1	H	238	GLN	2.8
1	F	455	MET	2.8
1	A	461	ILE	2.8
1	C	204	GLU	2.8
1	G	9	ALA	2.8
1	E	489	GLN	2.8
1	G	454	PRO	2.8
1	D	364	ARG	2.8
1	E	208	ASP	2.8
1	K	494	GLN	2.8
1	L	487	GLN	2.8
1	D	491	LYS	2.8
1	I	420	GLU	2.8
1	K	489	GLN	2.7
1	E	463	LEU	2.7
1	A	458	ASP	2.7
1	F	456	ARG	2.7
1	I	419	LYS	2.7
1	M	481	ILE	2.7
1	D	490	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	456	ARG	2.7
1	C	364	ARG	2.7
1	D	420	GLU	2.7
1	L	4	LYS	2.7
1	G	492	MET	2.7
1	F	491	LYS	2.7
1	F	454	PRO	2.7
1	C	98	SER	2.7
1	H	198	VAL	2.7
1	K	101	ASP	2.7
1	L	96	LEU	2.7
1	G	452	LEU	2.6
1	H	221	GLU	2.6
1	J	211	ILE	2.6
1	F	208	ASP	2.6
1	C	3	GLU	2.6
1	J	421	ALA	2.6
1	C	365	THR	2.6
1	H	458	ASP	2.6
1	E	3	GLU	2.5
1	H	3	GLU	2.5
1	D	368	ARG	2.5
1	I	46	ASP	2.5
1	L	468	LEU	2.5
1	B	492	MET	2.5
1	I	232	VAL	2.5
1	H	105	LYS	2.5
1	C	460	ASP	2.5
1	K	367	GLU	2.5
1	M	482	LEU	2.5
1	H	194	ILE	2.5
1	I	88	ILE	2.5
1	H	8	LEU	2.5
1	D	460	ASP	2.5
1	B	96	LEU	2.5
1	F	204	GLU	2.5
1	A	100	PRO	2.5
1	L	478	THR	2.5
1	E	4	LYS	2.5
1	D	205	LYS	2.5
1	K	11	ASP	2.5
1	K	46	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	201	GLN	2.5
1	H	233	GLU	2.5
1	L	94	LYS	2.5
1	J	233	GLU	2.5
1	C	493	ALA	2.4
1	J	305	ILE	2.4
1	E	456	ARG	2.4
1	B	452	LEU	2.4
1	G	451	ALA	2.4
1	D	483	LEU	2.4
1	E	453	ALA	2.4
1	L	101	ASP	2.4
1	J	179	MET	2.4
1	E	189	ALA	2.4
1	E	485	GLU	2.4
1	F	452	LEU	2.4
1	C	206	LYS	2.3
1	F	233	GLU	2.3
1	G	489	GLN	2.3
1	B	481	ILE	2.3
1	G	100	PRO	2.3
1	A	420	GLU	2.3
1	J	231	GLU	2.3
1	M	490	GLN	2.3
1	A	486	GLU	2.3
1	L	493	ALA	2.3
1	H	178	GLN	2.3
1	G	7	GLY	2.3
1	L	479	SER	2.3
1	F	4	LYS	2.3
1	E	201	GLN	2.3
1	H	219	LEU	2.3
1	B	420	GLU	2.3
1	H	412	GLN	2.3
1	K	483	LEU	2.3
1	K	193	ASP	2.3
1	K	368	ARG	2.3
1	L	204	GLU	2.3
1	I	442	LEU	2.3
1	G	216	HIS	2.3
1	I	481	ILE	2.3
1	L	489	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	93	ALA	2.3
1	K	479	SER	2.3
1	A	365	THR	2.3
1	M	100	PRO	2.3
1	M	476	ILE	2.3
1	F	487	GLN	2.3
1	G	328	SER	2.3
1	D	482	LEU	2.2
1	I	417	LEU	2.2
1	G	485	GLU	2.2
1	H	203	GLY	2.2
1	E	328	SER	2.2
1	H	452	LEU	2.2
1	I	483	LEU	2.2
1	H	94	LYS	2.2
1	H	420	GLU	2.2
1	H	454	PRO	2.2
1	J	13	ALA	2.2
1	J	485	GLU	2.2
1	A	92	GLU	2.2
1	B	486	GLU	2.2
1	I	204	GLU	2.2
1	L	206	LYS	2.2
1	H	5	ARG	2.2
1	H	226	TYR	2.2
1	I	17	TYR	2.2
1	L	12	GLY	2.2
1	C	208	ASP	2.2
1	F	13	ALA	2.2
1	F	207	ALA	2.2
1	G	466	ILE	2.2
1	K	178	GLN	2.2
1	K	219	LEU	2.2
1	H	48	ASP	2.2
1	F	481	ILE	2.2
1	I	486	GLU	2.2
1	B	483	LEU	2.2
1	G	368	ARG	2.2
1	L	492	MET	2.2
1	H	201	GLN	2.2
1	H	494	GLN	2.2
1	K	455	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	466	ILE	2.2
1	K	93	ALA	2.1
1	E	494	GLN	2.1
1	J	191	PRO	2.1
1	D	492	MET	2.1
1	F	6	THR	2.1
1	H	6	THR	2.1
1	M	449	TRP	2.1
1	J	189	ALA	2.1
1	C	221	GLU	2.1
1	F	98	SER	2.1
1	G	494	GLN	2.1
1	D	189	ALA	2.1
1	G	493	ALA	2.1
1	K	365	THR	2.1
1	L	462	ASN	2.1
1	M	478	THR	2.1
1	D	5	ARG	2.1
1	G	461	ILE	2.1
1	M	97	LEU	2.1
1	L	467	LYS	2.1
1	H	489	GLN	2.1
1	B	456	ARG	2.1
1	E	46	ASP	2.1
1	K	460	ASP	2.1
1	D	9	ALA	2.1
1	M	456	ARG	2.1
1	A	151	GLU	2.1
1	A	8	LEU	2.1
1	B	463	LEU	2.1
1	M	452	LEU	2.1
1	G	13	ALA	2.1
1	D	487	GLN	2.1
1	G	363	GLN	2.1
1	A	488	LYS	2.1
1	E	491	LYS	2.1
1	F	479	SER	2.1
1	G	458	ASP	2.1
1	F	192	GLU	2.1
1	K	105	LYS	2.1
1	C	232	VAL	2.1
1	L	466	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	449	TRP	2.1
1	D	187	PHE	2.1
1	H	204	GLU	2.1
1	H	229	TYR	2.1
1	H	486	GLU	2.1
1	E	466	ILE	2.1
1	K	468	LEU	2.1
1	J	46	ASP	2.1
1	K	491	LYS	2.0
1	M	469	ARG	2.0
1	E	462	ASN	2.0
1	B	203	GLY	2.0
1	J	465	MET	2.0
1	L	460	ASP	2.0
1	M	101	ASP	2.0
1	F	367	GLU	2.0
1	F	218	TYR	2.0
1	H	189	ALA	2.0
1	L	445	CYS	2.0
1	M	493	ALA	2.0
1	I	366	GLY	2.0
1	D	367	GLU	2.0
1	L	449	TRP	2.0
1	J	462	ASN	2.0
1	D	216	HIS	2.0
1	F	421	ALA	2.0
1	H	370	THR	2.0
1	D	416	GLU	2.0
1	I	231	GLU	2.0
1	D	101	ASP	2.0
1	G	362	VAL	2.0
1	E	319	PHE	2.0
1	G	459	PRO	2.0
1	C	489	GLN	2.0
1	L	490	GLN	2.0
1	E	91	TYR	2.0
1	G	483	LEU	2.0

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

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.