Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2022 – 02:26 PM EST

PDB ID	:	4XVW
Title	:	Crystal structure of Proteus mirabilis ScsC in a compact conformation
Authors	:	Kurth, F.; Furlong, E.J.; Premkumar, L.; Martin, J.L.
Deposited on	:	2015-01-27
Resolution	:	2.60 Å(reported)

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

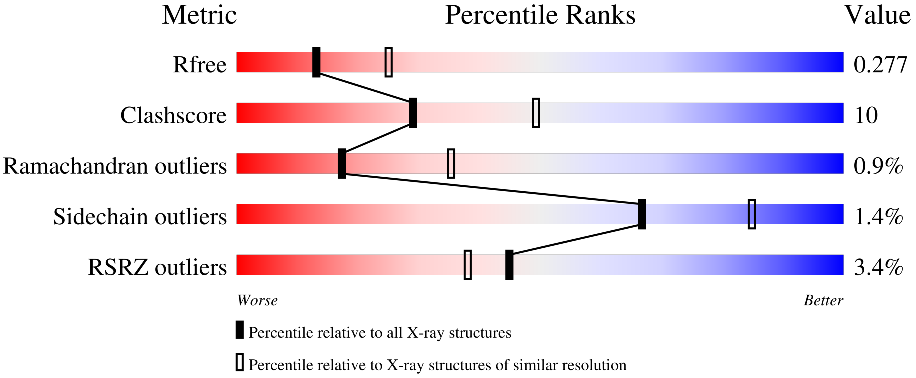
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

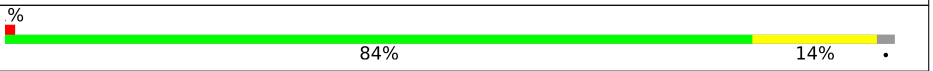
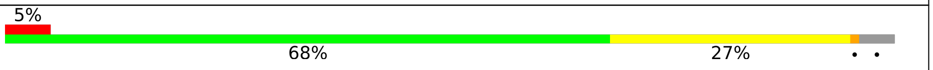
The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	224	 81% 18% •
1	B	224	 % 84% 14% •
1	C	224	 88% 11% ••
1	D	224	 86% 13% •
1	E	224	 5% 68% 27% • •

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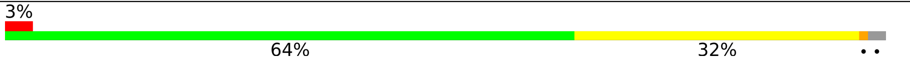
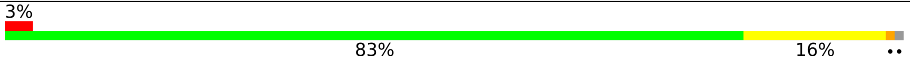
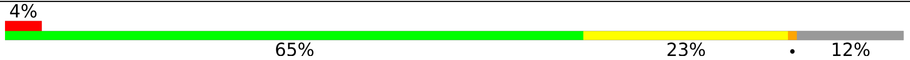
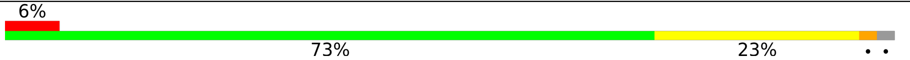
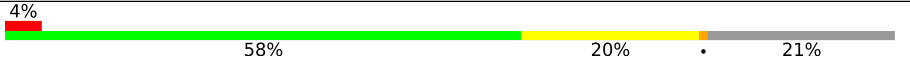
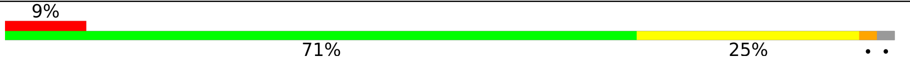
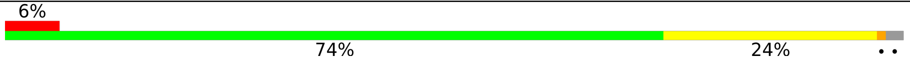
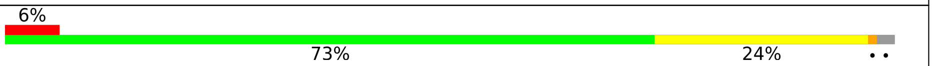
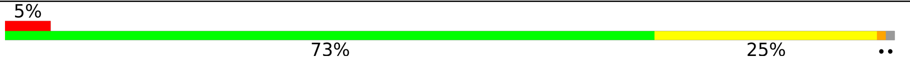
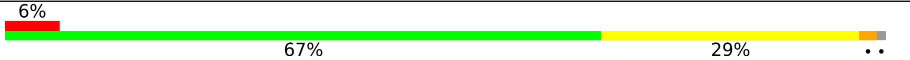
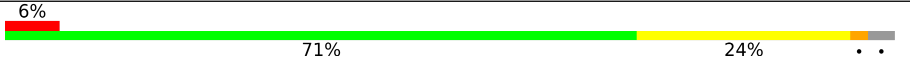
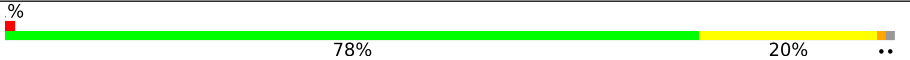
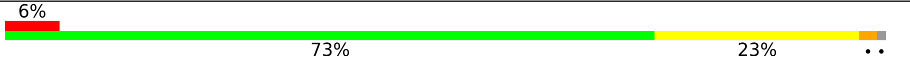
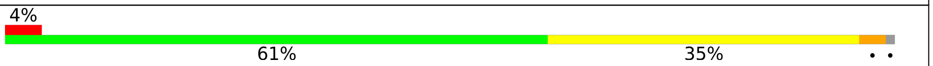
Mol	Chain	Length	Quality of chain
1	F	224	
1	G	224	
1	H	224	
1	I	224	
1	J	224	
1	K	224	
1	L	224	
1	M	224	
1	N	224	
1	O	224	
1	P	224	
1	Q	224	
1	R	224	
1	T	224	
1	U	224	
1	V	224	
1	W	224	
1	X	224	
1	Y	224	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 83204 atoms, of which 42074 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 DsbA-like protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	222	Total	C	H	N	O	S	Se	0	3	0
			3527	1095	1790	295	339	4	4			
1	B	220	Total	C	H	N	O	S	Se	0	5	0
			3500	1088	1774	292	337	4	5			
1	C	222	Total	C	H	N	O	S	Se	0	3	0
			3527	1095	1790	295	339	4	4			
1	D	222	Total	C	H	N	O	S	Se	0	3	0
			3527	1095	1790	295	339	4	4			
1	E	215	Total	C	H	N	O	S	Se	0	3	0
			3437	1068	1745	286	330	4	4			
1	F	222	Total	C	H	N	O	S	Se	0	3	0
			3527	1095	1790	295	339	4	4			
1	G	219	Total	C	H	N	O	S	Se	0	3	0
			3488	1083	1769	292	336	4	4			
1	H	222	Total	C	H	N	O	S	Se	0	3	0
			3527	1095	1790	295	339	4	4			
1	I	198	Total	C	H	N	O	S	Se	0	0	0
			3118	972	1579	261	300	2	4			
1	J	219	Total	C	H	N	O	S	Se	0	0	0
			3451	1074	1750	288	333	2	4			
1	K	220	Total	C	H	N	O	S	Se	0	5	0
			3500	1088	1774	292	337	4	5			
1	L	176	Total	C	H	N	O	S	Se	0	0	0
			2800	874	1428	224	268	2	4			
1	M	220	Total	C	H	N	O	S	Se	0	3	0
			3482	1083	1764	291	336	4	4			
1	N	220	Total	C	H	N	O	S	Se	0	0	0
			3473	1080	1763	290	334	2	4			
1	O	220	Total	C	H	N	O	S	Se	0	3	0
			3482	1083	1764	291	336	4	4			
1	P	222	Total	C	H	N	O	S	Se	0	0	0
			3506	1089	1781	293	337	2	4			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Q	221	Total C H N O S Se 3504 1089 1777 293 337 4 4	0	3	0
1	R	218	Total C H N O S Se 3474 1079 1763 290 334 4 4	0	3	0
1	T	221	Total C H N O S Se 3504 1089 1777 293 337 4 4	0	3	0
1	U	222	Total C H N O S Se 3527 1095 1790 295 339 4 4	0	3	0
1	V	221	Total C H N O S Se 3504 1089 1777 293 337 4 4	0	3	0
1	W	221	Total C H N O S Se 3504 1089 1777 293 337 4 4	0	3	0
1	X	222	Total C H N O S Se 3507 1089 1782 293 337 2 4	0	0	0
1	Y	222	Total C H N O S Se 3527 1095 1790 295 339 4 4	0	3	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP C2LPE2
A	2	ASN	-	expression tag	UNP C2LPE2
B	1	SER	-	expression tag	UNP C2LPE2
B	2	ASN	-	expression tag	UNP C2LPE2
C	1	SER	-	expression tag	UNP C2LPE2
C	2	ASN	-	expression tag	UNP C2LPE2
D	1	SER	-	expression tag	UNP C2LPE2
D	2	ASN	-	expression tag	UNP C2LPE2
E	1	SER	-	expression tag	UNP C2LPE2
E	2	ASN	-	expression tag	UNP C2LPE2
F	1	SER	-	expression tag	UNP C2LPE2
F	2	ASN	-	expression tag	UNP C2LPE2
G	1	SER	-	expression tag	UNP C2LPE2
G	2	ASN	-	expression tag	UNP C2LPE2
H	1	SER	-	expression tag	UNP C2LPE2
H	2	ASN	-	expression tag	UNP C2LPE2
I	1	SER	-	expression tag	UNP C2LPE2
I	2	ASN	-	expression tag	UNP C2LPE2
J	1	SER	-	expression tag	UNP C2LPE2
J	2	ASN	-	expression tag	UNP C2LPE2
K	1	SER	-	expression tag	UNP C2LPE2
K	2	ASN	-	expression tag	UNP C2LPE2
L	1	SER	-	expression tag	UNP C2LPE2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ASN	-	expression tag	UNP C2LPE2
M	1	SER	-	expression tag	UNP C2LPE2
M	2	ASN	-	expression tag	UNP C2LPE2
N	1	SER	-	expression tag	UNP C2LPE2
N	2	ASN	-	expression tag	UNP C2LPE2
O	1	SER	-	expression tag	UNP C2LPE2
O	2	ASN	-	expression tag	UNP C2LPE2
P	1	SER	-	expression tag	UNP C2LPE2
P	2	ASN	-	expression tag	UNP C2LPE2
Q	1	SER	-	expression tag	UNP C2LPE2
Q	2	ASN	-	expression tag	UNP C2LPE2
R	1	SER	-	expression tag	UNP C2LPE2
R	2	ASN	-	expression tag	UNP C2LPE2
T	1	SER	-	expression tag	UNP C2LPE2
T	2	ASN	-	expression tag	UNP C2LPE2
U	1	SER	-	expression tag	UNP C2LPE2
U	2	ASN	-	expression tag	UNP C2LPE2
V	1	SER	-	expression tag	UNP C2LPE2
V	2	ASN	-	expression tag	UNP C2LPE2
W	1	SER	-	expression tag	UNP C2LPE2
W	2	ASN	-	expression tag	UNP C2LPE2
X	1	SER	-	expression tag	UNP C2LPE2
X	2	ASN	-	expression tag	UNP C2LPE2
Y	1	SER	-	expression tag	UNP C2LPE2
Y	2	ASN	-	expression tag	UNP C2LPE2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	10	Total O 10 10	0	0
2	C	18	Total O 18 18	0	0
2	D	11	Total O 11 11	0	0
2	E	14	Total O 14 14	0	0
2	F	17	Total O 17 17	0	0
2	G	17	Total O 17 17	0	0

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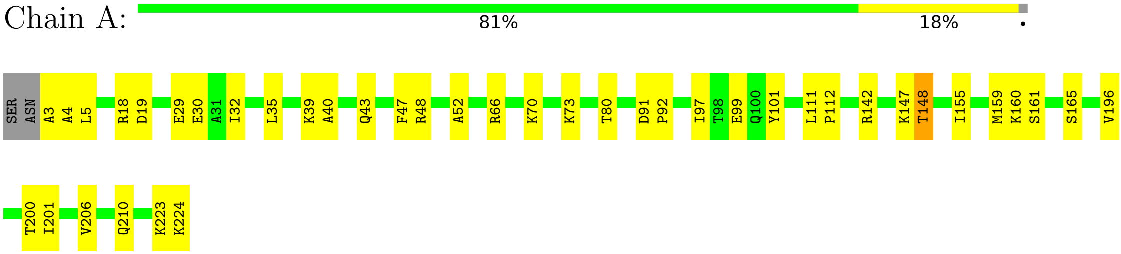
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	13	Total O 13 13	0	0
2	I	13	Total O 13 13	0	0
2	J	8	Total O 8 8	0	0
2	K	7	Total O 7 7	0	0
2	L	14	Total O 14 14	0	0
2	M	11	Total O 11 11	0	0
2	N	11	Total O 11 11	0	0
2	O	19	Total O 19 19	0	0
2	P	16	Total O 16 16	0	0
2	Q	17	Total O 17 17	0	0
2	R	9	Total O 9 9	0	0
2	T	10	Total O 10 10	0	0
2	U	6	Total O 6 6	0	0
2	V	9	Total O 9 9	0	0
2	W	6	Total O 6 6	0	0
2	X	9	Total O 9 9	0	0
2	Y	9	Total O 9 9	0	0

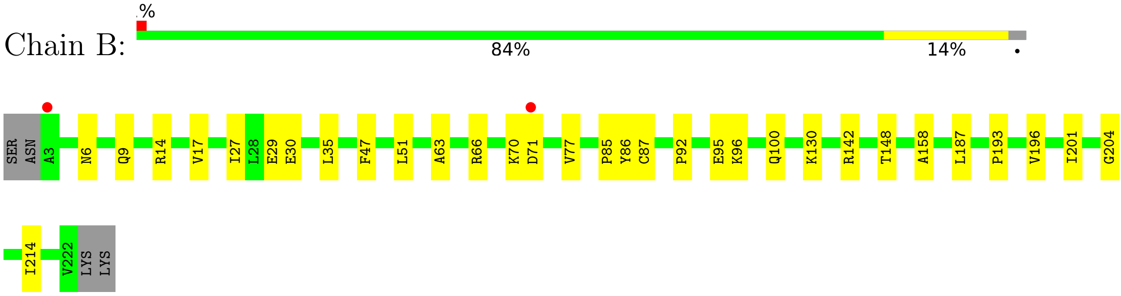
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

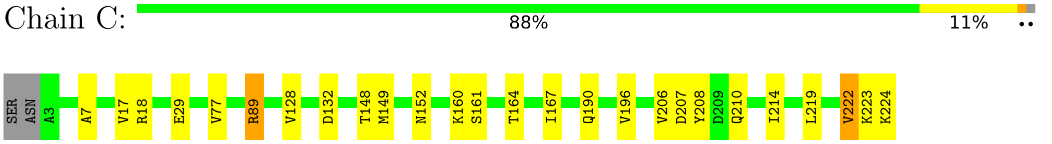
- Molecule 1: DsbA-like protein



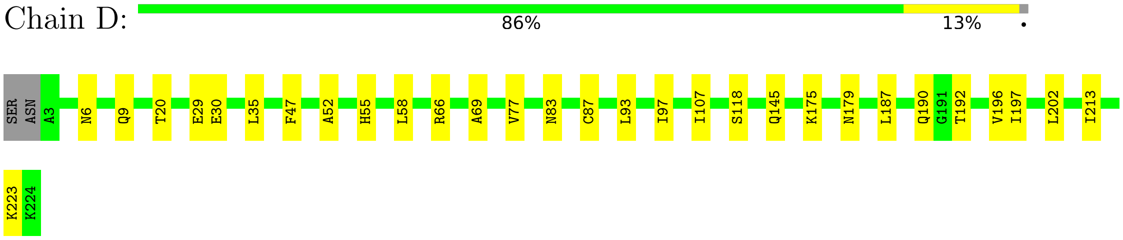
- Molecule 1: DsbA-like protein



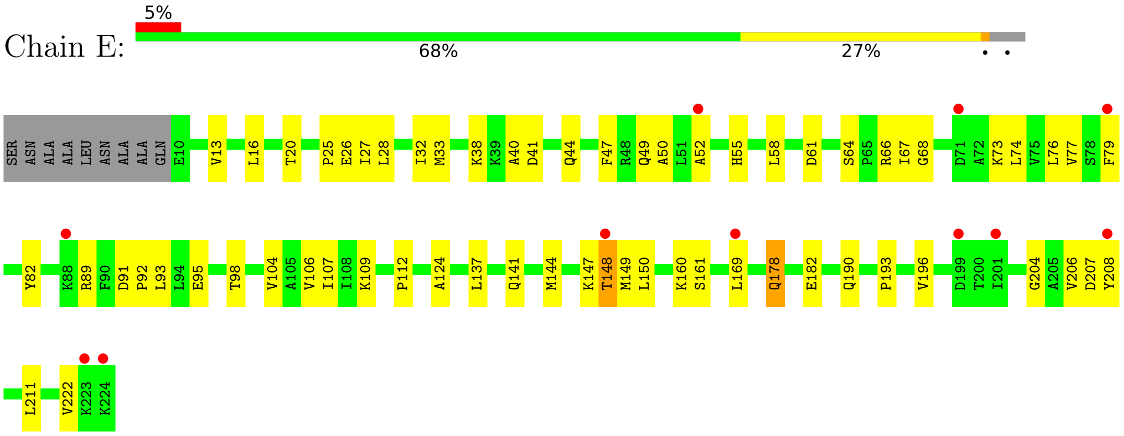
- Molecule 1: DsbA-like protein



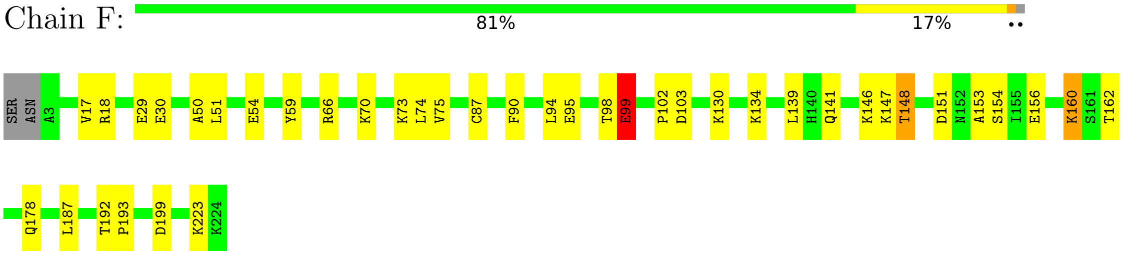
- Molecule 1: DsbA-like protein



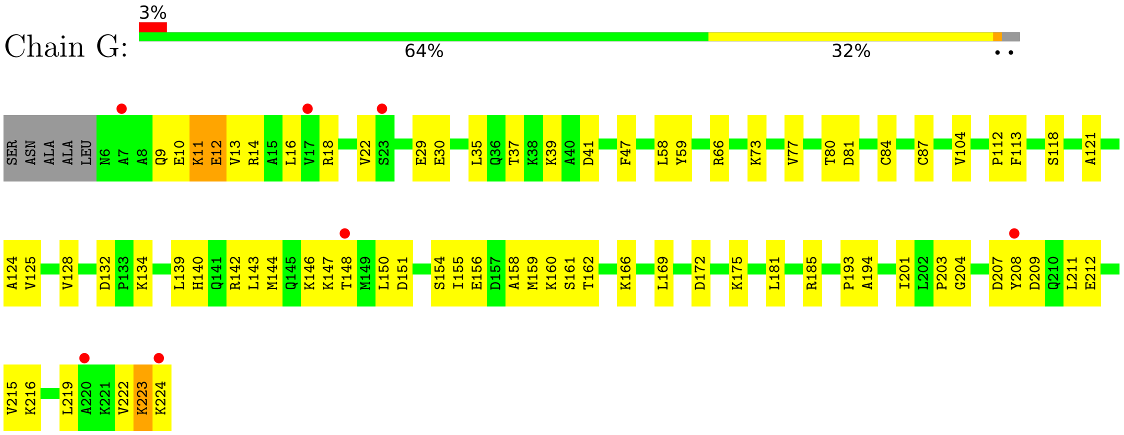
- Molecule 1: DsbA-like protein



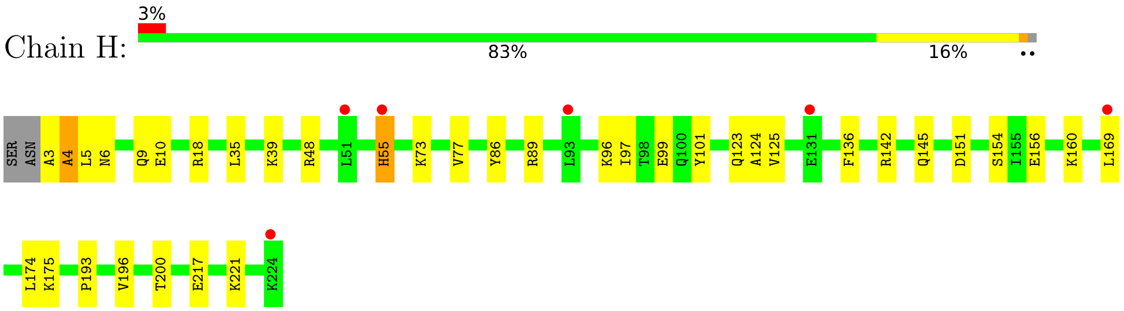
- Molecule 1: DsbA-like protein



- Molecule 1: DsbA-like protein

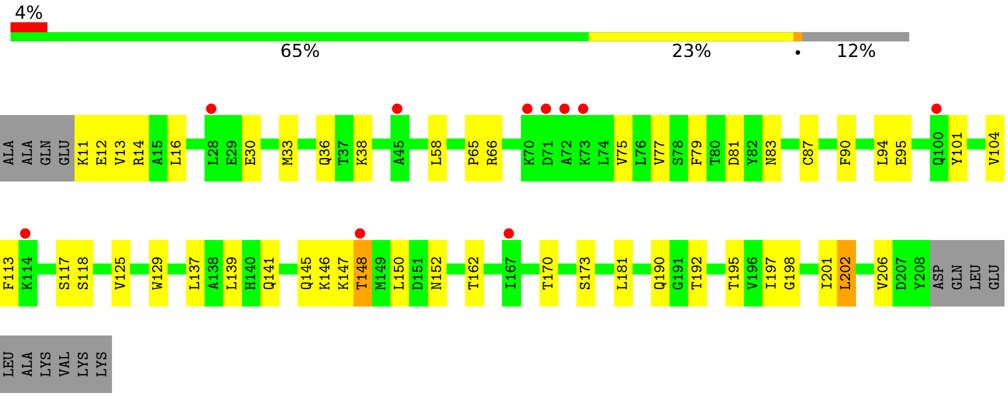


- Molecule 1: DsbA-like protein



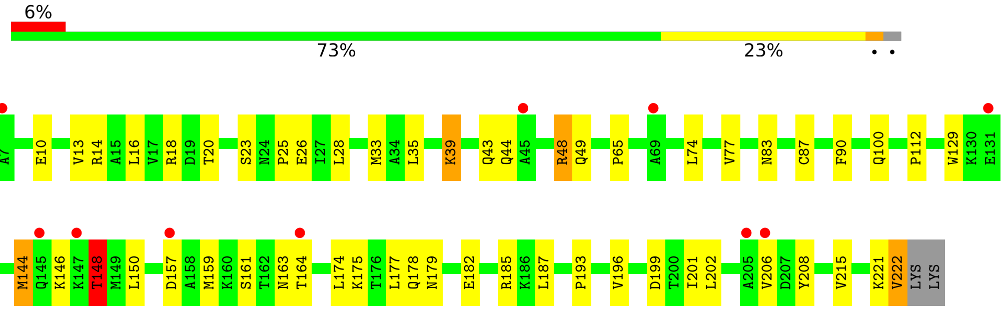
- Molecule 1: DsbA-like protein

Chain I:



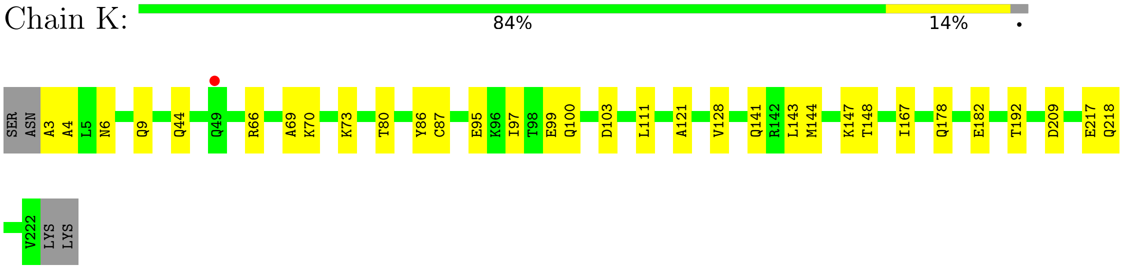
- Molecule 1: DsbA-like protein

Chain J:



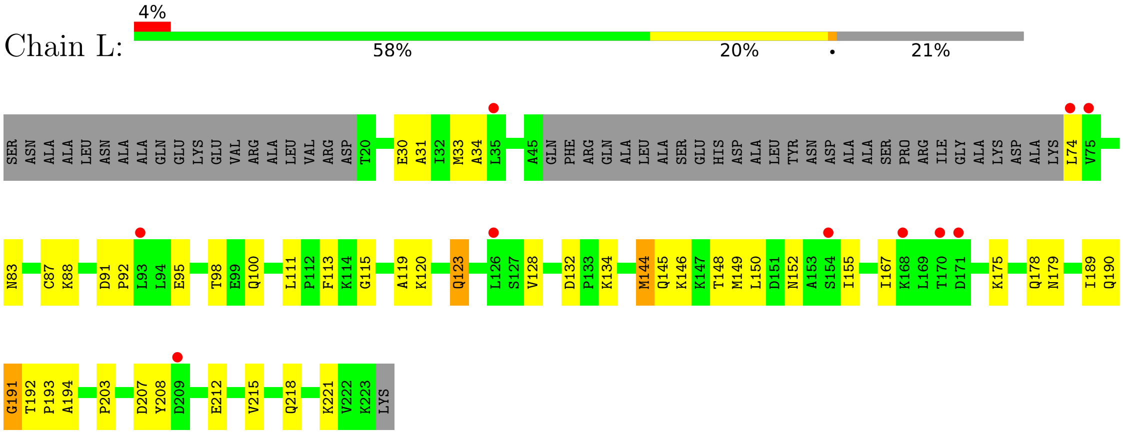
- Molecule 1: DsbA-like protein

Chain K:



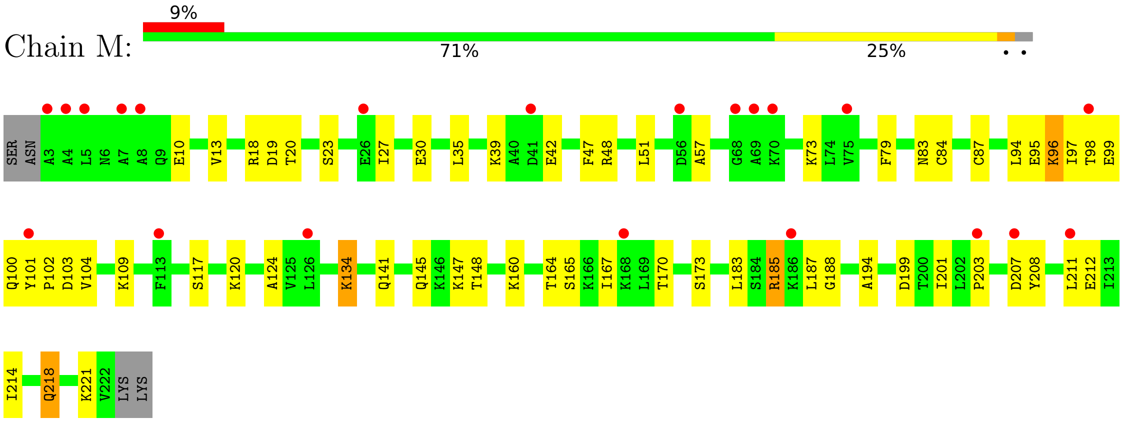
- Molecule 1: DsbA-like protein

Chain L:



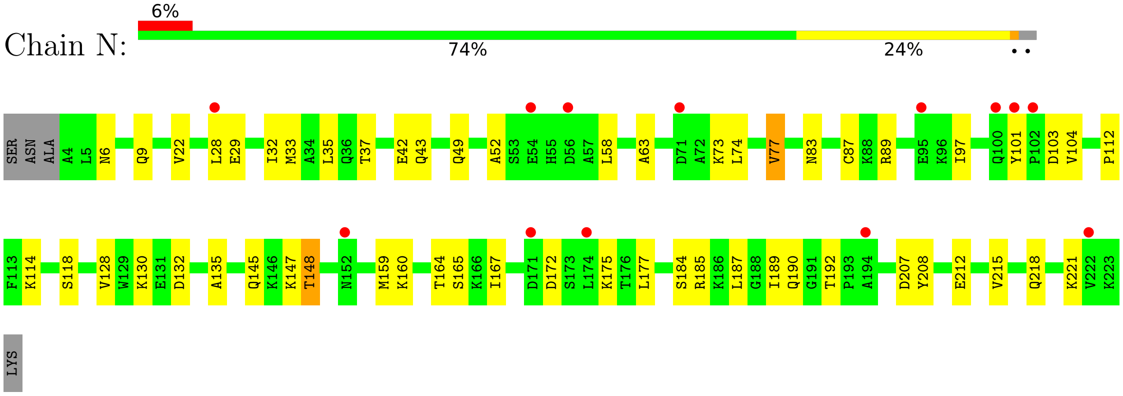
- Molecule 1: DsbA-like protein

Chain M:



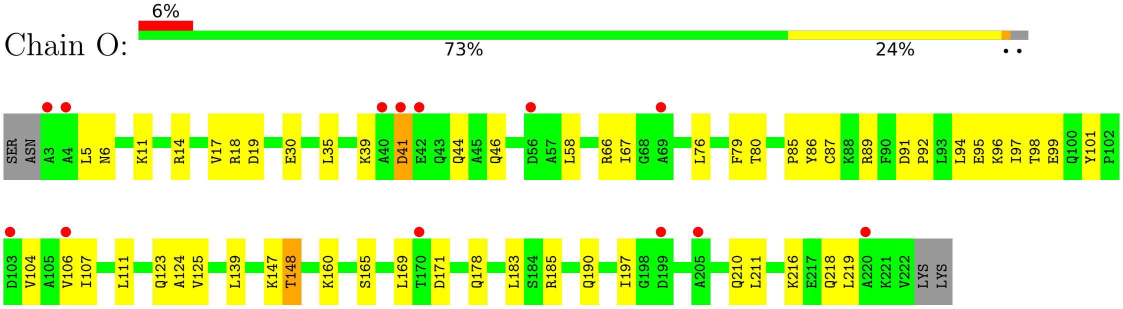
- Molecule 1: DsbA-like protein

Chain N:



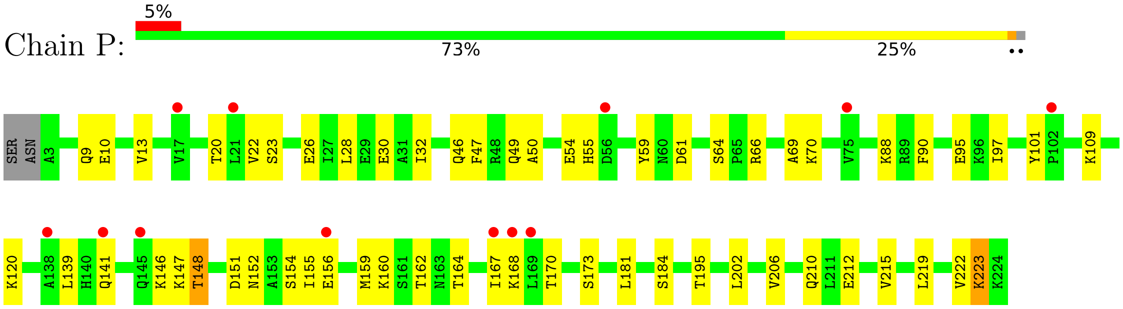
- Molecule 1: DsbA-like protein

Chain O:



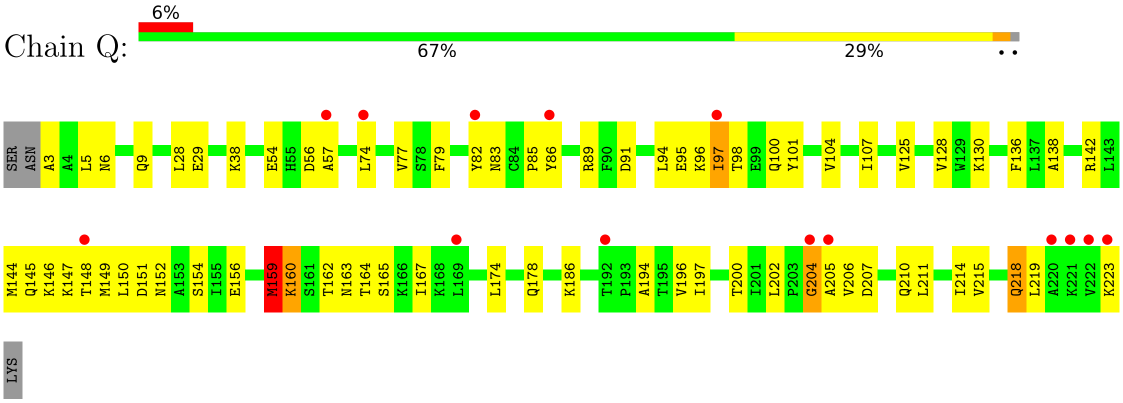
- Molecule 1: DsbA-like protein

Chain P:



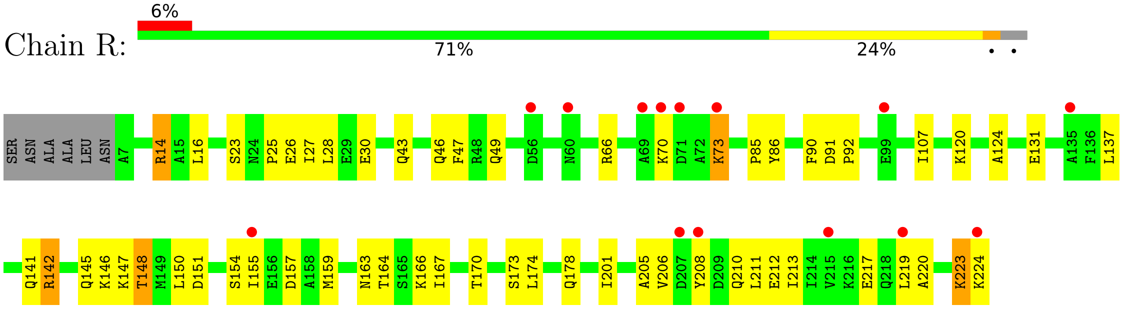
- Molecule 1: DsbA-like protein

Chain Q:



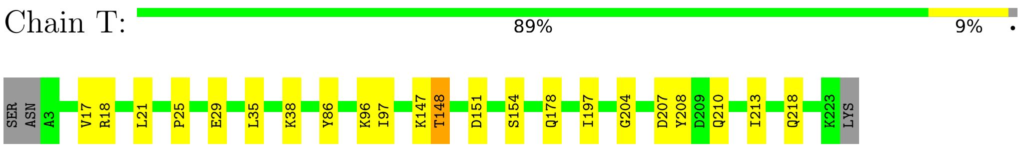
- Molecule 1: DsbA-like protein

Chain R:



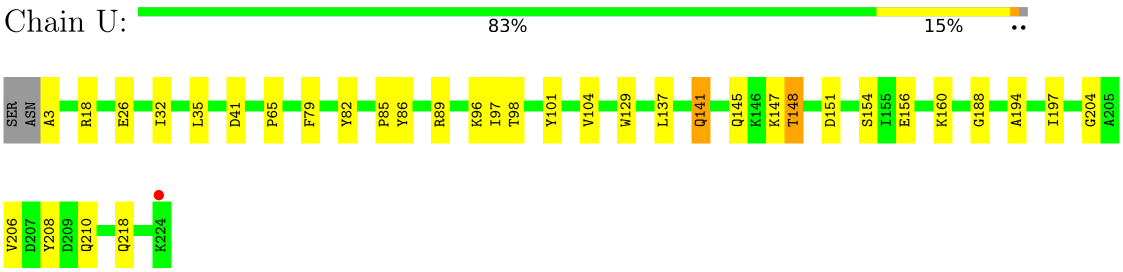
- Molecule 1: DsbA-like protein

Chain T:



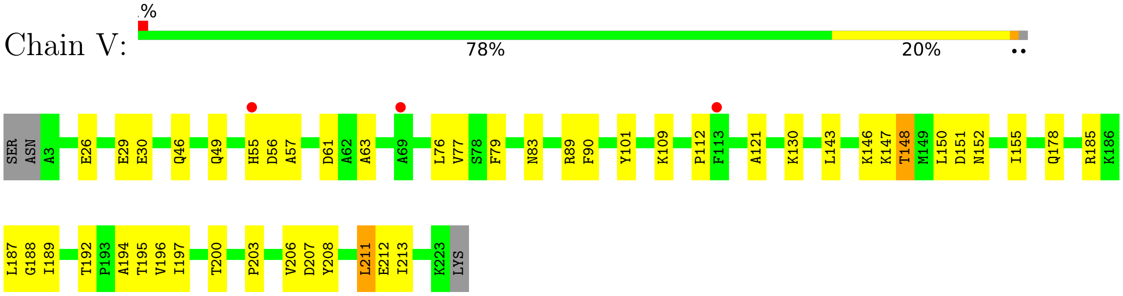
- Molecule 1: DsbA-like protein

Chain U:

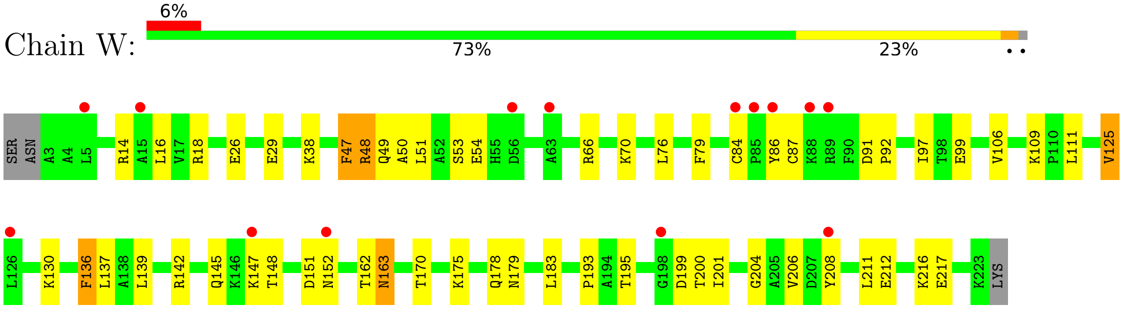


- Molecule 1: DsbA-like protein

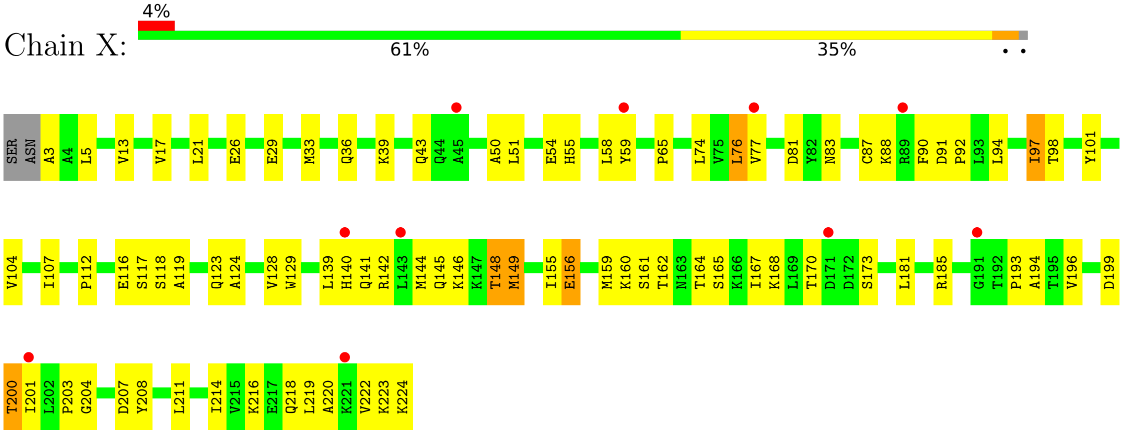
Chain V:



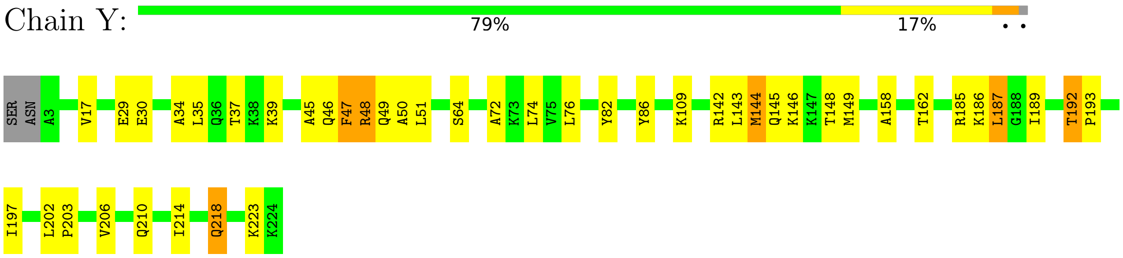
- Molecule 1: DsbA-like protein



- Molecule 1: DsbA-like protein



- Molecule 1: DsbA-like protein



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.47Å 163.88Å 181.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.15 – 2.60 64.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (91.15-2.60) 98.5 (64.30-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.248 , 0.282 0.245 , 0.277	Depositor DCC
R_{free} test set	12079 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 13.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for h,-k,-l	Depositor
Outliers	0 of 243406 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	83204	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1846e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	A	0.32	0/1765	0.56	0/2377
1	B	0.27	0/1762	0.50	0/2376
1	C	0.27	0/1765	0.53	0/2377
1	D	0.27	0/1765	0.51	0/2377
1	E	0.30	0/1720	0.62	0/2315
1	F	0.30	0/1765	0.55	0/2377
1	G	0.35	0/1747	0.68	0/2352
1	H	0.30	0/1765	0.59	0/2377
1	I	0.31	0/1558	0.65	0/2101
1	J	0.34	0/1720	0.63	0/2320
1	K	0.28	0/1763	0.51	0/2377
1	L	0.33	0/1386	0.59	0/1867
1	M	0.33	0/1746	0.67	0/2355
1	N	0.32	0/1729	0.61	0/2331
1	O	0.34	0/1746	0.63	1/2355 (0.0%)
1	P	0.30	0/1744	0.62	0/2349
1	Q	0.35	0/1755	0.70	1/2366 (0.0%)
1	R	0.31	0/1739	0.61	0/2341
1	T	0.26	0/1755	0.51	0/2366
1	U	0.29	0/1765	0.53	0/2377
1	V	0.27	0/1755	0.57	1/2366 (0.0%)
1	W	0.30	0/1755	0.64	3/2366 (0.1%)
1	X	0.33	0/1744	0.71	0/2349
1	Y	0.30	0/1765	0.62	3/2377 (0.1%)
All	All	0.31	0/41479	0.60	9/55891 (0.0%)

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	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	J	0	2
1	Q	0	1
1	X	0	1
All	All	0	6

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	47	PHE	N-CA-C	6.80	129.35	111.00
1	Y	187	LEU	CB-CG-CD1	6.50	122.06	111.00
1	Y	187	LEU	CA-CB-CG	6.37	129.95	115.30
1	Y	51	LEU	CA-CB-CG	6.15	129.45	115.30
1	O	41	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	V	211	LEU	CA-CB-CG	5.43	127.78	115.30
1	W	48	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	W	48	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	Q	204	GLY	N-CA-C	5.13	125.92	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	47	PHE	Peptide
1	F	99	GLU	Peptide
1	J	140	HIS	Peptide
1	J	144	MSE	Peptide
1	Q	149	MSE	Peptide
1	X	156	GLU	Peptide

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	1737	1790	1776	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1726	1774	1748	26	0
1	C	1737	1790	1776	18	2
1	D	1737	1790	1776	21	0
1	E	1692	1745	1731	54	0
1	F	1737	1790	1776	31	0
1	G	1719	1769	1755	69	2
1	H	1737	1790	1776	29	2
1	I	1539	1579	1579	36	0
1	J	1701	1750	1750	40	2
1	K	1726	1774	1751	23	0
1	L	1372	1428	1428	32	0
1	M	1718	1764	1750	50	1
1	N	1710	1763	1763	44	0
1	O	1718	1764	1750	51	0
1	P	1725	1781	1781	48	0
1	Q	1727	1777	1763	53	0
1	R	1711	1763	1749	41	0
1	T	1727	1777	1763	20	0
1	U	1737	1790	1776	25	1
1	V	1727	1777	1763	33	0
1	W	1727	1777	1763	38	0
1	X	1725	1782	1781	68	0
1	Y	1737	1790	1776	42	0
2	A	7	0	0	0	0
2	B	10	0	0	0	0
2	C	18	0	0	0	0
2	D	11	0	0	0	0
2	E	14	0	0	0	0
2	F	17	0	0	0	0
2	G	17	0	0	2	0
2	H	13	0	0	0	0
2	I	13	0	0	2	0
2	J	8	0	0	0	0
2	K	7	0	0	0	0
2	L	14	0	0	0	0
2	M	11	0	0	0	0
2	N	11	0	0	1	0
2	O	19	0	0	1	0
2	P	16	0	0	1	0
2	Q	17	0	0	1	0
2	R	9	0	0	1	0
2	T	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	6	0	0	0	0
2	V	9	0	0	0	0
2	W	6	0	0	0	0
2	X	9	0	0	1	0
2	Y	9	0	0	0	0
All	All	41130	42074	41800	796	5

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 10.

All (796) 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:O:124:ALA:HA	1:O:169:LEU:HD21	1.57	0.86
1:J:100:GLN:OE1	1:J:208:TYR:OH	1.97	0.83
1:I:95:GLU:OE2	1:I:141:GLN:NE2	2.11	0.83
1:O:14:ARG:NH2	1:P:23:SER:OG	2.14	0.81
1:M:57:ALA:O	1:M:109:LYS:NZ	2.13	0.81
1:Q:96:LYS:O	1:Q:98:THR:N	2.14	0.79
1:I:197:ILE:HB	1:I:198:GLY:HA3	1.65	0.78
1:I:87:CYS:SG	1:I:192:THR:OG1	2.41	0.77
1:G:18:ARG:NH2	1:L:30:GLU:OE1	2.17	0.77
1:J:178:GLN:NE2	1:J:182:GLU:OE2	2.18	0.77
1:F:187:LEU:O	1:K:86:TYR:OH	2.01	0.77
1:P:61:ASP:OD2	1:P:109:LYS:NZ	2.18	0.76
1:B:86:TYR:OH	1:D:187:LEU:O	2.02	0.76
1:L:144:MSE:O	1:L:146:LYS:N	2.20	0.75
1:T:38:LYS:NZ	1:X:26:GLU:OE1	2.20	0.75
1:M:187:LEU:O	1:O:86:TYR:OH	2.02	0.75
1:Q:89:ARG:NE	1:Q:145:GLN:OE1	2.20	0.74
1:R:43:GLN:O	1:W:86:TYR:OH	2.08	0.72
1:G:147:LYS:O	1:G:148:THR:OG1	2.07	0.71
1:E:124:ALA:HA	1:E:169:LEU:HD22	1.73	0.71
1:Y:142:ARG:NH2	1:Y:158:ALA:O	2.23	0.71
1:U:41:ASP:OD1	1:V:152:ASN:ND2	2.24	0.71
1:L:128:VAL:O	1:L:132:ASP:N	2.24	0.70
1:C:219:LEU:O	1:C:224:LYS:NZ	2.25	0.70
1:G:30:GLU:OE1	1:H:18:ARG:NH2	2.24	0.70
1:Q:151:ASP:OD1	1:Q:152:ASN:N	2.24	0.70
1:E:41:ASP:OD1	1:I:152:ASN:ND2	2.25	0.69
1:X:160:LYS:N	1:X:165:SER:OG	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:GLN:N	1:K:218:GLN:OE1	2.25	0.69
1:M:207:ASP:OD1	1:M:208:TYR:N	2.26	0.69
1:T:18:ARG:NH2	1:Y:30:GLU:OE1	2.26	0.68
1:A:160:LYS:HE3	1:A:165:SER:HB2	1.75	0.68
1:O:97:ILE:HG22	1:O:104:VAL:HG21	1.76	0.67
1:M:42:GLU:OE1	1:M:185:ARG:NH2	2.27	0.67
1:E:124:ALA:HA	1:E:169:LEU:CD2	2.24	0.67
1:O:101:TYR:HB2	1:O:104:VAL:HG22	1.75	0.67
1:O:18:ARG:NH2	1:W:175:LYS:HB2	2.09	0.67
1:M:94:LEU:O	1:M:98:THR:OG1	2.08	0.67
1:Y:187:LEU:HB3	1:Y:189:ILE:CD1	2.25	0.66
1:P:66:ARG:NH2	1:P:69:ALA:O	2.28	0.66
1:G:10:GLU:HA	1:G:13:VAL:HG22	1.78	0.66
1:U:156:GLU:O	1:U:160:LYS:N	2.27	0.66
1:Q:159:MSE:HE3	1:Q:165:SER:HA	1.77	0.66
1:F:95:GLU:O	1:F:98:THR:OG1	2.13	0.65
1:H:151:ASP:OD1	1:H:154:SER:N	2.29	0.65
1:L:175:LYS:O	1:L:179:ASN:ND2	2.28	0.65
1:O:123:GLN:HG2	1:O:169:LEU:HD22	1.79	0.65
1:R:205:ALA:O	1:W:200:THR:OG1	2.15	0.65
1:P:61:ASP:OD2	1:P:64:SER:OG	2.15	0.65
1:J:175:LYS:O	1:J:179:ASN:ND2	2.29	0.65
1:P:13:VAL:HG21	1:W:16:LEU:HD13	1.79	0.65
1:Q:163:ASN:OD1	2:Q:301:HOH:O	2.13	0.64
1:A:19:ASP:OD2	1:B:14:ARG:NH2	2.30	0.64
1:X:98:THR:HA	1:X:101:TYR:CD2	2.33	0.64
1:F:87[A]:CYS:SG	1:F:192:THR:HG22	2.38	0.64
1:M:201:ILE:HD11	1:O:86:TYR:CZ	2.33	0.64
1:X:159:MSE:O	1:X:164:THR:OG1	2.15	0.64
1:R:163:ASN:O	1:R:166:LYS:NZ	2.31	0.64
1:Q:147:LYS:O	1:Q:148:THR:OG1	2.13	0.63
1:F:160:LYS:HZ1	1:J:48:ARG:HB3	1.63	0.63
1:M:100:GLN:NE2	1:M:212:GLU:OE1	2.30	0.63
1:R:213:ILE:O	1:R:217:GLU:N	2.31	0.63
1:X:168:LYS:NZ	2:X:301:HOH:O	2.30	0.63
1:E:38:LYS:HD2	1:J:25:PRO:HD2	1.80	0.63
1:Q:200:THR:OG1	1:X:207:ASP:OD2	2.17	0.63
1:C:152:ASN:ND2	1:K:44:GLN:OE1	2.28	0.63
1:Q:91:ASP:O	1:Q:95:GLU:N	2.31	0.63
1:Y:187:LEU:HB3	1:Y:189:ILE:HD12	1.81	0.63
1:M:101:TYR:O	1:M:103:ASP:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ARG:HG2	1:D:107:ILE:HD13	1.81	0.62
1:U:26:GLU:OE1	1:V:178:GLN:NE2	2.32	0.62
1:G:29:GLU:OE2	1:L:178:GLN:NE2	2.33	0.62
1:Q:128:VAL:HG12	1:Q:167:ILE:HD11	1.82	0.62
1:A:3:ALA:HA	1:A:5:LEU:H	1.65	0.62
1:I:146:LYS:NZ	2:I:304:HOH:O	2.33	0.62
1:U:97:ILE:HG22	1:U:104:VAL:HG21	1.81	0.62
1:Y:197:ILE:O	1:Y:218:GLN:NE2	2.33	0.62
1:G:219:LEU:HA	1:G:222:VAL:HG12	1.83	0.61
1:P:170:THR:OG1	1:P:173:SER:OG	2.16	0.61
1:K:66:ARG:NH1	1:K:70:LYS:O	2.33	0.61
1:N:22:VAL:HG13	1:R:174:LEU:HD23	1.81	0.61
1:N:89:ARG:NH2	1:N:207:ASP:OD1	2.33	0.61
1:X:193:PRO:O	1:X:204:GLY:N	2.34	0.61
1:I:125:VAL:HG12	1:I:139:LEU:CD2	2.30	0.61
1:B:63:ALA:O	1:B:130:LYS:NZ	2.34	0.60
1:G:37:THR:O	1:G:41:ASP:N	2.33	0.60
1:P:46:GLN:HB2	1:P:49:GLN:HB3	1.83	0.60
1:U:147:LYS:O	1:U:148:THR:OG1	2.11	0.60
1:T:86:TYR:OH	1:V:187:LEU:O	2.17	0.60
1:G:142:ARG:HB3	1:G:146:LYS:NZ	2.16	0.60
1:J:48:ARG:NH1	1:J:199:ASP:OD1	2.34	0.60
1:G:22:VAL:HG13	1:L:34:ALA:HB2	1.82	0.60
1:I:201:ILE:O	2:I:301:HOH:O	2.16	0.60
1:K:128:VAL:HG22	1:K:167:ILE:HD13	1.84	0.60
1:I:112:PRO:HD2	1:I:181:LEU:HD13	1.83	0.60
1:D:29:GLU:OE2	1:K:178:GLN:NE2	2.34	0.59
1:U:101:TYR:O	1:U:104:VAL:HG22	2.02	0.59
1:Q:77:VAL:HG12	1:Q:107:ILE:HB	1.84	0.59
1:O:18:ARG:NH2	1:P:30:GLU:OE2	2.36	0.59
1:A:18:ARG:NH1	1:F:30:GLU:OE2	2.34	0.59
1:E:28:LEU:O	1:E:32:ILE:N	2.34	0.59
1:G:22:VAL:HG22	1:L:31:ALA:HA	1.85	0.59
1:O:5:LEU:CD1	1:P:9:GLN:HG2	2.32	0.59
1:Q:174:LEU:CD2	1:V:30:GLU:HG3	2.32	0.59
1:X:185:ARG:NH1	1:Y:29:GLU:OE2	2.34	0.59
1:R:142:ARG:HA	1:R:145:GLN:HG2	1.84	0.59
1:G:13:VAL:HG23	1:G:14:ARG:N	2.17	0.59
1:X:148:THR:HG22	1:X:149:MSE:H	1.68	0.59
1:H:96:LYS:HA	1:H:99:GLU:HG2	1.84	0.59
1:M:94:LEU:HA	1:M:97:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87[A]:CYS:SG	1:D:192:THR:OG1	2.59	0.59
1:G:58:LEU:CD2	1:G:77:VAL:HG21	2.33	0.59
1:G:146:LYS:NZ	1:G:158:ALA:HB2	2.17	0.59
1:J:39:LYS:HD3	1:J:39:LYS:N	2.17	0.59
1:P:46:GLN:O	1:P:50:ALA:N	2.36	0.59
1:Q:160:LYS:HA	1:Q:164:THR:H	1.68	0.59
1:A:48:ARG:NH2	1:E:161:SER:OG	2.36	0.58
1:I:30:GLU:HG3	1:J:174:LEU:HD22	1.85	0.58
1:J:35:LEU:HG	1:J:39:LYS:HE2	1.85	0.58
1:B:47:PHE:CE1	1:B:201:ILE:HG12	2.38	0.58
1:H:124:ALA:HA	1:H:169:LEU:CD2	2.33	0.58
1:R:147:LYS:O	1:R:148:THR:OG1	2.11	0.58
1:E:50:ALA:O	1:E:55:HIS:N	2.36	0.58
1:O:19:ASP:OD2	1:W:14:ARG:NH1	2.35	0.58
1:L:87:CYS:SG	1:L:192:THR:CG2	2.92	0.58
1:U:98:THR:HA	1:U:104:VAL:HG23	1.84	0.57
1:A:35:LEU:HD21	1:A:39:LYS:HE3	1.84	0.57
1:K:128:VAL:HG22	1:K:167:ILE:CD1	2.34	0.57
1:O:125:VAL:HG12	1:O:139:LEU:HD22	1.87	0.57
1:Q:74:LEU:HB2	1:Q:219:LEU:HD21	1.86	0.57
1:U:156:GLU:O	1:U:160:LYS:HG3	2.04	0.57
1:M:214:ILE:O	1:M:218:GLN:NE2	2.38	0.57
1:E:74:LEU:HD21	1:E:76:LEU:HD11	1.85	0.57
1:O:67:ILE:HB	1:O:106:VAL:CG2	2.35	0.57
1:A:147:LYS:O	1:A:148:THR:OG1	2.14	0.57
1:W:193:PRO:O	1:W:204:GLY:N	2.37	0.57
1:N:32:ILE:HD13	1:R:28:LEU:HD21	1.87	0.56
1:U:18:ARG:NH2	1:V:30:GLU:OE1	2.38	0.56
1:Y:144:MSE:O	1:Y:146:LYS:N	2.39	0.56
1:G:22:VAL:HG13	1:L:34:ALA:CB	2.36	0.56
1:G:66:ARG:NH2	2:G:301:HOH:O	2.39	0.56
1:M:47:PHE:CE2	1:O:85:PRO:HB2	2.39	0.56
1:M:147:LYS:O	1:M:148:THR:OG1	2.17	0.56
1:X:50:ALA:O	1:X:54:GLU:HB2	2.05	0.56
1:K:147:LYS:O	1:K:148:THR:OG1	2.22	0.56
1:Q:156:GLU:HA	1:Q:159:MSE:SE	2.56	0.56
1:C:207:ASP:OD1	1:C:208:TYR:N	2.38	0.56
1:O:11:LYS:HA	1:O:14:ARG:HB2	1.88	0.56
1:Y:35:LEU:CD2	1:Y:39:LYS:HE3	2.35	0.56
1:G:222:VAL:HG13	1:G:223:LYS:H	1.71	0.56
1:D:66:ARG:HG2	1:D:107:ILE:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:79:PHE:HB3	1:O:111:LEU:HD11	1.89	0.55
1:J:10:GLU:HA	1:J:13:VAL:HG22	1.88	0.55
1:R:66:ARG:HE	1:R:107:ILE:HD11	1.70	0.55
1:V:56:ASP:OD1	1:V:57:ALA:N	2.38	0.55
1:C:210:GLN:O	1:C:214:ILE:HD12	2.06	0.55
1:F:146:LYS:NZ	1:F:154:SER:O	2.40	0.55
1:G:58:LEU:HD22	1:G:59:TYR:CE2	2.42	0.55
1:G:142:ARG:NH2	1:G:161:SER:OG	2.39	0.55
1:U:197:ILE:O	1:U:218:GLN:NE2	2.40	0.55
1:E:73:LYS:HE3	1:E:222:VAL:HG22	1.89	0.55
1:P:26:GLU:OE2	2:P:301:HOH:O	2.18	0.55
1:G:11:LYS:HE2	1:H:4:ALA:HB2	1.89	0.55
1:X:216:LYS:HA	1:X:219:LEU:HD12	1.89	0.55
1:D:52:ALA:O	1:D:55:HIS:ND1	2.40	0.55
1:N:97:ILE:HD12	1:N:215:VAL:HG21	1.88	0.55
1:Q:207:ASP:H	1:X:200:THR:HG21	1.72	0.55
1:Q:206:VAL:HG22	1:Q:210:GLN:HB2	1.88	0.54
1:X:156:GLU:HA	1:X:159:MSE:CG	2.37	0.54
1:E:13:VAL:HG21	1:I:16:LEU:HD13	1.89	0.54
1:U:85:PRO:O	1:U:89:ARG:NH1	2.40	0.54
1:M:95:GLU:OE1	1:M:141:GLN:NE2	2.36	0.54
1:D:66:ARG:NH2	1:D:69:ALA:O	2.40	0.54
1:A:196:VAL:HG22	1:A:201:ILE:HD12	1.89	0.54
1:M:10:GLU:O	1:M:13:VAL:HG22	2.07	0.54
1:W:130:LYS:NZ	1:W:170:THR:OG1	2.39	0.54
1:A:73:LYS:HE2	1:A:224:LYS:HD3	1.89	0.54
1:P:147:LYS:O	1:P:148:THR:OG1	2.25	0.54
1:B:30:GLU:OE1	1:F:18:ARG:NH2	2.41	0.54
1:E:58:LEU:HD22	1:E:77:VAL:HG11	1.89	0.54
1:G:73:LYS:HD2	1:G:223:LYS:HD3	1.89	0.54
1:L:88:LYS:HE3	1:L:144:MSE:O	2.08	0.54
1:M:120:LYS:HD3	1:N:37:THR:HG21	1.90	0.54
1:Q:160:LYS:O	1:Q:160:LYS:HG3	2.06	0.54
1:A:66:ARG:NH1	1:A:70:LYS:O	2.41	0.53
1:X:101:TYR:CD2	1:X:104:VAL:HG23	2.43	0.53
1:M:30:GLU:HB3	1:R:178:GLN:HG3	1.89	0.53
1:O:67:ILE:HG21	1:O:95:GLU:HG3	1.89	0.53
1:A:160:LYS:HG3	1:A:165:SER:HB2	1.91	0.53
1:K:95:GLU:OE1	1:K:141:GLN:NE2	2.40	0.53
1:Q:204:GLY:HA3	1:X:203:PRO:HD2	1.89	0.53
1:A:35:LEU:CD2	1:A:39:LYS:HE3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:LEU:O	1:G:215:VAL:HG22	2.09	0.53
1:K:66:ARG:NH2	1:K:69:ALA:O	2.42	0.53
1:X:88:LYS:O	1:X:144:MSE:HE1	2.09	0.53
1:L:128:VAL:HG12	1:L:167:ILE:HD13	1.91	0.53
1:B:196:VAL:HG22	1:B:201:ILE:CD1	2.38	0.53
1:F:147:LYS:O	1:F:148:THR:OG1	2.19	0.53
1:O:30:GLU:OE1	1:W:18:ARG:NH1	2.42	0.53
1:U:86:TYR:OH	1:Y:187:LEU:O	2.27	0.53
1:Y:192:THR:HG22	1:Y:193:PRO:HA	1.90	0.53
1:J:90:PHE:HE1	1:J:206:VAL:HG22	1.74	0.52
1:M:96:LYS:HE3	1:M:208:TYR:CE1	2.44	0.52
1:M:218:GLN:OE1	1:O:210:GLN:NE2	2.42	0.52
1:Y:142:ARG:NH2	1:Y:162:THR:HG23	2.24	0.52
1:P:164:THR:O	1:P:167:ILE:HG22	2.09	0.52
1:R:157:ASP:OD1	2:R:301:HOH:O	2.19	0.52
1:A:3:ALA:HA	1:A:4:ALA:HB3	1.91	0.52
1:G:18:ARG:HH21	1:H:175:LYS:HG3	1.75	0.52
1:G:194:ALA:HA	1:G:203:PRO:HA	1.92	0.52
1:M:120:LYS:O	1:M:124:ALA:N	2.41	0.52
1:Q:86:TYR:CD2	1:Q:205:ALA:HB1	2.44	0.52
1:X:222:VAL:O	1:X:224:LYS:N	2.42	0.52
1:Q:142:ARG:O	1:Q:146:LYS:HE2	2.09	0.52
1:X:58:LEU:HB3	1:X:59:TYR:CD1	2.45	0.52
1:X:141:GLN:O	1:X:145:GLN:N	2.42	0.52
1:I:66:ARG:HB3	1:I:107:ILE:HD13	1.91	0.52
1:T:178:GLN:NE2	1:X:29:GLU:OE2	2.39	0.52
1:Y:64:SER:OG	1:Y:109:LYS:NZ	2.40	0.52
1:G:16:LEU:HD11	1:H:10:GLU:HG3	1.90	0.52
1:G:207:ASP:OD1	1:G:208:TYR:N	2.43	0.52
1:L:115:GLY:HA3	1:L:149:MSE:HE1	1.91	0.52
1:O:178:GLN:NE2	1:W:26:GLU:OE1	2.42	0.52
1:X:208:TYR:HA	1:X:211:LEU:HD13	1.91	0.52
1:J:83:ASN:HA	1:J:144:MSE:HG3	1.92	0.52
1:J:157:ASP:O	1:J:161:SER:N	2.41	0.52
1:C:17:VAL:HG11	1:D:20:THR:HG21	1.91	0.51
1:G:9:GLN:C	1:G:11:LYS:N	2.62	0.51
1:N:63:ALA:O	1:N:130:LYS:NZ	2.32	0.51
1:O:41:ASP:HA	1:O:44:GLN:HB2	1.91	0.51
1:X:142:ARG:HH21	1:X:162:THR:HG23	1.75	0.51
1:E:25:PRO:HD2	1:I:38:LYS:HD2	1.93	0.51
1:G:143:LEU:HD22	1:G:150:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:LEU:O	1:J:20:THR:OG1	2.23	0.51
1:J:196:VAL:HG12	1:J:201:ILE:HD12	1.92	0.51
1:N:58:LEU:HD22	1:N:77:VAL:HG21	1.91	0.51
1:X:194:ALA:HB1	1:X:201:ILE:HD11	1.92	0.51
1:D:93:LEU:O	1:D:97:ILE:HD12	2.09	0.51
1:L:128:VAL:HG12	1:L:167:ILE:HG21	1.92	0.51
1:Q:215:VAL:O	1:Q:218:GLN:NE2	2.43	0.51
1:W:84[B]:CYS:SG	1:W:87[B]:CYS:N	2.83	0.51
1:W:142:ARG:HA	1:W:145:GLN:HB2	1.92	0.51
1:E:178:GLN:NE2	1:J:26:GLU:O	2.44	0.51
1:N:184:SER:OG	1:N:189:ILE:O	2.28	0.51
1:X:50:ALA:O	1:X:54:GLU:N	2.43	0.51
1:G:151:ASP:H	1:G:154:SER:HB2	1.75	0.51
1:Q:160:LYS:HB3	1:Q:165:SER:OG	2.11	0.51
1:R:46:GLN:HB2	1:R:49:GLN:HE22	1.75	0.51
1:M:84[B]:CYS:SG	1:M:87[B]:CYS:N	2.83	0.51
1:G:11:LYS:HE2	1:H:4:ALA:CB	2.39	0.51
1:N:97:ILE:HG22	1:N:104:VAL:HG11	1.93	0.51
1:Y:47:PHE:O	1:Y:48:ARG:NH1	2.44	0.51
1:A:35:LEU:HD11	1:B:29:GLU:HB2	1.93	0.51
1:K:66:ARG:CZ	1:K:69:ALA:O	2.59	0.51
1:O:147:LYS:O	1:O:148:THR:OG1	2.29	0.51
1:E:95:GLU:O	1:E:98:THR:OG1	2.24	0.51
1:H:55:HIS:ND1	1:H:55:HIS:C	2.64	0.51
1:O:18:ARG:NH2	1:P:30:GLU:OE1	2.45	0.51
1:Q:138:ALA:HB3	1:Q:162:THR:HG23	1.92	0.51
1:X:160:LYS:HA	1:X:164:THR:H	1.75	0.51
1:C:89:ARG:O	1:C:89:ARG:HG3	2.10	0.50
1:M:47:PHE:CD2	1:O:86:TYR:CE1	2.99	0.50
1:V:63:ALA:O	1:V:130:LYS:NZ	2.42	0.50
1:F:51:LEU:HD22	1:F:199:ASP:HA	1.93	0.50
1:E:49:GLN:O	1:E:49:GLN:HG2	2.11	0.50
1:W:50:ALA:O	1:W:54:GLU:N	2.42	0.50
1:N:187:LEU:HB3	1:N:189:ILE:CD1	2.42	0.50
1:X:160:LYS:HB2	1:X:165:SER:HB2	1.94	0.50
1:F:73:LYS:HG3	1:F:74:LEU:N	2.26	0.50
1:L:87:CYS:SG	1:L:192:THR:HG22	2.52	0.50
1:E:20:THR:CG2	1:J:14:ARG:HG2	2.42	0.50
1:G:142:ARG:HB3	1:G:146:LYS:HZ1	1.77	0.50
1:P:139:LEU:HA	1:P:162:THR:HG21	1.93	0.50
1:C:18:ARG:NH2	1:D:30:GLU:OE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:TYR:CG	1:G:209:ASP:N	2.80	0.50
1:H:156:GLU:HB2	1:H:160:LYS:NZ	2.26	0.50
1:R:137:LEU:O	1:R:141:GLN:HG3	2.12	0.50
1:V:150:LEU:HD23	1:V:155:ILE:HD13	1.93	0.50
1:X:59:TYR:CE1	1:X:77:VAL:HG13	2.47	0.50
1:A:200:THR:HG21	1:C:207:ASP:HB2	1.94	0.50
1:G:10:GLU:HA	1:G:13:VAL:CG2	2.41	0.50
1:M:18:ARG:NH1	1:R:30:GLU:OE2	2.45	0.50
1:B:214:ILE:HG12	1:D:213:ILE:HD11	1.93	0.49
1:H:55:HIS:C	1:H:55:HIS:HD1	2.15	0.49
1:K:66:ARG:NE	1:K:69:ALA:O	2.44	0.49
1:O:197:ILE:HG22	1:O:218:GLN:HG3	1.94	0.49
1:Q:178:GLN:NE2	1:V:29:GLU:OE2	2.45	0.49
1:T:207:ASP:OD1	1:V:200:THR:OG1	2.29	0.49
1:X:51:LEU:O	1:X:55:HIS:NE2	2.44	0.49
1:P:66:ARG:NH1	1:P:70:LYS:O	2.44	0.49
1:X:139:LEU:HD11	1:X:159:MSE:SE	2.62	0.49
1:M:47:PHE:CE2	1:O:86:TYR:CE1	3.00	0.49
1:H:124:ALA:HA	1:H:169:LEU:HD21	1.93	0.49
1:A:30:GLU:HB2	1:F:178:GLN:HG3	1.93	0.49
1:X:98:THR:HA	1:X:101:TYR:CE2	2.48	0.49
1:Q:54:GLU:OE1	1:Q:186:LYS:NZ	2.46	0.49
1:B:196:VAL:HG22	1:B:201:ILE:HD12	1.94	0.49
1:L:100:GLN:NE2	1:L:212:GLU:OE2	2.38	0.49
1:N:97:ILE:CG2	1:N:104:VAL:HG11	2.42	0.49
1:R:27:ILE:HG23	1:R:28:LEU:N	2.27	0.49
1:H:124:ALA:CA	1:H:169:LEU:HD21	2.42	0.49
1:R:66:ARG:HH11	1:R:70:LYS:HA	1.77	0.49
1:C:206:VAL:HG22	1:C:210:GLN:HB2	1.93	0.49
1:E:178:GLN:O	1:E:182:GLU:N	2.41	0.49
1:G:13:VAL:HG23	1:G:14:ARG:HG3	1.94	0.49
1:A:160:LYS:CE	1:A:165:SER:HB2	2.42	0.48
1:E:64:SER:OG	1:E:109:LYS:NZ	2.31	0.48
1:Q:29:GLU:HB2	1:U:35:LEU:HD11	1.95	0.48
1:W:76:LEU:HD13	1:W:195:THR:HG23	1.95	0.48
1:G:10:GLU:CA	1:G:13:VAL:HG22	2.43	0.48
1:Y:74:LEU:CD2	1:Y:76:LEU:HD12	2.43	0.48
1:G:84[B]:CYS:SG	1:G:87[B]:CYS:N	2.81	0.48
1:Q:94:LEU:HD13	1:Q:211:LEU:HB3	1.96	0.48
1:X:83:ASN:OD1	1:X:117:SER:OG	2.18	0.48
1:Y:202:LEU:HD21	1:Y:206:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ILE:HB	1:E:106:VAL:HG23	1.95	0.48
1:N:87:CYS:SG	1:N:192:THR:HB	2.53	0.48
1:B:96:LYS:O	1:B:100:GLN:N	2.43	0.48
1:F:151:ASP:OD1	1:F:154:SER:N	2.39	0.48
1:G:139:LEU:HB2	1:G:162:THR:HG21	1.96	0.48
1:I:113:PHE:CE1	1:I:181:LEU:HD11	2.49	0.48
1:J:159:MSE:O	1:J:163:ASN:N	2.47	0.48
1:R:90:PHE:HE1	1:R:206:VAL:HG22	1.78	0.48
1:H:55:HIS:ND1	1:H:55:HIS:O	2.40	0.48
1:M:35:LEU:HD11	1:N:29:GLU:HB2	1.96	0.48
1:M:94:LEU:O	1:M:98:THR:N	2.44	0.48
1:M:101:TYR:C	1:M:103:ASP:H	2.17	0.48
1:M:170:THR:O	1:M:173:SER:OG	2.28	0.48
1:O:98:THR:HG21	1:O:106:VAL:HG22	1.96	0.48
1:P:159:MSE:O	1:P:164:THR:OG1	2.25	0.48
1:V:46:GLN:HB2	1:V:49:GLN:HE22	1.79	0.48
1:X:92:PRO:HD3	1:X:144:MSE:HE2	1.95	0.48
1:N:74:LEU:O	1:N:104:VAL:HA	2.13	0.48
1:R:223:LYS:HG3	1:R:224:LYS:H	1.79	0.48
1:I:11:LYS:HA	1:I:14:ARG:HB2	1.96	0.47
1:L:74:LEU:HD23	1:L:215:VAL:CG2	2.44	0.47
1:M:160:LYS:HG3	1:M:165:SER:OG	2.14	0.47
1:Q:28:LEU:HD21	1:U:32:ILE:HD13	1.96	0.47
1:X:167:ILE:O	1:X:167:ILE:HG13	2.12	0.47
1:B:66:ARG:HH11	1:B:70:LYS:HA	1.80	0.47
1:F:99:GLU:HA	1:F:102:PRO:HA	1.95	0.47
1:L:83:ASN:ND2	1:L:150:LEU:HD13	2.29	0.47
1:Q:210:GLN:NE2	1:X:199:ASP:OD1	2.46	0.47
1:V:77:VAL:HB	1:V:196:VAL:HB	1.96	0.47
1:M:20:THR:HG22	1:M:27:ILE:HD12	1.97	0.47
1:P:46:GLN:HB2	1:P:49:GLN:CB	2.44	0.47
1:Q:197:ILE:HD13	1:Q:202:LEU:HB2	1.97	0.47
1:R:219:LEU:HD12	1:R:220:ALA:N	2.29	0.47
1:J:144:MSE:HE2	1:J:146:LYS:HB3	1.96	0.47
1:N:83:ASN:OD1	1:N:118:SER:OG	2.24	0.47
1:X:116:GLU:OE2	1:Y:37:THR:HG22	2.13	0.47
1:E:149:MSE:HG3	1:E:150:LEU:H	1.80	0.47
1:F:130:LYS:HD2	1:F:130:LYS:O	2.15	0.47
1:G:166:LYS:H	1:G:166:LYS:HD2	1.80	0.47
1:H:125:VAL:HG13	1:H:136:PHE:CE1	2.49	0.47
1:V:79:PHE:HB2	1:V:194:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:48:ARG:NH1	1:W:200:THR:HA	2.30	0.47
1:Y:34:ALA:O	1:Y:37:THR:OG1	2.33	0.47
1:G:112:PRO:HA	1:G:118:SER:HB3	1.96	0.47
1:G:150:LEU:HD13	1:G:155:ILE:HD13	1.97	0.47
1:K:87[A]:CYS:SG	1:K:192:THR:HB	2.54	0.47
1:O:39:LYS:HG2	1:O:185:ARG:CZ	2.44	0.47
1:R:206:VAL:HG21	1:R:211:LEU:HB2	1.97	0.47
1:W:66:ARG:HH12	1:W:70:LYS:HD3	1.79	0.47
1:Y:142:ARG:CZ	1:Y:162:THR:HG23	2.45	0.47
1:D:223:LYS:HE3	1:L:134:LYS:HB3	1.96	0.47
1:F:139:LEU:HA	1:F:162:THR:HG21	1.97	0.47
1:Y:74:LEU:CD2	1:Y:76:LEU:CD1	2.93	0.47
1:M:83:ASN:ND2	1:M:117:SER:OG	2.47	0.47
1:E:20:THR:HG21	1:J:14:ARG:HG2	1.97	0.47
1:Y:48:ARG:NH2	1:Y:187:LEU:HG	2.29	0.47
1:A:200:THR:HG22	1:A:201:ILE:N	2.30	0.46
1:D:58:LEU:HD21	1:D:187:LEU:HD11	1.96	0.46
1:T:147:LYS:O	1:T:148:THR:OG1	2.19	0.46
1:W:179:ASN:O	1:W:183:LEU:N	2.45	0.46
1:C:222:VAL:HG23	1:C:224:LYS:HZ1	1.79	0.46
1:L:119:ALA:O	1:L:123:GLN:HG3	2.15	0.46
1:M:221:LYS:HB3	1:Q:138:ALA:HB2	1.97	0.46
1:N:159:MSE:O	1:N:164:THR:OG1	2.30	0.46
1:T:29:GLU:OE1	1:Y:185:ARG:NH1	2.48	0.46
1:V:206:VAL:HG13	1:V:211:LEU:HD11	1.96	0.46
1:W:79:PHE:CE2	1:W:183:LEU:HD22	2.50	0.46
1:A:142:ARG:NH1	1:A:161:SER:OG	2.49	0.46
1:E:27:ILE:HG12	1:J:18:ARG:HA	1.97	0.46
1:E:147:LYS:O	1:E:148:THR:HB	2.15	0.46
1:J:77:VAL:HB	1:J:196:VAL:HG22	1.97	0.46
1:M:79:PHE:HZ	1:M:183:LEU:HD22	1.79	0.46
1:G:58:LEU:HD21	1:G:77:VAL:HG21	1.98	0.46
1:Q:215:VAL:O	1:Q:215:VAL:HG13	2.16	0.46
1:Y:48:ARG:HG3	1:Y:50:ALA:HB3	1.97	0.46
1:T:25:PRO:O	1:Y:35:LEU:HD12	2.16	0.46
1:A:159:MSE:HB2	1:A:165:SER:OG	2.15	0.46
1:B:47:PHE:CZ	1:B:201:ILE:HG12	2.51	0.46
1:F:66:ARG:HB3	1:F:66:ARG:NH1	2.30	0.46
1:G:156:GLU:O	1:G:160:LYS:HG2	2.15	0.46
1:O:91:ASP:HB3	1:O:92:PRO:HD3	1.97	0.46
1:P:152:ASN:HA	1:P:155:ILE:HG12	1.97	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:G:121:ALA:HB2	1:G:155:ILE:HD12	1.97	0.46
1:X:87:CYS:SG	1:X:193:PRO:HB3	2.56	0.46
1:B:47:PHE:HE1	1:B:201:ILE:HG12	1.81	0.46
1:E:67:ILE:HB	1:E:106:VAL:CG2	2.46	0.46
1:E:76:LEU:HB2	1:E:106:VAL:HG12	1.97	0.46
1:I:170:THR:HG23	1:I:173:SER:H	1.80	0.46
1:K:6:ASN:OD1	1:K:9:GLN:N	2.44	0.46
1:E:190:GLN:N	1:E:190:GLN:OE1	2.48	0.46
1:F:134:LYS:HE2	1:J:222:VAL:HG12	1.98	0.46
1:G:224:LYS:NZ	1:K:99:GLU:OE1	2.45	0.46
1:N:101:TYR:HB2	1:N:104:VAL:HG12	1.96	0.46
1:B:92:PRO:O	1:B:95:GLU:HG2	2.15	0.46
1:E:76:LEU:HD12	1:E:76:LEU:N	2.31	0.46
1:P:168:LYS:CD	1:P:168:LYS:H	2.28	0.46
1:R:151:ASP:H	1:R:154:SER:HB2	1.80	0.46
1:I:75:VAL:HG12	1:I:105:ALA:HB3	1.98	0.45
1:O:96:LYS:O	1:O:99:GLU:HG2	2.16	0.45
1:X:90:PHE:O	1:X:94:LEU:HD12	2.16	0.45
1:I:195:THR:HG23	1:I:202:LEU:HB2	1.98	0.45
1:J:182:GLU:HG2	1:J:185:ARG:NH2	2.32	0.45
1:N:73:LYS:HG2	1:N:103:ASP:HB3	1.99	0.45
1:U:65:PRO:HA	1:U:129:TRP:CE2	2.52	0.45
1:Q:82:TYR:HD1	1:Q:144:MSE:HG2	1.81	0.45
1:Q:214:ILE:HG12	1:X:214:ILE:HG12	1.98	0.45
1:F:50:ALA:O	1:F:54:GLU:N	2.50	0.45
1:H:86:TYR:HB2	1:H:193:PRO:HD3	1.98	0.45
1:J:144:MSE:HE3	1:J:150:LEU:CD1	2.46	0.45
1:W:76:LEU:HD11	1:W:106:VAL:HG22	1.97	0.45
1:B:92:PRO:O	1:B:96:LYS:HD3	2.17	0.45
1:E:74:LEU:HD22	1:E:104:VAL:HG22	1.98	0.45
1:L:74:LEU:HD23	1:L:215:VAL:HG22	1.98	0.45
1:N:112:PRO:HD3	1:N:177:LEU:HD11	1.98	0.45
1:P:168:LYS:CD	1:P:168:LYS:N	2.80	0.45
1:Q:211:LEU:O	1:Q:215:VAL:HG12	2.17	0.45
1:T:197:ILE:HG22	1:T:218:GLN:HG3	1.98	0.45
1:U:204:GLY:HA3	1:Y:203:PRO:HG2	1.98	0.45
1:E:77:VAL:HB	1:E:196:VAL:HB	1.99	0.45
1:P:168:LYS:N	1:P:168:LYS:HD2	2.32	0.45
1:Q:97:ILE:HG23	1:Q:101:TYR:HD2	1.82	0.45
1:R:47:PHE:CZ	1:R:201:ILE:HG12	2.52	0.45
1:D:197:ILE:HD13	1:D:202:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:148:THR:HG22	1:X:149:MSE:N	2.30	0.45
1:B:193:PRO:HD2	1:B:204:GLY:HA2	1.98	0.45
1:H:142:ARG:HA	1:H:145:GLN:HG2	1.98	0.45
1:O:14:ARG:HA	1:O:17:VAL:HG12	1.99	0.45
1:W:179:ASN:O	1:W:183:LEU:HB2	2.16	0.45
1:X:13:VAL:O	1:X:17:VAL:HG23	2.17	0.45
1:X:65:PRO:HA	1:X:129:TRP:CE2	2.52	0.45
1:Y:148:THR:OG1	1:Y:149:MSE:N	2.49	0.45
1:A:206:VAL:HG12	1:A:210:GLN:HB2	1.98	0.45
1:O:18:ARG:NH2	1:P:30:GLU:CD	2.70	0.45
1:Q:97:ILE:HA	1:Q:100:GLN:HB2	1.99	0.45
1:Y:48:ARG:CD	1:Y:186:LYS:HB3	2.47	0.45
1:A:40:ALA:HA	1:A:43:GLN:HB3	1.98	0.44
1:A:80:THR:O	1:A:111:LEU:N	2.48	0.44
1:C:128:VAL:O	1:C:132:ASP:N	2.44	0.44
1:G:146:LYS:CD	1:G:150:LEU:HD21	2.47	0.44
1:J:43:GLN:HG3	1:J:44:GLN:HG3	2.00	0.44
1:T:17:VAL:HG21	1:Y:17:VAL:HA	1.99	0.44
1:T:210:GLN:HE22	1:V:197:ILE:HD12	1.82	0.44
1:C:222:VAL:HG23	1:C:224:LYS:NZ	2.32	0.44
1:E:82:TYR:CD1	1:E:144:MSE:HE3	2.52	0.44
1:E:193:PRO:O	1:E:204:GLY:N	2.50	0.44
1:F:59:TYR:CD1	1:F:75:VAL:HG23	2.52	0.44
1:I:58:LEU:CD2	1:I:77:VAL:HG21	2.47	0.44
1:N:28:LEU:O	1:N:32:ILE:HG12	2.17	0.44
1:Q:79:PHE:HB2	1:Q:194:ALA:HB3	1.98	0.44
1:U:151:ASP:H	1:U:154:SER:HB2	1.82	0.44
1:X:140:HIS:O	1:X:144:MSE:HB3	2.18	0.44
1:I:33:MSE:HA	1:I:36:GLN:HB2	1.99	0.44
1:M:39:LYS:HD3	1:M:185:ARG:CZ	2.47	0.44
1:M:194:ALA:HA	1:M:203:PRO:HA	1.99	0.44
1:O:76:LEU:HD22	1:O:197:ILE:HD13	1.99	0.44
1:R:73:LYS:HE2	1:R:224:LYS:HD2	1.99	0.44
1:A:91:ASP:HB3	1:A:92:PRO:HD3	2.00	0.44
1:B:35:LEU:HD21	1:F:29:GLU:HB3	1.99	0.44
1:E:74:LEU:HD21	1:E:76:LEU:CD1	2.48	0.44
1:E:137:LEU:HD21	1:E:141:GLN:NE2	2.33	0.44
1:G:104:VAL:HG22	1:G:219:LEU:HD21	1.99	0.44
1:G:212:GLU:O	1:G:216:LYS:N	2.44	0.44
1:I:77:VAL:HG22	1:I:107:ILE:HB	2.00	0.44
1:L:207:ASP:OD1	1:L:208:TYR:N	2.50	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:E:66:ARG:HB2	1:E:107:ILE:HD13	2.00	0.44
1:I:190:GLN:O	1:I:190:GLN:HG2	2.17	0.44
1:N:147:LYS:O	1:N:148:THR:OG1	2.26	0.44
1:O:80:THR:HG1	1:O:87[B]:CYS:HB3	1.83	0.44
1:B:142:ARG:HE	1:B:158:ALA:HA	1.83	0.44
1:F:98:THR:C	1:F:99:GLU:HG2	2.37	0.44
1:I:125:VAL:HG12	1:I:139:LEU:HD22	1.97	0.44
1:M:120:LYS:HD3	1:N:37:THR:CG2	2.47	0.44
1:N:6:ASN:OD1	1:N:9:GLN:N	2.43	0.44
1:N:83:ASN:HB2	1:N:114:LYS:HB3	1.99	0.44
1:P:97:ILE:HD13	1:P:215:VAL:HG21	1.99	0.44
1:T:21:LEU:HD21	1:X:21:LEU:CD1	2.47	0.44
1:X:139:LEU:HD12	1:X:164:THR:OG1	2.17	0.44
1:C:29:GLU:HB3	1:D:35:LEU:HD21	2.00	0.44
1:F:66:ARG:HB3	1:F:66:ARG:CZ	2.48	0.44
1:V:207:ASP:OD1	1:V:208:TYR:N	2.50	0.44
1:E:222:VAL:HG22	1:E:222:VAL:O	2.18	0.44
1:F:73:LYS:HG2	1:F:103:ASP:CG	2.37	0.44
1:I:13:VAL:CG2	1:J:16:LEU:HD13	2.47	0.44
1:I:83:ASN:HD21	1:I:150:LEU:HG	1.83	0.44
1:K:217:GLU:HB3	1:K:218:GLN:OE1	2.18	0.44
1:N:172:ASP:O	1:N:175:LYS:HB3	2.18	0.44
1:P:146:LYS:NZ	1:P:147:LYS:O	2.51	0.44
1:P:181:LEU:O	1:P:184:SER:OG	2.27	0.44
1:W:139:LEU:HA	1:W:162:THR:HG21	1.99	0.44
1:E:16:LEU:O	1:E:20:THR:HG23	2.18	0.43
1:E:206:VAL:HG23	1:E:211:LEU:HB2	1.99	0.43
1:F:141:GLN:OE1	1:J:221:LYS:HD3	2.18	0.43
1:G:223:LYS:HE2	1:G:224:LYS:HD3	1.99	0.43
1:J:87:CYS:HA	1:J:193:PRO:HG3	2.00	0.43
1:K:73:LYS:HD3	1:K:103:ASP:HB3	1.99	0.43
1:M:48:ARG:NH2	1:O:89:ARG:HD3	2.33	0.43
1:N:49:GLN:HG3	1:N:52:ALA:HB3	2.00	0.43
1:N:89:ARG:HD2	1:N:89:ARG:O	2.19	0.43
1:N:218:GLN:HA	1:N:221:LYS:HG3	1.99	0.43
1:R:14:ARG:HB3	1:R:14:ARG:CZ	2.47	0.43
1:X:3:ALA:O	1:X:5:LEU:N	2.46	0.43
1:X:81:ASP:OD1	1:X:118:SER:OG	2.29	0.43
1:A:3:ALA:CA	1:A:4:ALA:HB3	2.47	0.43
1:E:61:ASP:OD2	1:E:64:SER:OG	2.37	0.43
1:M:19:ASP:O	1:M:23:SER:OG	2.33	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:O:97:ILE:HD12	1:O:211:LEU:HG	2.00	0.43
1:U:79:PHE:N	1:U:194:ALA:O	2.43	0.43
1:Y:187:LEU:HD23	1:Y:189:ILE:HD13	2.00	0.43
1:I:147:LYS:O	1:I:148:THR:HG22	2.18	0.43
1:M:199:ASP:OD1	1:Q:160:LYS:NZ	2.51	0.43
1:O:94:LEU:HD23	1:O:211:LEU:HD21	2.00	0.43
1:T:35:LEU:HD21	1:X:29:GLU:HB3	2.00	0.43
1:V:151:ASP:O	1:V:155:ILE:HG12	2.18	0.43
1:X:128:VAL:HG21	1:X:139:LEU:HD13	2.00	0.43
1:E:89:ARG:O	1:E:89:ARG:HG3	2.17	0.43
1:G:13:VAL:CG2	1:G:14:ARG:N	2.82	0.43
1:G:125:VAL:O	1:G:128:VAL:HG22	2.18	0.43
1:O:5:LEU:HD11	1:P:9:GLN:HG2	2.00	0.43
1:P:219:LEU:O	1:P:223:LYS:N	2.47	0.43
1:Q:146:LYS:HD2	1:Q:150:LEU:HD11	2.00	0.43
1:B:87[A]:CYS:HA	1:B:193:PRO:HG3	2.01	0.43
1:C:164:THR:HA	1:C:167:ILE:CD1	2.49	0.43
1:Q:6:ASN:OD1	1:Q:9:GLN:N	2.47	0.43
1:R:25:PRO:HA	1:R:27:ILE:HG22	2.01	0.43
1:B:27:ILE:HG23	1:F:18:ARG:HG3	2.00	0.43
1:E:89:ARG:NH1	1:E:93:LEU:CD1	2.81	0.43
1:E:207:ASP:OD1	1:E:208:TYR:N	2.51	0.43
1:L:95:GLU:O	1:L:98:THR:OG1	2.29	0.43
1:M:214:ILE:HG12	1:O:210:GLN:HB3	2.00	0.43
1:N:128:VAL:HA	1:N:167:ILE:HG21	2.01	0.43
1:U:188:GLY:O	1:Y:86:TYR:OH	2.23	0.43
1:X:112:PRO:HD2	1:X:181:LEU:HD13	2.01	0.43
1:Y:35:LEU:HD21	1:Y:39:LYS:HE3	1.99	0.43
1:E:91:ASP:N	1:E:92:PRO:HD2	2.33	0.43
1:H:3:ALA:HA	1:H:5:LEU:N	2.34	0.43
1:N:101:TYR:HB2	1:N:104:VAL:CG1	2.48	0.43
1:Q:38:LYS:HZ1	1:V:26:GLU:N	2.17	0.43
1:T:29:GLU:HB3	1:Y:35:LEU:HD11	2.00	0.43
1:X:141:GLN:HA	1:X:144:MSE:HB3	2.00	0.43
1:X:218:GLN:C	1:X:220:ALA:N	2.72	0.43
1:D:83:ASN:OD1	1:D:118:SER:OG	2.28	0.43
1:G:185:ARG:NH1	2:G:304:HOH:O	2.50	0.43
1:H:89:ARG:O	1:H:89:ARG:HG2	2.19	0.43
1:P:222:VAL:HG13	1:P:223:LYS:N	2.34	0.43
1:R:131:GLU:OE2	1:R:167:ILE:HD12	2.19	0.43
1:G:113:PHE:HE1	1:G:181:LEU:HD21	1.84	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:N:97:ILE:HD13	1:N:208:TYR:OH	2.19	0.43
1:P:151:ASP:H	1:P:154:SER:HB2	1.84	0.43
1:R:170:THR:O	1:R:173:SER:OG	2.36	0.43
1:T:97:ILE:HG23	1:T:208:TYR:HE1	1.84	0.43
1:W:109:LYS:O	1:W:111:LEU:HD13	2.18	0.43
1:X:88:LYS:HA	1:X:144:MSE:HE1	2.00	0.43
1:C:148:THR:HG22	1:C:149:MSE:H	1.84	0.42
1:G:80:THR:CG2	1:G:144:MSE:SE	3.17	0.42
1:G:132:ASP:OD1	1:G:134:LYS:HE2	2.19	0.42
1:K:97:ILE:HA	1:K:100:GLN:HB2	2.01	0.42
1:N:208:TYR:O	1:N:212:GLU:N	2.42	0.42
1:P:26:GLU:O	1:W:178:GLN:NE2	2.34	0.42
1:P:28:LEU:O	1:P:32:ILE:HG13	2.18	0.42
1:P:202:LEU:HD21	1:P:206:VAL:HG21	2.01	0.42
1:V:83:ASN:OD1	1:V:150:LEU:N	2.47	0.42
1:B:77:VAL:HB	1:B:196:VAL:HB	2.01	0.42
1:G:35:LEU:O	1:G:39:LYS:N	2.44	0.42
1:J:65:PRO:HA	1:J:129:TRP:CE2	2.54	0.42
1:J:74:LEU:CD2	1:J:215:VAL:HG13	2.49	0.42
1:J:202:LEU:CD2	1:J:206:VAL:HG11	2.49	0.42
1:W:49:GLN:O	1:W:53:SER:N	2.52	0.42
1:E:89:ARG:NH1	1:E:92:PRO:HG2	2.34	0.42
1:G:193:PRO:O	1:G:204:GLY:N	2.53	0.42
1:L:74:LEU:CD2	1:L:218:GLN:HB3	2.49	0.42
1:L:111:LEU:HD23	1:L:113:PHE:CZ	2.55	0.42
1:O:171:ASP:HB2	1:P:22:VAL:HG12	2.00	0.42
1:R:25:PRO:C	1:R:27:ILE:N	2.73	0.42
1:B:87[B]:CYS:HA	1:B:193:PRO:HG3	2.01	0.42
1:D:77:VAL:HB	1:D:196:VAL:HB	2.02	0.42
1:D:175:LYS:O	1:D:179:ASN:ND2	2.43	0.42
1:E:58:LEU:HD21	1:E:79:PHE:HZ	1.84	0.42
1:H:97:ILE:HG23	1:H:101:TYR:CD2	2.55	0.42
1:I:90:PHE:CE2	1:I:94:LEU:HD11	2.54	0.42
1:M:47:PHE:CE1	1:M:188:GLY:HA3	2.54	0.42
1:M:97:ILE:HD13	1:M:211:LEU:HD21	2.01	0.42
1:O:66:ARG:HG2	1:O:107:ILE:HG12	2.02	0.42
1:R:210:GLN:HA	1:W:217:GLU:OE1	2.19	0.42
1:X:112:PRO:HB3	1:X:119:ALA:HB2	2.01	0.42
1:Y:74:LEU:HD11	1:Y:218:GLN:HB3	2.01	0.42
1:C:148:THR:HG22	1:C:149:MSE:N	2.34	0.42
1:G:47:PHE:CD1	1:G:201:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:LEU:HD23	1:H:39:LYS:HE2	2.01	0.42
1:I:137:LEU:O	1:I:141:GLN:HG3	2.19	0.42
1:N:132:ASP:O	1:N:135:ALA:HB3	2.20	0.42
1:G:80:THR:HG22	1:G:81:ASP:N	2.34	0.42
1:G:222:VAL:HG13	1:G:223:LYS:N	2.35	0.42
1:H:6:ASN:OD1	1:H:9:GLN:N	2.43	0.42
1:H:77:VAL:HB	1:H:196:VAL:HB	2.00	0.42
1:I:145:GLN:O	1:I:145:GLN:HG2	2.19	0.42
1:M:98:THR:C	1:M:99:GLU:HG3	2.39	0.42
1:N:160:LYS:HB2	1:N:165:SER:OG	2.18	0.42
1:O:58:LEU:CD2	1:O:183:LEU:HD21	2.49	0.42
1:P:26:GLU:HB3	1:W:38:LYS:NZ	2.35	0.42
1:P:159:MSE:O	1:P:164:THR:N	2.49	0.42
1:R:120:LYS:O	1:R:124:ALA:N	2.49	0.42
1:T:96:LYS:HE3	1:T:208:TYR:CZ	2.55	0.42
1:G:140:HIS:CE1	1:G:144:MSE:HE1	2.55	0.42
1:L:194:ALA:HA	1:L:203:PRO:HA	2.01	0.42
1:M:164:THR:HB	1:M:167:ILE:HD12	2.01	0.42
1:X:142:ARG:HH22	1:X:161:SER:HB3	1.84	0.42
1:A:52:ALA:HB2	1:E:160:LYS:HB3	2.01	0.42
1:L:189:ILE:C	1:L:191:GLY:HA2	2.40	0.42
1:Q:160:LYS:C	1:Q:162:THR:H	2.22	0.42
1:V:101:TYR:OH	1:V:212:GLU:OE2	2.38	0.42
1:V:185:ARG:C	1:V:188:GLY:H	2.23	0.42
1:X:77:VAL:HA	1:X:107:ILE:O	2.19	0.42
1:X:91:ASP:N	1:X:92:PRO:CD	2.83	0.42
1:G:124:ALA:HA	1:G:169:LEU:HG	2.02	0.42
1:G:146:LYS:HD2	1:G:150:LEU:HD21	2.01	0.42
1:G:159:MSE:HE1	1:G:169:LEU:CD1	2.50	0.42
1:I:101:TYR:O	1:I:104:VAL:HG12	2.20	0.42
1:M:47:PHE:CE2	1:O:86:TYR:CZ	3.07	0.42
1:O:216:LYS:HA	1:O:219:LEU:HG	2.02	0.42
1:P:95:GLU:OE1	1:P:141:GLN:NE2	2.53	0.42
1:Y:45:ALA:O	1:Y:47:PHE:N	2.53	0.42
1:C:77:VAL:HB	1:C:196:VAL:HB	2.02	0.42
1:C:148:THR:OG1	1:F:151:ASP:OD2	2.37	0.42
1:G:146:LYS:HZ3	1:G:158:ALA:HB2	1.83	0.42
1:I:111:LEU:HD22	1:I:181:LEU:HD12	2.01	0.42
1:J:144:MSE:HE3	1:J:150:LEU:HD12	2.02	0.42
1:U:96:LYS:HD2	1:U:208:TYR:CZ	2.55	0.42
1:W:76:LEU:HD11	1:W:106:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ARG:O	1:G:146:LYS:N	2.53	0.41
1:H:174:LEU:HD11	1:L:33:MSE:HG2	2.02	0.41
1:J:174:LEU:HA	1:J:177:LEU:HB3	2.02	0.41
1:L:221:LYS:O	1:L:221:LYS:HG2	2.20	0.41
1:W:208:TYR:O	1:W:212:GLU:N	2.53	0.41
1:X:170:THR:O	1:X:173:SER:OG	2.37	0.41
1:E:32:ILE:HA	1:J:28:LEU:CD2	2.49	0.41
1:E:49:GLN:CG	1:E:52:ALA:HB3	2.51	0.41
1:G:172:ASP:O	1:G:175:LYS:HG2	2.20	0.41
1:I:139:LEU:HB2	1:I:162:THR:HG21	2.02	0.41
1:M:208:TYR:O	1:M:212:GLU:HG2	2.20	0.41
1:N:29:GLU:HG2	1:N:33:MSE:HE3	2.02	0.41
1:N:32:ILE:CD1	1:R:28:LEU:HD21	2.50	0.41
1:P:55:HIS:O	1:P:59:TYR:N	2.42	0.41
1:Q:150:LEU:HG	1:Q:154:SER:HB2	2.01	0.41
1:V:76:LEU:HD21	1:V:195:THR:HG23	2.02	0.41
1:Y:202:LEU:HD21	1:Y:206:VAL:HG21	2.02	0.41
1:B:51:LEU:HD12	1:B:187:LEU:HD22	2.01	0.41
1:B:85:PRO:HG2	1:D:47:PHE:CE2	2.55	0.41
1:D:6:ASN:OD1	1:D:9:GLN:N	2.47	0.41
1:G:12:GLU:HB3	1:H:5:LEU:HD12	2.03	0.41
1:G:121:ALA:HB2	1:G:155:ILE:CD1	2.50	0.41
1:I:79:PHE:HB3	1:I:111:LEU:HD11	2.02	0.41
1:J:139:LEU:HD13	1:J:159:MSE:HA	2.02	0.41
1:O:89:ARG:O	1:O:89:ARG:HG2	2.20	0.41
1:Q:56:ASP:OD1	1:Q:57:ALA:N	2.53	0.41
1:U:206:VAL:HG22	1:U:210:GLN:HB2	2.02	0.41
1:V:89:ARG:O	1:V:89:ARG:HG2	2.21	0.41
1:V:121:ALA:HB1	1:V:143:LEU:HD13	2.02	0.41
1:W:48:ARG:HD2	1:W:199:ASP:O	2.19	0.41
1:Y:48:ARG:HD3	1:Y:186:LYS:HB3	2.02	0.41
1:Y:202:LEU:CD1	1:Y:214:ILE:HD13	2.50	0.41
1:I:81:ASP:OD1	1:I:118:SER:OG	2.30	0.41
1:M:96:LYS:C	1:M:96:LYS:HD2	2.41	0.41
1:Q:74:LEU:CD2	1:Q:104:VAL:HG23	2.50	0.41
1:R:208:TYR:CE2	1:R:212:GLU:HB2	2.54	0.41
1:Y:202:LEU:HD12	1:Y:214:ILE:HD13	2.02	0.41
1:E:112:PRO:HG3	1:J:33:MSE:HE1	2.02	0.41
1:F:90:PHE:CE2	1:F:94:LEU:HD21	2.55	0.41
1:F:192:THR:HG23	1:F:193:PRO:HA	2.03	0.41
1:G:156:GLU:HG3	1:G:159:MSE:HG2	2.02	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:H:124:ALA:CA	1:H:169:LEU:CD2	2.99	0.41
1:K:178:GLN:HE21	1:K:182:GLU:CG	2.34	0.41
1:M:96:LYS:HE3	1:M:208:TYR:HE1	1.81	0.41
1:O:124:ALA:CA	1:O:169:LEU:HD21	2.40	0.41
1:P:10:GLU:HA	1:P:13:VAL:HG22	2.03	0.41
1:U:97:ILE:HG13	1:U:208:TYR:HE1	1.85	0.41
1:A:155:ILE:O	1:A:159:MSE:HG3	2.21	0.41
1:K:80:THR:O	1:K:111:LEU:N	2.53	0.41
1:P:101:TYR:OH	1:P:212:GLU:OE2	2.35	0.41
1:P:120:LYS:HD3	1:P:152:ASN:OD1	2.20	0.41
1:V:61:ASP:C	1:V:63:ALA:H	2.23	0.41
1:W:212:GLU:O	1:W:216:LYS:NZ	2.41	0.41
1:X:76:LEU:N	1:X:76:LEU:CD1	2.84	0.41
1:X:97:ILE:HB	1:X:101:TYR:CE1	2.56	0.41
1:A:29:GLU:HA	1:A:32:ILE:HD12	2.02	0.41
1:E:40:ALA:O	1:E:44:GLN:HG2	2.20	0.41
1:E:58:LEU:HD23	1:E:109:LYS:HE3	2.03	0.41
1:I:65:PRO:HA	1:I:129:TRP:CE2	2.55	0.41
1:N:221:LYS:NZ	2:N:303:HOH:O	2.50	0.41
1:W:97:ILE:HD11	1:W:211:LEU:HG	2.02	0.41
1:X:124:ALA:HB1	1:X:159:MSE:HE1	2.02	0.41
1:B:17:VAL:HA	1:F:17:VAL:HG21	2.02	0.41
1:I:83:ASN:OD1	1:I:117:SER:OG	2.15	0.41
1:J:77:VAL:H	1:J:196:VAL:HG22	1.85	0.41
1:M:13:VAL:HG21	1:R:16:LEU:HD13	2.03	0.41
1:P:90:PHE:HZ	1:P:195:THR:HG1	1.68	0.41
1:R:146:LYS:CE	1:R:154:SER:HB3	2.51	0.41
1:V:147:LYS:O	1:V:148:THR:OG1	2.20	0.41
1:E:28:LEU:O	1:E:32:ILE:HG13	2.20	0.41
1:E:38:LYS:HE3	1:J:23:SER:O	2.21	0.41
1:K:73:LYS:N	1:K:73:LYS:HD2	2.36	0.41
1:L:190:GLN:N	1:L:191:GLY:HA2	2.36	0.41
1:N:32:ILE:HD13	1:R:28:LEU:CD2	2.50	0.41
1:N:35:LEU:HD22	1:R:28:LEU:HD23	2.03	0.41
1:N:42:GLU:OE1	1:N:185:ARG:NE	2.48	0.41
1:O:17:VAL:HG11	1:P:20:THR:HG21	2.02	0.41
1:O:190:GLN:O	1:O:190:GLN:HG2	2.20	0.41
1:P:88:LYS:HE2	1:P:88:LYS:HB3	1.93	0.41
1:P:206:VAL:HG12	1:P:210:GLN:HB2	2.02	0.41
1:Q:96:LYS:NZ	1:Q:100:GLN:N	2.69	0.41
1:Q:125:VAL:HG13	1:Q:136:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:159:MSE:HE2	1:R:164:THR:O	2.21	0.41
1:T:86:TYR:OH	1:V:188:GLY:O	2.38	0.41
1:W:51:LEU:HD11	1:W:201:ILE:HD11	2.03	0.41
1:W:91:ASP:N	1:W:92:PRO:CD	2.84	0.41
1:W:125:VAL:HG13	1:W:136:PHE:CD1	2.55	0.41
1:X:77:VAL:HG22	1:X:196:VAL:HB	2.02	0.41
1:X:211:LEU:HD12	1:X:211:LEU:H	1.86	0.41
1:H:217:GLU:O	1:H:221:LYS:HG3	2.21	0.41
1:L:91:ASP:N	1:L:92:PRO:HD2	2.35	0.41
1:O:6:ASN:ND2	2:O:307:HOH:O	2.52	0.41
1:Q:3:ALA:O	1:Q:5:LEU:N	2.48	0.41
1:Q:219:LEU:O	1:Q:223:LYS:N	2.53	0.41
1:R:150:LEU:HD23	1:R:155:ILE:HG12	2.03	0.41
1:U:137:LEU:HG	1:U:141:GLN:HE21	1.86	0.41
1:A:97:ILE:HG23	1:A:101:TYR:HD2	1.85	0.40
1:K:3:ALA:HA	1:K:4:ALA:HA	1.86	0.40
1:K:121:ALA:HB1	1:K:143:LEU:HD13	2.03	0.40
1:L:150:LEU:HD23	1:L:155:ILE:HG12	2.04	0.40
1:P:47:PHE:H	1:P:47:PHE:HD2	1.69	0.40
1:V:90:PHE:CZ	1:V:211:LEU:HD21	2.55	0.40
1:V:189:ILE:HD13	1:V:194:ALA:CB	2.50	0.40
1:W:151:ASP:OD1	1:W:152:ASN:N	2.55	0.40
1:X:39:LYS:O	1:X:43:GLN:HG3	2.21	0.40
1:X:74:LEU:HD22	1:X:222:VAL:CG1	2.51	0.40
1:F:66:ARG:NH1	1:F:70:LYS:HE2	2.37	0.40
1:J:135:ALA:HB1	1:J:164:THR:CG2	2.52	0.40
1:N:101:TYR:CB	1:N:104:VAL:HG12	2.52	0.40
1:O:35:LEU:HD21	1:W:29:GLU:HB2	2.02	0.40
1:R:91:ASP:N	1:R:92:PRO:CD	2.83	0.40
1:T:151:ASP:H	1:T:154:SER:HB2	1.85	0.40
1:T:213:ILE:HD13	1:V:213:ILE:HG12	2.02	0.40
1:X:33:MSE:HA	1:X:36:GLN:HG2	2.02	0.40
1:X:119:ALA:O	1:X:123:GLN:N	2.45	0.40
1:Y:206:VAL:HG12	1:Y:210:GLN:HB2	2.02	0.40
1:M:98:THR:O	1:M:104:VAL:O	2.39	0.40
1:N:145:GLN:OE1	1:N:147:LYS:NZ	2.49	0.40
1:P:156:GLU:HA	1:P:159:MSE:HB2	2.03	0.40
1:R:86:TYR:OH	1:W:47:PHE:HB3	2.22	0.40
1:T:204:GLY:HA3	1:V:203:PRO:HD2	2.02	0.40
1:V:77:VAL:HG13	1:V:109:LYS:HD3	2.04	0.40
1:W:91:ASP:N	1:W:92:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:163:ASN:O	1:W:163:ASN:ND2	2.49	0.40
1:A:47:PHE:CZ	1:A:201:ILE:HG12	2.57	0.40
1:H:125:VAL:HG13	1:H:136:PHE:HE1	1.86	0.40
1:L:87:CYS:SG	1:L:193:PRO:HB3	2.62	0.40
1:N:97:ILE:HG22	1:N:104:VAL:CG1	2.50	0.40
1:O:160:LYS:CE	1:O:165:SER:HB3	2.51	0.40
1:P:61:ASP:CG	1:P:64:SER:HG	2.18	0.40
1:Q:98:THR:HA	1:Q:104:VAL:CG1	2.52	0.40
1:B:6:ASN:OD1	1:B:9:GLN:N	2.48	0.40
1:E:66:ARG:NH1	1:E:68:GLY:O	2.55	0.40
1:F:153:ALA:O	1:F:156:GLU:HG2	2.21	0.40
1:G:142:ARG:NH2	1:G:161:SER:CB	2.85	0.40
1:H:123:GLN:HG2	1:H:169:LEU:HD22	2.04	0.40
1:I:83:ASN:ND2	1:I:148:THR:O	2.54	0.40
1:N:147:LYS:O	1:N:148:THR:HG23	2.21	0.40
1:Q:77:VAL:CG2	1:Q:196:VAL:HB	2.52	0.40
1:X:87:CYS:HA	1:X:90:PHE:HB3	2.04	0.40
1:X:164:THR:O	1:X:167:ILE:HG12	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:SER:OG	1:H:99:GLU:OE2[1_655]	1.95	0.25
1:H:86:TYR:OH	1:J:187:LEU:O[1_455]	2.12	0.08
1:G:134:LYS:NZ	1:M:134:LYS:O[2_456]	2.13	0.07
1:G:148:THR:OG1	1:J:148:THR:OG1[1_455]	2.17	0.03
1:C:7:ALA:H	1:U:3:ALA:O[1_554]	1.59	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/224 (100%)	212 (95%)	8 (4%)	3 (1%)	12	24
1	B	223/224 (100%)	216 (97%)	6 (3%)	1 (0%)	34	57
1	C	223/224 (100%)	214 (96%)	8 (4%)	1 (0%)	34	57
1	D	223/224 (100%)	216 (97%)	7 (3%)	0	100	100
1	E	216/224 (96%)	203 (94%)	12 (6%)	1 (0%)	29	52
1	F	223/224 (100%)	214 (96%)	7 (3%)	2 (1%)	17	35
1	G	220/224 (98%)	208 (94%)	10 (4%)	2 (1%)	17	35
1	H	223/224 (100%)	212 (95%)	9 (4%)	2 (1%)	17	35
1	I	196/224 (88%)	188 (96%)	6 (3%)	2 (1%)	15	32
1	J	217/224 (97%)	210 (97%)	5 (2%)	2 (1%)	17	35
1	K	223/224 (100%)	215 (96%)	8 (4%)	0	100	100
1	L	172/224 (77%)	162 (94%)	6 (4%)	4 (2%)	6	11
1	M	221/224 (99%)	210 (95%)	10 (4%)	1 (0%)	29	52
1	N	218/224 (97%)	210 (96%)	7 (3%)	1 (0%)	29	52
1	O	221/224 (99%)	213 (96%)	7 (3%)	1 (0%)	29	52
1	P	220/224 (98%)	210 (96%)	8 (4%)	2 (1%)	17	35
1	Q	222/224 (99%)	198 (89%)	20 (9%)	4 (2%)	8	16
1	R	219/224 (98%)	208 (95%)	7 (3%)	4 (2%)	8	16
1	T	222/224 (99%)	216 (97%)	5 (2%)	1 (0%)	29	52
1	U	223/224 (100%)	214 (96%)	8 (4%)	1 (0%)	34	57
1	V	222/224 (99%)	211 (95%)	9 (4%)	2 (1%)	17	35
1	W	222/224 (99%)	211 (95%)	10 (4%)	1 (0%)	29	52
1	X	220/224 (98%)	196 (89%)	20 (9%)	4 (2%)	8	16
1	Y	223/224 (100%)	206 (92%)	10 (4%)	7 (3%)	4	6
All	All	5235/5376 (97%)	4973 (95%)	213 (4%)	49 (1%)	17	35

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	LYS
1	F	148	THR
1	I	148	THR
1	L	145	GLN
1	N	148	THR
1	O	148	THR

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Mol	Chain	Res	Type
1	P	148	THR
1	Q	97	ILE
1	Q	218	GLN
1	T	148	THR
1	V	148	THR
1	Y	46	GLN
1	Y	223	LYS
1	A	148	THR
1	B	148	THR
1	E	148	THR
1	H	48	ARG
1	J	148	THR
1	L	148	THR
1	L	191	GLY
1	P	223	LYS
1	U	148	THR
1	X	148	THR
1	X	155	ILE
1	Y	47	PHE
1	Y	145	GLN
1	A	223	LYS
1	F	223	LYS
1	G	11	LYS
1	Q	159	MSE
1	W	148	THR
1	X	149	MSE
1	M	102	PRO
1	R	148	THR
1	R	223	LYS
1	X	223	LYS
1	Y	48	ARG
1	G	223	LYS
1	R	23	SER
1	R	26	GLU
1	Y	72	ALA
1	Y	144	MSE
1	H	4	ALA
1	L	144	MSE
1	Q	85	PRO
1	I	206	VAL
1	V	112	PRO
1	A	112	PRO

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Mol	Chain	Res	Type
1	J	112	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	192/187 (103%)	191 (100%)	1 (0%)	88	96
1	B	192/187 (103%)	191 (100%)	1 (0%)	88	96
1	C	192/187 (103%)	188 (98%)	4 (2%)	53	77
1	D	192/187 (103%)	191 (100%)	1 (0%)	88	96
1	E	189/187 (101%)	186 (98%)	3 (2%)	62	82
1	F	192/187 (103%)	190 (99%)	2 (1%)	76	90
1	G	191/187 (102%)	190 (100%)	1 (0%)	88	96
1	H	192/187 (103%)	189 (98%)	3 (2%)	62	82
1	I	170/187 (91%)	168 (99%)	2 (1%)	71	87
1	J	187/187 (100%)	182 (97%)	5 (3%)	44	71
1	K	192/187 (103%)	189 (98%)	3 (2%)	62	82
1	L	156/187 (83%)	153 (98%)	3 (2%)	57	79
1	M	190/187 (102%)	184 (97%)	6 (3%)	39	65
1	N	188/187 (100%)	185 (98%)	3 (2%)	62	82
1	O	190/187 (102%)	189 (100%)	1 (0%)	88	96
1	P	189/187 (101%)	187 (99%)	2 (1%)	73	88
1	Q	191/187 (102%)	188 (98%)	3 (2%)	62	82
1	R	190/187 (102%)	187 (98%)	3 (2%)	62	82
1	T	191/187 (102%)	191 (100%)	0	100	100
1	U	192/187 (103%)	191 (100%)	1 (0%)	88	96
1	V	191/187 (102%)	189 (99%)	2 (1%)	76	90
1	W	191/187 (102%)	184 (96%)	7 (4%)	34	60
1	X	189/187 (101%)	185 (98%)	4 (2%)	53	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	192/187 (103%)	189 (98%)	3 (2%)	62	82
All	All	4521/4488 (101%)	4457 (99%)	64 (1%)	67	85

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	B	71	ASP
1	C	89	ARG
1	C	160	LYS
1	C	190	GLN
1	C	222	VAL
1	D	190	GLN
1	E	26	GLU
1	E	33	MSE
1	E	178	GLN
1	F	99	GLU
1	F	160	LYS
1	G	12	GLU
1	H	55	HIS
1	H	73	LYS
1	H	200	THR
1	I	12	GLU
1	I	202	LEU
1	J	39	LYS
1	J	48	ARG
1	J	49	GLN
1	J	148	THR
1	J	222	VAL
1	K	144[A]	MSE
1	K	144[B]	MSE
1	K	209	ASP
1	L	120	LYS
1	L	123	GLN
1	L	152	ASN
1	M	51	LEU
1	M	73	LYS
1	M	96	LYS
1	M	134	LYS
1	M	185	ARG
1	M	218	GLN
1	N	43	GLN

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Mol	Chain	Res	Type
1	N	77	VAL
1	N	190	GLN
1	O	46	GLN
1	P	54	GLU
1	P	160	LYS
1	Q	130	LYS
1	Q	159	MSE
1	Q	160	LYS
1	R	14	ARG
1	R	73	LYS
1	R	142	ARG
1	U	141	GLN
1	V	55	HIS
1	V	192	THR
1	W	99	GLU
1	W	125	VAL
1	W	136	PHE
1	W	137	LEU
1	W	147	LYS
1	W	163	ASN
1	W	206	VAL
1	X	76	LEU
1	X	97	ILE
1	X	146	LYS
1	X	200	THR
1	Y	49	GLN
1	Y	192	THR
1	Y	218	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	G	43	GLN
1	G	190	GLN
1	R	210	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	218/224 (97%)	-0.12	0	100	100	19, 39, 60, 83	0
1	B	216/224 (96%)	-0.02	2 (0%)	84	82	24, 42, 62, 90	0
1	C	218/224 (97%)	0.01	0	100	100	29, 47, 64, 82	0
1	D	218/224 (97%)	-0.03	0	100	100	26, 44, 62, 68	0
1	E	211/224 (94%)	0.23	11 (5%)	27	21	38, 66, 86, 99	0
1	F	218/224 (97%)	-0.13	0	100	100	26, 45, 70, 90	0
1	G	215/224 (95%)	0.30	7 (3%)	46	39	43, 67, 87, 104	0
1	H	218/224 (97%)	0.15	6 (2%)	53	46	40, 61, 90, 103	0
1	I	194/224 (86%)	0.22	10 (5%)	27	21	39, 66, 85, 100	0
1	J	215/224 (95%)	0.25	14 (6%)	18	14	45, 66, 93, 112	0
1	K	216/224 (96%)	-0.09	1 (0%)	91	89	25, 42, 68, 81	0
1	L	172/224 (76%)	0.27	10 (5%)	23	17	41, 62, 78, 88	0
1	M	216/224 (96%)	0.48	21 (9%)	7	5	45, 69, 91, 124	0
1	N	216/224 (96%)	0.43	13 (6%)	21	16	33, 71, 95, 122	0
1	O	216/224 (96%)	0.33	13 (6%)	21	16	42, 66, 94, 109	0
1	P	218/224 (97%)	0.36	12 (5%)	25	19	39, 70, 89, 102	0
1	Q	217/224 (96%)	0.42	14 (6%)	18	14	28, 66, 95, 107	0
1	R	214/224 (95%)	0.29	14 (6%)	18	14	45, 68, 91, 104	0
1	T	217/224 (96%)	-0.03	0	100	100	25, 47, 66, 81	0
1	U	218/224 (97%)	-0.02	1 (0%)	91	89	29, 48, 70, 96	0
1	V	217/224 (96%)	0.16	3 (1%)	75	71	31, 58, 84, 97	0
1	W	217/224 (96%)	0.32	14 (6%)	18	14	40, 66, 91, 124	0
1	X	218/224 (97%)	0.34	10 (4%)	32	26	29, 67, 90, 108	0
1	Y	218/224 (97%)	0.09	0	100	100	25, 48, 70, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	5131/5376 (95%)	0.17	176 (3%)	45	38	19, 59, 86, 124	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	88[A]	LYS	8.9
1	J	4	ALA	7.0
1	G	220	ALA	6.7
1	M	69	ALA	6.7
1	E	169	LEU	6.5
1	N	222	VAL	5.4
1	Q	205	ALA	5.4
1	L	170	THR	5.3
1	R	219	LEU	5.2
1	J	5	LEU	5.0
1	P	138	ALA	4.7
1	V	55	HIS	4.6
1	L	93	LEU	4.6
1	M	203	PRO	4.5
1	G	148	THR	4.3
1	N	71	ASP	4.3
1	P	21	LEU	4.1
1	O	103	ASP	4.1
1	X	191	GLY	4.0
1	O	170	THR	4.0
1	J	138	ALA	3.9
1	U	224	LYS	3.8
1	M	7	ALA	3.8
1	J	6	ASN	3.7
1	W	5	LEU	3.7
1	M	207	ASP	3.7
1	L	75	VAL	3.6
1	O	40	ALA	3.6
1	R	135	ALA	3.6
1	P	169	LEU	3.6
1	L	209	ASP	3.6
1	P	156	GLU	3.6
1	J	7	ALA	3.5
1	J	206	VAL	3.5
1	M	8	ALA	3.4
1	N	56	ASP	3.4
1	Q	220	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	W	84[A]	CYS	3.3
1	P	168	LYS	3.3
1	E	224	LYS	3.3
1	Q	86	TYR	3.3
1	P	145	GLN	3.3
1	E	71	ASP	3.3
1	P	56	ASP	3.2
1	M	211	LEU	3.2
1	J	145	GLN	3.2
1	M	56	ASP	3.2
1	H	51	LEU	3.1
1	L	168	LYS	3.1
1	N	95	GLU	3.1
1	P	141	GLN	3.1
1	Q	82	TYR	3.0
1	Q	169	LEU	3.0
1	V	113	PHE	3.0
1	N	152	ASN	3.0
1	E	79	PHE	3.0
1	P	75	VAL	3.0
1	M	3	ALA	3.0
1	W	198	GLY	3.0
1	Q	221	LYS	3.0
1	E	52	ALA	3.0
1	I	70	LYS	2.9
1	P	17	VAL	2.9
1	X	143	LEU	2.9
1	Q	223	LYS	2.9
1	I	114	LYS	2.9
1	O	3	ALA	2.9
1	M	126	LEU	2.9
1	J	164	THR	2.9
1	X	77	VAL	2.9
1	O	69	ALA	2.8
1	J	147	LYS	2.8
1	M	168	LYS	2.8
1	O	106	VAL	2.8
1	Q	222	VAL	2.8
1	X	89	ARG	2.8
1	J	69	ALA	2.8
1	L	35	LEU	2.7
1	L	171	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	148	THR	2.7
1	Q	192	THR	2.7
1	G	224	LYS	2.7
1	H	224	LYS	2.7
1	M	75	VAL	2.7
1	B	71	ASP	2.7
1	G	23	SER	2.6
1	W	63	ALA	2.6
1	B	3	ALA	2.6
1	M	70	LYS	2.6
1	X	201	ILE	2.6
1	H	55	HIS	2.6
1	M	186	LYS	2.6
1	N	102	PRO	2.5
1	E	201	ILE	2.5
1	W	15	ALA	2.5
1	N	54	GLU	2.5
1	N	194	ALA	2.5
1	O	205	ALA	2.5
1	X	171	ASP	2.5
1	I	148	THR	2.5
1	W	56	ASP	2.5
1	P	167	ILE	2.5
1	M	68	GLY	2.5
1	I	73	LYS	2.4
1	M	4	ALA	2.4
1	M	113	PHE	2.4
1	W	86	TYR	2.4
1	H	131	GLU	2.4
1	I	100	GLN	2.4
1	X	140	HIS	2.4
1	K	49	GLN	2.4
1	R	60	ASN	2.4
1	M	98	THR	2.4
1	Q	204	GLY	2.4
1	L	126	LEU	2.4
1	G	17	VAL	2.4
1	R	215	VAL	2.4
1	N	28	LEU	2.3
1	R	224	LYS	2.3
1	N	174	LEU	2.3
1	R	56	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	73	LYS	2.3
1	W	147	LYS	2.3
1	O	199	ASP	2.3
1	I	45	ALA	2.3
1	L	154	SER	2.3
1	L	74	LEU	2.3
1	R	69	ALA	2.3
1	O	4	ALA	2.3
1	E	208	TYR	2.3
1	O	220	ALA	2.3
1	M	41	ASP	2.3
1	H	93	LEU	2.3
1	I	28	LEU	2.3
1	N	100	GLN	2.3
1	J	45	ALA	2.3
1	W	89	ARG	2.2
1	M	101	TYR	2.2
1	N	101	TYR	2.2
1	J	157	ASP	2.2
1	O	56	ASP	2.2
1	V	69	ALA	2.2
1	P	102	PRO	2.2
1	Q	57	ALA	2.2
1	X	59	TYR	2.2
1	X	221	LYS	2.2
1	R	208	TYR	2.2
1	W	126	LEU	2.2
1	I	71	ASP	2.2
1	I	167	ILE	2.2
1	H	169	LEU	2.1
1	Q	97	ILE	2.1
1	Q	74	LEU	2.1
1	E	223	LYS	2.1
1	G	7	ALA	2.1
1	J	205	ALA	2.1
1	O	41	ASP	2.1
1	O	42	GLU	2.1
1	R	155	ILE	2.1
1	I	72	ALA	2.1
1	Q	148	THR	2.1
1	E	199	ASP	2.1
1	W	85	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	207	ASP	2.1
1	R	99	GLU	2.1
1	N	171	ASP	2.1
1	R	71	ASP	2.1
1	R	70	LYS	2.0
1	W	208	TYR	2.0
1	W	152	ASN	2.0
1	X	45	ALA	2.0
1	M	5	LEU	2.0
1	M	26	GLU	2.0
1	E	88[A]	LYS	2.0
1	G	208	TYR	2.0
1	J	131	GLU	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.