



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:09 PM UTC

PDB ID : 4D80 / pdb_00004d80
Title : Metallosphera sedula Vps4 crystal structure
Authors : Caillat, C.; Macheboeuf, P.; Wu, Y.; McCarthy, A.A.; Boeri-Erba, E.; Effantin, G.; Gottlinger, H.G.; Weissenhorn, W.; Renesto, P.
Deposited on : 2014-12-02
Resolution : 3.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

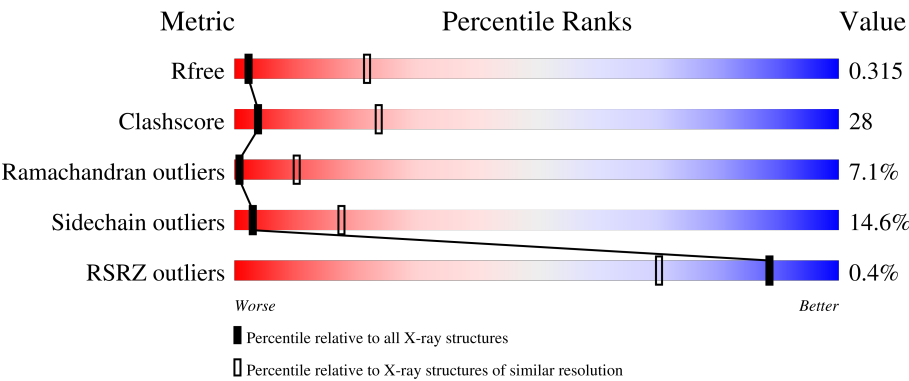
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	316	% 42%31%9%•15%
1	B	316	% 43%26%10%•19%
1	C	316	44%30%10%•14%
1	D	316	43%31%11%•14%
1	E	316	43%28%10%•17%

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Mol	Chain	Length	Quality of chain
1	F	316	41% 33% 11% • 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12875 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 AAA ATPASE, CENTRAL DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2152	1376	371	397	8			
1	B	257	Total	C	N	O	S	0	0	0
			2060	1319	356	377	8			
1	C	272	Total	C	N	O	S	0	0	0
			2177	1394	373	402	8			
1	D	273	Total	C	N	O	S	0	0	0
			2187	1400	376	403	8			
1	E	262	Total	C	N	O	S	0	0	0
			2106	1347	364	387	8			
1	F	274	Total	C	N	O	S	0	0	0
			2193	1405	378	402	8			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	expression tag	UNP A4YHC5
A	55	SER	-	expression tag	UNP A4YHC5
A	56	TYR	-	expression tag	UNP A4YHC5
A	57	TYR	-	expression tag	UNP A4YHC5
A	58	HIS	-	expression tag	UNP A4YHC5
A	59	HIS	-	expression tag	UNP A4YHC5
A	60	HIS	-	expression tag	UNP A4YHC5
A	61	HIS	-	expression tag	UNP A4YHC5
A	62	HIS	-	expression tag	UNP A4YHC5
A	63	HIS	-	expression tag	UNP A4YHC5
A	64	LEU	-	expression tag	UNP A4YHC5
A	65	GLU	-	expression tag	UNP A4YHC5
A	66	SER	-	expression tag	UNP A4YHC5
A	67	THR	-	expression tag	UNP A4YHC5
A	68	SER	-	expression tag	UNP A4YHC5
A	69	LEU	-	expression tag	UNP A4YHC5
A	70	TYR	-	expression tag	UNP A4YHC5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LYS	-	expression tag	UNP A4YHC5
A	72	LYS	-	expression tag	UNP A4YHC5
A	73	ALA	-	expression tag	UNP A4YHC5
A	74	GLY	-	expression tag	UNP A4YHC5
B	54	MET	-	expression tag	UNP A4YHC5
B	55	SER	-	expression tag	UNP A4YHC5
B	56	TYR	-	expression tag	UNP A4YHC5
B	57	TYR	-	expression tag	UNP A4YHC5
B	58	HIS	-	expression tag	UNP A4YHC5
B	59	HIS	-	expression tag	UNP A4YHC5
B	60	HIS	-	expression tag	UNP A4YHC5
B	61	HIS	-	expression tag	UNP A4YHC5
B	62	HIS	-	expression tag	UNP A4YHC5
B	63	HIS	-	expression tag	UNP A4YHC5
B	64	LEU	-	expression tag	UNP A4YHC5
B	65	GLU	-	expression tag	UNP A4YHC5
B	66	SER	-	expression tag	UNP A4YHC5
B	67	THR	-	expression tag	UNP A4YHC5
B	68	SER	-	expression tag	UNP A4YHC5
B	69	LEU	-	expression tag	UNP A4YHC5
B	70	TYR	-	expression tag	UNP A4YHC5
B	71	LYS	-	expression tag	UNP A4YHC5
B	72	LYS	-	expression tag	UNP A4YHC5
B	73	ALA	-	expression tag	UNP A4YHC5
B	74	GLY	-	expression tag	UNP A4YHC5
C	54	MET	-	expression tag	UNP A4YHC5
C	55	SER	-	expression tag	UNP A4YHC5
C	56	TYR	-	expression tag	UNP A4YHC5
C	57	TYR	-	expression tag	UNP A4YHC5
C	58	HIS	-	expression tag	UNP A4YHC5
C	59	HIS	-	expression tag	UNP A4YHC5
C	60	HIS	-	expression tag	UNP A4YHC5
C	61	HIS	-	expression tag	UNP A4YHC5
C	62	HIS	-	expression tag	UNP A4YHC5
C	63	HIS	-	expression tag	UNP A4YHC5
C	64	LEU	-	expression tag	UNP A4YHC5
C	65	GLU	-	expression tag	UNP A4YHC5
C	66	SER	-	expression tag	UNP A4YHC5
C	67	THR	-	expression tag	UNP A4YHC5
C	68	SER	-	expression tag	UNP A4YHC5
C	69	LEU	-	expression tag	UNP A4YHC5
C	70	TYR	-	expression tag	UNP A4YHC5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	71	LYS	-	expression tag	UNP A4YHC5
C	72	LYS	-	expression tag	UNP A4YHC5
C	73	ALA	-	expression tag	UNP A4YHC5
C	74	GLY	-	expression tag	UNP A4YHC5
D	54	MET	-	expression tag	UNP A4YHC5
D	55	SER	-	expression tag	UNP A4YHC5
D	56	TYR	-	expression tag	UNP A4YHC5
D	57	TYR	-	expression tag	UNP A4YHC5
D	58	HIS	-	expression tag	UNP A4YHC5
D	59	HIS	-	expression tag	UNP A4YHC5
D	60	HIS	-	expression tag	UNP A4YHC5
D	61	HIS	-	expression tag	UNP A4YHC5
D	62	HIS	-	expression tag	UNP A4YHC5
D	63	HIS	-	expression tag	UNP A4YHC5
D	64	LEU	-	expression tag	UNP A4YHC5
D	65	GLU	-	expression tag	UNP A4YHC5
D	66	SER	-	expression tag	UNP A4YHC5
D	67	THR	-	expression tag	UNP A4YHC5
D	68	SER	-	expression tag	UNP A4YHC5
D	69	LEU	-	expression tag	UNP A4YHC5
D	70	TYR	-	expression tag	UNP A4YHC5
D	71	LYS	-	expression tag	UNP A4YHC5
D	72	LYS	-	expression tag	UNP A4YHC5
D	73	ALA	-	expression tag	UNP A4YHC5
D	74	GLY	-	expression tag	UNP A4YHC5
E	54	MET	-	expression tag	UNP A4YHC5
E	55	SER	-	expression tag	UNP A4YHC5
E	56	TYR	-	expression tag	UNP A4YHC5
E	57	TYR	-	expression tag	UNP A4YHC5
E	58	HIS	-	expression tag	UNP A4YHC5
E	59	HIS	-	expression tag	UNP A4YHC5
E	60	HIS	-	expression tag	UNP A4YHC5
E	61	HIS	-	expression tag	UNP A4YHC5
E	62	HIS	-	expression tag	UNP A4YHC5
E	63	HIS	-	expression tag	UNP A4YHC5
E	64	LEU	-	expression tag	UNP A4YHC5
E	65	GLU	-	expression tag	UNP A4YHC5
E	66	SER	-	expression tag	UNP A4YHC5
E	67	THR	-	expression tag	UNP A4YHC5
E	68	SER	-	expression tag	UNP A4YHC5
E	69	LEU	-	expression tag	UNP A4YHC5
E	70	TYR	-	expression tag	UNP A4YHC5

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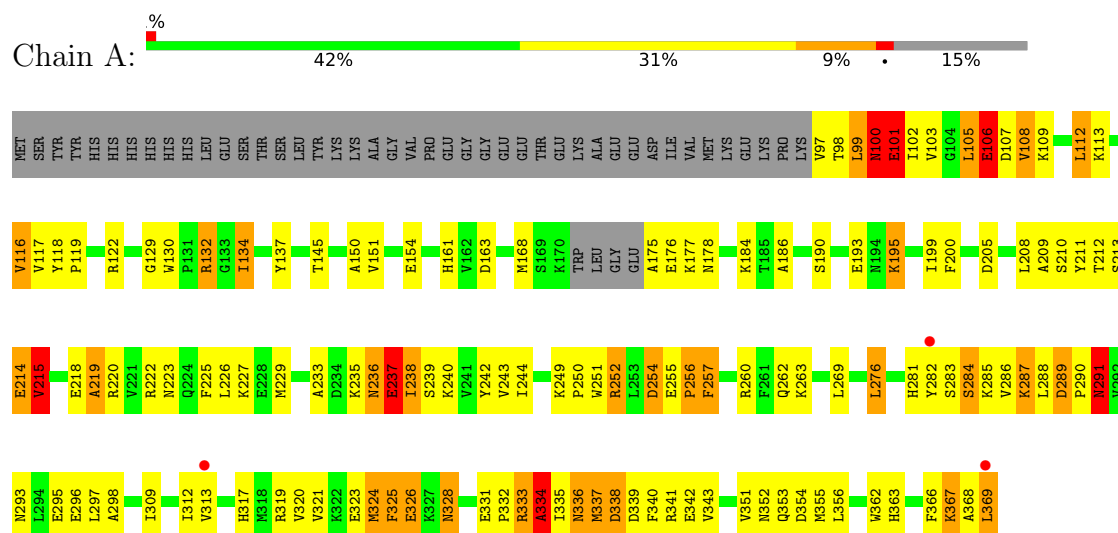
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Chain	Residue	Modelled	Actual	Comment	Reference
E	71	LYS	-	expression tag	UNP A4YHC5
E	72	LYS	-	expression tag	UNP A4YHC5
E	73	ALA	-	expression tag	UNP A4YHC5
E	74	GLY	-	expression tag	UNP A4YHC5
F	54	MET	-	expression tag	UNP A4YHC5
F	55	SER	-	expression tag	UNP A4YHC5
F	56	TYR	-	expression tag	UNP A4YHC5
F	57	TYR	-	expression tag	UNP A4YHC5
F	58	HIS	-	expression tag	UNP A4YHC5
F	59	HIS	-	expression tag	UNP A4YHC5
F	60	HIS	-	expression tag	UNP A4YHC5
F	61	HIS	-	expression tag	UNP A4YHC5
F	62	HIS	-	expression tag	UNP A4YHC5
F	63	HIS	-	expression tag	UNP A4YHC5
F	64	LEU	-	expression tag	UNP A4YHC5
F	65	GLU	-	expression tag	UNP A4YHC5
F	66	SER	-	expression tag	UNP A4YHC5
F	67	THR	-	expression tag	UNP A4YHC5
F	68	SER	-	expression tag	UNP A4YHC5
F	69	LEU	-	expression tag	UNP A4YHC5
F	70	TYR	-	expression tag	UNP A4YHC5
F	71	LYS	-	expression tag	UNP A4YHC5
F	72	LYS	-	expression tag	UNP A4YHC5
F	73	ALA	-	expression tag	UNP A4YHC5
F	74	GLY	-	expression tag	UNP A4YHC5

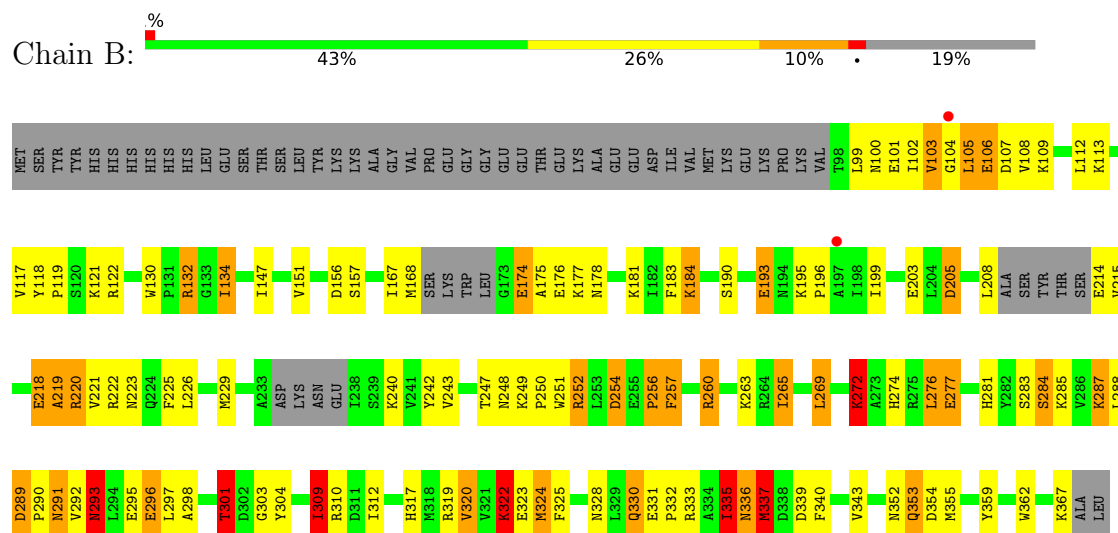
3 Residue-property plots

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: AAA ATPASE, CENTRAL DOMAIN PROTEIN

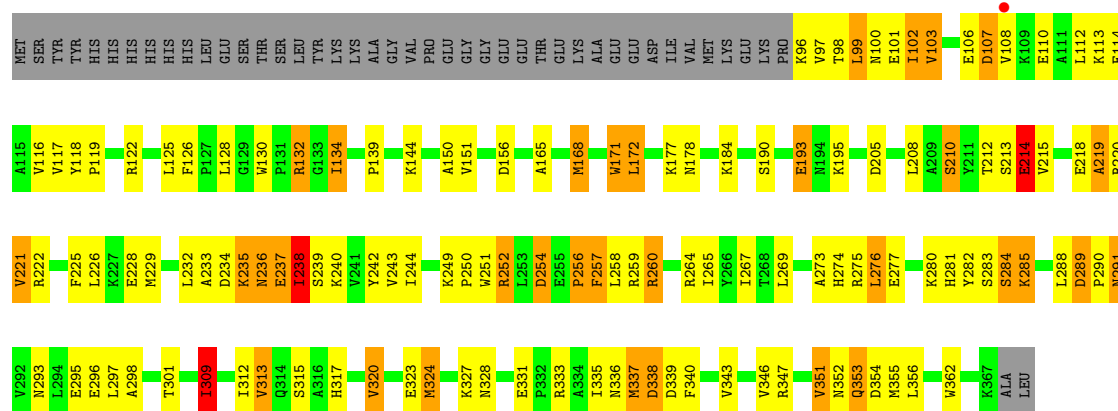


• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

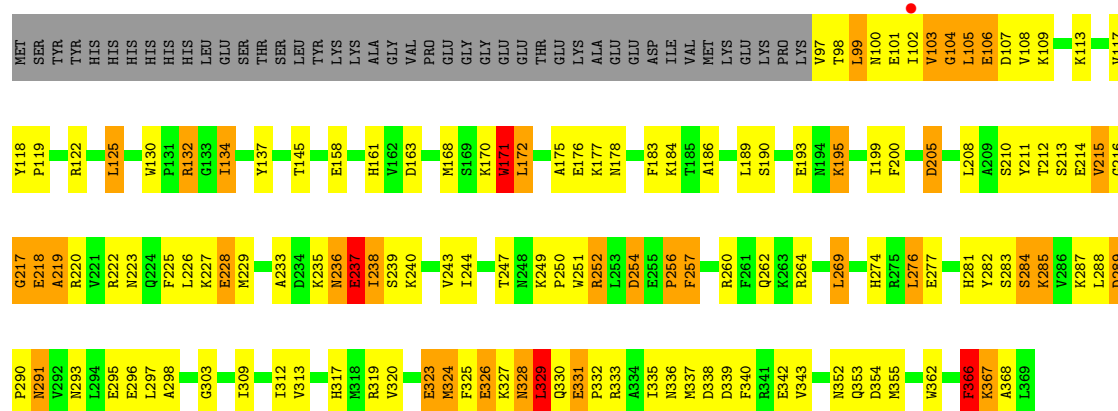


• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

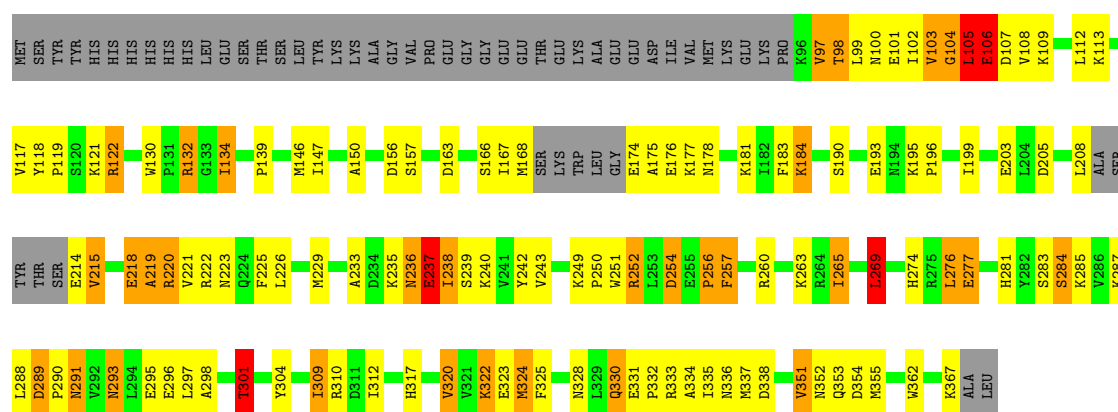




• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN



• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN



• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN



W362 H363 E364 K365 F366 K367 A368 L369	S284	S213	V117	MET
	K285	E214	Y118	SER
	V286	V215	P119	TVR
	K287	G216	S120	TVR
	L288	G217	K121	HIS
	D289	E218	R122	HIS
	P290	A219	L128	HIS
	N291	V221	G129	HIS
	V292	V222	W130	LEU
	N293	N223	F131	LEU
L294	Q224	P132	GLU	
E295	F225	G133	GLU	
S296	L226	T134	SER	
L297	K227	P139	SER	
A298	E228	L142	LEU	
	H229	K144	LEU	
T301	A233	T145	LYS	
S302	D234	M146	LYS	
G303	K235	A150	ALA	
L309	N236	V151	GLY	
	R237	A152	VAL	
L312	T238	N153	PRO	
V313	S239	D156	GLU	
K314	K240	E157	GLY	
S315	V243	E158	GLY	
A316	L244	A165	GLU	
H317	T247	S166	LYS	
K318	K248	I167	THR	
R319	R249	M168	GLU	
V320	P250	W171	LYS	
S321	K251	L172	ALA	
K322	R252	L178	GLU	
E323	L253	F183	GLU	
S324	D254	K184	LYS	
	E255	L189	GLU	
	E256	S190	LYS	
K330	P256	E193	PRO	
E331	F257	N194	K96	
	L258	K195	V97	
F332	R259	I198	T98	
K333	K260	S199	L99	
A334	R264	E101	N100	
N336		N102	Y103	
K337		I105	GL04	
D338		T106	L106	
L339		F200	D107	
S339		D205	V108	
F340		S210	K109	
K341		T211	E110	
E342		W212	A111	
F343		C282	K112	
			K113	
V351			K114	
K352			K115	
N353			K116	
K354			K117	
M355			K118	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 127.39Å 191.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.02 – 3.60 106.02 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (106.02-3.60) 99.7 (106.02-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.264 , 0.318 0.263 , 0.315	Depositor DCC
R_{free} test set	1464 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	110.9	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12875	wwPDB-VP
Average B, all atoms (Å ²)	142.0	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 36.23 % 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 5.1588e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.71	0/2191	1.11	10/2952 (0.3%)
1	B	0.70	1/2097 (0.0%)	1.08	10/2823 (0.4%)
1	C	0.75	0/2220	1.08	5/2995 (0.2%)
1	D	0.70	0/2230	1.07	6/3009 (0.2%)
1	E	0.71	0/2144	1.06	8/2887 (0.3%)
1	F	0.71	1/2236 (0.0%)	1.13	10/3016 (0.3%)
All	All	0.71	2/13118 (0.0%)	1.09	49/17682 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	251	TRP	CA-CB	5.58	1.61	1.53
1	B	335	ILE	CA-C	5.23	1.58	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	104	GLY	N-CA-C	-9.20	97.53	111.42
1	C	108	VAL	N-CA-C	8.80	118.87	110.42
1	F	102	ILE	N-CA-C	8.72	119.56	111.45
1	B	335	ILE	O-C-N	-8.04	114.74	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	MET	N-CA-C	-7.76	97.98	110.32
1	F	108	VAL	N-CA-C	7.76	117.87	110.42
1	C	237	GLU	N-CA-C	-7.32	103.19	112.93
1	B	335	ILE	N-CA-C	7.19	118.24	108.17
1	B	301	THR	CB-CA-C	-7.13	102.30	111.50
1	D	367	LYS	N-CA-C	7.11	120.52	107.73
1	A	100	ASN	CA-C-N	7.06	135.03	121.54
1	A	100	ASN	C-N-CA	7.06	135.03	121.54
1	E	301	THR	CB-CA-C	-7.04	102.42	111.50
1	D	331	GLU	N-CA-C	-7.00	100.97	110.36
1	A	324	MET	CB-CA-C	-6.85	100.54	110.06
1	A	336	ASN	N-CA-C	6.63	118.83	108.96
1	E	330	GLN	N-CA-C	-6.26	98.53	108.73
1	B	309	ILE	N-CA-C	-6.21	105.77	111.67
1	E	134	ILE	CB-CA-C	-6.21	100.47	110.28
1	B	337	MET	CB-CG-SD	6.20	131.29	112.70
1	F	267	ILE	CB-CA-C	6.17	118.34	111.80
1	F	309	ILE	N-CA-C	-6.12	105.86	111.67
1	B	134	ILE	CB-CA-C	-6.01	100.78	110.28
1	E	322	LYS	N-CA-CB	6.01	118.89	109.94
1	A	103	VAL	CB-CA-C	5.98	116.51	110.65
1	B	330	GLN	N-CA-C	-5.90	99.11	108.73
1	B	322	LYS	CB-CA-C	-5.83	101.47	110.81
1	F	355	MET	CB-CA-C	5.67	121.12	110.63
1	B	272	LYS	CB-CG-CD	-5.62	98.36	111.30
1	C	309	ILE	CB-CA-C	5.58	118.38	111.80
1	A	338	ASP	N-CA-CB	5.55	119.87	110.49
1	F	221	VAL	CB-CA-C	-5.52	103.16	112.16
1	E	269	LEU	CA-C-N	-5.49	114.06	119.99
1	E	269	LEU	C-N-CA	-5.49	114.06	119.99
1	C	238	ILE	N-CA-C	5.48	120.74	109.34
1	D	195	LYS	N-CA-C	-5.48	100.72	109.04
1	C	221	VAL	CB-CA-C	-5.44	103.29	112.16
1	A	195	LYS	N-CA-C	-5.44	100.78	109.04
1	A	291	ASN	CB-CA-C	-5.43	104.45	109.83
1	F	251	TRP	N-CA-CB	5.39	117.83	110.01
1	E	296	GLU	CA-CB-CG	-5.35	103.39	114.10
1	D	366	PHE	N-CA-C	-5.33	99.45	110.80
1	D	323	GLU	CB-CA-C	5.29	119.11	110.96
1	F	99	LEU	CA-CB-CG	5.29	134.80	116.30
1	A	106	GLU	N-CA-C	5.14	121.74	110.80
1	D	366	PHE	CB-CG-CD1	5.13	129.42	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	313	VAL	CB-CA-C	-5.01	105.45	112.02
1	F	198	ILE	CB-CA-C	5.01	117.50	110.99
1	B	337	MET	CG-SD-CE	5.00	111.91	100.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ALA	Peptide
1	B	335	ILE	Peptide
1	C	107	ASP	Peptide
1	D	170	LYS	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	2152	0	2201	153	0
1	B	2060	0	2106	121	0
1	C	2177	0	2219	121	1
1	D	2187	0	2233	130	0
1	E	2106	0	2155	109	0
1	F	2193	0	2244	140	1
All	All	12875	0	13158	737	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (737) 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:287:LYS:O	1:A:335:ILE:CG2	1.68	1.38
1:A:210:SER:HB3	1:A:211:TYR:N	1.54	1.19
1:B:288:LEU:O	1:B:335:ILE:O	1.66	1.11
1:A:287:LYS:O	1:A:335:ILE:HG21	0.96	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD22	1:A:151:VAL:HG11	1.35	1.08
1:E:100:ASN:HB2	1:E:101:GLU:HA	1.39	1.04
1:B:292:VAL:HA	1:B:337:MET:HG3	1.40	1.01
1:B:100:ASN:HB2	1:B:101:GLU:HA	1.40	1.00
1:A:324:MET:O	1:A:325:PHE:HB2	1.64	0.97
1:F:273:ALA:O	1:F:277:GLU:OE1	1.85	0.94
1:D:328:ASN:O	1:D:329:LEU:HB2	1.68	0.94
1:D:336:ASN:OD1	1:D:337:MET:N	2.02	0.93
1:E:336:ASN:OD1	1:E:337:MET:N	2.02	0.92
1:C:144:LYS:HG2	1:C:267:ILE:HD11	1.50	0.92
1:D:215:VAL:HG13	1:D:216:GLY:H	1.36	0.91
1:A:210:SER:CB	1:A:211:TYR:N	2.34	0.90
1:B:287:LYS:HE2	1:B:332:PRO:HG2	1.54	0.89
1:A:210:SER:HB3	1:A:211:TYR:CA	2.02	0.89
1:A:289:ASP:HB3	1:A:335:ILE:O	1.73	0.89
1:D:329:LEU:HD12	1:D:331:GLU:O	1.72	0.88
1:B:103:VAL:HG13	1:B:277:GLU:HB2	1.54	0.87
1:C:336:ASN:OD1	1:C:339:ASP:CG	2.18	0.86
1:B:99:LEU:HA	1:B:101:GLU:HB2	1.58	0.86
1:F:336:ASN:OD1	1:F:339:ASP:CG	2.19	0.86
1:C:234:ASP:O	1:C:236:ASN:N	2.08	0.86
1:B:292:VAL:HA	1:B:337:MET:CG	2.05	0.86
1:E:103:VAL:HG13	1:E:277:GLU:HB2	1.56	0.86
1:F:144:LYS:NZ	1:F:248:ASN:OD1	2.09	0.85
1:D:100:ASN:O	1:D:101:GLU:HG2	1.77	0.85
1:A:215:VAL:HG21	1:F:211:TYR:CZ	2.12	0.84
1:A:99:LEU:HG	1:A:109:LYS:CE	2.06	0.84
1:A:112:LEU:CD2	1:A:151:VAL:HG11	2.05	0.84
1:A:289:ASP:OD1	1:A:290:PRO:O	1.94	0.84
1:B:289:ASP:OD1	1:B:290:PRO:O	1.96	0.84
1:C:289:ASP:OD1	1:C:290:PRO:O	1.95	0.84
1:F:289:ASP:OD1	1:F:290:PRO:O	1.95	0.84
1:E:289:ASP:OD1	1:E:290:PRO:O	1.97	0.83
1:B:134:ILE:HD13	1:B:263:LYS:HB3	1.59	0.83
1:E:134:ILE:HD13	1:E:263:LYS:HB3	1.59	0.82
1:A:99:LEU:HD11	1:A:154:GLU:HB2	1.59	0.82
1:D:289:ASP:OD1	1:D:290:PRO:O	1.97	0.82
1:E:214:GLU:N	1:E:214:GLU:OE1	2.13	0.82
1:A:99:LEU:CD1	1:A:154:GLU:HB2	2.09	0.82
1:D:175:ALA:O	1:D:178:ASN:OD1	1.96	0.81
1:A:175:ALA:O	1:A:178:ASN:OD1	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:O	1:B:293:ASN:ND2	2.12	0.81
1:D:362:TRP:CH2	1:D:367:LYS:HE3	2.15	0.81
1:E:99:LEU:HA	1:E:101:GLU:HB2	1.63	0.81
1:B:214:GLU:OE1	1:B:214:GLU:N	2.14	0.80
1:D:339:ASP:O	1:D:343:VAL:HG13	1.81	0.80
1:A:333:ARG:N	1:A:334:ALA:HB2	1.98	0.78
1:A:324:MET:SD	1:A:332:PRO:CA	2.72	0.77
1:E:199:ILE:CG2	1:E:243:VAL:HG22	2.15	0.77
1:B:199:ILE:CG2	1:B:243:VAL:HG22	2.15	0.77
1:D:328:ASN:O	1:D:329:LEU:CB	2.34	0.76
1:A:215:VAL:HG21	1:F:211:TYR:CE1	2.22	0.75
1:A:287:LYS:O	1:A:287:LYS:HG2	1.85	0.74
1:D:211:TYR:HB3	1:D:217:GLY:HA3	1.70	0.74
1:A:215:VAL:HG11	1:F:211:TYR:CD2	2.23	0.73
1:F:99:LEU:HD13	1:F:99:LEU:O	1.88	0.73
1:B:287:LYS:CE	1:B:332:PRO:HG2	2.17	0.73
1:A:333:ARG:HB3	1:A:334:ALA:HA	1.71	0.73
1:F:214:GLU:O	1:F:215:VAL:HB	1.88	0.73
1:A:112:LEU:HD22	1:A:151:VAL:CG1	2.18	0.72
1:A:105:LEU:O	1:A:105:LEU:HD22	1.90	0.72
1:E:100:ASN:CB	1:E:101:GLU:HA	2.17	0.72
1:A:214:GLU:O	1:A:215:VAL:HB	1.88	0.72
1:D:215:VAL:HG13	1:D:216:GLY:N	2.05	0.71
1:F:183:PHE:CD2	1:F:228:GLU:HG2	2.24	0.71
1:D:183:PHE:CD2	1:D:228:GLU:HG2	2.25	0.71
1:C:260:ARG:HH11	1:C:260:ARG:HG3	1.55	0.71
1:A:320:VAL:HB	1:A:334:ALA:HB1	1.73	0.70
1:A:324:MET:CG	1:A:332:PRO:HA	2.21	0.70
1:D:362:TRP:CZ2	1:D:367:LYS:HE3	2.27	0.70
1:A:324:MET:SD	1:A:332:PRO:HA	2.31	0.70
1:B:291:ASN:OD1	1:B:336:ASN:O	2.10	0.70
1:B:260:ARG:HG3	1:B:260:ARG:HH11	1.57	0.69
1:A:105:LEU:CD2	1:A:108:VAL:HB	2.21	0.69
1:C:235:LYS:HB2	1:C:237:GLU:OE1	1.92	0.69
1:D:216:GLY:C	1:D:218:GLU:H	1.99	0.69
1:D:330:GLN:O	1:E:122:ARG:NH2	2.24	0.69
1:B:102:ILE:O	1:B:103:VAL:HG23	1.93	0.69
1:C:102:ILE:O	1:C:103:VAL:HG23	1.93	0.69
1:D:362:TRP:CH2	1:D:367:LYS:CE	2.75	0.69
1:B:99:LEU:HD13	1:B:109:LYS:CE	2.24	0.68
1:F:146:MET:SD	1:F:146:MET:C	2.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ILE:O	1:E:103:VAL:HG23	1.92	0.68
1:E:287:LYS:O	1:E:335:ILE:HG22	1.94	0.68
1:F:223:ASN:OD1	1:F:224:GLN:N	2.27	0.68
1:A:105:LEU:HD22	1:A:105:LEU:C	2.19	0.68
1:D:186:ALA:HB2	1:D:199:ILE:HD11	1.76	0.67
1:A:186:ALA:HB2	1:A:199:ILE:HD11	1.77	0.67
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.59	0.67
1:E:163:ASP:OD1	1:E:166:SER:OG	2.12	0.67
1:F:287:LYS:O	1:F:335:ILE:HG22	1.94	0.67
1:B:293:ASN:ND2	1:B:296:GLU:OE1	2.27	0.67
1:B:102:ILE:O	1:B:103:VAL:CB	2.42	0.67
1:B:102:ILE:O	1:B:103:VAL:HB	1.95	0.66
1:D:287:LYS:O	1:D:335:ILE:HG22	1.94	0.66
1:A:132:ARG:HG2	1:A:132:ARG:HH11	1.59	0.66
1:C:132:ARG:HG2	1:C:132:ARG:HH11	1.59	0.66
1:A:319:ARG:HH11	1:A:339:ASP:HA	1.61	0.66
1:B:323:GLU:OE1	1:B:333:ARG:NE	2.29	0.66
1:B:199:ILE:HG21	1:B:243:VAL:HG22	1.77	0.66
1:B:310:ARG:NH2	1:C:128:LEU:O	2.29	0.66
1:F:132:ARG:HG2	1:F:132:ARG:HH11	1.59	0.66
1:A:324:MET:O	1:A:325:PHE:CB	2.41	0.65
1:E:199:ILE:HG21	1:E:243:VAL:HG22	1.78	0.65
1:F:218:GLU:HA	1:F:222:ARG:NE	2.12	0.65
1:A:210:SER:C	1:A:211:TYR:N	2.55	0.65
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.59	0.65
1:D:319:ARG:HH11	1:D:339:ASP:HA	1.62	0.65
1:F:249:LYS:HE3	1:F:252:ARG:NH1	2.11	0.65
1:F:319:ARG:HH12	1:F:342:GLU:HB2	1.61	0.65
1:A:289:ASP:CB	1:A:335:ILE:O	2.45	0.65
1:B:287:LYS:O	1:B:335:ILE:HG22	1.96	0.64
1:E:132:ARG:HG2	1:E:132:ARG:HH11	1.59	0.64
1:A:333:ARG:HB3	1:A:334:ALA:CA	2.26	0.64
1:E:199:ILE:HG22	1:E:242:TYR:O	1.97	0.64
1:F:150:ALA:O	1:F:153:ASN:OD1	2.16	0.64
1:B:100:ASN:CB	1:B:101:GLU:HA	2.18	0.64
1:C:118:TYR:HB2	1:C:119:PRO:HD3	1.80	0.64
1:C:297:LEU:HD11	1:C:337:MET:HE1	1.80	0.64
1:F:118:TYR:HB2	1:F:119:PRO:HD3	1.80	0.64
1:F:226:LEU:HD21	1:F:260:ARG:NH1	2.12	0.64
1:A:363:HIS:O	1:A:367:LYS:HD3	1.98	0.64
1:A:333:ARG:CB	1:A:334:ALA:HA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:CG1	1:D:277:GLU:HB3	2.28	0.63
1:F:297:LEU:HD11	1:F:337:MET:HE1	1.80	0.63
1:E:323:GLU:OE1	1:E:333:ARG:NE	2.30	0.63
1:F:319:ARG:HH11	1:F:339:ASP:HA	1.64	0.63
1:A:226:LEU:HG	1:A:260:ARG:HD3	1.80	0.63
1:B:225:PHE:CZ	1:B:229:MET:HE3	2.33	0.63
1:F:144:LYS:CE	1:F:248:ASN:OD1	2.46	0.63
1:D:226:LEU:HG	1:D:260:ARG:HD3	1.80	0.63
1:B:199:ILE:HG22	1:B:242:TYR:O	1.98	0.63
1:E:225:PHE:CZ	1:E:229:MET:HE3	2.34	0.63
1:A:99:LEU:HD12	1:A:150:ALA:O	1.98	0.63
1:F:336:ASN:OD1	1:F:339:ASP:OD2	2.15	0.63
1:D:262:GLN:N	1:D:262:GLN:OE1	2.32	0.62
1:F:319:ARG:NH1	1:F:339:ASP:HA	2.14	0.62
1:B:134:ILE:CD1	1:B:263:LYS:HB3	2.28	0.62
1:D:118:TYR:HB2	1:D:119:PRO:HD3	1.82	0.62
1:B:269:LEU:HD21	1:B:303:GLY:HA2	1.81	0.62
1:E:134:ILE:CD1	1:E:263:LYS:HB3	2.28	0.62
1:D:102:ILE:O	1:D:103:VAL:HG22	2.00	0.62
1:B:287:LYS:O	1:B:287:LYS:HG2	1.97	0.62
1:F:237:GLU:O	1:F:239:SER:N	2.33	0.62
1:F:269:LEU:HD21	1:F:303:GLY:HA2	1.81	0.62
1:C:336:ASN:OD1	1:C:339:ASP:OD2	2.16	0.62
1:A:118:TYR:HB2	1:A:119:PRO:HD3	1.82	0.62
1:C:277:GLU:HA	1:C:280:LYS:HE2	1.81	0.62
1:E:226:LEU:HG	1:E:260:ARG:HD3	1.81	0.62
1:C:102:ILE:O	1:C:103:VAL:CB	2.47	0.62
1:D:323:GLU:OE1	1:D:333:ARG:NE	2.31	0.62
1:E:118:TYR:HB2	1:E:119:PRO:HD3	1.82	0.61
1:A:225:PHE:CZ	1:A:229:MET:HE3	2.35	0.61
1:A:319:ARG:NH1	1:A:339:ASP:HA	2.15	0.61
1:E:293:ASN:OD1	1:E:293:ASN:O	2.19	0.61
1:B:118:TYR:HB2	1:B:119:PRO:HD3	1.82	0.61
1:F:167:ILE:HD11	1:F:178:ASN:HB3	1.82	0.61
1:D:325:PHE:O	1:D:326:GLU:HG2	2.01	0.61
1:A:262:GLN:N	1:A:262:GLN:OE1	2.33	0.61
1:C:226:LEU:HG	1:C:260:ARG:HD3	1.82	0.61
1:A:237:GLU:O	1:A:239:SER:N	2.34	0.61
1:B:102:ILE:O	1:B:103:VAL:CG2	2.49	0.61
1:C:212:THR:HA	1:D:215:VAL:HG11	1.83	0.61
1:D:237:GLU:O	1:D:239:SER:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:PHE:HA	1:D:343:VAL:HG22	1.83	0.61
1:A:211:TYR:CE1	1:A:218:GLU:OE2	2.53	0.61
1:A:333:ARG:CA	1:A:334:ALA:HB2	2.31	0.61
1:B:317:HIS:NE2	1:C:125:LEU:O	2.28	0.61
1:F:256:PRO:C	1:F:260:ARG:NH1	2.59	0.61
1:E:102:ILE:O	1:E:103:VAL:CB	2.47	0.60
1:D:269:LEU:HD21	1:D:303:GLY:HA2	1.82	0.60
1:F:226:LEU:HG	1:F:260:ARG:HD3	1.83	0.60
1:C:260:ARG:HH11	1:C:260:ARG:CG	2.14	0.60
1:D:186:ALA:CB	1:D:199:ILE:HD11	2.32	0.60
1:D:319:ARG:NH1	1:D:339:ASP:HA	2.16	0.60
1:D:225:PHE:CZ	1:D:229:MET:HE3	2.36	0.60
1:A:220:ARG:HE	1:F:212:THR:CG2	2.13	0.60
1:E:237:GLU:O	1:E:239:SER:N	2.35	0.60
1:F:354:ASP:OD1	1:F:355:MET:N	2.35	0.60
1:E:301:THR:HG21	1:E:309:ILE:CD1	2.32	0.60
1:C:225:PHE:CZ	1:C:229:MET:HE3	2.36	0.60
1:F:225:PHE:CZ	1:F:229:MET:HE3	2.36	0.59
1:C:346:VAL:HG22	1:D:368:ALA:O	2.03	0.59
1:C:229:MET:CE	1:C:243:VAL:HG11	2.33	0.59
1:A:186:ALA:CB	1:A:199:ILE:HD11	2.32	0.59
1:A:320:VAL:CG1	1:A:334:ALA:HB1	2.32	0.59
1:D:229:MET:CE	1:D:243:VAL:HG11	2.33	0.59
1:C:229:MET:HE2	1:C:243:VAL:HG11	1.85	0.59
1:B:301:THR:HG21	1:B:309:ILE:CD1	2.32	0.59
1:C:269:LEU:HD11	1:C:356:LEU:HD21	1.85	0.59
1:F:229:MET:CE	1:F:243:VAL:HG11	2.33	0.59
1:C:102:ILE:O	1:C:103:VAL:HB	2.02	0.59
1:E:102:ILE:O	1:E:103:VAL:CG2	2.51	0.58
1:C:193:GLU:CG	1:C:193:GLU:O	2.51	0.58
1:E:229:MET:CE	1:E:243:VAL:HG11	2.33	0.58
1:A:229:MET:CE	1:A:243:VAL:HG11	2.33	0.58
1:C:315:SER:OG	1:C:343:VAL:HG21	2.03	0.58
1:C:102:ILE:O	1:C:103:VAL:CG2	2.51	0.58
1:E:99:LEU:HD13	1:E:109:LYS:HE3	1.86	0.58
1:E:226:LEU:HD11	1:E:257:PHE:HA	1.86	0.58
1:F:291:ASN:C	1:F:291:ASN:OD1	2.47	0.58
1:C:238:ILE:HG22	1:C:239:SER:O	2.02	0.58
1:E:102:ILE:O	1:E:103:VAL:HB	2.04	0.58
1:A:333:ARG:H	1:A:334:ALA:HB2	1.68	0.58
1:C:193:GLU:O	1:C:193:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:MET:HE2	1:F:243:VAL:HG11	1.86	0.58
1:F:193:GLU:O	1:F:193:GLU:CG	2.52	0.58
1:F:144:LYS:HB3	1:F:267:ILE:HD11	1.86	0.58
1:F:193:GLU:O	1:F:193:GLU:HG2	2.04	0.58
1:B:226:LEU:HD11	1:B:257:PHE:HA	1.86	0.58
1:B:229:MET:CE	1:B:243:VAL:HG11	2.33	0.58
1:F:97:VAL:O	1:F:153:ASN:ND2	2.37	0.58
1:B:287:LYS:NZ	1:B:332:PRO:HG2	2.18	0.57
1:B:324:MET:HE2	1:B:332:PRO:CA	2.34	0.57
1:C:291:ASN:C	1:C:291:ASN:OD1	2.47	0.57
1:B:193:GLU:CG	1:B:193:GLU:O	2.52	0.57
1:F:118:TYR:HB2	1:F:119:PRO:CD	2.34	0.57
1:C:118:TYR:HB2	1:C:119:PRO:CD	2.34	0.57
1:C:234:ASP:C	1:C:236:ASN:N	2.62	0.57
1:A:354:ASP:OD1	1:A:355:MET:N	2.37	0.57
1:B:193:GLU:O	1:B:193:GLU:HG2	2.04	0.57
1:E:229:MET:HE2	1:E:243:VAL:HG11	1.86	0.57
1:B:99:LEU:HD13	1:B:109:LYS:HE3	1.84	0.57
1:B:229:MET:HE2	1:B:243:VAL:HG11	1.86	0.57
1:E:98:THR:O	1:E:101:GLU:OE1	2.22	0.57
1:C:208:LEU:HD21	1:C:254:ASP:HB3	1.87	0.57
1:C:347:ARG:HA	1:D:368:ALA:HB1	1.85	0.57
1:F:315:SER:OG	1:F:343:VAL:HG21	2.05	0.57
1:A:229:MET:HE2	1:A:243:VAL:HG11	1.87	0.57
1:A:324:MET:SD	1:A:332:PRO:HB3	2.44	0.57
1:B:317:HIS:HA	1:B:335:ILE:HD12	1.85	0.57
1:E:291:ASN:OD1	1:E:291:ASN:C	2.47	0.57
1:F:144:LYS:HB3	1:F:267:ILE:CD1	2.35	0.57
1:A:269:LEU:HD11	1:A:356:LEU:HD21	1.87	0.57
1:D:354:ASP:OD1	1:D:355:MET:N	2.38	0.57
1:E:203:GLU:OE2	1:F:259:ARG:NH2	2.38	0.57
1:D:118:TYR:HB2	1:D:119:PRO:CD	2.35	0.56
1:F:317:HIS:HA	1:F:335:ILE:HD12	1.87	0.56
1:A:99:LEU:HG	1:A:109:LYS:HE2	1.87	0.56
1:A:319:ARG:HH12	1:A:342:GLU:HB2	1.69	0.56
1:E:118:TYR:HB2	1:E:119:PRO:CD	2.36	0.56
1:A:321:VAL:O	1:A:324:MET:O	2.24	0.56
1:B:99:LEU:HD13	1:B:109:LYS:HE2	1.88	0.56
1:B:118:TYR:HB2	1:B:119:PRO:CD	2.36	0.56
1:C:168:MET:HE1	1:C:221:VAL:HB	1.87	0.56
1:D:229:MET:HE2	1:D:243:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LYS:HG2	1:D:252:ARG:HD2	1.87	0.56
1:E:324:MET:HE2	1:E:332:PRO:CA	2.35	0.56
1:A:99:LEU:CD2	1:A:109:LYS:HE3	2.36	0.56
1:A:249:LYS:HG2	1:A:252:ARG:HD2	1.88	0.56
1:B:249:LYS:HG2	1:B:252:ARG:HD2	1.87	0.56
1:C:226:LEU:HD11	1:C:257:PHE:HA	1.87	0.56
1:A:118:TYR:HB2	1:A:119:PRO:CD	2.35	0.56
1:A:226:LEU:HD11	1:A:257:PHE:HA	1.87	0.56
1:A:320:VAL:CB	1:A:334:ALA:HB1	2.35	0.56
1:B:336:ASN:O	1:B:337:MET:HB2	2.04	0.56
1:C:324:MET:HE3	1:C:331:GLU:C	2.30	0.56
1:D:319:ARG:HH12	1:D:342:GLU:HB2	1.70	0.56
1:A:333:ARG:CB	1:A:334:ALA:CA	2.82	0.56
1:D:176:GLU:OE1	1:D:220:ARG:NH1	2.39	0.56
1:A:176:GLU:OE1	1:A:220:ARG:NH1	2.39	0.55
1:A:255:GLU:OE2	1:F:355:MET:HE2	2.06	0.55
1:C:171:TRP:O	1:C:172:LEU:C	2.47	0.55
1:D:226:LEU:HD11	1:D:257:PHE:HA	1.87	0.55
1:B:291:ASN:OD1	1:B:291:ASN:C	2.49	0.55
1:C:249:LYS:HG2	1:C:252:ARG:HD2	1.88	0.55
1:A:333:ARG:HB3	1:A:334:ALA:CB	2.36	0.55
1:B:102:ILE:HD12	1:B:147:ILE:HG13	1.88	0.55
1:D:103:VAL:HG12	1:D:277:GLU:HB3	1.87	0.55
1:F:218:GLU:HA	1:F:222:ARG:HE	1.71	0.55
1:A:208:LEU:HD21	1:A:254:ASP:HB3	1.88	0.55
1:D:291:ASN:OD1	1:D:291:ASN:C	2.48	0.55
1:F:226:LEU:HD11	1:F:257:PHE:HA	1.88	0.55
1:D:264:ARG:HD3	1:D:367:LYS:HD3	1.88	0.55
1:D:264:ARG:NH1	1:D:367:LYS:HE2	2.22	0.55
1:F:319:ARG:NH1	1:F:342:GLU:HB2	2.21	0.55
1:D:208:LEU:HD21	1:D:254:ASP:HB3	1.88	0.55
1:A:99:LEU:HG	1:A:109:LYS:NZ	2.22	0.55
1:A:209:ALA:O	1:A:210:SER:HB2	2.07	0.54
1:A:324:MET:SD	1:A:332:PRO:N	2.79	0.54
1:F:102:ILE:HD13	1:F:277:GLU:HB3	1.89	0.54
1:E:269:LEU:HD11	1:E:351:VAL:HG21	1.89	0.54
1:B:132:ARG:HH11	1:B:132:ARG:CG	2.20	0.54
1:E:317:HIS:HA	1:E:335:ILE:HD12	1.88	0.54
1:F:103:VAL:O	1:F:105:LEU:N	2.40	0.54
1:F:144:LYS:HZ1	1:F:248:ASN:CG	2.13	0.54
1:F:249:LYS:HG2	1:F:252:ARG:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ARG:NH2	1:E:254:ASP:OD2	2.40	0.54
1:C:320:VAL:HG22	1:C:333:ARG:HB3	1.88	0.54
1:B:291:ASN:O	1:B:337:MET:HG3	2.08	0.54
1:B:203:GLU:OE2	1:C:259:ARG:NH2	2.41	0.54
1:D:101:GLU:CD	1:D:104:GLY:HA2	2.33	0.54
1:B:272:LYS:NZ	1:B:272:LYS:HB3	2.23	0.54
1:C:132:ARG:HH11	1:C:132:ARG:CG	2.21	0.54
1:D:317:HIS:O	1:D:320:VAL:HG22	2.08	0.53
1:A:132:ARG:HH11	1:A:132:ARG:CG	2.21	0.53
1:A:324:MET:SD	1:A:332:PRO:CB	2.96	0.53
1:B:319:ARG:O	1:B:322:LYS:HB2	2.08	0.53
1:F:324:MET:HE3	1:F:331:GLU:C	2.33	0.53
1:F:132:ARG:HH11	1:F:132:ARG:CG	2.21	0.53
1:D:132:ARG:HH11	1:D:132:ARG:CG	2.21	0.53
1:A:212:THR:HG22	1:B:218:GLU:CD	2.33	0.53
1:A:317:HIS:O	1:A:320:VAL:HG22	2.09	0.53
1:D:250:PRO:HB2	1:D:362:TRP:CZ2	2.43	0.53
1:A:100:ASN:OD1	1:A:102:ILE:N	2.42	0.53
1:E:132:ARG:HH11	1:E:132:ARG:CG	2.21	0.53
1:B:222:ARG:NH2	1:B:254:ASP:OD2	2.41	0.53
1:D:222:ARG:NH2	1:D:254:ASP:OD2	2.41	0.53
1:E:320:VAL:HG22	1:E:333:ARG:HB3	1.90	0.53
1:B:208:LEU:HD21	1:B:254:ASP:HB3	1.89	0.53
1:F:112:LEU:HD12	1:F:134:ILE:HD11	1.90	0.53
1:B:320:VAL:HG22	1:B:333:ARG:HB3	1.91	0.52
1:E:156:ASP:O	1:E:195:LYS:HD3	2.09	0.52
1:F:320:VAL:HG22	1:F:333:ARG:HB3	1.90	0.52
1:C:234:ASP:C	1:C:236:ASN:H	2.17	0.52
1:D:317:HIS:HA	1:D:335:ILE:HD12	1.91	0.52
1:E:208:LEU:HD21	1:E:254:ASP:HB3	1.89	0.52
1:B:284:SER:OG	1:B:285:LYS:N	2.42	0.52
1:F:319:ARG:O	1:F:322:LYS:HG2	2.09	0.52
1:C:336:ASN:OD1	1:C:339:ASP:OD1	2.28	0.52
1:B:112:LEU:HD13	1:B:265:ILE:CD1	2.39	0.52
1:C:269:LEU:HD21	1:C:351:VAL:HG21	1.92	0.52
1:F:144:LYS:HD3	1:F:267:ILE:HD11	1.90	0.52
1:C:317:HIS:HA	1:C:335:ILE:CD1	2.39	0.52
1:A:129:GLY:C	1:F:314:GLN:HE21	2.17	0.51
1:E:97:VAL:HG21	1:E:146:MET:HE1	1.92	0.51
1:A:227:LYS:HE2	1:F:165:ALA:HB3	1.92	0.51
1:C:234:ASP:O	1:C:235:LYS:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:ASN:OD1	1:F:339:ASP:OD1	2.29	0.51
1:A:284:SER:OG	1:A:285:LYS:N	2.43	0.51
1:F:101:GLU:HB3	1:F:109:LYS:HD3	1.91	0.51
1:A:99:LEU:HD23	1:A:109:LYS:HE3	1.93	0.51
1:E:112:LEU:HD13	1:E:265:ILE:CD1	2.40	0.51
1:A:100:ASN:OD1	1:A:101:GLU:N	2.43	0.51
1:E:301:THR:HG21	1:E:309:ILE:HD13	1.92	0.51
1:A:116:VAL:HG23	1:A:242:TYR:CD2	2.46	0.51
1:F:213:SER:O	1:F:214:GLU:C	2.54	0.51
1:F:284:SER:OG	1:F:285:LYS:N	2.42	0.51
1:A:269:LEU:HD21	1:A:351:VAL:HG11	1.91	0.51
1:C:210:SER:CB	1:D:219:ALA:HB1	2.41	0.51
1:D:214:GLU:CD	1:E:215:VAL:HG23	2.36	0.51
1:F:139:PRO:CB	1:F:351:VAL:HG11	2.40	0.51
1:B:336:ASN:HD22	1:B:339:ASP:CG	2.18	0.51
1:C:323:GLU:HG2	1:C:327:LYS:CG	2.41	0.50
1:F:219:ALA:O	1:F:220:ARG:C	2.54	0.50
1:A:219:ALA:O	1:A:220:ARG:C	2.53	0.50
1:F:364:GLU:HA	1:F:367:LYS:HD3	1.94	0.50
1:D:284:SER:OG	1:D:285:LYS:N	2.44	0.50
1:E:301:THR:HG21	1:E:309:ILE:HD11	1.93	0.50
1:F:144:LYS:CD	1:F:267:ILE:HD11	2.42	0.50
1:C:171:TRP:O	1:C:172:LEU:O	2.29	0.50
1:E:99:LEU:CA	1:E:101:GLU:HB2	2.38	0.50
1:F:102:ILE:CD1	1:F:277:GLU:HB3	2.42	0.50
1:A:130:TRP:HA	1:F:314:GLN:NE2	2.26	0.50
1:A:250:PRO:HB2	1:A:362:TRP:CZ2	2.46	0.50
1:A:337:MET:HE2	1:A:341:ARG:NH2	2.27	0.50
1:E:324:MET:HE2	1:E:332:PRO:N	2.26	0.50
1:B:105:LEU:O	1:B:106:GLU:C	2.55	0.50
1:B:301:THR:HG21	1:B:309:ILE:HD13	1.93	0.50
1:B:322:LYS:HE3	1:C:114:GLU:HB2	1.94	0.50
1:D:324:MET:HE2	1:D:332:PRO:HA	1.94	0.50
1:C:139:PRO:CB	1:C:351:VAL:HG11	2.41	0.49
1:C:219:ALA:O	1:C:220:ARG:C	2.53	0.49
1:C:284:SER:OG	1:C:285:LYS:N	2.44	0.49
1:C:113:LYS:CA	1:C:117:VAL:HG12	2.42	0.49
1:D:219:ALA:O	1:D:220:ARG:C	2.54	0.49
1:D:211:TYR:O	1:D:212:THR:OG1	2.28	0.49
1:F:99:LEU:O	1:F:99:LEU:CD1	2.59	0.49
1:F:113:LYS:CA	1:F:117:VAL:HG12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:MET:HE2	1:B:332:PRO:N	2.27	0.49
1:E:105:LEU:HG	1:E:274:HIS:HD2	1.78	0.49
1:E:336:ASN:OD1	1:E:338:ASP:N	2.43	0.49
1:C:103:VAL:HG11	1:C:274:HIS:N	2.28	0.49
1:B:301:THR:HG21	1:B:309:ILE:HD11	1.93	0.49
1:D:327:LYS:O	1:D:328:ASN:HB2	2.12	0.49
1:F:151:VAL:HG23	1:F:198:ILE:HD13	1.95	0.49
1:F:211:TYR:CG	1:F:217:GLY:HA3	2.48	0.49
1:B:113:LYS:HA	1:B:117:VAL:HG13	1.95	0.49
1:B:301:THR:HG22	1:B:304:TYR:HB2	1.95	0.49
1:E:105:LEU:O	1:E:106:GLU:C	2.55	0.49
1:F:226:LEU:CD2	1:F:260:ARG:NH1	2.76	0.49
1:A:324:MET:HE3	1:A:331:GLU:C	2.37	0.49
1:E:249:LYS:HG3	1:E:251:TRP:HE3	1.78	0.49
1:B:105:LEU:HG	1:B:274:HIS:HD2	1.78	0.48
1:E:113:LYS:HA	1:E:117:VAL:HG13	1.95	0.48
1:B:219:ALA:O	1:B:220:ARG:C	2.56	0.48
1:C:96:LYS:N	1:C:150:ALA:O	2.46	0.48
1:C:276:LEU:HD11	1:C:295:GLU:HG2	1.95	0.48
1:D:336:ASN:OD1	1:D:336:ASN:C	2.56	0.48
1:F:249:LYS:HZ3	1:F:251:TRP:CD1	2.30	0.48
1:A:213:SER:O	1:A:214:GLU:C	2.56	0.48
1:D:113:LYS:CA	1:D:117:VAL:HG12	2.44	0.48
1:E:219:ALA:O	1:E:220:ARG:C	2.56	0.48
1:B:293:ASN:HD21	1:B:296:GLU:CD	2.21	0.48
1:C:165:ALA:HB3	1:D:227:LYS:HE2	1.94	0.48
1:C:301:THR:HG21	1:C:309:ILE:HD11	1.95	0.48
1:F:276:LEU:HD11	1:F:295:GLU:HG2	1.95	0.48
1:A:99:LEU:H	1:A:99:LEU:HD13	1.78	0.48
1:C:116:VAL:HG21	1:C:151:VAL:HG11	1.96	0.48
1:D:105:LEU:HG	1:D:274:HIS:HD2	1.77	0.48
1:A:113:LYS:CA	1:A:117:VAL:HG12	2.43	0.48
1:D:213:SER:O	1:D:214:GLU:C	2.57	0.48
1:D:105:LEU:O	1:D:106:GLU:C	2.56	0.48
1:D:130:TRP:CH2	1:D:132:ARG:CZ	2.97	0.48
1:B:113:LYS:HB3	1:B:118:TYR:HE1	1.78	0.48
1:B:249:LYS:HG3	1:B:251:TRP:HE3	1.79	0.48
1:F:256:PRO:CB	1:F:260:ARG:HH12	2.26	0.48
1:E:297:LEU:O	1:E:298:ALA:C	2.56	0.47
1:C:112:LEU:O	1:C:116:VAL:HG22	2.14	0.47
1:C:144:LYS:CG	1:C:267:ILE:HD11	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:LYS:HB3	1:F:118:TYR:HE1	1.79	0.47
1:B:156:ASP:O	1:B:195:LYS:HD3	2.14	0.47
1:E:113:LYS:HB3	1:E:118:TYR:HE1	1.79	0.47
1:F:256:PRO:HB3	1:F:260:ARG:HH12	1.80	0.47
1:A:249:LYS:HG3	1:A:251:TRP:HE3	1.80	0.47
1:B:112:LEU:HD13	1:B:265:ILE:HD11	1.97	0.47
1:A:323:GLU:HA	1:A:326:GLU:HG2	1.97	0.47
1:A:333:ARG:CG	1:A:334:ALA:HA	2.45	0.47
1:C:113:LYS:HB3	1:C:118:TYR:HE1	1.79	0.47
1:C:229:MET:HA	1:C:232:LEU:HD13	1.96	0.47
1:D:235:LYS:O	1:D:236:ASN:C	2.57	0.47
1:F:338:ASP:OD1	1:F:338:ASP:C	2.58	0.47
1:F:264:ARG:HD2	1:F:368:ALA:HB3	1.97	0.47
1:A:263:LYS:NZ	1:A:369:LEU:HD23	2.30	0.47
1:D:336:ASN:OD1	1:D:338:ASP:N	2.47	0.47
1:E:139:PRO:CB	1:E:351:VAL:HG11	2.44	0.47
1:F:158:GLU:CG	1:F:189:LEU:HD21	2.45	0.47
1:C:99:LEU:HD12	1:C:150:ALA:HB1	1.97	0.47
1:C:338:ASP:OD1	1:C:338:ASP:C	2.58	0.47
1:E:301:THR:HG22	1:E:304:TYR:HB2	1.96	0.47
1:B:297:LEU:O	1:B:298:ALA:C	2.58	0.46
1:B:352:ASN:HB3	1:B:355:MET:HG3	1.98	0.46
1:C:97:VAL:CG1	1:C:100:ASN:HD21	2.28	0.46
1:E:284:SER:OG	1:E:285:LYS:N	2.43	0.46
1:A:130:TRP:CH2	1:A:132:ARG:CZ	2.98	0.46
1:A:219:ALA:HB1	1:F:210:SER:HB3	1.97	0.46
1:A:99:LEU:HG	1:A:109:LYS:HE3	1.93	0.46
1:B:130:TRP:CH2	1:B:132:ARG:CZ	2.98	0.46
1:C:323:GLU:O	1:C:324:MET:C	2.59	0.46
1:A:333:ARG:HB3	1:A:334:ALA:HB2	1.97	0.46
1:D:276:LEU:HD11	1:D:295:GLU:HG2	1.98	0.46
1:E:112:LEU:HD13	1:E:265:ILE:HD11	1.98	0.46
1:F:139:PRO:HB3	1:F:351:VAL:HG11	1.97	0.46
1:A:276:LEU:HD11	1:A:295:GLU:HG2	1.98	0.46
1:A:297:LEU:O	1:A:298:ALA:C	2.59	0.46
1:B:225:PHE:CZ	1:B:229:MET:CE	2.98	0.46
1:E:287:LYS:HE2	1:E:334:ALA:HB2	1.98	0.46
1:E:362:TRP:CD1	1:E:362:TRP:C	2.93	0.46
1:F:297:LEU:O	1:F:298:ALA:C	2.58	0.46
1:C:297:LEU:O	1:C:298:ALA:C	2.58	0.46
1:D:216:GLY:C	1:D:218:GLU:N	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:ASP:OD1	1:F:247:THR:OG1	2.25	0.46
1:A:210:SER:CA	1:A:211:TYR:N	2.79	0.46
1:E:283:SER:O	1:E:285:LYS:N	2.49	0.46
1:F:352:ASN:OD1	1:F:353:GLN:N	2.49	0.46
1:C:113:LYS:HA	1:C:117:VAL:HG12	1.97	0.46
1:B:176:GLU:HG2	1:B:221:VAL:HG12	1.97	0.46
1:C:352:ASN:OD1	1:C:353:GLN:N	2.49	0.46
1:E:235:LYS:O	1:E:236:ASN:C	2.58	0.46
1:F:105:LEU:O	1:F:107:ASP:N	2.49	0.46
1:F:113:LYS:HA	1:F:117:VAL:HG12	1.97	0.46
1:F:158:GLU:HG3	1:F:189:LEU:HG	1.98	0.46
1:A:254:ASP:OD1	1:A:256:PRO:HD2	2.16	0.46
1:C:323:GLU:HG2	1:C:327:LYS:HG3	1.98	0.46
1:D:205:ASP:OD1	1:D:247:THR:OG1	2.25	0.46
1:E:176:GLU:HG2	1:E:221:VAL:HG12	1.97	0.46
1:A:105:LEU:HD21	1:A:108:VAL:CG1	2.46	0.45
1:A:105:LEU:HD21	1:A:108:VAL:HB	1.97	0.45
1:D:297:LEU:O	1:D:298:ALA:C	2.59	0.45
1:D:324:MET:HE2	1:D:332:PRO:CA	2.47	0.45
1:D:352:ASN:OD1	1:D:353:GLN:N	2.49	0.45
1:E:97:VAL:HG21	1:E:146:MET:CE	2.46	0.45
1:E:225:PHE:CZ	1:E:229:MET:CE	2.99	0.45
1:D:215:VAL:HG22	1:D:216:GLY:N	2.30	0.45
1:E:97:VAL:O	1:E:97:VAL:HG13	2.16	0.45
1:E:104:GLY:O	1:E:105:LEU:HB2	2.16	0.45
1:A:352:ASN:OD1	1:A:353:GLN:N	2.49	0.45
1:C:250:PRO:O	1:C:362:TRP:CH2	2.70	0.45
1:C:324:MET:HE3	1:C:331:GLU:O	2.16	0.45
1:D:158:GLU:CG	1:D:189:LEU:HD21	2.46	0.45
1:E:130:TRP:CH2	1:E:132:ARG:CZ	2.99	0.45
1:A:235:LYS:O	1:A:236:ASN:C	2.58	0.45
1:A:323:GLU:O	1:A:324:MET:C	2.60	0.45
1:C:106:GLU:O	1:C:107:ASP:CB	2.64	0.45
1:E:283:SER:O	1:E:284:SER:C	2.59	0.45
1:E:288:LEU:HA	1:E:335:ILE:CG2	2.47	0.45
1:A:97:VAL:HG13	1:A:97:VAL:O	2.17	0.45
1:B:276:LEU:HD11	1:B:295:GLU:HG2	1.99	0.45
1:D:216:GLY:HA3	1:D:218:GLU:CD	2.42	0.45
1:D:250:PRO:HB2	1:D:362:TRP:CH2	2.51	0.45
1:B:283:SER:O	1:B:284:SER:C	2.60	0.45
1:C:139:PRO:HB3	1:C:351:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LYS:O	1:C:236:ASN:C	2.59	0.45
1:F:362:TRP:CD1	1:F:362:TRP:C	2.94	0.45
1:A:109:LYS:HA	1:A:109:LYS:HD3	1.83	0.45
1:A:352:ASN:HB3	1:A:355:MET:HG3	1.98	0.45
1:B:283:SER:O	1:B:285:LYS:N	2.49	0.45
1:C:282:TYR:HB3	1:C:313:VAL:HG11	1.98	0.45
1:D:254:ASP:OD1	1:D:256:PRO:HD2	2.17	0.45
1:D:320:VAL:HG11	1:D:335:ILE:HA	1.98	0.45
1:F:283:SER:O	1:F:285:LYS:N	2.50	0.45
1:A:320:VAL:HG11	1:A:335:ILE:HA	1.99	0.45
1:B:254:ASP:OD1	1:B:256:PRO:HD2	2.17	0.45
1:B:352:ASN:OD1	1:B:353:GLN:N	2.50	0.45
1:C:228:GLU:O	1:C:232:LEU:HD13	2.16	0.45
1:C:254:ASP:OD1	1:C:256:PRO:HD2	2.17	0.45
1:C:352:ASN:HB3	1:C:355:MET:HG3	1.98	0.45
1:D:325:PHE:HE2	1:E:121:LYS:CD	2.30	0.45
1:E:310:ARG:NH2	1:F:128:LEU:O	2.50	0.45
1:F:97:VAL:O	1:F:97:VAL:HG13	2.16	0.45
1:F:258:LEU:HD11	1:F:362:TRP:HH2	1.82	0.45
1:A:116:VAL:HG23	1:A:242:TYR:CE2	2.51	0.45
1:A:281:HIS:O	1:A:284:SER:HB3	2.17	0.45
1:E:208:LEU:HD22	1:E:252:ARG:O	2.17	0.45
1:D:249:LYS:HG3	1:D:251:TRP:HE3	1.81	0.44
1:E:276:LEU:HD11	1:E:295:GLU:HG2	1.99	0.44
1:E:336:ASN:OD1	1:E:336:ASN:C	2.58	0.44
1:F:235:LYS:O	1:F:236:ASN:C	2.59	0.44
1:F:324:MET:HE3	1:F:331:GLU:O	2.17	0.44
1:F:327:LYS:O	1:F:328:ASN:HB2	2.16	0.44
1:A:134:ILE:HG23	1:A:244:ILE:HG12	1.99	0.44
1:A:227:LYS:HE2	1:F:165:ALA:CB	2.47	0.44
1:B:99:LEU:CA	1:B:101:GLU:HB2	2.38	0.44
1:D:106:GLU:O	1:D:107:ASP:C	2.59	0.44
1:F:134:ILE:HG23	1:F:244:ILE:HG12	1.98	0.44
1:F:156:ASP:O	1:F:195:LYS:HD2	2.18	0.44
1:B:288:LEU:O	1:B:289:ASP:HB3	2.17	0.44
1:B:325:PHE:CG	1:C:118:TYR:CE2	3.06	0.44
1:B:330:GLN:O	1:B:331:GLU:HB2	2.17	0.44
1:D:137:TYR:CD2	1:D:362:TRP:HZ3	2.36	0.44
1:F:254:ASP:OD1	1:F:256:PRO:HD2	2.17	0.44
1:A:98:THR:OG1	1:A:99:LEU:N	2.50	0.44
1:C:352:ASN:OD1	1:C:352:ASN:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ASP:OD1	1:E:256:PRO:HD2	2.17	0.44
1:B:157:SER:OG	1:B:196:PRO:O	2.33	0.44
1:D:158:GLU:HG3	1:D:189:LEU:HG	1.98	0.44
1:E:157:SER:OG	1:E:196:PRO:O	2.33	0.44
1:E:323:GLU:O	1:E:324:MET:C	2.60	0.44
1:B:99:LEU:CD1	1:B:109:LYS:HE2	2.48	0.44
1:B:352:ASN:OD1	1:B:352:ASN:C	2.61	0.44
1:C:156:ASP:O	1:C:195:LYS:HD2	2.18	0.44
1:C:327:LYS:O	1:C:328:ASN:HB2	2.16	0.44
1:D:171:TRP:CZ2	1:D:177:LYS:HD3	2.53	0.44
1:F:97:VAL:C	1:F:153:ASN:ND2	2.75	0.44
1:F:337:MET:HE3	1:F:337:MET:HA	1.98	0.44
1:D:281:HIS:O	1:D:284:SER:HB3	2.18	0.44
1:A:106:GLU:O	1:A:107:ASP:C	2.61	0.44
1:C:134:ILE:HG23	1:C:244:ILE:HG12	1.98	0.44
1:C:337:MET:HA	1:C:337:MET:HE3	1.98	0.44
1:D:134:ILE:HG23	1:D:244:ILE:HG12	1.99	0.44
1:E:99:LEU:HD23	1:E:150:ALA:HB1	2.00	0.44
1:E:269:LEU:CD1	1:E:351:VAL:HG21	2.47	0.44
1:A:113:LYS:HB3	1:A:118:TYR:HE1	1.83	0.44
1:A:212:THR:CG2	1:B:218:GLU:CD	2.91	0.44
1:B:249:LYS:HE2	1:B:252:ARG:NH1	2.33	0.44
1:D:249:LYS:HE2	1:D:252:ARG:NH1	2.33	0.44
1:E:139:PRO:HB3	1:E:351:VAL:HG11	2.00	0.44
1:F:229:MET:HE2	1:F:243:VAL:HG21	2.00	0.44
1:A:161:HIS:HE1	1:A:163:ASP:OD1	2.01	0.43
1:B:287:LYS:HZ3	1:B:332:PRO:HG2	1.82	0.43
1:C:249:LYS:HE2	1:C:252:ARG:NH1	2.33	0.43
1:D:98:THR:OG1	1:D:99:LEU:N	2.50	0.43
1:D:177:LYS:HG3	1:D:178:ASN:N	2.32	0.43
1:E:330:GLN:O	1:E:331:GLU:HB2	2.17	0.43
1:F:275:ARG:HD3	1:F:301:THR:HG23	1.99	0.43
1:A:100:ASN:O	1:A:101:GLU:HB2	2.17	0.43
1:A:249:LYS:HE2	1:A:252:ARG:NH1	2.33	0.43
1:A:287:LYS:O	1:A:335:ILE:HG22	1.96	0.43
1:C:229:MET:HE2	1:C:243:VAL:HG21	2.00	0.43
1:D:113:LYS:HB3	1:D:118:TYR:HE1	1.83	0.43
1:F:352:ASN:OD1	1:F:352:ASN:C	2.61	0.43
1:A:99:LEU:HB3	1:A:150:ALA:HB1	2.00	0.43
1:C:258:LEU:HD11	1:C:362:TRP:HH2	1.83	0.43
1:E:352:ASN:HB3	1:E:355:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:GLU:HG3	1:F:189:LEU:CD2	2.49	0.43
1:A:113:LYS:HA	1:A:117:VAL:HG12	1.99	0.43
1:A:352:ASN:OD1	1:A:352:ASN:C	2.61	0.43
1:B:362:TRP:CD1	1:B:362:TRP:C	2.95	0.43
1:D:113:LYS:HA	1:D:117:VAL:HG12	1.99	0.43
1:D:352:ASN:HB3	1:D:355:MET:HG3	1.99	0.43
1:C:362:TRP:CD1	1:C:362:TRP:C	2.95	0.43
1:D:340:PHE:HA	1:D:343:VAL:CG2	2.48	0.43
1:F:110:GLU:HA	1:F:113:LYS:HE3	2.01	0.43
1:F:158:GLU:HG3	1:F:189:LEU:HD21	2.00	0.43
1:F:223:ASN:OD1	1:F:223:ASN:C	2.61	0.43
1:F:288:LEU:HA	1:F:335:ILE:CG2	2.48	0.43
1:A:208:LEU:HD22	1:A:252:ARG:O	2.18	0.43
1:B:208:LEU:HD22	1:B:252:ARG:O	2.18	0.43
1:C:260:ARG:CG	1:C:260:ARG:NH1	2.80	0.43
1:C:275:ARG:HD3	1:C:301:THR:HG23	1.99	0.43
1:D:282:TYR:HB3	1:D:313:VAL:HG21	2.00	0.43
1:D:340:PHE:O	1:D:343:VAL:HG22	2.18	0.43
1:D:352:ASN:OD1	1:D:352:ASN:C	2.61	0.43
1:E:166:SER:HA	1:F:223:ASN:ND2	2.33	0.43
1:E:288:LEU:O	1:E:289:ASP:HB3	2.17	0.43
1:F:102:ILE:HD11	1:F:277:GLU:HG2	2.00	0.43
1:F:145:THR:HG23	1:F:200:PHE:CE2	2.53	0.43
1:A:210:SER:HB3	1:A:211:TYR:CB	2.48	0.43
1:B:174:GLU:O	1:B:175:ALA:HB3	2.19	0.43
1:C:96:LYS:HB2	1:C:150:ALA:HA	1.99	0.43
1:C:264:ARG:C	1:C:265:ILE:HD13	2.43	0.43
1:D:208:LEU:HD22	1:D:252:ARG:O	2.18	0.43
1:D:288:LEU:HA	1:D:335:ILE:CG2	2.49	0.43
1:E:166:SER:HA	1:F:223:ASN:HD21	1.84	0.43
1:E:325:PHE:CG	1:F:118:TYR:CE2	3.06	0.43
1:F:287:LYS:HE2	1:F:334:ALA:HB2	1.99	0.43
1:A:175:ALA:C	1:A:178:ASN:OD1	2.60	0.43
1:B:292:VAL:HA	1:B:337:MET:HG2	1.96	0.43
1:C:97:VAL:HG13	1:C:97:VAL:O	2.17	0.43
1:C:250:PRO:HB2	1:C:362:TRP:CE2	2.54	0.43
1:D:161:HIS:HE1	1:D:163:ASP:OD1	2.02	0.43
1:F:283:SER:O	1:F:284:SER:C	2.61	0.43
1:A:129:GLY:C	1:F:314:GLN:NE2	2.77	0.43
1:A:225:PHE:CZ	1:A:229:MET:CE	3.00	0.43
1:A:283:SER:O	1:A:285:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:CD1	1:B:109:LYS:CE	2.94	0.43
1:C:118:TYR:CB	1:C:119:PRO:CD	2.97	0.43
1:E:229:MET:HE2	1:E:243:VAL:HG21	2.00	0.43
1:F:130:TRP:CH2	1:F:132:ARG:CZ	3.01	0.43
1:F:288:LEU:O	1:F:289:ASP:HB3	2.18	0.43
1:A:116:VAL:CG2	1:A:242:TYR:CD2	3.02	0.43
1:A:177:LYS:HG3	1:A:178:ASN:N	2.32	0.43
1:A:282:TYR:HB3	1:A:313:VAL:HG21	2.01	0.43
1:D:288:LEU:O	1:D:289:ASP:HB3	2.19	0.43
1:E:106:GLU:O	1:E:107:ASP:C	2.61	0.43
1:B:287:LYS:O	1:B:287:LYS:CG	2.63	0.42
1:E:281:HIS:O	1:E:284:SER:HB3	2.19	0.42
1:E:297:LEU:HG	1:E:337:MET:HE1	2.01	0.42
1:C:130:TRP:CH2	1:C:132:ARG:CZ	3.01	0.42
1:C:281:HIS:O	1:C:284:SER:HB3	2.19	0.42
1:D:323:GLU:O	1:D:324:MET:C	2.62	0.42
1:D:362:TRP:CZ3	1:D:367:LYS:HG3	2.55	0.42
1:A:283:SER:O	1:A:284:SER:C	2.62	0.42
1:A:288:LEU:O	1:A:289:ASP:HB3	2.20	0.42
1:B:250:PRO:O	1:B:362:TRP:CH2	2.72	0.42
1:E:105:LEU:O	1:E:107:ASP:N	2.53	0.42
1:F:118:TYR:CB	1:F:119:PRO:CD	2.98	0.42
1:F:225:PHE:CZ	1:F:229:MET:CE	3.01	0.42
1:F:281:HIS:O	1:F:284:SER:HB3	2.19	0.42
1:F:323:GLU:O	1:F:324:MET:C	2.63	0.42
1:B:323:GLU:O	1:B:324:MET:C	2.61	0.42
1:F:250:PRO:O	1:F:362:TRP:CH2	2.73	0.42
1:C:97:VAL:O	1:C:98:THR:OG1	2.23	0.42
1:D:175:ALA:C	1:D:178:ASN:OD1	2.59	0.42
1:F:105:LEU:HD23	1:F:110:GLU:HB3	2.01	0.42
1:A:215:VAL:HG11	1:F:211:TYR:CE2	2.55	0.42
1:A:323:GLU:HA	1:A:326:GLU:CG	2.49	0.42
1:A:333:ARG:NH2	1:A:334:ALA:O	2.52	0.42
1:C:225:PHE:CZ	1:C:229:MET:CE	3.01	0.42
1:D:225:PHE:CZ	1:D:229:MET:CE	3.02	0.42
1:E:250:PRO:O	1:E:362:TRP:CH2	2.72	0.42
1:F:139:PRO:HB2	1:F:351:VAL:HG11	1.99	0.42
1:A:116:VAL:CG1	1:A:117:VAL:N	2.82	0.42
1:C:208:LEU:HD22	1:C:252:ARG:O	2.19	0.42
1:C:249:LYS:HG3	1:C:251:TRP:HE3	1.84	0.42
1:D:99:LEU:C	1:D:101:GLU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD11	1:D:109:LYS:HG3	2.02	0.42
1:D:340:PHE:CA	1:D:343:VAL:HG22	2.49	0.42
1:C:139:PRO:HB2	1:C:351:VAL:HG11	2.00	0.42
1:D:212:THR:CB	1:E:218:GLU:HG3	2.49	0.42
1:D:229:MET:HE2	1:D:243:VAL:HG21	2.00	0.42
1:D:362:TRP:CH2	1:D:367:LYS:CD	3.02	0.42
1:A:290:PRO:O	1:A:291:ASN:CG	2.63	0.42
1:B:118:TYR:O	1:B:121:LYS:HG3	2.19	0.42
1:B:281:HIS:O	1:B:284:SER:HB3	2.20	0.42
1:C:100:ASN:C	1:C:102:ILE:H	2.28	0.42
1:C:213:SER:O	1:C:214:GLU:C	2.63	0.42
1:C:283:SER:O	1:C:284:SER:C	2.62	0.42
1:D:158:GLU:HG3	1:D:189:LEU:CD2	2.49	0.42
1:E:229:MET:HE1	1:E:243:VAL:HG11	2.02	0.42
1:B:106:GLU:O	1:B:107:ASP:C	2.62	0.42
1:B:229:MET:HE2	1:B:243:VAL:HG21	2.01	0.42
1:E:102:ILE:HD12	1:E:147:ILE:HG13	2.02	0.42
1:E:174:GLU:O	1:E:175:ALA:HB3	2.20	0.42
1:F:144:LYS:HE3	1:F:248:ASN:OD1	2.20	0.42
1:D:103:VAL:HB	1:D:274:HIS:CE1	2.55	0.41
1:D:158:GLU:HG3	1:D:189:LEU:HD21	2.01	0.41
1:C:110:GLU:HA	1:C:113:LYS:HE3	2.02	0.41
1:C:171:TRP:NE1	1:C:177:LYS:HE2	2.35	0.41
1:C:288:LEU:O	1:C:289:ASP:HB3	2.19	0.41
1:A:229:MET:HE2	1:A:243:VAL:HG21	2.01	0.41
1:C:103:VAL:HG21	1:C:273:ALA:C	2.45	0.41
1:C:116:VAL:HG12	1:C:242:TYR:CD2	2.55	0.41
1:C:106:GLU:O	1:C:107:ASP:HB3	2.21	0.41
1:C:177:LYS:HG3	1:C:178:ASN:N	2.35	0.41
1:D:283:SER:O	1:D:284:SER:C	2.64	0.41
1:A:250:PRO:HB2	1:A:362:TRP:CH2	2.55	0.41
1:B:205:ASP:OD1	1:B:247:THR:OG1	2.25	0.41
1:D:218:GLU:O	1:D:220:ARG:N	2.54	0.41
1:A:137:TYR:CD2	1:A:362:TRP:HZ3	2.39	0.41
1:A:145:THR:HG23	1:A:200:PHE:CE2	2.55	0.41
1:B:181:LYS:HA	1:B:184:LYS:HB2	2.03	0.41
1:C:324:MET:SD	1:D:125:LEU:HD21	2.61	0.41
1:E:97:VAL:CG2	1:E:101:GLU:OE2	2.68	0.41
1:E:181:LYS:HA	1:E:184:LYS:HB2	2.02	0.41
1:B:322:LYS:HA	1:B:322:LYS:HD3	1.89	0.41
1:C:340:PHE:HA	1:C:343:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:GLU:OE1	1:E:215:VAL:HG23	2.21	0.41
1:F:105:LEU:O	1:F:106:GLU:C	2.63	0.41
1:A:290:PRO:O	1:A:291:ASN:CB	2.68	0.41
1:C:283:SER:O	1:C:285:LYS:N	2.54	0.41
1:D:212:THR:OG1	1:E:218:GLU:HG3	2.20	0.41
1:E:118:TYR:CB	1:E:119:PRO:CD	2.99	0.41
1:F:340:PHE:HA	1:F:343:VAL:HG12	2.02	0.41
1:D:106:GLU:O	1:D:109:LYS:N	2.54	0.40
1:D:145:THR:HG23	1:D:200:PHE:CE2	2.56	0.40
1:E:177:LYS:HG3	1:E:178:ASN:N	2.35	0.40
1:E:218:GLU:O	1:E:220:ARG:N	2.54	0.40
1:F:218:GLU:O	1:F:220:ARG:N	2.54	0.40
1:F:250:PRO:HB2	1:F:362:TRP:CE2	2.56	0.40
1:A:218:GLU:O	1:A:220:ARG:N	2.54	0.40
1:B:105:LEU:O	1:B:107:ASP:N	2.54	0.40
1:D:103:VAL:O	1:D:105:LEU:N	2.54	0.40
1:D:118:TYR:CB	1:D:119:PRO:CD	2.99	0.40
1:D:264:ARG:NH1	1:D:366:PHE:O	2.54	0.40
1:D:297:LEU:HG	1:D:337:MET:HE1	2.02	0.40
1:A:340:PHE:HA	1:A:343:VAL:HG12	2.03	0.40
1:B:112:LEU:HG	1:B:151:VAL:HG11	2.02	0.40
1:B:183:PHE:O	1:B:184:LYS:C	2.64	0.40
1:B:248:ASN:O	1:B:359:TYR:OH	2.34	0.40
1:B:260:ARG:HD2	1:B:260:ARG:N	2.36	0.40
1:B:291:ASN:OD1	1:B:337:MET:HB2	2.21	0.40
1:B:324:MET:CE	1:C:125:LEU:HD21	2.51	0.40
1:A:286:VAL:O	1:A:286:VAL:HG23	2.21	0.40
1:B:177:LYS:HG3	1:B:178:ASN:N	2.36	0.40
1:B:340:PHE:HA	1:B:343:VAL:HG12	2.02	0.40
1:F:158:GLU:HG3	1:F:189:LEU:CG	2.52	0.40
1:F:256:PRO:O	1:F:260:ARG:NH1	2.55	0.40
1:A:336:ASN:OD1	1:A:337:MET:N	2.53	0.40
1:B:218:GLU:O	1:B:220:ARG:N	2.54	0.40
1:C:317:HIS:HA	1:C:335:ILE:HD11	2.03	0.40
1:E:183:PHE:O	1:E:184:LYS:C	2.65	0.40
1:F:286:VAL:HG23	1:F:286:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:PHE:O	1:F:330:GLN:NE2[2_665]	2.19	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	263/316 (83%)	207 (79%)	34 (13%)	22 (8%)	0	7
1	B	249/316 (79%)	204 (82%)	31 (12%)	14 (6%)	1	14
1	C	270/316 (85%)	218 (81%)	35 (13%)	17 (6%)	1	12
1	D	271/316 (86%)	210 (78%)	38 (14%)	23 (8%)	0	7
1	E	256/316 (81%)	207 (81%)	32 (12%)	17 (7%)	1	12
1	F	272/316 (86%)	214 (79%)	39 (14%)	19 (7%)	1	10
All	All	1581/1896 (83%)	1260 (80%)	209 (13%)	112 (7%)	1	10

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	101	GLU
1	A	106	GLU
1	A	215	VAL
1	A	238	ILE
1	A	284	SER
1	A	328	ASN
1	B	103	VAL
1	B	106	GLU
1	B	174	GLU
1	B	284	SER
1	B	337	MET
1	C	103	VAL
1	C	172	LEU
1	C	235	LYS

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Mol	Chain	Res	Type
1	C	284	SER
1	D	104	GLY
1	D	106	GLU
1	D	172	LEU
1	D	238	ILE
1	D	284	SER
1	D	329	LEU
1	D	366	PHE
1	E	103	VAL
1	E	106	GLU
1	E	238	ILE
1	E	284	SER
1	F	104	GLY
1	F	106	GLU
1	F	172	LEU
1	F	215	VAL
1	F	238	ILE
1	F	284	SER
1	A	219	ALA
1	A	233	ALA
1	A	236	ASN
1	A	237	GLU
1	A	325	PHE
1	A	334	ALA
1	B	219	ALA
1	C	171	TRP
1	C	219	ALA
1	C	233	ALA
1	C	236	ASN
1	C	293	ASN
1	D	171	TRP
1	D	219	ALA
1	D	233	ALA
1	D	236	ASN
1	D	237	GLU
1	D	293	ASN
1	D	328	ASN
1	E	219	ALA
1	E	233	ALA
1	E	236	ASN
1	E	237	GLU
1	F	171	TRP

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Mol	Chain	Res	Type
1	F	210	SER
1	F	219	ALA
1	F	233	ALA
1	F	236	ASN
1	F	237	GLU
1	A	193	GLU
1	A	240	LYS
1	A	293	ASN
1	A	333	ARG
1	A	338	ASP
1	B	193	GLU
1	B	240	LYS
1	B	293	ASN
1	C	193	GLU
1	C	210	SER
1	C	214	GLU
1	C	240	LYS
1	D	193	GLU
1	D	210	SER
1	D	240	LYS
1	D	326	GLU
1	E	193	GLU
1	E	240	LYS
1	E	293	ASN
1	F	193	GLU
1	F	240	LYS
1	F	293	ASN
1	A	289	ASP
1	A	368	ALA
1	B	184	LYS
1	B	289	ASP
1	B	336	ASN
1	C	289	ASP
1	D	215	VAL
1	D	289	ASP
1	E	98	THR
1	E	184	LYS
1	E	289	ASP
1	F	289	ASP
1	F	184	LYS
1	A	184	LYS
1	C	99	LEU

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Mol	Chain	Res	Type
1	C	184	LYS
1	D	184	LYS
1	D	217	GLY
1	E	97	VAL
1	E	105	LEU
1	A	256	PRO
1	B	104	GLY
1	C	256	PRO
1	D	256	PRO
1	F	256	PRO
1	B	256	PRO
1	E	256	PRO
1	F	97	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/273 (85%)	199 (86%)	33 (14%)	3	19
1	B	221/273 (81%)	185 (84%)	36 (16%)	2	15
1	C	234/273 (86%)	203 (87%)	31 (13%)	4	21
1	D	235/273 (86%)	203 (86%)	32 (14%)	3	20
1	E	227/273 (83%)	193 (85%)	34 (15%)	3	17
1	F	235/273 (86%)	199 (85%)	36 (15%)	3	16
All	All	1384/1638 (84%)	1182 (85%)	202 (15%)	3	18

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	101	GLU
1	A	105	LEU
1	A	108	VAL
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	116	VAL
1	A	122	ARG
1	A	132	ARG
1	A	134	ILE
1	A	168	MET
1	A	190	SER
1	A	195	LYS
1	A	205	ASP
1	A	214	GLU
1	A	215	VAL
1	A	222	ARG
1	A	223	ASN
1	A	237	GLU
1	A	238	ILE
1	A	252	ARG
1	A	254	ASP
1	A	257	PHE
1	A	276	LEU
1	A	287	LYS
1	A	291	ASN
1	A	296	GLU
1	A	309	ILE
1	A	312	ILE
1	A	326	GLU
1	A	328	ASN
1	A	366	PHE
1	A	367	LYS
1	A	369	LEU
1	B	105	LEU
1	B	108	VAL
1	B	122	ARG
1	B	132	ARG
1	B	167	ILE
1	B	168	MET
1	B	190	SER
1	B	205	ASP
1	B	215	VAL
1	B	218	GLU
1	B	220	ARG
1	B	223	ASN
1	B	252	ARG
1	B	254	ASP

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Mol	Chain	Res	Type
1	B	257	PHE
1	B	260	ARG
1	B	265	ILE
1	B	269	LEU
1	B	272	LYS
1	B	276	LEU
1	B	277	GLU
1	B	287	LYS
1	B	291	ASN
1	B	293	ASN
1	B	296	GLU
1	B	301	THR
1	B	309	ILE
1	B	312	ILE
1	B	320	VAL
1	B	322	LYS
1	B	324	MET
1	B	328	ASN
1	B	337	MET
1	B	353	GLN
1	B	354	ASP
1	B	367	LYS
1	C	101	GLU
1	C	102	ILE
1	C	122	ARG
1	C	132	ARG
1	C	134	ILE
1	C	168	MET
1	C	190	SER
1	C	205	ASP
1	C	214	GLU
1	C	215	VAL
1	C	218	GLU
1	C	222	ARG
1	C	238	ILE
1	C	252	ARG
1	C	254	ASP
1	C	257	PHE
1	C	260	ARG
1	C	276	LEU
1	C	285	LYS
1	C	291	ASN

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Mol	Chain	Res	Type
1	C	296	GLU
1	C	309	ILE
1	C	312	ILE
1	C	313	VAL
1	C	320	VAL
1	C	324	MET
1	C	337	MET
1	C	338	ASP
1	C	351	VAL
1	C	353	GLN
1	C	354	ASP
1	D	97	VAL
1	D	99	LEU
1	D	103	VAL
1	D	105	LEU
1	D	108	VAL
1	D	122	ARG
1	D	125	LEU
1	D	132	ARG
1	D	134	ILE
1	D	168	MET
1	D	171	TRP
1	D	172	LEU
1	D	190	SER
1	D	195	LYS
1	D	205	ASP
1	D	218	GLU
1	D	223	ASN
1	D	228	GLU
1	D	237	GLU
1	D	238	ILE
1	D	252	ARG
1	D	254	ASP
1	D	257	PHE
1	D	269	LEU
1	D	276	LEU
1	D	285	LYS
1	D	291	ASN
1	D	296	GLU
1	D	309	ILE
1	D	312	ILE
1	D	324	MET

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Mol	Chain	Res	Type
1	D	329	LEU
1	E	105	LEU
1	E	106	GLU
1	E	108	VAL
1	E	122	ARG
1	E	132	ARG
1	E	167	ILE
1	E	168	MET
1	E	190	SER
1	E	205	ASP
1	E	215	VAL
1	E	218	GLU
1	E	220	ARG
1	E	223	ASN
1	E	237	GLU
1	E	238	ILE
1	E	252	ARG
1	E	254	ASP
1	E	257	PHE
1	E	265	ILE
1	E	269	LEU
1	E	276	LEU
1	E	277	GLU
1	E	291	ASN
1	E	301	THR
1	E	309	ILE
1	E	312	ILE
1	E	320	VAL
1	E	322	LYS
1	E	324	MET
1	E	328	ASN
1	E	351	VAL
1	E	353	GLN
1	E	354	ASP
1	E	367	LYS
1	F	99	LEU
1	F	102	ILE
1	F	121	LYS
1	F	122	ARG
1	F	132	ARG
1	F	134	ILE
1	F	144	LYS

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Mol	Chain	Res	Type
1	F	146	MET
1	F	168	MET
1	F	171	TRP
1	F	172	LEU
1	F	190	SER
1	F	205	ASP
1	F	215	VAL
1	F	218	GLU
1	F	223	ASN
1	F	228	GLU
1	F	237	GLU
1	F	251	TRP
1	F	252	ARG
1	F	254	ASP
1	F	257	PHE
1	F	269	LEU
1	F	276	LEU
1	F	285	LYS
1	F	291	ASN
1	F	309	ILE
1	F	312	ILE
1	F	320	VAL
1	F	322	LYS
1	F	324	MET
1	F	337	MET
1	F	338	ASP
1	F	351	VAL
1	F	365	LYS
1	F	369	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	B	100	ASN
1	C	100	ASN
1	C	328	ASN
1	D	161	HIS
1	D	274	HIS
1	E	274	HIS
1	F	100	ASN
1	F	328	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	210:SER	C	211:TYR	N	2.55

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	269/316 (85%)	-0.10	3 (1%) 78 52	84, 149, 228, 279	0
1	B	257/316 (81%)	-0.13	2 (0%) 82 58	71, 135, 218, 262	0
1	C	272/316 (86%)	-0.21	1 (0%) 88 70	86, 134, 200, 216	0
1	D	273/316 (86%)	-0.30	1 (0%) 88 70	81, 135, 208, 251	0
1	E	262/316 (82%)	-0.20	0 100 100	61, 133, 216, 275	0
1	F	274/316 (86%)	-0.30	0 100 100	73, 126, 193, 246	0
All	All	1607/1896 (84%)	-0.21	7 (0%) 88 70	61, 134, 214, 279	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	VAL	3.0
1	D	102	ILE	3.0
1	B	197	ALA	2.7
1	B	104	GLY	2.4
1	A	369	LEU	2.3
1	A	282	TYR	2.2
1	C	108	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.