



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:11 PM GMT

PDB ID : 4BP9
Title : Oligopeptidase B from Trypanosoma brucei with covalently bound antipain - closed form
Authors : Canning, P.; Rea, D.; Morty, R.; Fulop, V.
Deposited on : 2013-05-23
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

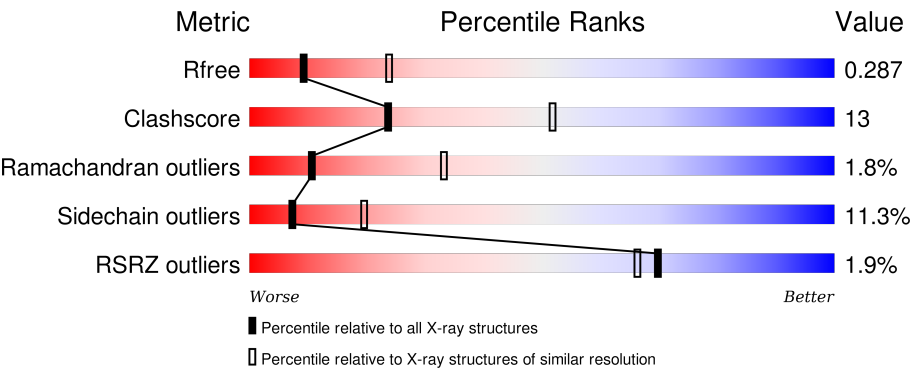
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.85 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	715	<div><div></div><div>66%28% . .</div></div>
1	B	715	<div><div>%</div><div>66%28% . .</div></div>
1	C	715	<div><div>2%</div><div>66%29% . .</div></div>
1	D	715	<div><div>%</div><div>68%28% . .</div></div>
1	E	715	<div><div>3%</div><div>66%30% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	F	715	
2	G	4	
2	H	4	
2	I	4	
2	J	4	
2	K	4	
2	L	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OAR	G	4	X	-	-	-
2	OAR	H	4	X	-	-	-
2	OAR	I	4	X	-	-	-
2	OAR	J	4	X	-	-	-
2	OAR	K	4	X	-	-	-
2	OAR	L	4	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34406 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 OLIGOPEPTIDASSE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	B	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	C	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	D	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	E	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			
1	F	710	Total	C	N	O	S	0	0	0
			5634	3568	976	1059	31			

- Molecule 2 is a protein called ANTIPAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	H	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	I	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	J	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	K	4	Total	C	N	O	0	0	0
			43	27	10	6			
2	L	4	Total	C	N	O	0	0	0
			43	27	10	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	4	OAR	RGL	CONFLICT	NOR NOR00664

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Chain	Residue	Modelled	Actual	Comment	Reference
H	4	OAR	RGL	CONFLICT	NOR NOR00664
I	4	OAR	RGL	CONFLICT	NOR NOR00664
J	4	OAR	RGL	CONFLICT	NOR NOR00664
K	4	OAR	RGL	CONFLICT	NOR NOR00664
L	4	OAR	RGL	CONFLICT	NOR NOR00664

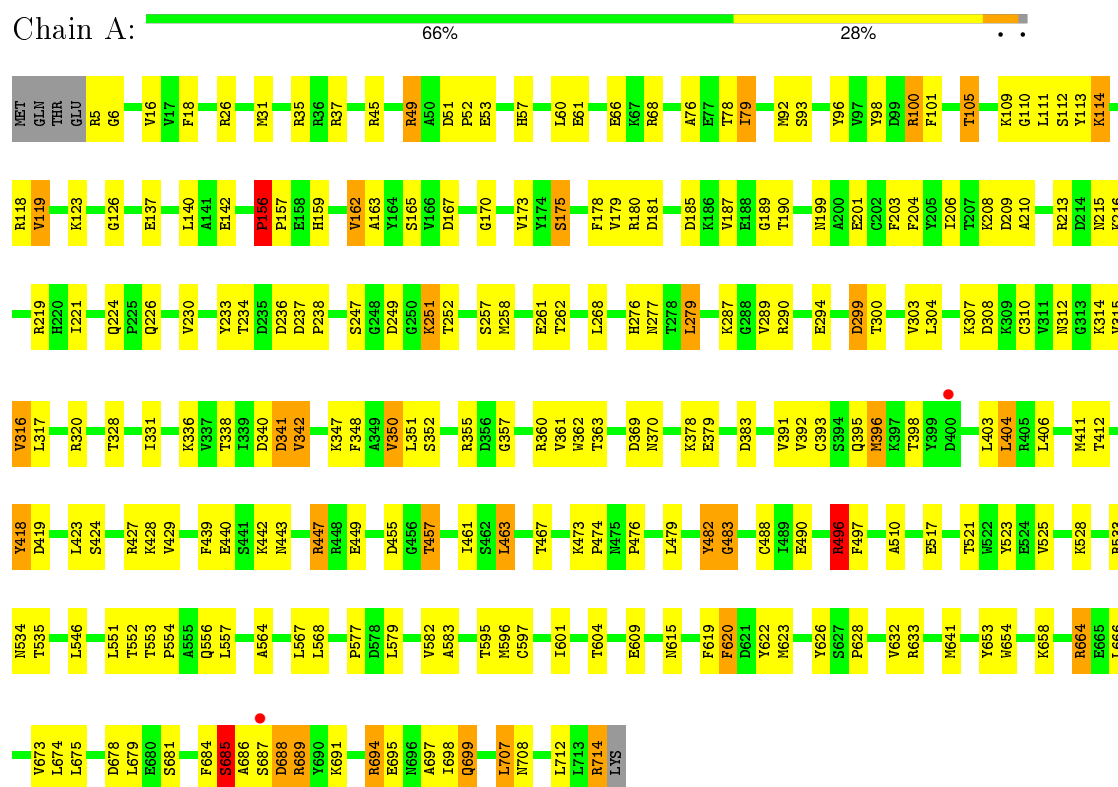
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	B	75	Total O 75 75	0	0
3	C	36	Total O 36 36	0	0
3	D	39	Total O 39 39	0	0
3	E	37	Total O 37 37	0	0
3	F	48	Total O 48 48	0	0

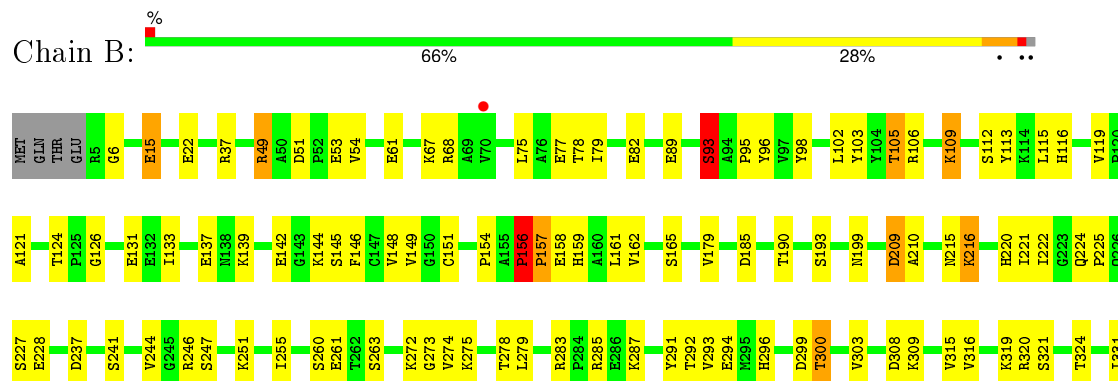
3 Residue-property plots

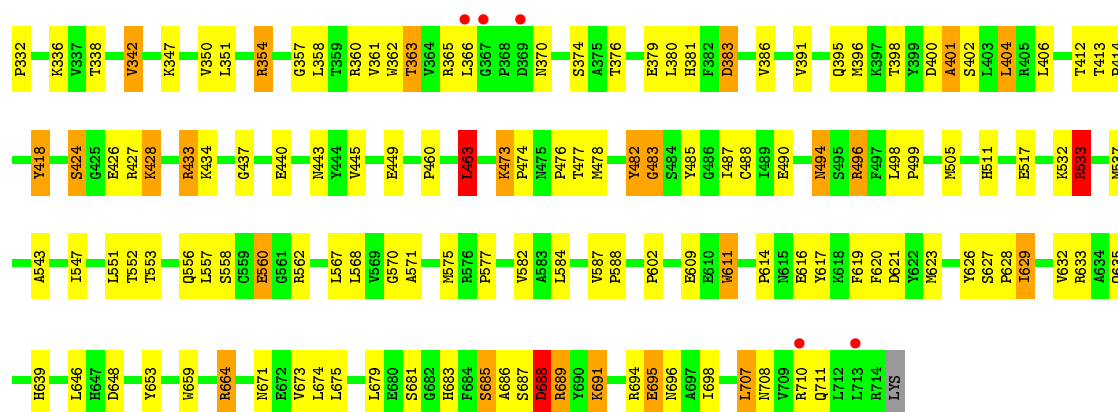
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: OLIGOPEPTIDASSE B

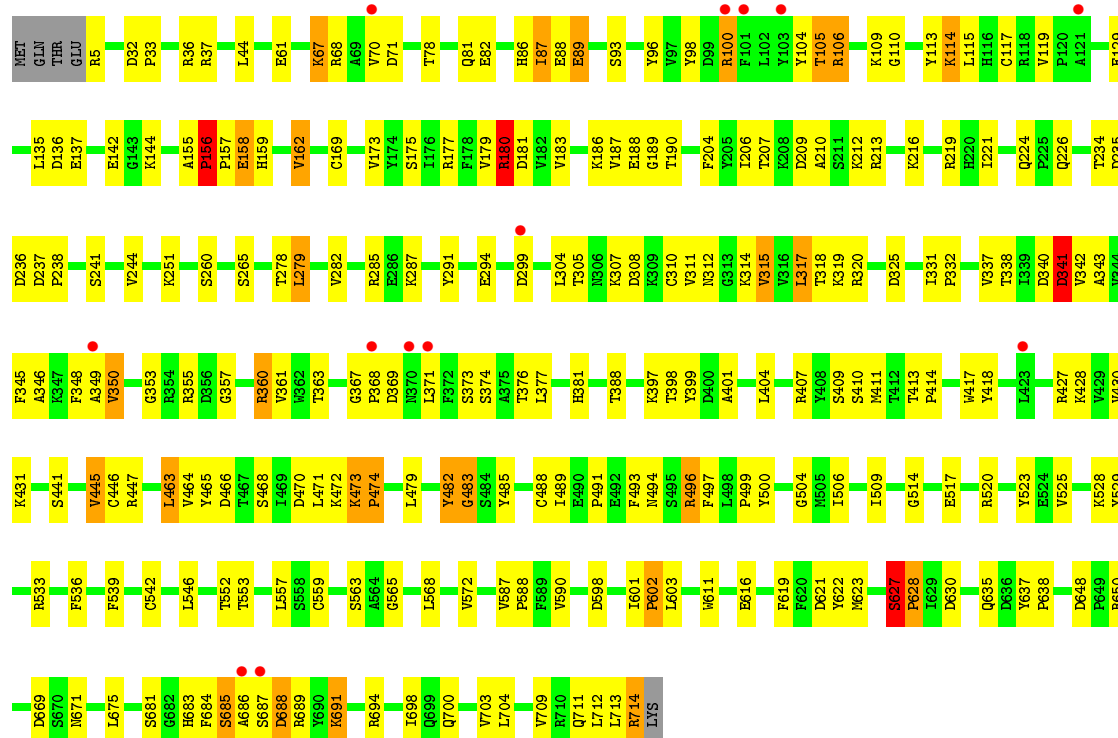


• Molecule 1: OLIGOPEPTIDASSE B

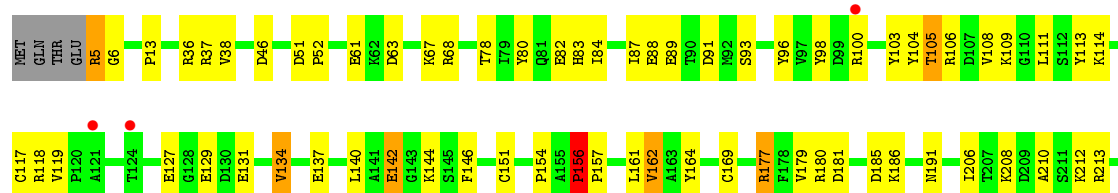


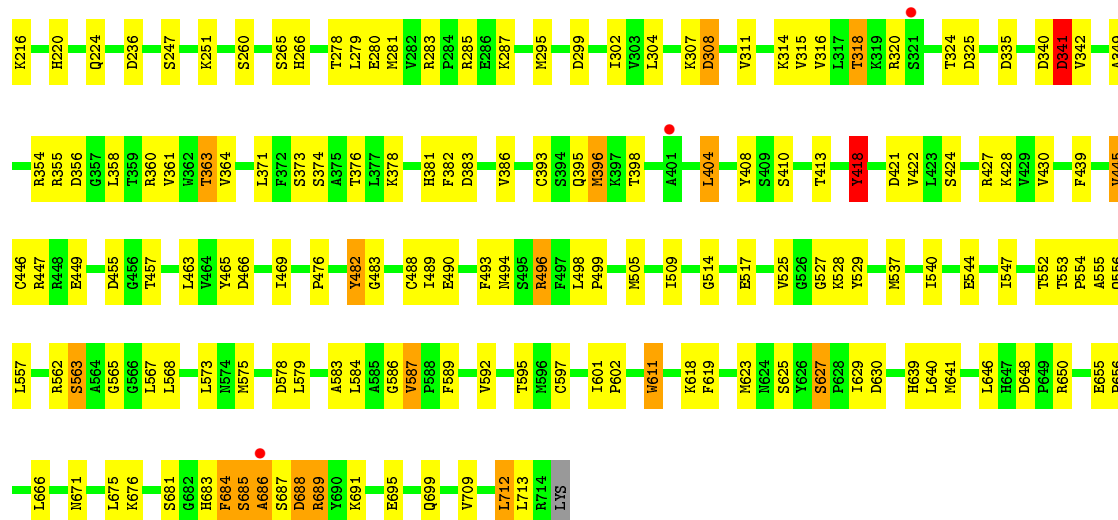


● Molecule 1: OLIGOPEPTIDASSE B

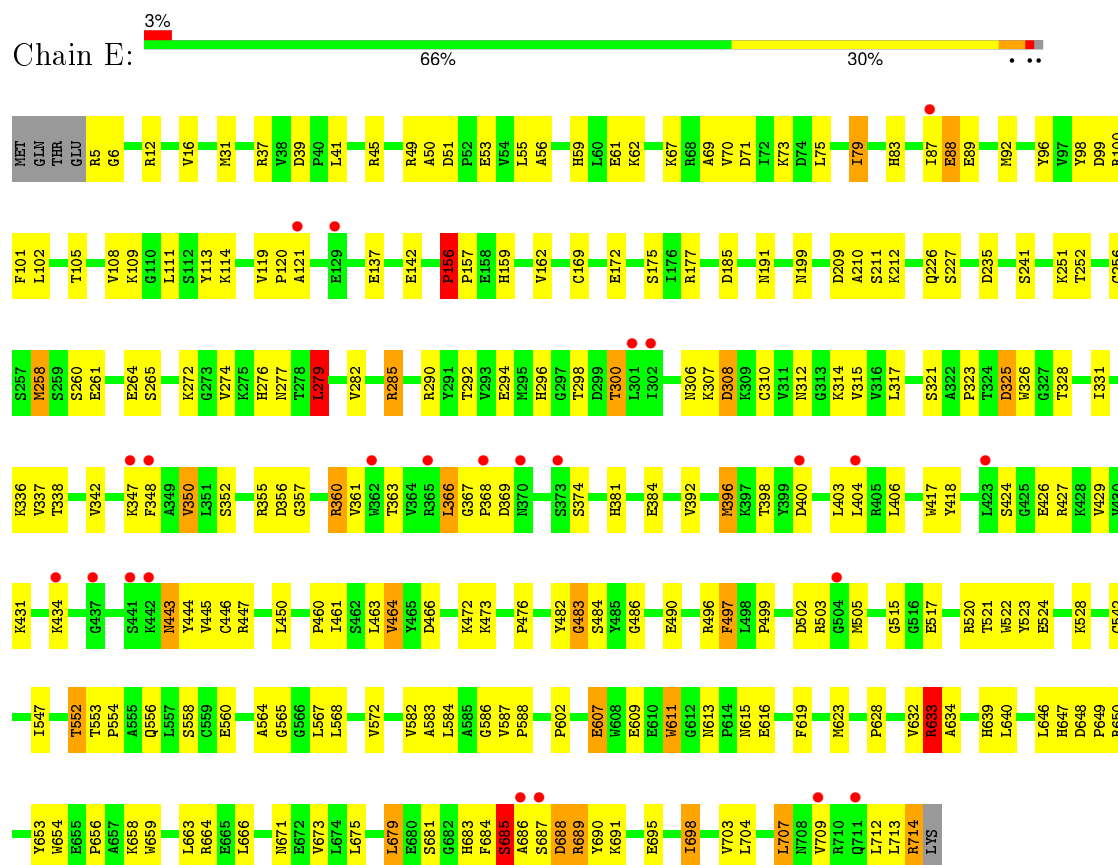


● Molecule 1: OLIGOPEPTIDASSE B

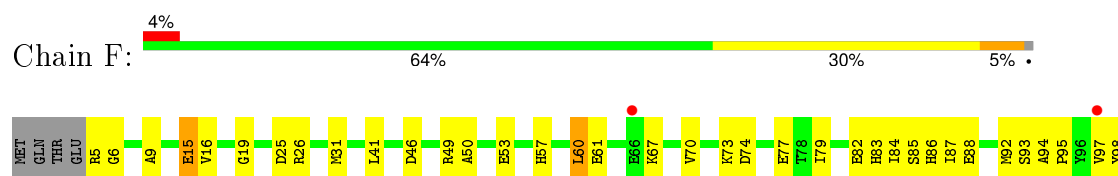


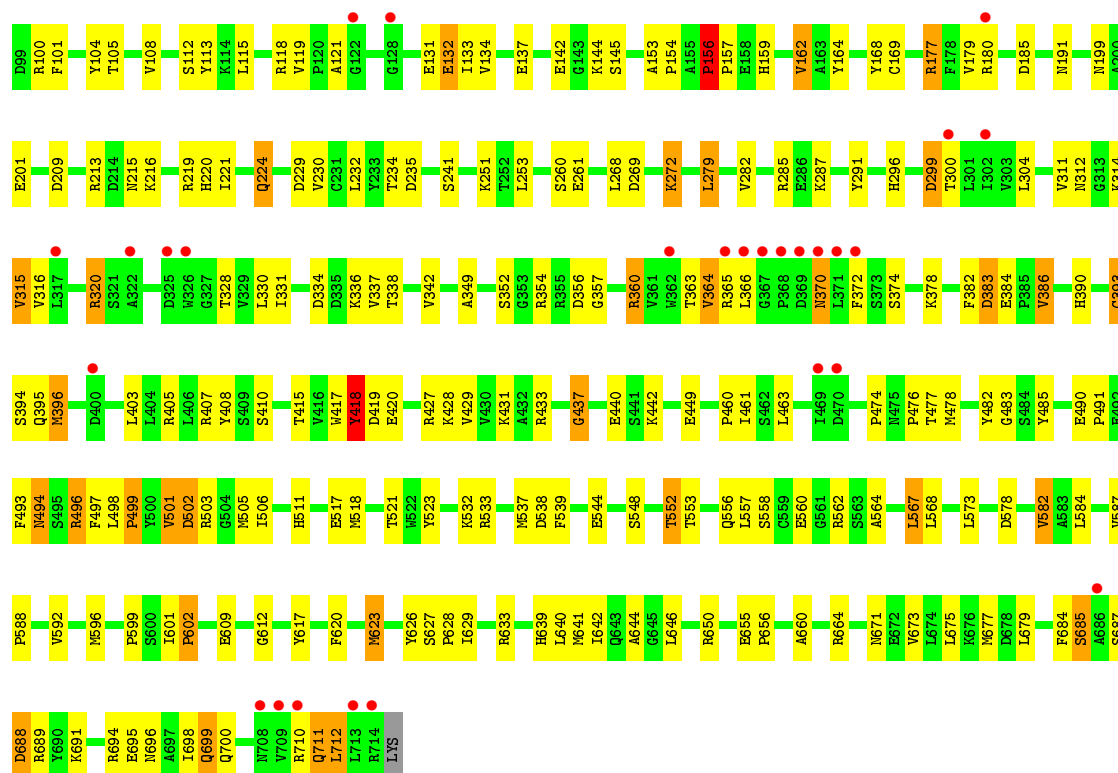


• Molecule 1: OLIGOPEPTIDASSE B



• Molecule 1: OLIGOPEPTIDASSE B





● Molecule 2: ANTIPAIN



● Molecule 2: ANTIPAIN



● Molecule 2: ANTIPAIN



● Molecule 2: ANTIPAIN



● Molecule 2: ANTIPAIN





● Molecule 2: ANTIPAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.80 Å 148.80 Å 268.00 Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	58.59 – 2.85 58.59 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (58.59-2.85) 96.7 (58.59-2.85)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.281 0.222 , 0.287	Depositor DCC
R_{free} test set	5162 reflections (4.23%)	DCC
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 127053 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34406	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 45.78 % 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 1.2588e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FC0, OAR

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	0.76	1/5772 (0.0%)	0.88	8/7832 (0.1%)
1	B	0.75	2/5772 (0.0%)	0.88	10/7832 (0.1%)
1	C	0.65	0/5772	0.79	2/7832 (0.0%)
1	D	0.69	0/5772	0.81	1/7832 (0.0%)
1	E	0.66	0/5772	0.80	3/7832 (0.0%)
1	F	0.69	0/5772	0.83	8/7832 (0.1%)
2	G	1.29	0/17	1.36	0/21
2	H	1.53	0/17	1.88	1/21 (4.8%)
2	I	1.35	0/17	1.72	0/21
2	J	1.33	0/17	1.28	0/21
2	K	1.21	0/17	1.50	0/21
2	L	1.49	0/17	1.73	0/21
All	All	0.70	3/34734 (0.0%)	0.83	33/47118 (0.1%)

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	2
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	2
1	F	0	2
2	G	1	2
2	H	1	1
2	I	1	1
2	J	1	1
2	K	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	1	2
All	All	6	26

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ASP	CB-CG	5.88	1.64	1.51
1	A	678	ASP	CB-CG	5.53	1.63	1.51
1	B	560	GLU	CG-CD	5.25	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	B	49	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	463	LEU	CA-CB-CG	7.20	131.85	115.30
1	B	49	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	E	279	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	49	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	483	GLY	N-CA-C	-6.57	96.67	113.10
1	A	350	VAL	CB-CA-C	-6.37	99.30	111.40
1	A	496	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	664	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	482	TYR	CA-C-N	6.05	128.31	116.20
1	B	483	GLY	N-CA-C	-6.04	97.99	113.10
1	F	533	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	E	483	GLY	N-CA-C	-5.99	98.12	113.10
1	F	360	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	482	TYR	C-N-CA	5.95	134.80	122.30
1	F	623	MET	CG-SD-CE	-5.89	90.77	100.20
1	B	664	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	418	TYR	CA-CB-CG	5.65	124.14	113.40
1	F	418	TYR	CA-CB-CG	5.64	124.12	113.40
1	B	567	LEU	CA-CB-CG	5.59	128.16	115.30
1	C	279	LEU	CA-CB-CG	5.54	128.04	115.30
1	E	633	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	C	483	GLY	N-CA-C	-5.24	100.00	113.10
1	F	360	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	26	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	F	567	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	354	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	F	418	TYR	N-CA-C	5.12	124.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	237	ASP	CB-CG-OD1	5.06	122.86	118.30
1	F	538	ASP	CB-CG-OD1	5.04	122.84	118.30
2	H	2	ARG	CA-CB-CG	-5.03	102.34	113.40

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	4	OAR	CA
2	H	4	OAR	CA
2	I	4	OAR	CA
2	J	4	OAR	CA
2	K	4	OAR	CA
2	L	4	OAR	CA

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	PRO	Peptide
1	A	685	SER	Peptide
1	B	156	PRO	Peptide
1	B	482	TYR	Peptide
1	B	685	SER	Peptide
1	B	688	ASP	Peptide
1	C	110	GLY	Peptide
1	C	156	PRO	Peptide
1	C	482	TYR	Peptide
1	C	685	SER	Peptide
1	D	156	PRO	Peptide
1	D	482	TYR	Peptide
1	D	684	PHE	Peptide
1	D	685	SER	Peptide
1	E	156	PRO	Peptide
1	E	685	SER	Peptide
1	F	156	PRO	Peptide
1	F	685	SER	Peptide
2	G	2	ARG	Sidechain,Peptide
2	H	2	ARG	Sidechain
2	I	2	ARG	Sidechain
2	J	2	ARG	Sidechain
2	K	2	ARG	Sidechain
2	L	2	ARG	Sidechain,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	5634	0	5522	156	0
1	B	5634	0	5522	139	0
1	C	5634	0	5522	148	0
1	D	5634	0	5522	129	0
1	E	5634	0	5522	147	0
1	F	5634	0	5522	166	0
2	G	43	0	41	1	0
2	H	43	0	40	1	0
2	I	43	0	41	1	0
2	J	43	0	42	4	0
2	K	43	0	42	2	0
2	L	43	0	41	1	0
3	A	109	0	0	12	0
3	B	75	0	0	15	0
3	C	36	0	0	7	0
3	D	39	0	0	6	0
3	E	37	0	0	4	0
3	F	48	0	0	3	0
All	All	34406	0	33379	889	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (889) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:GLU:HG2	1:C:675:LEU:HD23	1.13	1.12
1:E:61:GLU:HG2	1:E:675:LEU:HD23	1.34	1.05
1:A:496:ARG:HH11	1:A:496:ARG:HG2	1.19	1.05
1:D:619:PHE:HB3	1:D:623:MET:HE2	1.38	1.03
1:D:681:SER:HB2	1:D:685:SER:CB	1.87	1.02
1:F:87:ILE:HG13	1:F:88:GLU:H	1.24	1.01
1:A:681:SER:HB2	1:A:685:SER:HB2	1.44	0.98
1:D:681:SER:HB2	1:D:685:SER:HB2	1.43	0.97
1:F:494:ASN:HD21	1:F:496:ARG:HD3	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.29	0.96
1:E:315:VAL:HG12	1:E:331:ILE:HB	1.47	0.96
1:A:418:TYR:HB2	1:A:428:LYS:O	1.66	0.95
1:B:552:THR:HG22	1:B:553:THR:N	1.84	0.92
1:D:340:ASP:O	1:D:341:ASP:HB3	1.68	0.91
1:A:61:GLU:HG2	1:A:675:LEU:HD23	1.53	0.91
1:C:494:ASN:ND2	1:C:496:ARG:HB2	1.86	0.91
1:D:619:PHE:HB3	1:D:623:MET:CE	2.02	0.89
1:F:87:ILE:HG13	1:F:88:GLU:N	1.88	0.89
1:B:61:GLU:HG2	1:B:675:LEU:HD23	1.53	0.89
1:A:688:ASP:OD1	1:A:688:ASP:N	2.06	0.89
1:E:366:LEU:H	1:E:366:LEU:HD12	1.39	0.87
1:B:93:SER:O	1:B:95:PRO:HD3	1.74	0.87
1:E:632:VAL:HG12	1:E:666:LEU:HD12	1.55	0.85
1:F:418:TYR:HB2	1:F:428:LYS:O	1.76	0.85
1:F:482:TYR:HB3	1:F:483:GLY:HA2	1.59	0.85
1:C:340:ASP:O	1:C:341:ASP:HB3	1.75	0.85
1:B:93:SER:HB3	1:B:105:THR:HG22	1.58	0.84
1:E:5:ARG:HG2	1:E:6:GLY:H	1.44	0.83
1:D:154:PRO:O	1:D:156:PRO:HD3	1.78	0.83
1:E:619:PHE:HB3	1:E:623:MET:CE	2.10	0.82
1:A:496:ARG:HG2	1:A:496:ARG:NH1	1.93	0.82
1:D:488:CYS:HB3	1:D:517:GLU:HG3	1.62	0.82
1:A:619:PHE:HB3	1:A:623:MET:CE	2.11	0.81
1:A:496:ARG:CG	1:A:496:ARG:HH11	1.92	0.81
1:A:315:VAL:HG12	1:A:331:ILE:HB	1.62	0.81
1:D:496:ARG:HG2	1:D:496:ARG:HH11	1.44	0.81
1:B:552:THR:CG2	1:B:553:THR:N	2.44	0.80
1:E:619:PHE:HB3	1:E:623:MET:HE2	1.64	0.80
1:C:367:GLY:O	1:C:369:ASP:N	2.13	0.80
1:B:381:HIS:O	1:B:427:ARG:NH2	2.15	0.79
1:B:688:ASP:N	1:B:688:ASP:OD1	2.15	0.79
1:F:104:TYR:OH	1:F:131:GLU:HG3	1.82	0.79
1:B:246:ARG:HD2	3:B:2027:HOH:O	1.81	0.79
1:E:681:SER:HB2	1:E:685:SER:CB	2.10	0.79
1:A:418:TYR:HB3	1:A:429:VAL:HA	1.64	0.79
1:E:482:TYR:HB3	1:E:483:GLY:HA2	1.64	0.79
1:F:688:ASP:N	1:F:688:ASP:OD1	2.14	0.78
1:C:315:VAL:HG13	1:C:331:ILE:HB	1.64	0.78
1:D:363:THR:HG22	1:D:378:LYS:HB3	1.64	0.78
1:D:618:LYS:HE2	3:D:2038:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ASN:ND2	1:C:338:THR:OG1	2.15	0.77
1:E:357:GLY:HA2	1:E:517:GLU:O	1.85	0.77
1:E:490:GLU:OE1	1:E:490:GLU:HA	1.83	0.77
1:C:175:SER:HB3	1:C:188:GLU:OE1	1.84	0.77
1:A:112:SER:HB3	1:A:689:ARG:HG2	1.66	0.77
1:A:619:PHE:HB3	1:A:623:MET:HE3	1.67	0.77
1:A:689:ARG:HB3	1:A:691:LYS:H	1.47	0.76
1:E:400:ASP:HB2	3:E:2023:HOH:O	1.84	0.76
1:C:681:SER:HB2	1:C:685:SER:CB	2.16	0.76
1:B:209:ASP:OD1	1:B:210:ALA:N	2.15	0.76
1:A:681:SER:HB2	1:A:685:SER:CB	2.15	0.75
1:F:83:HIS:CE1	1:F:499:PRO:HG2	2.21	0.75
1:A:439:PHE:HA	3:A:2065:HOH:O	1.84	0.75
1:C:210:ALA:HA	3:C:2012:HOH:O	1.85	0.75
1:B:293:VAL:HG22	1:B:303:VAL:HG22	1.67	0.75
1:F:279:LEU:H	1:F:279:LEU:HD22	1.52	0.75
1:F:711:GLN:HE21	1:F:711:GLN:HA	1.49	0.75
1:F:677:MET:O	1:F:677:MET:HG3	1.86	0.75
1:F:664:ARG:NH2	1:F:673:VAL:O	2.14	0.74
1:C:619:PHE:HB3	1:C:623:MET:HE2	1.68	0.74
1:D:5:ARG:HG3	1:D:6:GLY:H	1.52	0.74
1:D:648:ASP:OD1	1:D:683:HIS:HB2	1.87	0.74
1:F:213:ARG:NH2	1:F:235:ASP:O	2.20	0.74
1:C:598:ASP:HB3	1:C:601:ILE:HD12	1.69	0.74
1:F:168:TYR:HE2	1:F:177:ARG:NH2	1.84	0.73
1:E:681:SER:HB2	1:E:685:SER:HB2	1.70	0.73
1:C:648:ASP:OD1	1:C:683:HIS:HB2	1.89	0.73
1:F:494:ASN:ND2	1:F:496:ARG:H	1.85	0.73
1:F:582:VAL:HG23	1:F:639:HIS:HB2	1.69	0.73
2:J:1:FC0:HE2	2:J:2:ARG:NH2	2.03	0.73
1:F:334:ASP:HB3	1:F:337:VAL:HB	1.70	0.73
1:A:310:CYS:SG	1:A:314:LYS:HD3	2.29	0.73
1:C:93:SER:HB3	1:C:105:THR:HG22	1.69	0.73
1:E:444:TYR:OH	1:E:502:ASP:OD1	2.06	0.72
1:C:482:TYR:HB3	1:C:483:GLY:HA2	1.69	0.72
1:C:621:ASP:OD2	1:D:575:MET:HG2	1.90	0.72
1:D:689:ARG:NH1	1:D:691:LYS:HG2	2.06	0.71
1:A:45:ARG:HD2	1:A:654:TRP:CZ2	2.24	0.71
1:F:279:LEU:N	1:F:279:LEU:HD22	2.06	0.71
1:E:588:PRO:HD2	1:E:656:PRO:HG3	1.73	0.71
1:C:106:ARG:HB3	1:C:106:ARG:HH11	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:SER:HB2	1:C:685:SER:HB2	1.71	0.70
1:B:413:THR:HG22	1:B:414:PRO:O	1.91	0.70
1:D:681:SER:CB	1:D:685:SER:HB2	2.19	0.70
1:B:552:THR:CG2	1:B:553:THR:H	2.04	0.70
1:B:426:GLU:HA	3:B:2043:HOH:O	1.91	0.70
1:B:22:GLU:HG3	3:B:2002:HOH:O	1.90	0.70
1:C:209:ASP:OD1	1:C:210:ALA:N	2.23	0.70
1:B:315:VAL:CG1	1:B:331:ILE:HB	2.22	0.70
1:C:588:PRO:O	1:C:590:VAL:HG22	1.92	0.70
1:F:655:GLU:HB2	1:F:656:PRO:HD3	1.72	0.69
1:A:113:TYR:HB3	1:A:137:GLU:HB2	1.75	0.69
1:E:381:HIS:O	1:E:427:ARG:NH2	2.26	0.68
1:B:418:TYR:HB3	1:B:428:LYS:O	1.94	0.68
1:F:494:ASN:HD22	1:F:496:ARG:H	1.38	0.68
1:A:632:VAL:HG12	1:A:666:LEU:HD12	1.75	0.68
1:B:358:LEU:HB2	1:B:360:ARG:NH1	2.08	0.68
1:A:93:SER:HB3	1:A:105:THR:HG22	1.75	0.68
1:D:482:TYR:HB3	1:D:483:GLY:HA2	1.75	0.68
1:A:447:ARG:NH1	1:A:449:GLU:OE2	2.27	0.68
1:A:221:ILE:HB	1:A:224:GLN:HE21	1.58	0.68
1:B:112:SER:HB3	1:B:689:ARG:HE	1.58	0.67
1:C:346:ALA:HB2	1:C:399:TYR:CE2	2.29	0.67
1:B:474:PRO:HB2	1:B:556:GLN:HE22	1.59	0.67
1:B:331:ILE:HD13	1:B:351:LEU:HD21	1.75	0.67
2:G:1:FC0:HA	2:G:2:ARG:HB2	1.76	0.67
1:D:553:THR:OG1	1:D:556:GLN:HG3	1.95	0.67
1:E:12:ARG:NH2	1:E:53:GLU:OE1	2.27	0.67
1:F:15:GLU:HG3	1:F:15:GLU:O	1.94	0.67
1:A:664:ARG:NH2	1:A:673:VAL:O	2.28	0.67
1:B:209:ASP:CG	1:B:210:ALA:H	1.97	0.66
1:D:650:ARG:NH2	1:D:684:PHE:HE2	1.93	0.66
1:C:113:TYR:HB3	1:C:137:GLU:HB2	1.77	0.66
1:A:483:GLY:HA2	3:A:2074:HOH:O	1.94	0.66
1:F:644:ALA:HB3	1:F:677:MET:HE2	1.75	0.66
1:B:400:ASP:O	1:B:401:ALA:O	2.13	0.66
1:C:319:LYS:HB3	3:C:2016:HOH:O	1.96	0.66
1:C:221:ILE:HB	1:C:224:GLN:NE2	2.09	0.66
1:F:269:ASP:OD2	1:F:272:LYS:HE2	1.96	0.66
1:F:420:GLU:OE1	1:F:427:ARG:NE	2.28	0.66
1:A:304:LEU:CD2	1:A:341:ASP:HA	2.25	0.66
1:B:619:PHE:HB3	1:B:623:MET:HE2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:CD2	1:A:551:LEU:HD12	2.25	0.65
1:E:607:GLU:HG2	1:E:611:TRP:NE1	2.10	0.65
1:B:614:PRO:HD3	1:B:623:MET:HE1	1.78	0.65
1:D:496:ARG:HG2	1:D:496:ARG:NH1	2.10	0.65
1:E:476:PRO:HB2	1:E:505:MET:HG2	1.78	0.65
1:F:477:THR:HB	1:F:557:LEU:HD12	1.78	0.65
1:A:53:GLU:HG3	3:A:2016:HOH:O	1.95	0.65
1:F:70:VAL:O	1:F:73:LYS:HG2	1.97	0.65
1:F:696:ASN:HA	1:F:699:GLN:HB2	1.78	0.65
1:F:474:PRO:HB2	1:F:556:GLN:HE22	1.62	0.65
1:E:315:VAL:CG1	1:E:331:ILE:HB	2.23	0.65
1:C:650:ARG:NH2	1:C:684:PHE:HE2	1.93	0.65
1:C:688:ASP:OD1	1:C:688:ASP:N	2.30	0.65
1:B:112:SER:OG	1:B:689:ARG:NH2	2.30	0.64
1:A:564:ALA:O	1:A:567:LEU:HB3	1.96	0.64
2:J:1:FC0:CE2	2:J:2:ARG:HH21	2.10	0.64
1:D:93:SER:HB3	1:D:105:THR:HG22	1.79	0.64
1:C:213:ARG:HH22	1:C:236:ASP:HA	1.62	0.64
1:C:294:GLU:HG3	1:C:342:VAL:HG23	1.80	0.64
1:A:315:VAL:CG1	1:A:331:ILE:HB	2.27	0.63
1:F:478:MET:SD	1:F:560:GLU:HB2	2.38	0.63
1:E:307:LYS:HE2	1:E:308:ASP:OD1	1.99	0.63
1:C:61:GLU:HG2	1:C:675:LEU:CD2	2.08	0.63
1:F:209:ASP:OD2	1:F:215:ASN:ND2	2.31	0.63
1:A:100:ARG:HG2	1:A:100:ARG:NH1	2.06	0.63
2:J:1:FC0:HE2	2:J:2:ARG:HH21	1.62	0.63
1:F:712:LEU:H	1:F:712:LEU:HD12	1.63	0.63
1:A:61:GLU:CG	1:A:675:LEU:HD23	2.27	0.62
1:F:209:ASP:HB2	1:F:215:ASN:CG	2.20	0.62
1:D:78:THR:O	1:D:82:GLU:HG3	2.00	0.62
1:F:279:LEU:CD2	1:F:279:LEU:H	2.11	0.62
1:D:104:TYR:CE1	1:D:117:CYS:HB2	2.34	0.62
1:A:262:THR:HA	1:A:289:VAL:O	1.98	0.62
1:F:330:LEU:HG	1:F:331:ILE:HG13	1.81	0.62
1:D:627:SER:HB3	1:D:630:ASP:HB2	1.81	0.62
1:A:5:ARG:HG2	1:A:6:GLY:H	1.64	0.61
1:C:180:ARG:HB2	1:C:180:ARG:NH1	2.13	0.61
1:F:640:LEU:HD23	1:F:673:VAL:HG13	1.83	0.61
1:D:61:GLU:HG2	1:D:675:LEU:HD23	1.81	0.61
1:B:494:ASN:HD22	1:B:496:ARG:H	1.48	0.61
1:B:315:VAL:HG13	1:B:331:ILE:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:TYR:HE2	1:F:177:ARG:HH21	1.48	0.61
1:B:577:PRO:HG3	1:B:635:GLN:NE2	2.16	0.61
1:E:210:ALA:O	1:E:211:SER:HB2	2.00	0.61
1:E:639:HIS:CE1	1:E:671:ASN:HB3	2.36	0.61
1:C:488:CYS:HB3	1:C:517:GLU:HG3	1.83	0.61
1:A:92:MET:HE1	1:A:126:GLY:HA2	1.81	0.61
1:F:168:TYR:CE2	1:F:177:ARG:NH2	2.67	0.60
1:B:543:ALA:O	1:B:547:ILE:HD12	2.00	0.60
1:C:619:PHE:HB3	1:C:623:MET:CE	2.31	0.60
1:E:5:ARG:CG	1:E:6:GLY:H	2.15	0.60
1:D:421:ASP:HB3	1:D:424:SER:OG	2.01	0.60
1:C:536:PHE:CE1	1:C:568:LEU:HA	2.37	0.60
1:A:219:ARG:NH2	1:A:276:HIS:O	2.35	0.60
1:C:712:LEU:H	1:C:712:LEU:HD12	1.67	0.60
1:D:568:LEU:HD23	1:D:568:LEU:C	2.22	0.60
1:F:395:GLN:OE1	1:F:405:ARG:HG2	2.01	0.60
1:B:681:SER:HB2	1:B:685:SER:HB2	1.83	0.60
1:E:79:ILE:HD11	1:E:499:PRO:HB3	1.84	0.60
1:E:61:GLU:OE2	1:E:664:ARG:NH2	2.35	0.59
1:F:61:GLU:HG2	1:F:675:LEU:HD23	1.83	0.59
1:E:689:ARG:HH11	1:E:691:LYS:HG2	1.67	0.59
1:A:216:LYS:HG3	1:A:234:THR:HG23	1.83	0.59
1:D:681:SER:HB2	1:D:685:SER:HB3	1.83	0.59
1:C:713:LEU:O	1:C:714:ARG:HD2	2.02	0.59
1:E:355:ARG:HG2	1:E:355:ARG:HH11	1.66	0.59
1:F:87:ILE:CG1	1:F:88:GLU:H	2.07	0.59
1:E:547:ILE:CD1	1:E:554:PRO:HD3	2.33	0.59
1:C:470:ASP:C	1:C:472:LYS:H	2.06	0.59
1:C:466:ASP:OD1	1:C:468:SER:OG	2.20	0.59
1:A:623:MET:HA	1:A:626:TYR:CE2	2.37	0.59
1:F:261:GLU:HG2	1:F:609:GLU:OE1	2.02	0.59
1:F:494:ASN:ND2	1:F:496:ARG:HD3	2.10	0.59
1:A:712:LEU:HD12	3:A:2109:HOH:O	2.02	0.59
1:E:325:ASP:O	1:E:326:TRP:HD1	1.86	0.59
1:F:476:PRO:HB2	1:F:505:MET:HG2	1.85	0.58
1:B:685:SER:HB3	1:B:687:SER:HA	1.85	0.58
1:F:584:LEU:HD13	1:F:699:GLN:HG2	1.85	0.58
1:A:404:LEU:HD21	1:A:406:LEU:HD21	1.85	0.58
1:C:552:THR:HG21	1:C:557:LEU:HB2	1.86	0.58
1:B:478:MET:SD	1:B:560:GLU:HB2	2.43	0.58
1:F:499:PRO:HB2	1:F:700:GLN:HE22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:689:ARG:HD3	1:E:691:LYS:H	1.69	0.58
1:D:108:VAL:HB	1:D:111:LEU:HD12	1.86	0.58
1:B:357:GLY:HA2	1:B:517:GLU:O	2.04	0.58
1:D:650:ARG:NH2	1:D:684:PHE:CE2	2.71	0.58
1:F:5:ARG:HG2	1:F:6:GLY:H	1.69	0.58
1:F:687:SER:HB2	1:F:689:ARG:HG3	1.84	0.58
1:A:691:LYS:HE2	1:A:694:ARG:HD3	1.86	0.58
1:C:71:ASP:OD1	1:C:71:ASP:N	2.34	0.58
1:E:619:PHE:HB3	1:E:623:MET:HE3	1.86	0.58
1:F:417:TRP:CE3	1:F:431:LYS:HD3	2.39	0.58
1:F:365:ARG:HH21	1:F:378:LYS:HB2	1.69	0.57
1:D:611:TRP:HB2	3:D:2037:HOH:O	2.02	0.57
1:F:655:GLU:HB2	1:F:656:PRO:CD	2.34	0.57
1:B:691:LYS:HG3	3:B:2074:HOH:O	2.04	0.57
1:B:96:TYR:CD2	1:B:395:GLN:HG2	2.39	0.57
1:B:639:HIS:ND1	1:B:671:ASN:HB3	2.19	0.57
1:B:115:LEU:HD23	1:B:133:ILE:HG21	1.87	0.57
1:C:552:THR:HG22	1:C:553:THR:O	2.04	0.57
1:A:357:GLY:HA2	1:A:517:GLU:O	2.04	0.57
1:A:163:ALA:HB2	1:A:178:PHE:CE2	2.40	0.57
1:E:113:TYR:HB3	1:E:137:GLU:HB3	1.87	0.57
1:D:340:ASP:HB2	3:D:2022:HOH:O	2.04	0.57
1:F:696:ASN:O	1:F:700:GLN:HG3	2.05	0.57
1:E:582:VAL:HG22	1:E:583:ALA:N	2.19	0.57
1:B:15:GLU:O	1:B:15:GLU:HG3	2.02	0.57
1:A:418:TYR:CB	1:A:428:LYS:O	2.46	0.57
1:B:553:THR:OG1	1:B:556:GLN:NE2	2.26	0.57
1:D:304:LEU:CD2	1:D:341:ASP:HA	2.35	0.57
1:B:209:ASP:HB2	1:B:215:ASN:CG	2.25	0.57
1:F:131:GLU:HG2	1:F:132:GLU:H	1.70	0.57
1:E:653:TYR:O	1:E:656:PRO:HD2	2.05	0.57
1:F:552:THR:HG22	1:F:553:THR:H	1.68	0.57
1:D:280:GLU:HB3	3:D:2018:HOH:O	2.03	0.57
1:E:639:HIS:ND1	1:E:671:ASN:HB3	2.20	0.56
1:A:213:ARG:HD3	3:A:2040:HOH:O	2.04	0.56
1:E:564:ALA:O	1:E:567:LEU:HB3	2.05	0.56
1:F:485:TYR:OH	2:L:4:OAR:HA	2.05	0.56
1:E:294:GLU:HG3	1:E:342:VAL:HG23	1.87	0.56
1:F:685:SER:HB3	1:F:687:SER:HA	1.86	0.56
1:B:614:PRO:CD	1:B:623:MET:HE1	2.34	0.56
1:C:180:ARG:HH11	1:C:180:ARG:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:GLU:HB3	1:E:109:LYS:HA	1.86	0.56
1:A:114:LYS:HG2	3:A:2023:HOH:O	2.04	0.56
1:D:447:ARG:NH1	1:D:449:GLU:OE2	2.38	0.56
1:F:162:VAL:O	1:F:179:VAL:HG23	2.06	0.56
1:E:235:ASP:OD2	1:E:285:ARG:NH2	2.39	0.56
1:D:455:ASP:CG	1:D:457:THR:HG1	2.07	0.56
1:B:358:LEU:HB2	1:B:360:ARG:HH11	1.70	0.56
1:D:87:ILE:O	1:D:88:GLU:HG2	2.05	0.56
1:A:173:VAL:CG1	1:A:189:GLY:HA2	2.35	0.56
1:B:477:THR:HB	1:B:557:LEU:CD1	2.35	0.56
1:D:639:HIS:ND1	1:D:671:ASN:HB3	2.20	0.56
1:F:221:ILE:O	1:F:224:GLN:HG3	2.04	0.56
1:F:79:ILE:HD11	1:F:499:PRO:HB3	1.88	0.56
1:B:292:THR:HG22	3:B:2032:HOH:O	2.05	0.56
1:C:204:PHE:CE1	1:C:219:ARG:HG3	2.40	0.56
1:F:539:PHE:CG	1:F:568:LEU:HD21	2.40	0.56
1:A:316:VAL:HG22	1:A:328:THR:O	2.06	0.56
1:F:711:GLN:NE2	1:F:711:GLN:HA	2.20	0.56
1:E:560:GLU:HG3	1:E:584:LEU:HB2	1.87	0.56
1:D:340:ASP:O	1:D:341:ASP:CB	2.47	0.55
1:A:112:SER:CB	1:A:689:ARG:HG2	2.35	0.55
1:C:601:ILE:O	1:C:603:LEU:N	2.39	0.55
1:E:461:ILE:HD11	1:E:542:CYS:HB3	1.88	0.55
1:B:629:ILE:O	1:B:632:VAL:HG23	2.05	0.55
1:D:88:GLU:HG3	1:D:91:ASP:HB2	1.88	0.55
1:B:482:TYR:HB3	1:B:483:GLY:HA2	1.89	0.55
1:F:25:ASP:O	1:F:599:PRO:HG3	2.05	0.55
1:B:332:PRO:HD2	3:B:2036:HOH:O	2.07	0.55
1:C:87:ILE:O	1:C:88:GLU:HG2	2.06	0.55
1:E:688:ASP:N	1:E:688:ASP:OD1	2.40	0.55
1:A:496:ARG:CG	1:A:496:ARG:NH1	2.61	0.55
1:C:81:GLN:HA	1:C:81:GLN:OE1	2.06	0.55
1:C:61:GLU:CG	1:C:675:LEU:HD23	2.09	0.55
1:B:681:SER:HB2	1:B:685:SER:CB	2.37	0.55
2:K:1:FC0:HA	2:K:2:ARG:HB2	1.88	0.55
1:A:461:ILE:HG22	1:A:463:LEU:HD23	1.89	0.55
1:E:646:LEU:HD22	1:E:679:LEU:HB3	1.87	0.54
1:C:685:SER:C	1:C:687:SER:N	2.60	0.54
1:D:247:SER:HB2	1:D:295:MET:HB2	1.89	0.54
1:F:366:LEU:HD13	1:F:370:ASN:HA	1.89	0.54
1:F:85:SER:O	1:F:437:GLY:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:ILE:CG1	1:F:499:PRO:HB3	2.38	0.54
1:A:304:LEU:HD22	1:A:341:ASP:HA	1.89	0.54
1:C:371:LEU:HD23	3:C:2017:HOH:O	2.06	0.54
1:C:312:ASN:HD22	1:C:338:THR:HG1	1.51	0.54
1:A:221:ILE:HB	1:A:224:GLN:NE2	2.22	0.54
1:B:664:ARG:NH2	1:B:673:VAL:O	2.36	0.54
1:F:230:VAL:HG23	3:F:2020:HOH:O	2.07	0.54
1:B:77:GLU:OE1	1:B:694:ARG:NH2	2.41	0.54
1:E:523:TYR:OH	1:E:528:LYS:NZ	2.41	0.54
1:E:256:CYS:SG	1:E:258:MET:SD	2.99	0.54
1:D:482:TYR:O	1:D:565:GLY:HA2	2.08	0.54
1:C:650:ARG:CZ	1:C:684:PHE:HE2	2.20	0.54
1:C:144:LYS:HE2	3:C:2007:HOH:O	2.08	0.54
1:F:82:GLU:O	1:F:86:HIS:ND1	2.41	0.54
1:A:110:GLY:C	1:A:111:LEU:HD23	2.29	0.54
1:B:619:PHE:HB3	1:B:623:MET:CE	2.38	0.53
1:E:568:LEU:O	1:E:572:VAL:HG23	2.08	0.53
1:C:310:CYS:SG	1:C:314:LYS:HD3	2.48	0.53
1:A:455:ASP:OD1	1:A:457:THR:OG1	2.21	0.53
1:E:685:SER:C	1:E:687:SER:N	2.62	0.53
1:F:57:HIS:O	1:F:60:LEU:HB2	2.08	0.53
1:C:482:TYR:O	1:C:565:GLY:HA2	2.08	0.53
1:A:474:PRO:HB2	1:A:556:GLN:HE22	1.73	0.53
1:E:482:TYR:HB3	1:E:483:GLY:CA	2.36	0.53
1:C:563:SER:HA	1:C:587:VAL:O	2.09	0.53
1:A:418:TYR:CZ	1:A:427:ARG:HD3	2.44	0.53
1:F:365:ARG:NH2	1:F:378:LYS:HB2	2.23	0.53
1:A:482:TYR:HB3	1:A:483:GLY:HA2	1.91	0.53
1:E:647:HIS:O	1:E:649:PRO:HD3	2.09	0.53
1:C:82:GLU:O	1:C:86:HIS:ND1	2.42	0.53
1:C:711:GLN:HG3	1:C:712:LEU:O	2.09	0.52
1:D:113:TYR:HB3	1:D:137:GLU:HB2	1.92	0.52
1:A:362:TRP:CD1	1:A:379:GLU:HA	2.45	0.52
1:A:633:ARG:NH2	1:B:621:ASP:OD2	2.41	0.52
1:D:354:ARG:NH2	1:D:490:GLU:OE2	2.42	0.52
1:A:681:SER:CB	1:A:685:SER:HB2	2.28	0.52
1:E:482:TYR:CB	1:E:483:GLY:HA2	2.38	0.52
1:F:641:MET:HE2	1:F:699:GLN:HA	1.91	0.52
1:A:340:ASP:O	1:A:341:ASP:HB3	2.09	0.52
1:E:582:VAL:CG2	1:E:583:ALA:N	2.72	0.52
1:A:577:PRO:HG2	3:A:2103:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:CYS:HA	1:A:396:MET:HG3	1.92	0.52
1:D:466:ASP:O	1:D:469:ILE:HG12	2.09	0.52
1:A:209:ASP:OD1	1:A:210:ALA:N	2.41	0.52
1:A:383:ASP:HA	3:A:2060:HOH:O	2.10	0.52
1:A:209:ASP:HB2	1:A:215:ASN:OD1	2.10	0.52
1:C:67:LYS:O	1:C:70:VAL:HG23	2.10	0.52
1:E:296:HIS:O	1:E:300:THR:HG23	2.09	0.52
1:F:113:TYR:HB3	1:F:137:GLU:CB	2.40	0.52
1:B:383:ASP:OD1	1:B:383:ASP:N	2.33	0.52
1:B:112:SER:HB2	1:B:113:TYR:CD1	2.45	0.52
1:E:547:ILE:HD13	1:E:554:PRO:HD3	1.91	0.52
1:F:113:TYR:HB3	1:F:137:GLU:HB3	1.92	0.52
1:A:355:ARG:O	1:A:360:ARG:NH1	2.43	0.52
1:D:562:ARG:O	1:D:565:GLY:N	2.43	0.52
1:A:209:ASP:OD2	1:A:215:ASN:ND2	2.43	0.52
1:F:296:HIS:CD2	1:F:372:PHE:HE1	2.28	0.52
1:A:57:HIS:HA	1:A:60:LEU:HD12	1.90	0.52
1:A:68:ARG:HG2	1:A:674:LEU:HD21	1.91	0.52
1:A:100:ARG:CG	1:A:100:ARG:HH11	2.14	0.51
1:E:613:ASN:HB3	1:E:616:GLU:HG3	1.92	0.51
1:B:685:SER:C	1:B:687:SER:N	2.63	0.51
1:C:650:ARG:NH2	1:C:684:PHE:CE2	2.75	0.51
1:D:381:HIS:O	1:D:427:ARG:NH2	2.41	0.51
1:B:558:SER:HA	1:B:582:VAL:O	2.09	0.51
1:A:362:TRP:NE1	1:A:379:GLU:HG3	2.25	0.51
1:C:304:LEU:CD2	1:C:341:ASP:HA	2.40	0.51
1:D:688:ASP:C	1:D:689:ARG:HG3	2.29	0.51
1:A:347:LYS:O	1:A:348:PHE:HB3	2.11	0.51
1:E:306:ASN:HA	1:E:310:CYS:O	2.10	0.51
1:A:552:THR:HG21	1:A:557:LEU:HB2	1.93	0.51
1:F:131:GLU:HG2	1:F:132:GLU:N	2.25	0.51
1:E:499:PRO:O	1:E:503:ARG:HD2	2.10	0.51
1:E:558:SER:CB	1:E:582:VAL:HG13	2.40	0.51
1:F:626:TYR:O	1:F:627:SER:C	2.49	0.51
1:E:113:TYR:HB3	1:E:137:GLU:CB	2.40	0.51
1:A:312:ASN:HB3	1:A:338:THR:HA	1.93	0.51
1:D:489:ILE:HG22	1:D:509:ILE:HD13	1.92	0.51
1:E:681:SER:CB	1:E:685:SER:HB2	2.39	0.51
1:A:483:GLY:CA	3:A:2074:HOH:O	2.56	0.51
1:F:134:VAL:O	1:F:179:VAL:HG11	2.11	0.51
1:B:686:ALA:HB1	1:B:695:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:NH2	1:C:236:ASP:HA	2.24	0.51
1:F:644:ALA:HB3	1:F:677:MET:CE	2.41	0.50
1:B:342:VAL:HG23	3:B:2032:HOH:O	2.10	0.50
1:C:291:TYR:HA	1:C:304:LEU:O	2.11	0.50
1:A:331:ILE:HD13	1:A:351:LEU:HD21	1.93	0.50
1:F:482:TYR:HB3	1:F:483:GLY:CA	2.36	0.50
1:E:92:MET:O	1:E:431:LYS:NZ	2.45	0.50
1:F:440:GLU:OE1	1:F:442:LYS:HE2	2.12	0.50
1:D:80:TYR:O	1:D:84:ILE:HG12	2.10	0.50
1:E:640:LEU:HB3	1:E:673:VAL:HG22	1.93	0.50
1:A:424:SER:HB2	1:D:308:ASP:HB3	1.92	0.50
1:C:704:LEU:HD22	1:C:709:VAL:HG23	1.93	0.50
1:B:587:VAL:N	1:B:588:PRO:HD3	2.27	0.50
1:F:338:THR:HB	1:F:354:ARG:HB2	1.93	0.50
1:F:499:PRO:HB2	1:F:700:GLN:NE2	2.26	0.50
1:E:558:SER:HB3	1:E:582:VAL:HG13	1.94	0.50
1:F:460:PRO:HG3	1:F:518:MET:SD	2.52	0.50
1:E:337:VAL:HG22	1:E:355:ARG:HB2	1.93	0.50
1:C:489:ILE:HG22	1:C:509:ILE:HD13	1.93	0.50
1:E:586:GLY:O	1:E:587:VAL:C	2.49	0.50
1:F:349:ALA:HB3	1:F:364:VAL:HG12	1.92	0.50
1:C:318:THR:HB	1:C:325:ASP:O	2.11	0.50
1:B:485:TYR:OH	2:H:4:OAR:HG2	2.12	0.50
1:F:496:ARG:HB2	1:F:496:ARG:HH11	1.77	0.49
1:E:367:GLY:C	1:E:369:ASP:H	2.14	0.49
1:D:552:THR:HG21	1:D:557:LEU:HB2	1.93	0.49
1:C:173:VAL:HG13	1:C:189:GLY:HA2	1.94	0.49
1:A:79:ILE:HG22	1:A:697:ALA:HB1	1.94	0.49
1:B:418:TYR:CB	1:B:428:LYS:O	2.59	0.49
1:C:536:PHE:HE1	1:C:568:LEU:HA	1.75	0.49
1:F:312:ASN:HB3	1:F:338:THR:HA	1.93	0.49
1:D:213:ARG:HH22	1:D:236:ASP:HA	1.77	0.49
1:C:539:PHE:CD2	1:C:572:VAL:HG21	2.48	0.49
1:E:272:LYS:HB2	1:E:276:HIS:CD2	2.48	0.49
1:A:76:ALA:HB1	1:A:698:ILE:HD12	1.93	0.49
2:K:2:ARG:O	2:K:2:ARG:HG3	2.12	0.49
1:A:476:PRO:HA	1:A:556:GLN:HB3	1.94	0.49
1:D:445:VAL:HG12	3:D:2028:HOH:O	2.12	0.49
1:C:398:THR:O	1:C:401:ALA:HB2	2.12	0.49
1:B:338:THR:HG21	3:B:2037:HOH:O	2.13	0.49
1:D:439:PHE:HA	3:D:2027:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASP:CG	1:B:210:ALA:N	2.65	0.49
1:E:83:HIS:HE1	1:E:499:PRO:HG2	1.76	0.49
1:D:567:LEU:HB2	1:D:589:PHE:O	2.12	0.49
1:C:446:CYS:HA	1:C:463:LEU:O	2.12	0.49
1:E:366:LEU:N	1:E:366:LEU:HD12	2.19	0.49
1:C:470:ASP:C	1:C:472:LYS:N	2.66	0.49
1:E:695:GLU:O	1:E:698:ILE:HG22	2.13	0.49
1:B:283:ARG:HG3	1:B:324:THR:HG22	1.95	0.49
1:F:220:HIS:ND1	1:F:229:ASP:OD1	2.39	0.49
1:E:264:GLU:HB2	1:E:285:ARG:HB3	1.95	0.49
1:B:225:PRO:O	1:B:228:GLU:HB2	2.12	0.49
1:D:404:LEU:HD22	1:D:422:VAL:HG22	1.93	0.49
1:F:357:GLY:HA2	1:F:517:GLU:O	2.13	0.49
1:C:689:ARG:NH2	1:C:691:LYS:HG2	2.27	0.49
1:B:708:ASN:ND2	1:B:710:ARG:HH12	2.10	0.49
1:A:685:SER:O	1:A:686:ALA:HB3	2.13	0.49
1:C:494:ASN:HD21	1:C:496:ARG:HB2	1.72	0.48
1:F:418:TYR:CB	1:F:429:VAL:HA	2.42	0.48
1:B:113:TYR:HB3	1:B:137:GLU:CB	2.43	0.48
1:A:303:VAL:HB	1:A:316:VAL:HG12	1.95	0.48
1:C:485:TYR:CE2	2:I:3:VAL:HB	2.48	0.48
1:A:249:ASP:O	1:A:251:LYS:HD3	2.12	0.48
1:B:68:ARG:HD2	3:B:2007:HOH:O	2.13	0.48
1:F:552:THR:HG22	1:F:553:THR:N	2.28	0.48
1:E:211:SER:O	1:E:602:PRO:HA	2.13	0.48
1:C:500:TYR:CZ	1:C:700:GLN:HG2	2.48	0.48
1:C:635:GLN:HG2	1:C:637:TYR:CE1	2.48	0.48
1:A:568:LEU:C	1:A:568:LEU:HD23	2.33	0.48
1:C:338:THR:O	1:C:353:GLY:HA3	2.13	0.48
1:F:641:MET:CE	1:F:699:GLN:HA	2.43	0.48
1:B:646:LEU:HD22	1:B:679:LEU:HD22	1.94	0.48
1:F:482:TYR:CB	1:F:483:GLY:HA2	2.35	0.48
1:F:382:PHE:HB3	1:F:408:TYR:HE2	1.79	0.48
1:B:51:ASP:OD2	1:B:54:VAL:HG23	2.13	0.48
1:F:383:ASP:OD1	1:F:383:ASP:N	2.46	0.48
1:D:554:PRO:O	1:D:556:GLN:N	2.47	0.48
1:A:552:THR:HG22	1:A:553:THR:N	2.28	0.48
1:F:544:GLU:HB2	3:F:2036:HOH:O	2.14	0.48
1:F:564:ALA:O	1:F:567:LEU:HB3	2.14	0.48
1:D:476:PRO:HB2	1:D:505:MET:HG2	1.94	0.48
1:D:355:ARG:HB3	1:D:360:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:LEU:CD2	1:F:279:LEU:N	2.72	0.48
1:B:112:SER:CB	1:B:689:ARG:HH21	2.27	0.48
1:F:70:VAL:HA	1:F:73:LYS:HE2	1.96	0.48
1:B:146:PHE:CZ	1:B:148:VAL:HG23	2.48	0.48
1:C:407:ARG:HD2	1:C:417:TRP:CZ2	2.48	0.48
1:C:465:TYR:HB3	1:C:506:ILE:HG23	1.94	0.48
1:F:494:ASN:C	1:F:494:ASN:HD22	2.17	0.48
1:A:707:LEU:HA	1:A:707:LEU:HD12	1.68	0.48
1:B:61:GLU:HG3	1:B:675:LEU:HB3	1.95	0.48
1:B:363:THR:HG22	3:B:2040:HOH:O	2.13	0.48
1:D:483:GLY:O	1:D:514:GLY:HA3	2.13	0.48
1:C:357:GLY:HA2	1:C:517:GLU:O	2.14	0.48
1:C:177:ARG:HD3	1:C:186:LYS:CG	2.44	0.48
1:F:154:PRO:O	1:F:156:PRO:HD3	2.13	0.48
1:D:373:SER:HB3	1:D:376:THR:HG23	1.94	0.48
1:F:164:TYR:OH	1:F:177:ARG:HD2	2.14	0.48
1:E:654:TRP:O	1:E:658:LYS:HG3	2.14	0.48
1:B:149:VAL:HG13	1:B:165:SER:O	2.14	0.48
1:F:299:ASP:O	1:F:320:ARG:HB2	2.14	0.48
1:C:183:VAL:HB	3:C:2010:HOH:O	2.13	0.48
1:B:568:LEU:HD23	1:B:568:LEU:C	2.34	0.48
1:B:6:GLY:HA3	1:B:664:ARG:HD3	1.96	0.47
1:D:646:LEU:O	1:D:646:LEU:HD12	2.14	0.47
1:E:175:SER:OG	1:E:177:ARG:NH2	2.47	0.47
1:B:474:PRO:HA	1:B:551:LEU:O	2.13	0.47
1:B:113:TYR:HB3	1:B:137:GLU:HB2	1.96	0.47
1:C:650:ARG:CZ	1:C:684:PHE:CE2	2.97	0.47
1:F:410:SER:O	1:F:493:PHE:HB2	2.14	0.47
1:B:476:PRO:HB2	1:B:505:MET:HG2	1.95	0.47
1:A:45:ARG:HD2	1:A:654:TRP:CE2	2.48	0.47
1:E:521:THR:C	1:E:523:TYR:N	2.68	0.47
1:A:392:VAL:O	1:A:396:MET:HG2	2.14	0.47
1:E:56:ALA:O	1:E:59:HIS:HB3	2.14	0.47
1:F:612:GLY:C	1:F:623:MET:CE	2.83	0.47
1:E:87:ILE:HD13	3:E:2025:HOH:O	2.13	0.47
1:F:498:LEU:HB2	1:F:499:PRO:HD3	1.97	0.47
1:D:691:LYS:HD3	1:D:691:LYS:HA	1.69	0.47
1:C:413:THR:HG22	1:C:414:PRO:O	2.14	0.47
1:F:650:ARG:NH2	1:F:684:PHE:HE2	2.12	0.47
1:D:83:HIS:HE1	1:D:496:ARG:HA	1.78	0.47
1:F:260:SER:HB3	1:F:609:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:OD2	1:A:170:GLY:HA2	2.14	0.47
1:C:32:ASP:HA	1:C:33:PRO:C	2.34	0.47
1:D:396:MET:HE3	1:D:396:MET:HA	1.97	0.47
1:A:490:GLU:HA	1:A:490:GLU:OE1	2.15	0.47
1:D:554:PRO:C	1:D:556:GLN:H	2.18	0.47
1:B:487:ILE:CG2	1:B:488:CYS:N	2.78	0.47
1:B:362:TRP:CD1	1:B:379:GLU:HB2	2.49	0.47
1:C:367:GLY:C	1:C:369:ASP:H	2.11	0.47
1:A:233:TYR:HA	3:A:2044:HOH:O	2.14	0.47
1:C:312:ASN:ND2	1:C:520:ARG:H	2.13	0.46
1:E:210:ALA:O	1:E:211:SER:CB	2.62	0.46
1:E:31:MET:HG3	1:E:615:ASN:O	2.15	0.46
1:D:547:ILE:CD1	1:D:579:LEU:HD22	2.46	0.46
1:F:93:SER:O	1:F:95:PRO:HD3	2.14	0.46
1:A:557:LEU:HD23	1:A:579:LEU:O	2.15	0.46
1:D:355:ARG:O	1:D:360:ARG:NH1	2.47	0.46
1:B:440:GLU:O	1:B:443:ASN:HB2	2.15	0.46
1:B:347:LYS:O	1:B:366:LEU:HG	2.15	0.46
1:D:162:VAL:HG13	1:D:179:VAL:HG21	1.97	0.46
1:E:312:ASN:HB3	1:E:338:THR:HA	1.96	0.46
1:C:598:ASP:HB3	1:C:601:ILE:CD1	2.41	0.46
1:C:638:PRO:HA	1:C:671:ASN:HD22	1.79	0.46
1:C:100:ARG:O	1:C:100:ARG:HD3	2.16	0.46
1:E:607:GLU:HG2	1:E:611:TRP:HE1	1.80	0.46
1:C:445:VAL:O	1:C:464:VAL:HA	2.16	0.46
1:B:577:PRO:HG3	1:B:635:GLN:HE21	1.81	0.46
1:B:68:ARG:HG2	1:B:674:LEU:HD21	1.97	0.46
1:C:190:THR:HA	1:C:206:ILE:O	2.16	0.46
1:D:689:ARG:NH1	1:D:691:LYS:CG	2.77	0.46
1:B:294:GLU:HG2	3:B:2032:HOH:O	2.15	0.46
1:B:560:GLU:HG3	1:B:584:LEU:HD12	1.97	0.46
1:A:167:ASP:OD2	1:A:170:GLY:CA	2.63	0.46
1:C:114:LYS:C	1:C:115:LEU:HD12	2.36	0.46
1:D:106:ARG:NH2	1:D:127:GLU:HG3	2.31	0.46
1:C:355:ARG:HB3	1:C:360:ARG:HH11	1.81	0.46
1:F:639:HIS:ND1	1:F:671:ASN:HB3	2.31	0.46
1:D:308:ASP:OD2	1:D:314:LYS:NZ	2.48	0.46
1:D:177:ARG:HG2	1:D:186:LYS:HG2	1.98	0.46
1:D:393:CYS:C	1:D:395:GLN:H	2.19	0.46
1:D:349:ALA:HB3	1:D:364:VAL:HG12	1.96	0.46
1:A:685:SER:HB3	1:A:687:SER:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:553:THR:OG1	1:F:556:GLN:NE2	2.47	0.46
1:C:213:ARG:NH2	1:C:235:ASP:O	2.49	0.46
1:A:552:THR:CG2	1:A:557:LEU:HB2	2.46	0.46
1:E:39:ASP:OD2	1:E:658:LYS:NZ	2.48	0.46
1:D:685:SER:O	1:D:686:ALA:HB3	2.16	0.45
1:E:49:ARG:HE	1:E:653:TYR:HE2	1.64	0.45
1:A:111:LEU:HD23	1:A:111:LEU:N	2.30	0.45
1:B:498:LEU:HB2	1:B:499:PRO:HD3	1.98	0.45
1:C:685:SER:O	1:C:687:SER:N	2.49	0.45
1:A:552:THR:CG2	1:A:553:THR:N	2.79	0.45
1:D:676:LYS:HE3	1:D:695:GLU:HG2	1.98	0.45
1:A:443:ASN:CG	1:A:714:ARG:HH12	2.20	0.45
1:F:9:ALA:HB3	1:F:41:LEU:HD22	1.98	0.45
1:B:533:ARG:HD3	3:B:2057:HOH:O	2.17	0.45
1:F:291:TYR:HA	1:F:304:LEU:O	2.17	0.45
1:F:403:LEU:HD22	1:F:419:ASP:HB3	1.98	0.45
1:D:266:HIS:CE1	1:D:281:MET:CE	2.99	0.45
1:A:685:SER:C	1:A:687:SER:N	2.69	0.45
1:F:588:PRO:HD2	1:F:656:PRO:HG3	1.98	0.45
1:D:104:TYR:OH	1:D:131:GLU:HG3	2.17	0.45
1:F:612:GLY:C	1:F:623:MET:HE1	2.37	0.45
1:F:710:ARG:HB2	1:F:710:ARG:HH11	1.80	0.45
1:F:418:TYR:HB3	1:F:429:VAL:HA	1.98	0.45
1:F:558:SER:HA	1:F:582:VAL:O	2.16	0.45
1:C:317:LEU:HD21	3:C:2017:HOH:O	2.16	0.45
1:E:406:LEU:O	1:E:417:TRP:HA	2.17	0.45
1:C:689:ARG:CZ	1:C:691:LYS:HG2	2.47	0.45
1:D:103:TYR:CZ	1:D:118:ARG:HG3	2.52	0.45
1:E:714:ARG:HB3	3:E:2037:HOH:O	2.16	0.45
1:F:711:GLN:CA	1:F:711:GLN:HE21	2.23	0.45
1:C:689:ARG:NH1	1:C:691:LYS:HG2	2.31	0.45
1:B:532:LYS:HE2	1:B:611:TRP:HZ3	1.81	0.45
1:D:151:CYS:O	1:D:164:TYR:HA	2.17	0.45
1:F:499:PRO:O	1:F:503:ARG:HD2	2.16	0.45
1:C:588:PRO:HB2	1:C:590:VAL:HG13	1.99	0.45
1:E:325:ASP:C	1:E:326:TRP:HD1	2.18	0.45
1:D:641:MET:CE	1:D:699:GLN:HG2	2.47	0.45
1:D:318:THR:HB	1:D:325:ASP:O	2.17	0.45
1:F:601:ILE:HA	1:F:602:PRO:HD3	1.79	0.45
1:E:497:PHE:CD1	1:E:497:PHE:C	2.90	0.45
1:B:473:LYS:HB2	1:B:474:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:O	1:C:499:PRO:HD2	2.16	0.45
1:E:337:VAL:CG2	1:E:355:ARG:HD3	2.47	0.45
1:D:354:ARG:NH2	1:D:490:GLU:CD	2.70	0.45
1:F:463:LEU:HD12	1:F:506:ILE:HG21	1.98	0.45
1:E:96:TYR:O	1:E:102:LEU:HA	2.17	0.45
1:C:563:SER:HB2	1:C:683:HIS:CE1	2.52	0.45
1:F:216:LYS:HD3	1:F:234:THR:OG1	2.17	0.45
1:C:681:SER:CB	1:C:685:SER:HB2	2.45	0.45
1:C:113:TYR:HB3	1:C:137:GLU:CB	2.45	0.45
1:A:641:MET:CE	1:A:699:GLN:HE21	2.29	0.45
1:F:386:VAL:HG22	1:F:386:VAL:O	2.17	0.45
1:A:173:VAL:HG13	1:A:189:GLY:HA2	1.97	0.45
1:F:19:GLY:O	1:F:26:ARG:HG3	2.17	0.45
1:C:158:GLU:O	1:C:159:HIS:HB2	2.16	0.45
1:B:354:ARG:NH2	1:B:490:GLU:OE2	2.50	0.45
1:F:501:VAL:C	1:F:503:ARG:H	2.20	0.44
1:E:355:ARG:O	1:E:360:ARG:NH1	2.50	0.44
1:C:78:THR:O	1:C:82:GLU:HG3	2.16	0.44
1:E:101:PHE:HD1	1:E:120:PRO:HA	1.82	0.44
1:D:528:LYS:HG3	1:D:529:TYR:N	2.31	0.44
1:A:101:PHE:CE1	1:A:118:ARG:HD3	2.52	0.44
1:C:89:GLU:HB3	1:C:109:LYS:HA	1.98	0.44
1:B:552:THR:HG23	1:B:553:THR:H	1.81	0.44
1:C:648:ASP:CG	1:C:683:HIS:HB2	2.37	0.44
1:B:342:VAL:HG12	1:B:351:LEU:HD12	1.99	0.44
1:A:237:ASP:HA	1:A:238:PRO:HD2	1.61	0.44
1:E:484:SER:O	1:E:486:GLY:N	2.50	0.44
1:F:460:PRO:HG2	1:F:511:HIS:HB2	2.00	0.44
1:E:520:ARG:HG3	1:E:524:GLU:HG3	1.99	0.44
1:B:112:SER:HB3	1:B:689:ARG:NE	2.31	0.44
1:F:712:LEU:N	1:F:712:LEU:HD12	2.29	0.44
1:E:172:GLU:HB2	1:E:649:PRO:HG3	1.99	0.44
1:F:46:ASP:OD2	1:F:50:ALA:N	2.44	0.44
1:F:642:ILE:CD1	1:F:660:ALA:HB2	2.47	0.44
1:C:162:VAL:O	1:C:179:VAL:HG23	2.17	0.44
1:E:88:GLU:HG3	1:E:88:GLU:O	2.17	0.44
1:F:112:SER:HB3	1:F:689:ARG:HA	1.99	0.44
1:D:88:GLU:O	1:D:88:GLU:CG	2.66	0.44
1:E:707:LEU:HA	1:E:707:LEU:HD12	1.85	0.44
1:E:69:ALA:O	1:E:71:ASP:N	2.51	0.44
1:B:263:SER:CB	1:B:291:TYR:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:PHE:CD1	1:C:348:PHE:C	2.90	0.44
1:C:177:ARG:HD3	1:C:186:LYS:HG3	1.99	0.44
1:A:175:SER:HA	1:A:187:VAL:O	2.17	0.44
1:A:18:PHE:CE2	1:A:597:CYS:HB3	2.52	0.44
1:C:627:SER:HB3	1:C:630:ASP:HB2	1.98	0.44
1:A:261:GLU:HG2	1:A:609:GLU:OE1	2.18	0.44
1:A:521:THR:O	1:A:525:VAL:HG22	2.18	0.44
1:C:96:TYR:HE2	1:C:397:LYS:HG3	1.82	0.44
1:A:119:VAL:HG13	1:A:123:LYS:HB2	1.99	0.44
1:D:413:THR:O	1:D:493:PHE:HB2	2.18	0.44
1:D:666:LEU:HA	1:D:666:LEU:HD23	1.78	0.44
1:A:96:TYR:CD1	1:A:395:GLN:HG2	2.52	0.44
1:A:488:CYS:HB3	1:A:517:GLU:HG3	1.98	0.44
1:E:342:VAL:HA	1:E:350:VAL:O	2.17	0.44
1:B:261:GLU:HG2	1:B:609:GLU:OE1	2.18	0.44
1:E:679:LEU:HD12	1:E:679:LEU:H	1.83	0.44
1:B:532:LYS:HE2	1:B:611:TRP:CZ3	2.53	0.44
1:D:584:LEU:HD23	1:D:641:MET:HB3	2.00	0.44
1:F:521:THR:C	1:F:523:TYR:N	2.70	0.44
1:D:563:SER:HA	1:D:587:VAL:O	2.18	0.43
1:A:482:TYR:HB3	3:A:2074:HOH:O	2.17	0.43
1:E:307:LYS:HG2	1:E:308:ASP:OD1	2.18	0.43
1:E:261:GLU:HA	1:E:290:ARG:HD2	2.00	0.43
1:F:573:LEU:HA	1:F:573:LEU:HD23	1.63	0.43
1:B:308:ASP:O	1:B:309:LYS:HB2	2.17	0.43
1:D:307:LYS:O	1:D:308:ASP:HB2	2.18	0.43
1:E:367:GLY:O	1:E:369:ASP:N	2.50	0.43
1:A:261:GLU:HA	1:A:290:ARG:HD2	2.00	0.43
1:F:219:ARG:HB2	1:F:232:LEU:HD11	2.00	0.43
1:C:411:MET:HE1	1:C:491:PRO:HB3	2.00	0.43
1:C:413:THR:O	1:C:493:PHE:HB2	2.17	0.43
1:A:479:LEU:HD11	1:A:510:ALA:HB2	2.00	0.43
1:A:299:ASP:OD1	1:A:299:ASP:N	2.50	0.43
1:C:473:LYS:HA	1:C:474:PRO:HD2	1.88	0.43
1:B:209:ASP:HB2	1:B:215:ASN:OD1	2.17	0.43
1:B:494:ASN:ND2	1:B:496:ARG:HB2	2.33	0.43
1:E:515:GLY:O	1:E:523:TYR:HB2	2.19	0.43
1:E:497:PHE:C	1:E:497:PHE:HD1	2.22	0.43
1:A:236:ASP:O	1:A:238:PRO:HD3	2.18	0.43
1:B:221:ILE:O	1:B:224:GLN:HG3	2.18	0.43
1:A:533:ARG:HG3	1:A:622:TYR:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLU:O	1:B:159:HIS:HB2	2.18	0.43
1:B:331:ILE:HA	1:B:332:PRO:HD3	1.85	0.43
1:C:504:GLY:HA3	1:C:713:LEU:HD12	2.01	0.43
1:E:41:LEU:O	1:E:658:LYS:HE2	2.18	0.43
1:E:650:ARG:NH2	1:E:684:PHE:HE2	2.16	0.43
1:D:210:ALA:C	1:D:212:LYS:N	2.71	0.43
1:F:74:ASP:O	1:F:77:GLU:HB3	2.18	0.43
1:D:446:CYS:O	1:D:446:CYS:SG	2.77	0.43
1:F:191:ASN:C	1:F:191:ASN:OD1	2.55	0.43
1:E:482:TYR:O	1:E:565:GLY:HA2	2.19	0.43
1:D:162:VAL:HG13	1:D:179:VAL:CG2	2.49	0.43
1:A:230:VAL:HG11	1:A:277:ASN:ND2	2.34	0.43
1:F:449:GLU:HB2	1:F:461:ILE:HB	2.00	0.43
1:A:179:VAL:O	1:A:181:ASP:N	2.52	0.43
1:F:100:ARG:O	1:F:121:ALA:HB2	2.18	0.43
1:E:613:ASN:O	1:E:619:PHE:HB2	2.18	0.43
1:A:113:TYR:HB3	1:A:137:GLU:CB	2.43	0.43
1:E:210:ALA:C	1:E:212:LYS:H	2.21	0.43
1:A:247:SER:HB3	1:A:252:THR:HB	2.00	0.43
1:D:595:THR:HG23	1:D:601:ILE:HD13	2.00	0.43
1:D:540:ILE:O	1:D:544:GLU:HG2	2.19	0.43
1:D:712:LEU:H	1:D:712:LEU:HD12	1.83	0.43
1:B:116:HIS:HB3	3:B:2012:HOH:O	2.18	0.43
1:D:283:ARG:HG3	1:D:324:THR:HG22	1.99	0.43
1:A:61:GLU:HG2	1:A:675:LEU:CD2	2.36	0.43
2:J:1:FC0:CD2	2:J:2:ARG:HH21	2.31	0.43
1:A:204:PHE:CE1	1:A:219:ARG:HG3	2.53	0.43
1:F:61:GLU:HG2	1:F:675:LEU:HB3	2.01	0.43
1:F:153:ALA:HA	1:F:154:PRO:HD3	1.85	0.43
1:F:689:ARG:HB2	1:F:691:LYS:H	1.84	0.43
1:C:483:GLY:O	1:C:514:GLY:HA3	2.19	0.43
1:E:209:ASP:OD1	1:E:210:ALA:N	2.51	0.43
1:D:51:ASP:HA	1:D:52:PRO:HD3	1.91	0.43
1:A:35:ARG:NH1	1:A:620:PHE:CD2	2.87	0.43
1:F:115:LEU:HD23	1:F:133:ILE:HG12	2.00	0.43
1:E:400:ASP:CB	3:E:2023:HOH:O	2.57	0.43
1:B:685:SER:O	1:B:686:ALA:HB3	2.19	0.43
1:B:689:ARG:HD3	3:B:2074:HOH:O	2.18	0.43
1:A:294:GLU:HG3	1:A:342:VAL:HG23	2.01	0.43
1:B:154:PRO:O	1:B:156:PRO:HD3	2.19	0.43
1:C:44:LEU:HA	1:C:44:LEU:HD23	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:GLN:O	1:E:226:GLN:HG3	2.18	0.43
1:C:479:LEU:O	1:C:559:CYS:HA	2.19	0.43
1:C:104:TYR:CE2	1:C:117:CYS:HB2	2.53	0.43
1:E:366:LEU:H	1:E:366:LEU:CD1	2.14	0.42
1:D:496:ARG:HH11	1:D:496:ARG:CG	2.21	0.42
1:C:523:TYR:OH	1:C:528:LYS:NZ	2.48	0.42
1:C:343:ALA:HB1	1:C:345:PHE:HE1	1.82	0.42
1:B:222:ILE:H	1:B:222:ILE:HG12	1.60	0.42
1:B:95:PRO:HA	1:B:103:TYR:O	2.19	0.42
1:A:307:LYS:HG2	1:A:308:ASP:N	2.34	0.42
1:E:108:VAL:HB	1:E:111:LEU:HD12	2.02	0.42
1:F:494:ASN:C	1:F:494:ASN:ND2	2.73	0.42
1:F:712:LEU:H	1:F:712:LEU:CD1	2.28	0.42
1:B:396:MET:HE3	1:B:404:LEU:HA	2.01	0.42
1:B:570:GLY:O	1:B:571:ALA:C	2.56	0.42
1:B:244:VAL:HG23	1:B:255:ILE:HG12	2.01	0.42
1:C:542:CYS:O	1:C:546:LEU:HG	2.18	0.42
1:D:563:SER:HB2	1:D:683:HIS:CE1	2.55	0.42
1:E:83:HIS:CE1	1:E:499:PRO:HG2	2.54	0.42
1:E:689:ARG:HB2	1:E:690:TYR:H	1.59	0.42
1:C:447:ARG:HG3	1:C:463:LEU:HD21	2.01	0.42
1:D:162:VAL:HG13	1:D:179:VAL:HB	2.00	0.42
1:B:89:GLU:OE1	1:B:109:LYS:HE2	2.19	0.42
1:A:689:ARG:HD3	1:A:691:LYS:HG2	1.99	0.42
1:E:446:CYS:HB3	1:E:464:VAL:HG23	2.02	0.42
1:C:305:THR:OG1	1:C:307:LYS:HB2	2.20	0.42
1:D:220:HIS:HE1	1:D:224:GLN:O	2.01	0.42
1:C:533:ARG:HG3	1:C:622:TYR:CZ	2.54	0.42
1:F:592:VAL:O	1:F:596:MET:HB2	2.19	0.42
1:D:685:SER:C	1:D:687:SER:N	2.73	0.42
1:A:675:LEU:O	1:A:675:LEU:HG	2.18	0.42
1:A:619:PHE:HB3	1:A:623:MET:HE2	1.95	0.42
1:D:96:TYR:CD1	1:D:395:GLN:HG2	2.55	0.42
1:F:396:MET:HB3	1:F:396:MET:HE2	1.98	0.42
1:D:89:GLU:OE1	1:D:109:LYS:HE3	2.20	0.42
1:B:449:GLU:HG3	1:B:463:LEU:HD21	2.00	0.42
1:A:109:LYS:O	1:A:109:LYS:HG2	2.20	0.42
1:C:381:HIS:O	1:C:427:ARG:NH2	2.42	0.42
1:E:400:ASP:OD1	1:E:400:ASP:O	2.37	0.42
1:F:79:ILE:CD1	1:F:499:PRO:HB3	2.48	0.42
1:B:424:SER:OG	1:B:426:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:VAL:HB	1:D:627:SER:OG	2.20	0.42
1:C:162:VAL:HG12	3:C:2009:HOH:O	2.18	0.42
1:E:321:SER:O	1:E:323:PRO:HD3	2.19	0.42
1:D:618:LYS:HD3	1:D:619:PHE:CE2	2.55	0.42
1:B:687:SER:HB2	1:B:689:ARG:HG3	2.01	0.42
1:D:61:GLU:CG	1:D:675:LEU:HB3	2.50	0.42
1:C:637:TYR:N	1:C:669:ASP:OD2	2.40	0.42
1:F:612:GLY:CA	1:F:623:MET:HE1	2.50	0.42
1:F:393:CYS:HA	1:F:396:MET:HG3	2.02	0.42
1:B:220:HIS:HE1	1:B:224:GLN:O	2.03	0.42
1:B:126:GLY:O	1:B:131:GLU:HB2	2.20	0.42
1:E:443:ASN:O	1:E:466:ASP:HA	2.19	0.42
1:E:659:TRP:CE2	1:E:663:LEU:HD11	2.55	0.42
1:A:363:THR:HG22	1:A:378:LYS:HB3	2.02	0.42
1:F:199:ASN:HB2	1:F:201:GLU:HG3	2.02	0.42
1:D:418:TYR:HB3	1:D:428:LYS:O	2.20	0.42
1:E:426:GLU:HG3	1:E:426:GLU:O	2.20	0.42
1:D:586:GLY:O	1:D:587:VAL:C	2.58	0.42
1:C:528:LYS:O	1:C:529:TYR:C	2.58	0.42
1:A:534:ASN:O	1:A:535:THR:C	2.57	0.42
1:E:396:MET:HE1	1:E:404:LEU:HA	2.02	0.42
1:D:382:PHE:HB3	1:D:408:TYR:CE1	2.55	0.42
1:A:268:LEU:HD13	1:A:279:LEU:HD13	2.02	0.42
1:D:421:ASP:HB3	1:D:424:SER:HG	1.83	0.42
1:D:639:HIS:CE1	1:D:671:ASN:HB3	2.55	0.42
1:C:539:PHE:HD2	1:C:572:VAL:HG21	1.83	0.42
1:E:713:LEU:O	1:E:714:ARG:NE	2.43	0.42
1:C:373:SER:O	1:C:376:THR:OG1	2.36	0.42
1:E:50:ALA:O	1:E:51:ASP:C	2.59	0.42
1:B:616:GLU:O	1:B:617:TYR:C	2.58	0.42
1:F:101:PHE:CD1	1:F:118:ARG:HD3	2.55	0.42
1:A:206:ILE:HG22	1:A:206:ILE:O	2.20	0.41
1:C:418:TYR:HA	1:C:428:LYS:O	2.20	0.41
1:B:78:THR:O	1:B:82:GLU:HG3	2.19	0.41
1:F:498:LEU:HB2	1:F:499:PRO:CD	2.50	0.41
1:F:501:VAL:HG12	1:F:502:ASP:N	2.35	0.41
1:F:304:LEU:HD12	1:F:314:LYS:O	2.19	0.41
1:A:31:MET:HG3	1:A:615:ASN:O	2.21	0.41
1:C:216:LYS:HG2	1:C:234:THR:HG23	2.02	0.41
1:A:369:ASP:O	1:A:370:ASN:HB2	2.20	0.41
1:A:203:PHE:C	1:A:203:PHE:CD1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:CG	1:A:100:ARG:NH1	2.77	0.41
1:B:614:PRO:N	1:B:623:MET:HE1	2.35	0.41
1:E:476:PRO:HD3	1:E:556:GLN:OE1	2.20	0.41
1:E:648:ASP:OD1	1:E:683:HIS:HB2	2.21	0.41
1:D:134:VAL:HG12	1:D:162:VAL:HG11	2.02	0.41
1:E:703:VAL:HG12	1:E:707:LEU:HD22	2.02	0.41
1:A:595:THR:HA	1:A:601:ILE:HD12	2.00	0.41
1:C:331:ILE:HA	1:C:332:PRO:HD3	1.88	0.41
1:F:315:VAL:HG13	1:F:331:ILE:HB	2.02	0.41
1:E:310:CYS:SG	1:E:314:LYS:HE2	2.60	0.41
1:F:408:TYR:O	1:F:415:THR:HA	2.20	0.41
1:C:479:LEU:HD12	1:C:479:LEU:HA	1.87	0.41
1:B:648:ASP:OD1	1:B:683:HIS:HB2	2.21	0.41
1:E:260:SER:HB3	1:E:609:GLU:HB3	2.02	0.41
1:F:532:LYS:HG3	1:F:532:LYS:O	2.20	0.41
1:F:418:TYR:HB2	1:F:429:VAL:HA	2.02	0.41
1:F:5:ARG:CG	1:F:6:GLY:H	2.31	0.41
1:D:489:ILE:HA	1:D:489:ILE:HD13	1.88	0.41
1:E:587:VAL:HG21	1:E:683:HIS:CE1	2.56	0.41
1:C:500:TYR:OH	1:C:703:VAL:HG21	2.20	0.41
1:D:655:GLU:HB2	1:D:656:PRO:CD	2.50	0.41
1:B:460:PRO:HB2	1:B:511:HIS:CD2	2.55	0.41
1:C:187:VAL:HA	1:C:226:GLN:OE1	2.20	0.41
1:B:380:LEU:HD23	1:B:406:LEU:HD11	2.02	0.41
1:B:75:LEU:O	1:B:79:ILE:HD13	2.20	0.41
1:E:632:VAL:CG1	1:E:666:LEU:HD12	2.36	0.41
1:E:482:TYR:CD2	1:E:483:GLY:HA2	2.55	0.41
1:E:45:ARG:HD2	1:E:654:TRP:CZ2	2.56	0.41
1:F:612:GLY:N	1:F:623:MET:HE1	2.36	0.41
1:D:89:GLU:HB3	1:D:109:LYS:HA	2.02	0.41
1:D:583:ALA:O	1:D:640:LEU:HA	2.21	0.41
1:C:681:SER:HB2	1:C:685:SER:HB3	1.98	0.41
1:E:347:LYS:O	1:E:348:PHE:HB3	2.20	0.41
1:E:99:ASP:HB2	1:E:159:HIS:NE2	2.36	0.41
1:A:582:VAL:HG22	1:A:583:ALA:N	2.36	0.41
1:E:191:ASN:OD1	1:E:191:ASN:C	2.59	0.41
1:D:573:LEU:HD23	1:D:573:LEU:HA	1.75	0.41
1:D:552:THR:HG22	1:D:553:THR:N	2.35	0.41
1:E:355:ARG:HB3	1:E:360:ARG:HD3	2.03	0.41
1:B:629:ILE:HD11	1:B:659:TRP:N	2.36	0.41
1:A:165:SER:HA	1:A:175:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:MET:SD	1:F:617:TYR:CD1	3.13	0.41
1:D:498:LEU:O	1:D:499:PRO:C	2.58	0.41
1:B:273:GLY:O	1:B:275:LYS:N	2.54	0.41
1:B:49:ARG:HH11	1:B:653:TYR:HD2	1.67	0.41
1:F:407:ARG:NE	3:F:2026:HOH:O	2.53	0.41
1:B:707:LEU:HA	1:B:707:LEU:HD12	1.93	0.41
1:B:296:HIS:O	1:B:300:THR:HG23	2.21	0.41
1:A:684:PHE:O	1:A:685:SER:O	2.39	0.41
1:C:601:ILE:HA	1:C:602:PRO:HD3	1.91	0.41
1:C:691:LYS:HD3	1:C:691:LYS:HA	1.52	0.41
1:A:707:LEU:O	1:A:708:ASN:CB	2.69	0.41
1:C:348:PHE:CD1	1:C:349:ALA:N	2.89	0.41
1:C:135:LEU:HD12	1:C:136:ASP:H	1.85	0.41
1:A:653:TYR:CD1	1:A:653:TYR:C	2.94	0.41
1:D:619:PHE:CB	1:D:623:MET:CE	2.89	0.41
1:A:691:LYS:HA	1:A:691:LYS:HD3	1.86	0.41
1:E:476:PRO:HG2	1:E:709:VAL:HG11	2.02	0.41
1:A:206:ILE:HA	1:A:216:LYS:O	2.20	0.41
1:F:382:PHE:HB3	1:F:408:TYR:CE2	2.55	0.41
1:D:220:HIS:CE1	1:D:224:GLN:O	2.73	0.41
1:A:554:PRO:HD2	3:A:2084:HOH:O	2.20	0.41
1:D:146:PHE:HE1	1:D:685:SER:HG	1.67	0.40
1:D:688:ASP:N	1:D:688:ASP:OD1	2.54	0.40
1:E:704:LEU:HD22	1:E:709:VAL:HG23	2.02	0.40
1:C:704:LEU:CD2	1:C:709:VAL:HG23	2.50	0.40
1:E:552:THR:CG2	1:E:553:THR:N	2.84	0.40
1:B:626:TYR:O	1:B:627:SER:C	2.59	0.40
1:C:155:ALA:HA	1:C:156:PRO:HD2	1.95	0.40
1:A:596:MET:HA	1:A:604:THR:HG23	2.01	0.40
1:A:396:MET:HA	1:A:396:MET:HE3	2.01	0.40
1:E:450:LEU:HD23	1:E:460:PRO:HA	2.03	0.40
1:C:237:ASP:HA	1:C:238:PRO:HD2	1.92	0.40
1:B:433:ARG:HG3	1:B:434:LYS:N	2.36	0.40
1:A:51:ASP:HA	1:A:52:PRO:HD3	1.93	0.40
1:E:633:ARG:HH11	1:E:633:ARG:HD3	1.65	0.40
1:F:687:SER:HB2	1:F:688:ASP:H	1.77	0.40
1:C:88:GLU:O	1:C:88:GLU:CG	2.70	0.40
1:A:118:ARG:NH2	1:A:159:HIS:O	2.54	0.40
1:A:162:VAL:HG22	1:A:179:VAL:HG23	2.03	0.40
1:E:277:ASN:O	1:E:279:LEU:HD13	2.22	0.40
1:D:191:ASN:ND2	1:D:206:ILE:HB	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:VAL:HG13	1:B:179:VAL:CG2	2.50	0.40
1:D:494:ASN:OD1	1:D:496:ARG:HB2	2.22	0.40
1:A:654:TRP:O	1:A:658:LYS:HG3	2.21	0.40
1:C:342:VAL:HA	1:C:350:VAL:O	2.22	0.40
1:E:558:SER:HA	1:E:582:VAL:O	2.21	0.40
1:E:417:TRP:CE3	1:E:431:LYS:HD3	2.56	0.40
1:D:445:VAL:HG23	1:D:465:TYR:CE1	2.56	0.40
1:C:463:LEU:CD2	1:C:463:LEU:N	2.84	0.40
1:F:396:MET:HE1	1:F:403:LEU:O	2.22	0.40
1:B:106:ARG:NH2	1:B:131:GLU:OE1	2.47	0.40
1:F:253:LEU:HB3	1:F:268:LEU:HB3	2.04	0.40
1:B:139:LYS:HE3	3:B:2014:HOH:O	2.22	0.40
1:A:523:TYR:OH	1:A:528:LYS:NZ	2.44	0.40
1:F:490:GLU:HA	1:F:491:PRO:HD3	1.96	0.40
1:E:62:LYS:HB3	1:E:62:LYS:HE2	1.69	0.40
1:A:403:LEU:HD22	1:A:419:ASP:HB3	2.02	0.40
1:B:215:ASN:OD1	1:B:216:LYS:HG2	2.22	0.40
1:B:115:LEU:HD23	1:B:133:ILE:HD13	2.02	0.40
1:F:646:LEU:HB3	1:F:679:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	708/715 (99%)	651 (92%)	48 (7%)	9 (1%)	15	42
1	B	708/715 (99%)	646 (91%)	51 (7%)	11 (2%)	12	36
1	C	708/715 (99%)	623 (88%)	69 (10%)	16 (2%)	8	26
1	D	708/715 (99%)	645 (91%)	49 (7%)	14 (2%)	9	30
1	E	708/715 (99%)	631 (89%)	63 (9%)	14 (2%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	708/715 (99%)	613 (87%)	82 (12%)	13 (2%)	11	33
All	All	4248/4290 (99%)	3809 (90%)	362 (8%)	77 (2%)	11	33

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	A	157	PRO
1	A	685	SER
1	B	157	PRO
1	B	274	VAL
1	B	401	ALA
1	C	156	PRO
1	C	157	PRO
1	D	156	PRO
1	D	157	PRO
1	E	70	VAL
1	E	121	ALA
1	E	156	PRO
1	E	157	PRO
1	F	142	GLU
1	F	157	PRO
1	A	180	ARG
1	B	93	SER
1	B	121	ALA
1	B	142	GLU
1	B	437	GLY
1	C	89	GLU
1	C	142	GLU
1	C	282	VAL
1	C	368	PRO
1	C	686	ALA
1	D	713	LEU
1	E	274	VAL
1	E	522	TRP
1	E	634	ALA
1	E	685	SER
1	F	159	HIS
1	A	142	GLU
1	B	620	PHE
1	C	341	ASP
1	C	471	LEU

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Mol	Chain	Res	Type
1	C	474	PRO
1	D	180	ARG
1	D	555	ALA
1	D	563	SER
1	D	686	ALA
1	D	689	ARG
1	E	142	GLU
1	E	368	PRO
1	F	156	PRO
1	F	578	ASP
1	A	467	THR
1	C	409	SER
1	C	602	PRO
1	E	88	GLU
1	E	282	VAL
1	E	686	ALA
1	F	84	ILE
1	F	370	ASN
1	F	620	PHE
1	A	208	LYS
1	A	411	MET
1	A	620	PHE
1	B	370	ASN
1	C	180	ARG
1	C	627	SER
1	C	628	PRO
1	D	63	ASP
1	D	142	GLU
1	D	308	ASP
1	E	429	VAL
1	F	437	GLY
1	F	502	ASP
1	C	181	ASP
1	D	341	ASP
1	B	156	PRO
1	F	282	VAL
1	F	94	ALA
1	B	628	PRO
1	D	13	PRO
1	D	527	GLY
1	F	628	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	614/619 (99%)	553 (90%)	61 (10%)	10	27
1	B	614/619 (99%)	537 (88%)	77 (12%)	6	15
1	C	614/619 (99%)	551 (90%)	63 (10%)	9	24
1	D	614/619 (99%)	542 (88%)	72 (12%)	7	17
1	E	614/619 (99%)	543 (88%)	71 (12%)	7	18
1	F	614/619 (99%)	542 (88%)	72 (12%)	7	17
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	3696/3726 (99%)	3277 (89%)	419 (11%)	7	19

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	37	ARG
1	A	49	ARG
1	A	66	GLU
1	A	78	THR
1	A	79	ILE
1	A	98	TYR
1	A	100	ARG
1	A	105	THR
1	A	114	LYS
1	A	119	VAL
1	A	140	LEU
1	A	156	PRO
1	A	162	VAL

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Mol	Chain	Res	Type
1	A	175	SER
1	A	185	ASP
1	A	190	THR
1	A	199	ASN
1	A	201	GLU
1	A	226	GLN
1	A	251	LYS
1	A	257	SER
1	A	258	MET
1	A	279	LEU
1	A	287	LYS
1	A	299	ASP
1	A	300	THR
1	A	316	VAL
1	A	317	LEU
1	A	320	ARG
1	A	336	LYS
1	A	341	ASP
1	A	342	VAL
1	A	350	VAL
1	A	352	SER
1	A	361	VAL
1	A	391	VAL
1	A	396	MET
1	A	398	THR
1	A	404	LEU
1	A	412	THR
1	A	418	TYR
1	A	423	LEU
1	A	440	GLU
1	A	442	LYS
1	A	447	ARG
1	A	457	THR
1	A	463	LEU
1	A	473	LYS
1	A	496	ARG
1	A	497	PHE
1	A	628	PRO
1	A	679	LEU
1	A	685	SER
1	A	688	ASP
1	A	689	ARG

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Mol	Chain	Res	Type
1	A	694	ARG
1	A	695	GLU
1	A	699	GLN
1	A	707	LEU
1	A	714	ARG
1	B	15	GLU
1	B	37	ARG
1	B	53	GLU
1	B	67	LYS
1	B	93	SER
1	B	98	TYR
1	B	102	LEU
1	B	105	THR
1	B	109	LYS
1	B	119	VAL
1	B	124	THR
1	B	144	LYS
1	B	145	SER
1	B	151	CYS
1	B	157	PRO
1	B	161	LEU
1	B	185	ASP
1	B	190	THR
1	B	193	SER
1	B	199	ASN
1	B	216	LYS
1	B	227	SER
1	B	241	SER
1	B	247	SER
1	B	251	LYS
1	B	260	SER
1	B	272	LYS
1	B	278	THR
1	B	279	LEU
1	B	285	ARG
1	B	287	LYS
1	B	299	ASP
1	B	300	THR
1	B	316	VAL
1	B	319	LYS
1	B	320	ARG
1	B	321	SER

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Mol	Chain	Res	Type
1	B	336	LYS
1	B	342	VAL
1	B	350	VAL
1	B	361	VAL
1	B	363	THR
1	B	365	ARG
1	B	374	SER
1	B	376	THR
1	B	383	ASP
1	B	386	VAL
1	B	391	VAL
1	B	398	THR
1	B	402	SER
1	B	404	LEU
1	B	412	THR
1	B	418	TYR
1	B	424	SER
1	B	428	LYS
1	B	433	ARG
1	B	445	VAL
1	B	463	LEU
1	B	473	LYS
1	B	494	ASN
1	B	496	ARG
1	B	533	ARG
1	B	537	MET
1	B	562	ARG
1	B	575	MET
1	B	602	PRO
1	B	611	TRP
1	B	629	ILE
1	B	633	ARG
1	B	688	ASP
1	B	689	ARG
1	B	691	LYS
1	B	695	GLU
1	B	696	ASN
1	B	698	ILE
1	B	707	LEU
1	B	711	GLN
1	C	5	ARG
1	C	36	ARG

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Mol	Chain	Res	Type
1	C	37	ARG
1	C	67	LYS
1	C	68	ARG
1	C	87	ILE
1	C	98	TYR
1	C	100	ARG
1	C	105	THR
1	C	106	ARG
1	C	114	LYS
1	C	119	VAL
1	C	129	GLU
1	C	158	GLU
1	C	162	VAL
1	C	169	CYS
1	C	180	ARG
1	C	207	THR
1	C	212	LYS
1	C	241	SER
1	C	244	VAL
1	C	251	LYS
1	C	260	SER
1	C	265	SER
1	C	278	THR
1	C	279	LEU
1	C	285	ARG
1	C	287	LYS
1	C	299	ASP
1	C	308	ASP
1	C	311	VAL
1	C	315	VAL
1	C	317	LEU
1	C	320	ARG
1	C	337	VAL
1	C	341	ASP
1	C	350	VAL
1	C	360	ARG
1	C	361	VAL
1	C	363	THR
1	C	374	SER
1	C	377	LEU
1	C	388	THR
1	C	404	LEU

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Mol	Chain	Res	Type
1	C	410	SER
1	C	430	VAL
1	C	431	LYS
1	C	441	SER
1	C	445	VAL
1	C	463	LEU
1	C	473	LYS
1	C	496	ARG
1	C	497	PHE
1	C	525	VAL
1	C	611	TRP
1	C	616	GLU
1	C	627	SER
1	C	628	PRO
1	C	688	ASP
1	C	691	LYS
1	C	694	ARG
1	C	698	ILE
1	C	714	ARG
1	D	5	ARG
1	D	36	ARG
1	D	37	ARG
1	D	38	VAL
1	D	46	ASP
1	D	67	LYS
1	D	68	ARG
1	D	98	TYR
1	D	100	ARG
1	D	105	THR
1	D	114	LYS
1	D	119	VAL
1	D	129	GLU
1	D	134	VAL
1	D	140	LEU
1	D	142	GLU
1	D	144	LYS
1	D	161	LEU
1	D	162	VAL
1	D	169	CYS
1	D	177	ARG
1	D	181	ASP
1	D	185	ASP

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Mol	Chain	Res	Type
1	D	208	LYS
1	D	216	LYS
1	D	251	LYS
1	D	260	SER
1	D	265	SER
1	D	278	THR
1	D	279	LEU
1	D	285	ARG
1	D	287	LYS
1	D	299	ASP
1	D	302	ILE
1	D	311	VAL
1	D	315	VAL
1	D	316	VAL
1	D	318	THR
1	D	320	ARG
1	D	335	ASP
1	D	341	ASP
1	D	342	VAL
1	D	356	ASP
1	D	358	LEU
1	D	361	VAL
1	D	363	THR
1	D	371	LEU
1	D	374	SER
1	D	383	ASP
1	D	386	VAL
1	D	396	MET
1	D	398	THR
1	D	404	LEU
1	D	410	SER
1	D	418	TYR
1	D	430	VAL
1	D	445	VAL
1	D	463	LEU
1	D	496	ARG
1	D	525	VAL
1	D	537	MET
1	D	578	ASP
1	D	587	VAL
1	D	597	CYS
1	D	602	PRO

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Mol	Chain	Res	Type
1	D	611	TRP
1	D	625	SER
1	D	627	SER
1	D	629	ILE
1	D	688	ASP
1	D	709	VAL
1	D	712	LEU
1	E	16	VAL
1	E	37	ARG
1	E	55	LEU
1	E	67	LYS
1	E	73	LYS
1	E	75	LEU
1	E	79	ILE
1	E	98	TYR
1	E	100	ARG
1	E	105	THR
1	E	114	LYS
1	E	119	VAL
1	E	156	PRO
1	E	162	VAL
1	E	169	CYS
1	E	185	ASP
1	E	199	ASN
1	E	227	SER
1	E	241	SER
1	E	251	LYS
1	E	252	THR
1	E	258	MET
1	E	265	SER
1	E	279	LEU
1	E	285	ARG
1	E	292	THR
1	E	298	THR
1	E	300	THR
1	E	308	ASP
1	E	317	LEU
1	E	325	ASP
1	E	328	THR
1	E	336	LYS
1	E	350	VAL
1	E	352	SER

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Mol	Chain	Res	Type
1	E	356	ASP
1	E	360	ARG
1	E	361	VAL
1	E	363	THR
1	E	366	LEU
1	E	374	SER
1	E	384	GLU
1	E	392	VAL
1	E	396	MET
1	E	398	THR
1	E	403	LEU
1	E	418	TYR
1	E	424	SER
1	E	434	LYS
1	E	443	ASN
1	E	445	VAL
1	E	447	ARG
1	E	463	LEU
1	E	464	VAL
1	E	472	LYS
1	E	473	LYS
1	E	496	ARG
1	E	497	PHE
1	E	552	THR
1	E	607	GLU
1	E	611	TRP
1	E	628	PRO
1	E	633	ARG
1	E	679	LEU
1	E	685	SER
1	E	688	ASP
1	E	689	ARG
1	E	698	ILE
1	E	707	LEU
1	E	712	LEU
1	E	714	ARG
1	F	15	GLU
1	F	16	VAL
1	F	49	ARG
1	F	53	GLU
1	F	60	LEU
1	F	67	LYS

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Mol	Chain	Res	Type
1	F	92	MET
1	F	97	VAL
1	F	98	TYR
1	F	105	THR
1	F	108	VAL
1	F	119	VAL
1	F	132	GLU
1	F	144	LYS
1	F	145	SER
1	F	162	VAL
1	F	169	CYS
1	F	177	ARG
1	F	180	ARG
1	F	185	ASP
1	F	224	GLN
1	F	241	SER
1	F	251	LYS
1	F	272	LYS
1	F	279	LEU
1	F	285	ARG
1	F	287	LYS
1	F	299	ASP
1	F	300	THR
1	F	311	VAL
1	F	315	VAL
1	F	316	VAL
1	F	320	ARG
1	F	328	THR
1	F	336	LYS
1	F	342	VAL
1	F	352	SER
1	F	356	ASP
1	F	360	ARG
1	F	363	THR
1	F	364	VAL
1	F	374	SER
1	F	383	ASP
1	F	384	GLU
1	F	386	VAL
1	F	390	HIS
1	F	393	CYS
1	F	394	SER

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Mol	Chain	Res	Type
1	F	396	MET
1	F	418	TYR
1	F	433	ARG
1	F	494	ASN
1	F	496	ARG
1	F	497	PHE
1	F	499	PRO
1	F	501	VAL
1	F	537	MET
1	F	548	SER
1	F	552	THR
1	F	562	ARG
1	F	582	VAL
1	F	587	VAL
1	F	602	PRO
1	F	629	ILE
1	F	633	ARG
1	F	688	ASP
1	F	694	ARG
1	F	695	GLU
1	F	698	ILE
1	F	699	GLN
1	F	711	GLN
1	F	712	LEU
2	H	2	ARG
2	I	2	ARG
2	L	2	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	224	GLN
1	A	443	ASN
1	A	556	GLN
1	A	699	GLN
1	A	708	ASN
1	B	14	HIS
1	B	224	GLN
1	B	266	HIS
1	B	494	ASN
1	B	556	GLN

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Mol	Chain	Res	Type
1	B	708	ASN
1	C	224	GLN
1	C	266	HIS
1	C	276	HIS
1	C	312	ASN
1	C	381	HIS
1	C	494	ASN
1	C	581	HIS
1	C	683	HIS
1	C	708	ASN
1	D	83	HIS
1	D	266	HIS
1	D	556	GLN
1	D	581	HIS
1	D	699	GLN
1	E	14	HIS
1	E	59	HIS
1	E	83	HIS
1	E	224	GLN
1	E	276	HIS
1	F	83	HIS
1	F	296	HIS
1	F	494	ASN
1	F	556	GLN
1	F	700	GLN
1	F	708	ASN
1	F	711	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FC0	G	1	2	11,14,15	0.89	0	13,17,19	1.58	1 (7%)
2	OAR	G	4	2	7,10,10	1.76	1 (14%)	5,11,11	1.17	1 (20%)
2	FC0	H	1	2	11,14,15	0.98	0	13,17,19	1.41	3 (23%)
2	OAR	H	4	2	7,10,10	1.64	1 (14%)	5,11,11	1.04	0
2	FC0	I	1	2	11,14,15	0.77	0	13,17,19	1.33	1 (7%)
2	OAR	I	4	2	7,10,10	1.72	1 (14%)	5,11,11	1.34	1 (20%)
2	FC0	J	1	2	11,14,15	1.23	0	13,17,19	1.42	2 (15%)
2	OAR	J	4	2	7,10,10	1.73	2 (28%)	5,11,11	2.26	2 (40%)
2	FC0	K	1	2	11,14,15	0.98	0	13,17,19	1.61	1 (7%)
2	OAR	K	4	2	7,10,10	1.56	1 (14%)	5,11,11	1.04	0
2	FC0	L	1	2	11,14,15	1.00	0	13,17,19	0.80	1 (7%)
2	OAR	L	4	2	7,10,10	1.68	1 (14%)	5,11,11	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FC0	G	1	2	-	1/7/11/12	0/1/1/1
2	OAR	G	4	2	1/1/2/3	0/7/9/9	0/0/0/0
2	FC0	H	1	2	-	0/7/11/12	0/1/1/1
2	OAR	H	4	2	1/1/2/3	0/7/9/9	0/0/0/0
2	FC0	I	1	2	-	1/7/11/12	0/1/1/1
2	OAR	I	4	2	1/1/2/3	0/7/9/9	0/0/0/0
2	FC0	J	1	2	-	1/7/11/12	0/1/1/1
2	OAR	J	4	2	1/1/2/3	0/7/9/9	0/0/0/0
2	FC0	K	1	2	-	0/7/11/12	0/1/1/1
2	OAR	K	4	2	1/1/2/3	0/7/9/9	0/0/0/0
2	FC0	L	1	2	-	1/7/11/12	0/1/1/1
2	OAR	L	4	2	1/1/2/3	0/7/9/9	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	OAR	O-C	-4.47	1.23	1.42
2	I	4	OAR	O-C	-4.27	1.23	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4	OAR	O-C	-4.24	1.24	1.42
2	H	4	OAR	O-C	-4.03	1.25	1.42
2	J	4	OAR	O-C	-3.98	1.25	1.42
2	K	4	OAR	O-C	-3.96	1.25	1.42
2	J	4	OAR	CB-CA	-2.02	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	FC0	O1-C1-N	-5.13	117.37	124.76
2	K	1	FC0	O1-C1-N	-5.01	117.54	124.76
2	I	1	FC0	O1-C1-N	-4.32	118.54	124.76
2	H	1	FC0	CA-N-C1	-3.72	116.82	122.97
2	J	4	OAR	CG-CB-CA	-3.64	103.28	115.16
2	J	1	FC0	O1-C1-N	-2.85	120.66	124.76
2	I	4	OAR	CG-CB-CA	-2.69	106.38	115.16
2	H	1	FC0	O1-C1-N	-2.36	121.36	124.76
2	L	1	FC0	CA-N-C1	-2.14	119.43	122.97
2	G	4	OAR	CG-CB-CA	-2.01	108.59	115.16
2	H	1	FC0	CB-CA-C	2.03	115.92	111.55
2	J	4	OAR	O-C-CA	2.95	119.57	111.84
2	J	1	FC0	CG-CB-CA	3.04	120.35	113.61

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	4	OAR	CA
2	I	4	OAR	CA
2	K	4	OAR	CA
2	L	4	OAR	CA
2	J	4	OAR	CA
2	H	4	OAR	CA

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	FC0	O1-C1-N-CA
2	G	1	FC0	O1-C1-N-CA
2	L	1	FC0	O1-C1-N-CA
2	J	1	FC0	O1-C1-N-CA

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	FC0	1	0
2	H	4	OAR	1	0
2	J	1	FC0	4	0
2	K	1	FC0	1	0
2	L	4	OAR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	710/715 (99%)	-0.11	2 (0%) 94 93	33, 45, 64, 79	0
1	B	710/715 (99%)	0.01	6 (0%) 87 86	34, 49, 78, 108	0
1	C	710/715 (99%)	0.16	13 (1%) 71 68	44, 62, 94, 109	0
1	D	710/715 (99%)	-0.03	6 (0%) 87 86	38, 54, 79, 93	0
1	E	710/715 (99%)	0.20	24 (3%) 49 41	37, 63, 106, 130	0
1	F	710/715 (99%)	0.26	29 (4%) 41 34	38, 66, 115, 144	0
2	G	2/4 (50%)	0.09	0 100 100	29, 29, 29, 58	0
2	H	2/4 (50%)	0.11	0 100 100	29, 29, 29, 55	0
2	I	2/4 (50%)	0.04	0 100 100	42, 42, 42, 66	0
2	J	2/4 (50%)	-0.08	0 100 100	38, 38, 38, 60	0
2	K	2/4 (50%)	0.15	0 100 100	33, 33, 33, 65	0
2	L	2/4 (50%)	-0.20	0 100 100	39, 39, 39, 62	0
All	All	4272/4314 (99%)	0.08	80 (1%) 70 66	29, 55, 97, 144	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	686	ALA	4.3
1	F	686	ALA	4.3
1	F	371	LEU	4.2
1	F	469	ILE	3.8
1	E	423	LEU	3.7
1	F	370	ASN	3.7
1	E	368	PRO	3.6
1	F	368	PRO	3.5
1	F	709	VAL	3.4
1	F	369	ASP	3.3
1	C	687	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	121	ALA	3.2
1	E	87	ILE	3.1
1	E	129	GLU	3.1
1	D	100	ARG	3.0
1	E	370	ASN	3.0
1	E	686	ALA	2.9
1	F	300	THR	2.9
1	C	100	ARG	2.9
1	E	365	ARG	2.9
1	D	686	ALA	2.8
1	A	400	ASP	2.8
1	F	470	ASP	2.7
1	E	687	SER	2.7
1	F	128	GLY	2.7
1	E	348	PHE	2.7
1	F	366	LEU	2.6
1	F	713	LEU	2.6
1	E	711	GLN	2.6
1	E	437	GLY	2.6
1	E	302	ILE	2.6
1	B	367	GLY	2.6
1	F	322	ALA	2.6
1	E	347	LYS	2.5
1	E	442	LYS	2.5
1	D	401	ALA	2.5
1	E	373	SER	2.5
1	C	368	PRO	2.4
1	E	404	LEU	2.4
1	E	121	ALA	2.4
1	F	362	TRP	2.4
1	F	367	GLY	2.4
1	C	370	ASN	2.4
1	C	70	VAL	2.4
1	E	301	LEU	2.4
1	C	423	LEU	2.4
1	F	710	ARG	2.4
1	C	299	ASP	2.4
1	D	124	THR	2.3
1	C	349	ALA	2.3
1	F	66	GLU	2.3
1	F	180	ARG	2.3
1	F	122	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	714	ARG	2.2
1	B	369	ASP	2.2
1	F	400	ASP	2.2
1	E	362	TRP	2.2
1	A	687	SER	2.2
1	F	708	ASN	2.2
1	F	317	LEU	2.2
1	F	302	ILE	2.2
1	F	326	TRP	2.2
1	E	504	GLY	2.2
1	E	709	VAL	2.2
1	F	372	PHE	2.2
1	F	97	VAL	2.2
1	D	321	SER	2.1
1	C	371	LEU	2.1
1	D	121	ALA	2.1
1	B	713	LEU	2.1
1	C	103	TYR	2.1
1	F	365	ARG	2.1
1	E	441	SER	2.1
1	B	70	VAL	2.1
1	E	400	ASP	2.1
1	F	325	ASP	2.1
1	E	434	LYS	2.1
1	C	101	PHE	2.0
1	B	710	ARG	2.0
1	B	366	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OAR	G	4	11/11	0.98	0.17	-	16,18,27,28	0
2	OAR	I	4	11/11	0.97	0.15	-	19,25,35,37	0
2	FC0	L	1	14/15	0.68	0.45	-	74,88,91,91	0
2	FC0	J	1	14/15	0.67	0.40	-	65,83,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	OAR	K	4	11/11	0.97	0.17	-	19,25,30,30	0
2	FC0	H	1	14/15	0.64	0.44	-	68,81,87,88	0
2	FC0	G	1	14/15	0.77	0.39	-	69,77,79,80	0
2	OAR	L	4	11/11	0.97	0.14	-	24,26,35,38	0
2	OAR	J	4	11/11	0.97	0.15	-	20,23,27,31	0
2	FC0	K	1	14/15	0.73	0.37	-	72,83,84,84	0
2	OAR	H	4	11/11	0.96	0.15	-	23,27,32,33	0
2	FC0	I	1	14/15	0.80	0.28	-	70,84,87,88	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.