



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:33 AM UTC

PDB ID : 2VHI / pdb_00002vhi
Title : Crystal structure of a pyrimidine degrading enzyme from *Drosophila melanogaster*
Authors : Lundgren, S.; Lohkamp, B.; Andersen, B.; Piskur, J.; Dobritsch, D.
Deposited on : 2007-11-21
Resolution : 3.30 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:

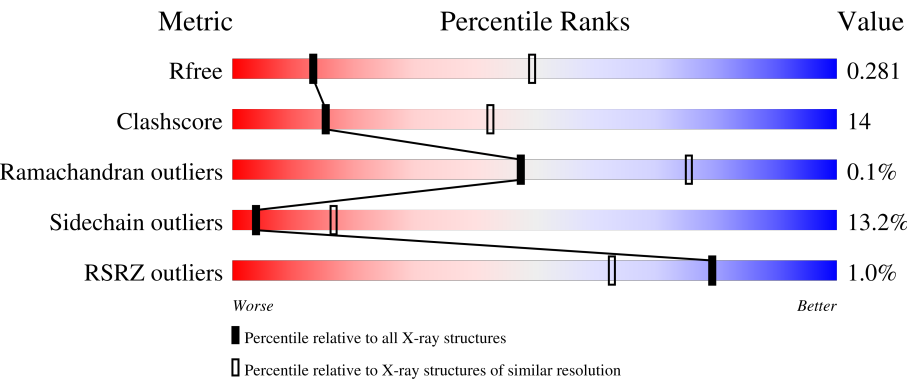
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	405	% 52%29%5%14%
1	B	405	59%30%6%
1	C	405	% 59%31%6%
1	D	405	% 60%28%6%6%
1	E	405	2% 60%29%6%

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Mol	Chain	Length	Quality of chain
1	F	405	63%26%6%
1	G	405	61%28%6%
1	H	405	%54%26%16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23689 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.

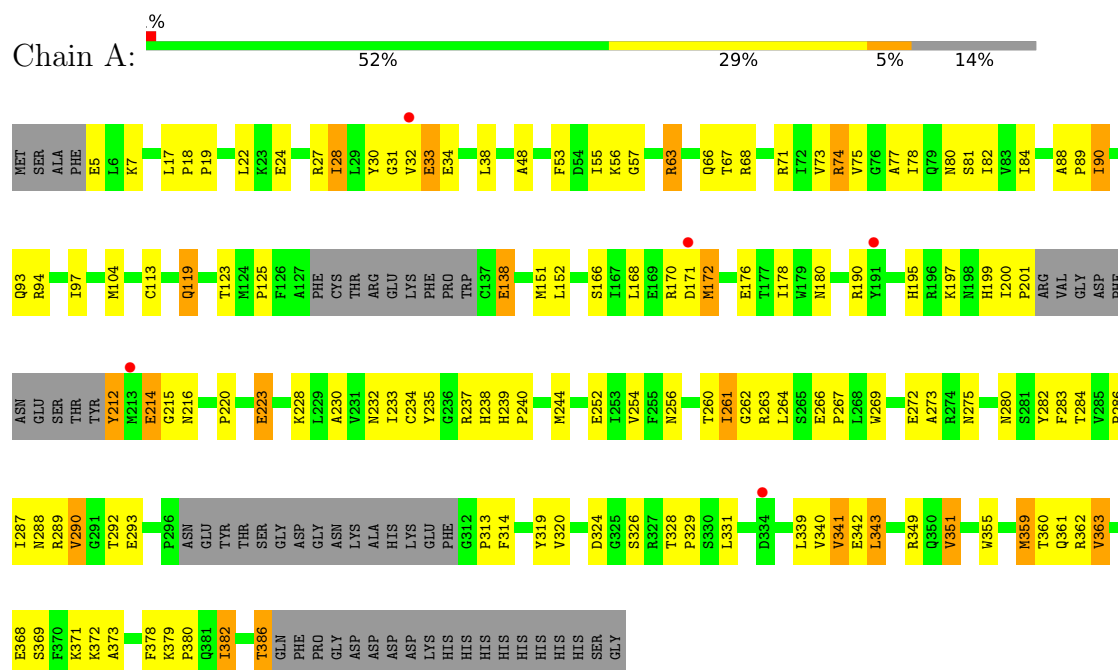
- Molecule 1 is a protein called CG3027-PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	1	0
			2774	1756	487	516	15			
1	B	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			
1	C	381	Total	C	N	O	S	0	0	0
			3044	1928	533	567	16			
1	D	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			
1	E	380	Total	C	N	O	S	0	0	0
			3036	1922	532	566	16			
1	F	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			
1	G	381	Total	C	N	O	S	0	0	0
			3044	1928	533	567	16			
1	H	342	Total	C	N	O	S	0	0	0
			2710	1712	478	505	15			

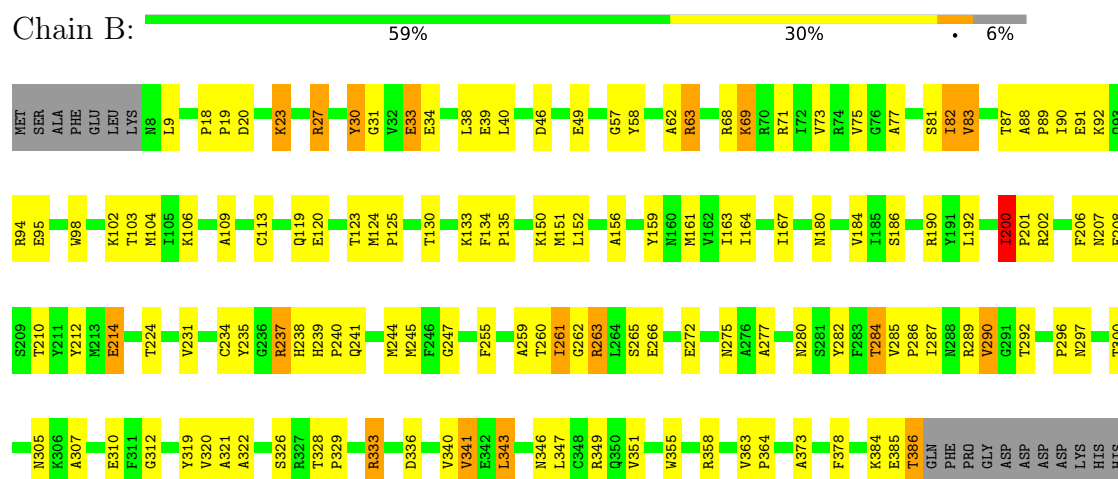
3 Residue-property plots

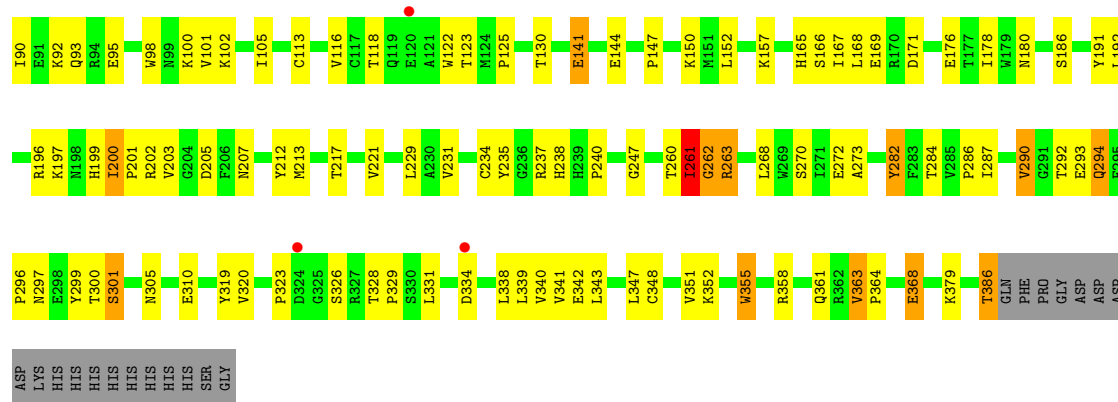
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CG3027-PA



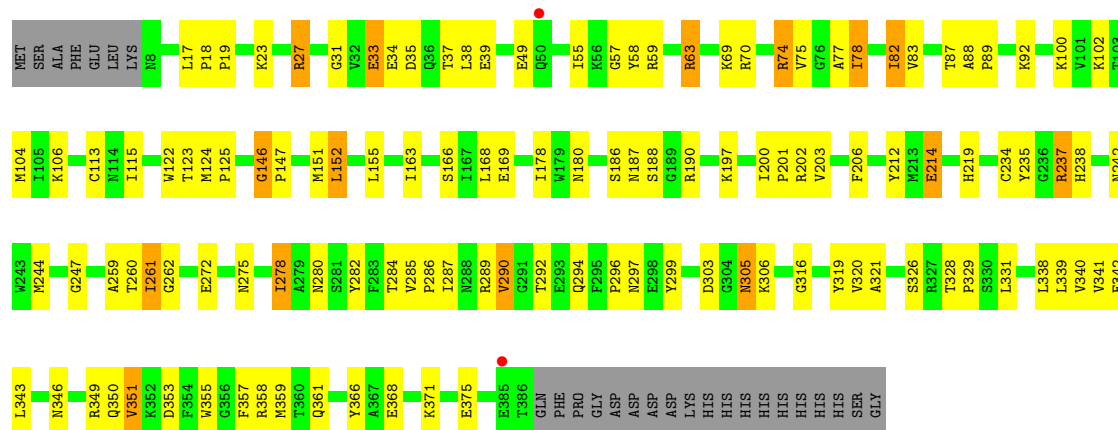
• Molecule 1: CG3027-PA





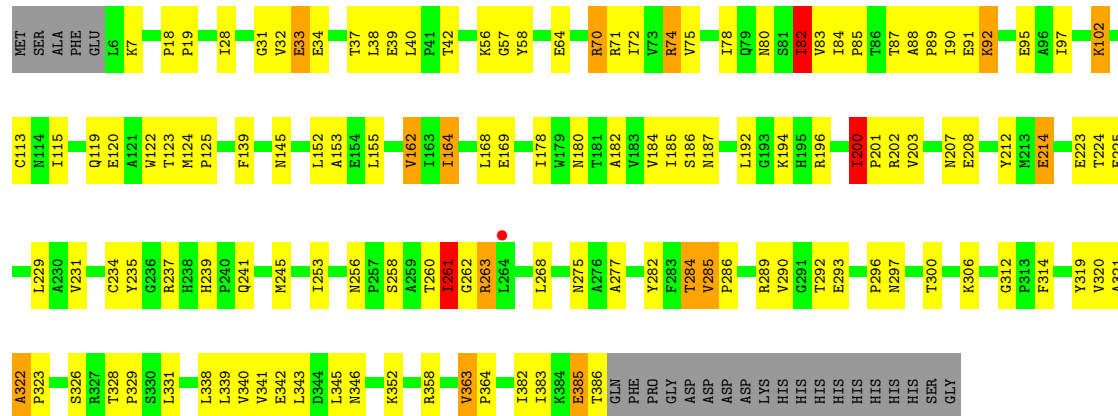
• Molecule 1: CG3027-PA

Chain F: 63% 26% 6%



• Molecule 1: CG3027-PA

Chain G: 61% 28% 6%



• Molecule 1: CG3027-PA

Chain H: 54% 26% 16%

1382	PHE	GLY	N99	MET
1383	PRO	ASP	K100	SER
K384	ASN	PHE	V101	ALA
E385	GLU	ASN	K102	PHE
T386	THR	GLU	T103	GLU
GLN	SER	THR	M104	LEU
PHE	GLY	TYR	I105	LYS
PRO	ASP	TYR	V116	N8
GLY	GLY	M213	Q119	L9
ASP	ASN	E214	E120	N10
ASP	LYS	T217	A121	D11
ASP	ALA	F222	A127	P18
LYS	HIS	E223	CYS	F19
HIS	LYS	PHE	THR	D20
HIS	GLU	V231	ARG	E21
HIS	PHE	N232	GLU	L22
HIS	GLY	I233	LYS	Y30
HIS	GLU	C234	PHE	G31
HIS	GLU	Y235	PRO	V32
HIS	GLY	G236	TRP	E33
SER	SER	R237	C137	E34
GLY	S326	H238	E142	L38
	R327	H239	M145	M51
	T328	P240	K150	K56
	S329	Q241	M151	G57
	L331	M244	L152	Y58
	R332	N245	A153	R59
	R333	L248	E154	R63
	D334	N256	I164	E64
	K335	T260	L168	K69
	D336	I261	E169	V73
	L339	G262	R170	R74
	V340	R263	D171	V75
	V341	E266	M172	G76
	E342	P267	E173	A77
	L343	E272	H174	I78
	L343	A273	E176	S81
	V351	N280	A182	I82
	V351	S281	V183	V83
	K355	Y282	V184	I84
	T360	T283	R190	A88
	V363	T284	K196	P89
	S369	V285	K197	K92
	A373	P286	G197	Q93
	S374	I287	P201	E94
	E375	G288	ARG	E95
	H376	R289	VAL	A96
	G377	V290		I97
	F378	Q294		W98
	K379			
	P380			
	Q381			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.86Å 95.05Å 199.31Å 90.00° 125.82° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.6 (30.00-3.30) 85.4 (30.00-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.282 0.229 , 0.281	Depositor DCC
R_{free} test set	2766 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23689	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	1/2835 (0.0%)	0.95	3/3833 (0.1%)
1	B	0.55	0/3101	0.92	5/4197 (0.1%)
1	C	0.58	0/3118	0.98	6/4219 (0.1%)
1	D	0.57	0/3101	0.92	2/4197 (0.0%)
1	E	0.59	0/3110	0.96	4/4208 (0.1%)
1	F	0.56	0/3101	0.92	4/4197 (0.1%)
1	G	0.59	0/3118	0.94	5/4219 (0.1%)
1	H	0.60	1/2768 (0.0%)	0.92	0/3742
All	All	0.58	2/24252 (0.0%)	0.94	29/32812 (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	1
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	VAL	CA-CB	5.39	1.56	1.54
1	H	363	VAL	CA-CB	5.05	1.56	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ILE	N-CA-C	-7.88	101.46	110.05
1	A	262	GLY	N-CA-C	-6.88	101.57	110.38
1	E	262	GLY	N-CA-C	-6.80	101.22	110.20
1	G	262	GLY	N-CA-C	-6.67	101.39	110.20
1	D	305	ASN	N-CA-C	6.60	118.52	110.41
1	E	261	ILE	N-CA-C	-6.40	100.56	109.45
1	C	262	GLY	N-CA-C	-6.35	101.82	110.20
1	E	200	ILE	N-CA-C	6.23	114.83	107.73
1	E	305	ASN	N-CA-C	6.01	118.46	110.53
1	C	8	ASN	N-CA-C	5.90	117.08	107.23
1	B	305	ASN	N-CA-C	5.86	118.11	110.43
1	F	305	ASN	N-CA-C	5.77	117.99	110.43
1	F	262	GLY	N-CA-C	5.69	119.06	110.97
1	B	262	GLY	N-CA-C	5.65	118.13	111.63
1	G	200	ILE	N-CA-C	5.46	113.96	107.73
1	C	124	MET	N-CA-C	5.35	113.04	108.22
1	G	261	ILE	N-CA-C	-5.32	100.72	109.12
1	D	262	GLY	N-CA-C	5.30	118.21	111.85
1	C	185	ILE	CB-CA-C	-5.27	103.76	110.98
1	B	200	ILE	N-CA-C	5.24	113.64	107.77
1	F	146	GLY	CA-C-N	5.21	124.66	119.24
1	F	146	GLY	C-N-CA	5.21	124.66	119.24
1	A	363	VAL	CB-CA-C	-5.21	108.75	113.70
1	C	146	GLY	CA-C-N	5.18	124.63	119.24
1	C	146	GLY	C-N-CA	5.18	124.63	119.24
1	B	322	ALA	CA-C-N	5.14	124.80	119.56
1	B	322	ALA	C-N-CA	5.14	124.80	119.56
1	G	322	ALA	CA-C-N	5.02	124.68	119.56
1	G	322	ALA	C-N-CA	5.02	124.68	119.56

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ILE	Peptide
1	B	261	ILE	Peptide
1	C	261	ILE	Peptide
1	C	82	ILE	Peptide
1	D	261	ILE	Peptide
1	D	82	ILE	Peptide
1	E	261	ILE	Peptide
1	F	261	ILE	Peptide
1	G	261	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	G	82	ILE	Peptide
1	H	261	ILE	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	2774	0	2738	89	0
1	B	3027	0	2958	93	0
1	C	3044	0	2982	95	0
1	D	3027	0	2958	91	0
1	E	3036	0	2971	85	0
1	F	3027	0	2958	72	0
1	G	3044	0	2982	83	0
1	H	2710	0	2678	92	0
All	All	23689	0	23225	634	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 14.

All (634) 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:63:ARG:HG3	1:C:350:GLN:OE1	1.58	1.04
1:B:63:ARG:HB2	1:B:63:ARG:HH11	1.17	1.04
1:A:172:MET:HE3	1:A:176:GLU:HG2	1.42	1.01
1:H:197:LYS:HA	1:H:233:ILE:HD13	1.42	1.01
1:G:87:THR:HG22	1:G:296:PRO:HG3	1.43	0.97
1:E:66:GLN:HE22	1:G:90:ILE:H	0.98	0.96
1:A:31:GLY:HA3	1:A:326:SER:HA	1.48	0.94
1:G:31:GLY:HA3	1:G:326:SER:HA	1.50	0.94
1:A:386:THR:HG22	1:B:190:ARG:HH22	1.32	0.93
1:H:31:GLY:HA3	1:H:326:SER:HA	1.49	0.92
1:D:31:GLY:HA3	1:D:326:SER:HA	1.48	0.92
1:A:33:GLU:CD	1:A:33:GLU:H	1.78	0.90
1:B:31:GLY:HA3	1:B:326:SER:HA	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:GLY:HA3	1:E:326:SER:HA	1.53	0.90
1:F:31:GLY:HA3	1:F:326:SER:HA	1.52	0.89
1:C:31:GLY:HA3	1:C:326:SER:HA	1.54	0.89
1:E:328:THR:HG22	1:E:329:PRO:O	1.73	0.88
1:G:284:THR:HG22	1:G:321:ALA:HB3	1.56	0.87
1:C:102:LYS:HE2	1:C:151:MET:HE2	1.57	0.86
1:C:234:CYS:O	1:C:237:ARG:HB2	1.76	0.86
1:A:74:ARG:HD2	1:A:342:GLU:HB2	1.58	0.85
1:D:263:ARG:H	1:D:263:ARG:HD2	1.40	0.84
1:B:300:THR:HG21	1:C:299:TYR:HA	1.62	0.82
1:D:201:PRO:HB3	1:D:235:TYR:CD1	2.15	0.81
1:G:328:THR:HG22	1:G:329:PRO:O	1.79	0.81
1:F:87:THR:HG22	1:F:296:PRO:HG3	1.61	0.81
1:E:263:ARG:H	1:E:263:ARG:CD	1.94	0.81
1:B:63:ARG:HH11	1:B:63:ARG:CB	1.93	0.81
1:G:74:ARG:HD2	1:G:342:GLU:HB2	1.63	0.81
1:B:285:VAL:HG22	1:B:320:VAL:HG22	1.62	0.80
1:E:386:THR:HG22	1:F:190:ARG:HH22	1.46	0.80
1:A:292:THR:HG22	1:A:313:PRO:HA	1.61	0.80
1:B:109:ALA:HA	1:B:161:MET:HE1	1.61	0.80
1:E:234:CYS:O	1:E:237:ARG:HB2	1.81	0.80
1:E:74:ARG:HD2	1:E:342:GLU:HB2	1.64	0.79
1:E:66:GLN:HE22	1:G:90:ILE:N	1.80	0.79
1:B:63:ARG:HB2	1:B:63:ARG:NH1	1.98	0.79
1:D:328:THR:HG22	1:D:329:PRO:O	1.82	0.79
1:C:55:ILE:HD12	1:C:338:LEU:HD23	1.63	0.79
1:G:284:THR:CG2	1:G:321:ALA:HB3	2.12	0.79
1:A:63:ARG:HH11	1:A:63:ARG:HB2	1.47	0.78
1:A:119:GLN:OE1	1:A:289:ARG:HA	1.84	0.78
1:E:201:PRO:HB3	1:E:235:TYR:CD1	2.19	0.78
1:F:124:MET:O	1:F:289:ARG:NH1	2.17	0.77
1:G:363:VAL:HG23	1:G:364:PRO:HD3	1.66	0.77
1:A:33:GLU:CD	1:A:33:GLU:N	2.42	0.76
1:H:172:MET:SD	1:H:176:GLU:HG2	2.24	0.76
1:F:284:THR:HG22	1:F:286:PRO:HD3	1.68	0.76
1:H:164:ILE:HG12	1:H:184:VAL:HG22	1.67	0.76
1:C:205:ASP:OD1	1:C:301:SER:HB3	1.84	0.76
1:B:124:MET:O	1:B:289:ARG:NH1	2.19	0.75
1:H:83:VAL:HG11	1:H:96:ALA:CB	2.16	0.75
1:G:275:ASN:ND2	1:H:272:GLU:HA	2.01	0.75
1:E:263:ARG:H	1:E:263:ARG:HD2	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:ARG:H	1:G:263:ARG:HD2	1.51	0.75
1:A:172:MET:HE3	1:A:176:GLU:CG	2.17	0.75
1:D:234:CYS:O	1:D:237:ARG:HB2	1.87	0.74
1:B:82:ILE:HG12	1:B:83:VAL:N	2.02	0.73
1:D:284:THR:HG22	1:D:286:PRO:HD3	1.70	0.73
1:H:331:LEU:HD11	1:H:339:LEU:HB2	1.70	0.73
1:D:261:ILE:HG21	1:D:312:GLY:HA2	1.71	0.73
1:D:263:ARG:HD2	1:D:263:ARG:N	2.04	0.72
1:C:63:ARG:HG2	1:C:63:ARG:HH11	1.54	0.72
1:C:263:ARG:HA	1:D:27:ARG:HH21	1.55	0.72
1:C:87:THR:HG22	1:C:296:PRO:HG3	1.72	0.71
1:C:286:PRO:HD2	1:C:319:TYR:O	1.90	0.71
1:H:83:VAL:HG11	1:H:96:ALA:HB1	1.73	0.71
1:H:233:ILE:HD12	1:H:233:ILE:H	1.56	0.70
1:F:200:ILE:HD13	1:F:214:GLU:HA	1.74	0.70
1:H:51:ASN:N	1:H:51:ASN:HD22	1.89	0.70
1:E:84:ILE:HD11	1:E:93:GLN:HA	1.72	0.70
1:B:328:THR:HG22	1:B:329:PRO:O	1.91	0.69
1:E:352:LYS:HD3	1:E:358:ARG:HG3	1.72	0.69
1:B:119:GLN:OE1	1:B:289:ARG:HA	1.91	0.69
1:B:234:CYS:O	1:B:237:ARG:HB3	1.92	0.69
1:E:386:THR:HG22	1:F:190:ARG:NH2	2.06	0.69
1:H:78:ILE:HD11	1:H:116:VAL:CG1	2.23	0.69
1:A:234:CYS:O	1:A:237:ARG:HB2	1.93	0.68
1:B:82:ILE:HG12	1:B:83:VAL:H	1.58	0.68
1:F:188:SER:OG	1:F:190:ARG:HG3	1.94	0.68
1:H:8:ASN:HD22	1:H:11:ASP:H	1.40	0.68
1:E:205:ASP:OD1	1:E:301:SER:HB3	1.94	0.68
1:E:273:ALA:HB1	1:E:286:PRO:HG3	1.76	0.68
1:A:190:ARG:HH22	1:B:386:THR:HG22	1.58	0.68
1:E:199:HIS:NE2	1:F:366:TYR:OH	2.26	0.67
1:B:27:ARG:HH11	1:B:27:ARG:HB3	1.58	0.67
1:F:234:CYS:O	1:F:237:ARG:HB3	1.94	0.67
1:F:328:THR:HG22	1:F:329:PRO:O	1.94	0.67
1:G:70:ARG:HA	1:G:346:ASN:HD21	1.60	0.67
1:H:351:VAL:HG13	1:H:355:TRP:HE3	1.58	0.67
1:E:261:ILE:HD12	1:E:262:GLY:HA3	1.76	0.67
1:G:285:VAL:HG13	1:G:320:VAL:HG22	1.76	0.67
1:A:84:ILE:HD11	1:A:93:GLN:HA	1.75	0.66
1:A:286:PRO:HD2	1:A:319:TYR:O	1.96	0.66
1:E:66:GLN:NE2	1:G:90:ILE:H	1.84	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:VAL:HG22	1:H:84:ILE:HG23	1.76	0.66
1:F:285:VAL:HG13	1:F:320:VAL:HG22	1.78	0.66
1:D:280:ASN:O	1:D:358:ARG:NH1	2.28	0.66
1:A:197:LYS:HE3	1:A:199:HIS:O	1.96	0.66
1:H:263:ARG:H	1:H:263:ARG:HD3	1.60	0.66
1:A:284:THR:HG22	1:A:286:PRO:HD3	1.79	0.65
1:H:142:GLU:OE2	1:H:172:MET:HG2	1.96	0.65
1:A:170:ARG:HD3	1:A:172:MET:HE1	1.78	0.65
1:F:63:ARG:HB3	1:F:350:GLN:OE1	1.97	0.65
1:B:156:ALA:HB2	1:B:163:ILE:HD12	1.79	0.65
1:H:328:THR:HG22	1:H:329:PRO:O	1.98	0.64
1:G:234:CYS:O	1:G:237:ARG:HB3	1.98	0.64
1:C:33:GLU:CD	1:C:33:GLU:H	2.06	0.64
1:A:171:ASP:O	1:A:176:GLU:HA	1.98	0.64
1:A:328:THR:HG22	1:A:329:PRO:O	1.98	0.64
1:D:63:ARG:HB3	1:D:350:GLN:OE1	1.98	0.64
1:C:66:GLN:HE22	1:E:90:ILE:H	1.46	0.63
1:F:238:HIS:HA	1:F:272:GLU:OE1	1.98	0.63
1:A:24:GLU:OE2	1:A:27:ARG:NH1	2.32	0.63
1:C:383:ILE:HD12	1:D:222:PHE:CE2	2.33	0.63
1:C:124:MET:O	1:C:289:ARG:NH1	2.32	0.63
1:D:197:LYS:HE3	1:D:234:CYS:HB3	1.79	0.63
1:B:87:THR:HG22	1:B:296:PRO:HG3	1.79	0.63
1:G:75:VAL:HG12	1:G:115:ILE:HB	1.79	0.63
1:H:84:ILE:HD11	1:H:93:GLN:HA	1.81	0.62
1:H:273:ALA:O	1:H:284:THR:HG21	1.98	0.62
1:C:230:ALA:HB3	1:C:254:VAL:HG22	1.81	0.62
1:H:81:SER:HB3	1:H:290:VAL:O	1.99	0.62
1:B:31:GLY:HA3	1:B:326:SER:CA	2.28	0.62
1:C:275:ASN:ND2	1:D:272:GLU:HA	2.13	0.62
1:D:292:THR:HG22	1:D:313:PRO:HB3	1.80	0.62
1:H:373:ALA:HA	1:H:378:PHE:CD1	2.33	0.62
1:B:286:PRO:HD2	1:B:319:TYR:O	1.99	0.62
1:B:27:ARG:HB3	1:B:27:ARG:NH1	2.15	0.62
1:G:239:HIS:HD2	1:G:241:GLN:HE22	1.47	0.62
1:H:170:ARG:HE	1:H:172:MET:HE1	1.64	0.62
1:H:59:ARG:HG3	1:H:342:GLU:HG2	1.80	0.61
1:C:66:GLN:HE22	1:E:89:PRO:HA	1.64	0.61
1:C:190:ARG:HH22	1:D:386:THR:HG22	1.64	0.61
1:A:66:GLN:HE22	1:C:90:ILE:H	1.48	0.61
1:B:284:THR:HG23	1:B:286:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:GLY:HA3	1:F:326:SER:CA	2.30	0.61
1:E:77:ALA:HB1	1:E:287:ILE:HG12	1.83	0.61
1:H:33:GLU:CD	1:H:33:GLU:N	2.58	0.60
1:A:190:ARG:HH21	1:B:385:GLU:HG2	1.66	0.60
1:B:23:LYS:HG2	1:B:33:GLU:HB2	1.83	0.60
1:F:82:ILE:HG12	1:F:83:VAL:N	2.17	0.60
1:E:268:LEU:HD22	1:F:278:ILE:HG21	1.84	0.60
1:G:33:GLU:H	1:G:33:GLU:CD	2.10	0.60
1:E:199:HIS:HE2	1:F:366:TYR:HH	1.49	0.60
1:A:94:ARG:HG3	1:A:123:THR:OG1	2.01	0.60
1:H:263:ARG:HD3	1:H:263:ARG:N	2.17	0.60
1:A:172:MET:CE	1:A:176:GLU:HG2	2.27	0.59
1:C:57:GLY:HA2	1:C:340:VAL:O	2.02	0.59
1:C:284:THR:HG22	1:C:286:PRO:HD3	1.84	0.59
1:C:328:THR:HG23	1:C:329:PRO:O	2.02	0.59
1:C:31:GLY:HA3	1:C:326:SER:CA	2.30	0.59
1:G:208:GLU:OE2	1:G:212:TYR:OH	2.18	0.59
1:A:380:PRO:HB2	1:A:382:ILE:HD12	1.85	0.59
1:G:115:ILE:HG23	1:G:162:VAL:HG12	1.84	0.59
1:G:162:VAL:HG22	1:G:186:SER:HA	1.83	0.59
1:H:121:ALA:O	1:H:289:ARG:NH2	2.36	0.59
1:F:55:ILE:HD12	1:F:338:LEU:HD23	1.85	0.58
1:G:120:GLU:CD	1:G:234:CYS:HB2	2.28	0.58
1:H:318:SER:HB2	1:H:331:LEU:HD12	1.85	0.58
1:C:363:VAL:HG23	1:C:364:PRO:HD3	1.84	0.58
1:A:178:ILE:HG22	1:A:212:TYR:HD1	1.68	0.58
1:B:82:ILE:HD12	1:B:125:PRO:HB3	1.85	0.58
1:E:31:GLY:HA3	1:E:326:SER:CA	2.28	0.58
1:E:286:PRO:HD2	1:E:319:TYR:O	2.04	0.57
1:H:78:ILE:HD11	1:H:116:VAL:HG13	1.85	0.57
1:C:287:ILE:HA	1:C:318:SER:OG	2.04	0.57
1:A:238:HIS:ND1	1:A:272:GLU:OE2	2.29	0.57
1:B:266:GLU:OE1	1:B:333:ARG:NH1	2.38	0.57
1:C:200:ILE:HD13	1:C:214:GLU:HA	1.85	0.57
1:C:275:ASN:HD22	1:D:271:ILE:HG22	1.70	0.57
1:H:83:VAL:HG12	1:H:97:ILE:HG13	1.85	0.57
1:E:118:THR:HG1	1:E:122:TRP:CD1	2.22	0.57
1:H:171:ASP:O	1:H:176:GLU:HA	2.04	0.57
1:C:100:LYS:O	1:C:103:THR:HG23	2.04	0.57
1:G:58:TYR:CD1	1:G:328:THR:HG23	2.40	0.57
1:C:275:ASN:HD21	1:D:272:GLU:HG2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ILE:HG12	1:E:293:GLU:HG2	1.87	0.57
1:F:57:GLY:HA2	1:F:340:VAL:O	2.05	0.57
1:B:263:ARG:H	1:B:263:ARG:HD2	1.70	0.56
1:D:31:GLY:HA3	1:D:326:SER:CA	2.29	0.56
1:E:273:ALA:CB	1:E:286:PRO:HG3	2.35	0.56
1:B:57:GLY:HA2	1:B:340:VAL:O	2.06	0.56
1:B:247:GLY:C	1:B:358:ARG:HH22	2.12	0.56
1:D:320:VAL:HG21	1:D:341:VAL:HG11	1.88	0.56
1:G:284:THR:HG22	1:G:321:ALA:CB	2.31	0.56
1:F:74:ARG:HG3	1:F:342:GLU:HB2	1.86	0.56
1:H:351:VAL:HG13	1:H:355:TRP:CE3	2.40	0.56
1:B:71:ARG:H	1:B:346:ASN:ND2	2.03	0.56
1:F:77:ALA:HB1	1:F:287:ILE:HG12	1.86	0.56
1:G:57:GLY:HA2	1:G:340:VAL:O	2.05	0.56
1:B:284:THR:HG22	1:B:321:ALA:HB3	1.88	0.56
1:D:57:GLY:HA2	1:D:340:VAL:O	2.05	0.55
1:E:197:LYS:NZ	1:E:234:CYS:HB3	2.21	0.55
1:H:83:VAL:HG22	1:H:84:ILE:N	2.20	0.55
1:H:263:ARG:HH11	1:H:263:ARG:HG2	1.70	0.55
1:H:320:VAL:HG21	1:H:341:VAL:HG11	1.88	0.55
1:H:286:PRO:HD2	1:H:319:TYR:O	2.07	0.55
1:B:33:GLU:H	1:B:33:GLU:CD	2.15	0.55
1:D:119:GLN:OE1	1:D:289:ARG:HA	2.06	0.55
1:G:164:ILE:HG21	1:G:231:VAL:HG21	1.88	0.55
1:A:151:MET:SD	1:A:152:LEU:HD12	2.47	0.55
1:B:164:ILE:HG21	1:B:231:VAL:HG21	1.87	0.55
1:G:364:PRO:HG3	1:H:374:SER:HB2	1.87	0.55
1:E:263:ARG:CD	1:E:263:ARG:N	2.68	0.55
1:G:164:ILE:HG23	1:G:184:VAL:HG22	1.89	0.55
1:A:273:ALA:HB1	1:A:284:THR:HG21	1.89	0.55
1:D:282:TYR:C	1:D:323:PRO:HG3	2.31	0.55
1:F:82:ILE:HD12	1:F:125:PRO:HB3	1.89	0.55
1:A:57:GLY:HA2	1:A:340:VAL:O	2.07	0.55
1:E:30:TYR:CD1	1:E:30:TYR:N	2.75	0.55
1:F:197:LYS:NZ	1:F:234:CYS:HB3	2.21	0.55
1:G:223:GLU:OE1	1:H:384:LYS:HE3	2.07	0.55
1:G:277:ALA:HB2	1:G:284:THR:HB	1.89	0.55
1:G:286:PRO:HD2	1:G:319:TYR:O	2.07	0.54
1:D:300:THR:HG21	1:E:299:TYR:HA	1.87	0.54
1:F:299:TYR:HA	1:G:300:THR:HG21	1.89	0.54
1:E:238:HIS:O	1:E:240:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:VAL:HG13	1:C:355:TRP:HE3	1.71	0.54
1:H:84:ILE:HD11	1:H:93:GLN:CA	2.37	0.54
1:E:40:LEU:HD13	1:E:55:ILE:HG12	1.88	0.54
1:E:205:ASP:CG	1:E:301:SER:HB3	2.32	0.54
1:H:77:ALA:HB1	1:H:287:ILE:HG12	1.90	0.54
1:E:144:GLU:HG3	1:E:191:TYR:CG	2.44	0.53
1:E:57:GLY:HA2	1:E:340:VAL:O	2.08	0.53
1:H:74:ARG:HG2	1:H:342:GLU:HB2	1.90	0.53
1:H:245:MET:HA	1:H:248:LEU:HD12	1.91	0.53
1:A:244:MET:HA	1:A:280:ASN:OD1	2.08	0.53
1:B:31:GLY:HA3	1:B:326:SER:CB	2.39	0.53
1:B:341:VAL:HG22	1:B:343:LEU:HD23	1.90	0.53
1:D:170:ARG:NH1	1:F:353:ASP:OD1	2.41	0.53
1:E:368:GLU:OE1	1:E:368:GLU:HA	2.08	0.53
1:H:33:GLU:N	1:H:33:GLU:OE2	2.41	0.53
1:E:43:SER:O	1:E:47:ILE:HD12	2.09	0.53
1:G:120:GLU:OE1	1:G:234:CYS:HB2	2.09	0.53
1:E:31:GLY:HA3	1:E:326:SER:CB	2.39	0.53
1:B:277:ALA:HB2	1:B:284:THR:HB	1.91	0.52
1:F:357:PHE:O	1:F:361:GLN:HG3	2.09	0.52
1:G:31:GLY:HA3	1:G:326:SER:CA	2.30	0.52
1:A:195:HIS:ND1	1:A:220:PRO:HD2	2.23	0.52
1:F:371:LYS:O	1:F:375:GLU:HG3	2.08	0.52
1:D:83:VAL:HG13	1:D:84:ILE:H	1.73	0.52
1:C:28:ILE:HD11	1:D:9:LEU:HD13	1.90	0.52
1:D:30:TYR:CD1	1:D:30:TYR:N	2.77	0.52
1:E:84:ILE:HD11	1:E:93:GLN:CA	2.39	0.52
1:H:31:GLY:HA3	1:H:326:SER:CA	2.30	0.52
1:H:83:VAL:HG13	1:H:84:ILE:H	1.74	0.52
1:C:319:TYR:HB2	1:C:328:THR:HG22	1.90	0.52
1:F:280:ASN:O	1:F:358:ARG:NH1	2.42	0.52
1:G:284:THR:HG23	1:G:286:PRO:HD3	1.92	0.52
1:H:88:ALA:O	1:H:89:PRO:C	2.53	0.52
1:B:373:ALA:HA	1:B:378:PHE:CD1	2.45	0.52
1:E:284:THR:HG22	1:E:286:PRO:HD3	1.92	0.52
1:E:294:GLN:HB3	1:E:310:GLU:HG3	1.90	0.52
1:A:232:ASN:O	1:A:256:ASN:ND2	2.32	0.52
1:A:272:GLU:HA	1:B:275:ASN:ND2	2.25	0.52
1:C:164:ILE:HG21	1:C:231:VAL:HG21	1.91	0.52
1:A:178:ILE:HG22	1:A:212:TYR:CD1	2.44	0.51
1:E:141:GLU:OE1	1:E:147:PRO:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LYS:HG2	1:C:155:LEU:HD11	1.92	0.51
1:D:172:MET:HE1	1:F:349:ARG:HH22	1.73	0.51
1:D:181:THR:CG2	1:D:194:LYS:HB2	2.39	0.51
1:G:78:ILE:HG12	1:G:338:LEU:HD13	1.91	0.51
1:D:230:ALA:HB3	1:D:254:VAL:HG22	1.93	0.51
1:B:30:TYR:CD1	1:B:30:TYR:N	2.79	0.51
1:D:39:GLU:HA	1:D:39:GLU:OE2	2.10	0.51
1:A:373:ALA:HA	1:A:378:PHE:CD1	2.45	0.51
1:F:31:GLY:CA	1:F:326:SER:HA	2.34	0.51
1:H:78:ILE:HD11	1:H:116:VAL:HG11	1.93	0.51
1:A:31:GLY:HA3	1:A:326:SER:CA	2.33	0.51
1:G:239:HIS:CD2	1:G:241:GLN:HE22	2.27	0.51
1:A:74:ARG:HB3	1:A:113:CYS:HA	1.92	0.50
1:C:75:VAL:HG12	1:C:115:ILE:HB	1.93	0.50
1:D:77:ALA:HB1	1:D:287:ILE:HG12	1.92	0.50
1:G:194:LYS:NZ	1:G:196:ARG:NH2	2.60	0.50
1:A:200:ILE:HD13	1:A:214:GLU:HA	1.94	0.50
1:A:292:THR:HG22	1:A:313:PRO:CA	2.37	0.50
1:H:51:ASN:N	1:H:51:ASN:ND2	2.60	0.50
1:H:284:THR:HG22	1:H:286:PRO:HD3	1.93	0.50
1:A:228:LYS:HB2	1:A:252:GLU:HG3	1.94	0.50
1:B:180:ASN:HB2	1:B:212:TYR:CE2	2.46	0.50
1:D:83:VAL:HG13	1:D:84:ILE:N	2.27	0.50
1:F:303:ASP:OD2	1:F:305:ASN:HB2	2.11	0.50
1:G:192:LEU:HD11	1:G:224:THR:HG22	1.94	0.50
1:G:256:ASN:HB3	1:G:286:PRO:HA	1.92	0.50
1:D:23:LYS:HD2	1:D:33:GLU:HB2	1.94	0.50
1:G:31:GLY:CA	1:G:326:SER:HA	2.33	0.50
1:G:320:VAL:H	1:G:328:THR:HB	1.77	0.50
1:D:74:ARG:HG3	1:D:342:GLU:HB2	1.93	0.50
1:A:283:PHE:CD2	1:A:343:LEU:HD22	2.47	0.50
1:C:82:ILE:HD13	1:C:125:PRO:HB3	1.93	0.50
1:C:324:ASP:HA	1:C:355:TRP:HZ3	1.77	0.50
1:C:374:SER:HB2	1:D:364:PRO:HG3	1.92	0.50
1:E:83:VAL:HG22	1:E:100:LYS:HD3	1.93	0.50
1:E:180:ASN:HB2	1:E:212:TYR:CZ	2.47	0.50
1:F:284:THR:HB	1:F:321:ALA:HB3	1.93	0.50
1:C:82:ILE:HG12	1:C:293:GLU:HG2	1.94	0.50
1:F:82:ILE:CG1	1:F:83:VAL:N	2.75	0.50
1:F:244:MET:HA	1:F:280:ASN:OD1	2.11	0.50
1:G:28:ILE:HD11	1:H:9:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:PRO:HB3	1:G:235:TYR:CD1	2.47	0.50
1:A:88:ALA:O	1:A:89:PRO:C	2.54	0.49
1:A:369:SER:HB3	1:B:245:MET:SD	2.52	0.49
1:C:256:ASN:HB3	1:C:286:PRO:HA	1.92	0.49
1:D:164:ILE:HG21	1:D:231:VAL:HG21	1.94	0.49
1:F:152:LEU:HG	1:F:163:ILE:HG21	1.93	0.49
1:F:320:VAL:HG21	1:F:341:VAL:HG11	1.93	0.49
1:E:351:VAL:HG13	1:E:355:TRP:HE3	1.77	0.49
1:H:38:LEU:HG	1:H:59:ARG:HB2	1.94	0.49
1:A:67:THR:HG22	1:C:91:GLU:OE1	2.12	0.49
1:E:98:TRP:O	1:E:102:LYS:HG3	2.13	0.49
1:G:200:ILE:HD13	1:G:214:GLU:HA	1.93	0.49
1:F:197:LYS:HE3	1:F:234:CYS:HB3	1.95	0.49
1:A:82:ILE:HD13	1:A:125:PRO:HB3	1.95	0.49
1:A:331:LEU:HD11	1:A:339:LEU:HB2	1.95	0.49
1:C:237:ARG:HG3	1:C:256:ASN:OD1	2.13	0.49
1:G:263:ARG:HD2	1:G:263:ARG:N	2.23	0.49
1:B:106:LYS:HG3	1:B:159:TYR:OH	2.12	0.49
1:G:74:ARG:HB3	1:G:113:CYS:HA	1.95	0.49
1:A:230:ALA:HB3	1:A:254:VAL:HG22	1.95	0.48
1:C:382:ILE:HA	1:D:221:VAL:O	2.13	0.48
1:D:238:HIS:ND1	1:D:272:GLU:OE1	2.44	0.48
1:E:323:PRO:HG2	1:E:347:LEU:HG	1.94	0.48
1:F:78:ILE:HG13	1:F:338:LEU:HD13	1.94	0.48
1:A:351:VAL:HG13	1:A:355:TRP:HE3	1.77	0.48
1:C:186:SER:HB2	1:C:192:LEU:HD21	1.96	0.48
1:E:290:VAL:HG22	1:E:334:ASP:HA	1.95	0.48
1:H:57:GLY:HA2	1:H:340:VAL:O	2.14	0.48
1:H:83:VAL:HG11	1:H:96:ALA:HB3	1.93	0.48
1:D:144:GLU:HG3	1:D:191:TYR:CG	2.47	0.48
1:F:169:GLU:O	1:F:178:ILE:HA	2.14	0.48
1:H:233:ILE:HD12	1:H:233:ILE:N	2.27	0.48
1:C:118:THR:OG1	1:C:165:HIS:HA	2.14	0.48
1:C:359:MET:O	1:E:213:MET:HG3	2.13	0.48
1:D:31:GLY:CA	1:D:326:SER:HA	2.32	0.48
1:D:184:VAL:HG21	1:D:222:PHE:CD1	2.48	0.48
1:D:299:TYR:HA	1:E:300:THR:HG21	1.95	0.48
1:C:284:THR:HB	1:C:321:ALA:HB3	1.96	0.48
1:C:18:PRO:HD2	1:D:16:HIS:CD2	2.48	0.48
1:H:151:MET:O	1:H:154:GLU:HB2	2.14	0.48
1:H:237:ARG:HH12	1:H:260:THR:HG21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:THR:HG22	1:D:124:MET:HE2	1.95	0.48
1:E:83:VAL:CG2	1:E:100:LYS:HD3	2.43	0.48
1:G:253:ILE:HD11	1:G:345:LEU:HD21	1.96	0.48
1:A:31:GLY:CA	1:A:326:SER:HA	2.34	0.47
1:A:55:ILE:HG23	1:A:55:ILE:O	2.13	0.47
1:A:349:ARG:NH2	1:C:176:GLU:OE2	2.46	0.47
1:B:201:PRO:HB3	1:B:235:TYR:CD1	2.49	0.47
1:D:108:ALA:HB2	1:D:338:LEU:HD11	1.95	0.47
1:D:150:LYS:HA	1:D:150:LYS:HE2	1.97	0.47
1:A:238:HIS:O	1:A:240:PRO:HD3	2.14	0.47
1:A:275:ASN:HD22	1:B:272:GLU:HA	1.78	0.47
1:E:78:ILE:HD11	1:E:116:VAL:HG13	1.96	0.47
1:G:119:GLN:OE1	1:G:289:ARG:HA	2.14	0.47
1:C:75:VAL:HG23	1:C:341:VAL:HG12	1.96	0.47
1:H:266:GLU:N	1:H:267:PRO:HD2	2.29	0.47
1:H:373:ALA:HA	1:H:378:PHE:CE1	2.49	0.47
1:F:75:VAL:HG12	1:F:115:ILE:HB	1.94	0.47
1:A:223:GLU:HG2	1:B:384:LYS:HG2	1.95	0.47
1:B:81:SER:HB3	1:B:290:VAL:O	2.13	0.47
1:C:30:TYR:HD2	1:C:327:ARG:HE	1.61	0.47
1:F:59:ARG:HG3	1:F:342:GLU:OE2	2.14	0.47
1:C:31:GLY:HA3	1:C:326:SER:CB	2.45	0.47
1:C:66:GLN:NE2	1:E:89:PRO:HA	2.29	0.47
1:D:144:GLU:HG3	1:D:191:TYR:CD2	2.49	0.47
1:H:58:TYR:CZ	1:H:329:PRO:HG2	2.49	0.47
1:C:82:ILE:HG21	1:C:125:PRO:HA	1.96	0.47
1:C:331:LEU:HD11	1:C:339:LEU:HB2	1.95	0.47
1:E:64:GLU:HG2	1:E:65:GLU:N	2.28	0.47
1:E:82:ILE:HG21	1:E:125:PRO:HA	1.96	0.47
1:E:88:ALA:O	1:E:89:PRO:C	2.58	0.47
1:E:31:GLY:CA	1:E:326:SER:HA	2.35	0.47
1:G:82:ILE:HD13	1:G:125:PRO:HB3	1.95	0.47
1:G:275:ASN:HD22	1:H:272:GLU:HA	1.78	0.47
1:B:82:ILE:CG1	1:B:83:VAL:H	2.27	0.47
1:E:272:GLU:HA	1:F:275:ASN:ND2	2.30	0.47
1:A:273:ALA:HB1	1:A:284:THR:CG2	2.44	0.47
1:C:90:ILE:HD13	1:C:138:GLU:HB2	1.97	0.47
1:D:221:VAL:HG22	1:D:230:ALA:HB2	1.96	0.47
1:C:151:MET:SD	1:C:151:MET:C	2.99	0.46
1:G:102:LYS:HG2	1:G:155:LEU:HD11	1.97	0.46
1:H:83:VAL:CG1	1:H:96:ALA:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HG21	1:B:312:GLY:HA2	1.97	0.46
1:D:286:PRO:HD2	1:D:319:TYR:O	2.16	0.46
1:E:82:ILE:HD13	1:E:125:PRO:HB3	1.98	0.46
1:G:82:ILE:HG21	1:G:125:PRO:HA	1.97	0.46
1:A:81:SER:HB3	1:A:290:VAL:O	2.15	0.46
1:C:31:GLY:CA	1:C:326:SER:HA	2.36	0.46
1:E:234:CYS:SG	1:E:235:TYR:N	2.89	0.46
1:F:351:VAL:HG13	1:F:355:TRP:HE3	1.80	0.46
1:G:386:THR:C	1:H:190:ARG:HH22	2.23	0.46
1:H:171:ASP:OD2	1:H:174:HIS:HB2	2.16	0.46
1:H:380:PRO:HB2	1:H:382:ILE:HD12	1.96	0.46
1:D:40:LEU:HD13	1:D:55:ILE:HG12	1.96	0.46
1:D:191:TYR:OH	1:D:194:LYS:HG2	2.15	0.46
1:D:238:HIS:O	1:D:240:PRO:HD3	2.15	0.46
1:E:48:ALA:HA	1:E:53:PHE:CE1	2.50	0.46
1:B:206:PHE:HE2	1:B:259:ALA:O	1.98	0.46
1:C:361:GLN:HB3	1:C:363:VAL:HG13	1.98	0.46
1:H:31:GLY:CA	1:H:326:SER:HA	2.34	0.46
1:A:77:ALA:HB1	1:A:287:ILE:HG12	1.97	0.46
1:C:364:PRO:HG3	1:D:374:SER:HB2	1.97	0.46
1:D:320:VAL:H	1:D:328:THR:HB	1.81	0.46
1:E:169:GLU:O	1:E:178:ILE:HA	2.16	0.46
1:F:88:ALA:O	1:F:89:PRO:C	2.56	0.46
1:B:98:TRP:CG	1:B:151:MET:HE2	2.51	0.46
1:A:84:ILE:HD11	1:A:93:GLN:CA	2.44	0.46
1:A:320:VAL:HG21	1:A:341:VAL:HG11	1.97	0.46
1:H:84:ILE:HD11	1:H:93:GLN:N	2.30	0.46
1:B:63:ARG:HH11	1:B:63:ARG:CG	2.28	0.46
1:G:89:PRO:HB2	1:G:92:LYS:HD2	1.97	0.46
1:H:83:VAL:CG1	1:H:96:ALA:CB	2.91	0.46
1:C:8:ASN:ND2	1:C:330:SER:O	2.48	0.46
1:E:87:THR:HG22	1:E:296:PRO:HG3	1.97	0.45
1:F:31:GLY:HA3	1:F:326:SER:CB	2.46	0.45
1:H:119:GLN:OE1	1:H:289:ARG:HA	2.16	0.45
1:B:88:ALA:O	1:B:89:PRO:C	2.57	0.45
1:B:320:VAL:H	1:B:328:THR:HB	1.81	0.45
1:C:148:THR:O	1:C:152:LEU:HB2	2.17	0.45
1:A:235:TYR:CE2	1:A:239:HIS:HE1	2.34	0.45
1:A:359:MET:HB2	1:A:359:MET:HE3	1.74	0.45
1:C:280:ASN:O	1:C:358:ARG:NH1	2.49	0.45
1:G:385:GLU:HG3	1:H:190:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HD11	1:B:9:LEU:HD22	1.99	0.45
1:A:66:GLN:HE21	1:A:66:GLN:HB3	1.63	0.45
1:A:90:ILE:HG12	1:A:138:GLU:HB3	1.99	0.45
1:E:358:ARG:HA	1:E:361:GLN:HG3	1.97	0.45
1:F:247:GLY:O	1:F:358:ARG:NH2	2.50	0.45
1:C:28:ILE:HD11	1:D:9:LEU:HD22	1.98	0.45
1:F:180:ASN:HB2	1:F:212:TYR:CZ	2.51	0.45
1:G:70:ARG:HA	1:G:346:ASN:ND2	2.28	0.45
1:F:33:GLU:CD	1:F:33:GLU:H	2.25	0.45
1:A:275:ASN:ND2	1:B:272:GLU:HA	2.32	0.45
1:B:31:GLY:CA	1:B:326:SER:HA	2.35	0.45
1:E:247:GLY:C	1:E:358:ARG:HH22	2.24	0.45
1:G:88:ALA:O	1:G:89:PRO:C	2.60	0.45
1:G:382:ILE:CG2	1:H:223:GLU:HB2	2.46	0.45
1:H:234:CYS:HB3	1:H:235:TYR:H	1.63	0.45
1:A:273:ALA:O	1:A:284:THR:HG21	2.17	0.45
1:B:40:LEU:HD21	1:B:57:GLY:HA3	1.99	0.45
1:E:74:ARG:HB3	1:E:113:CYS:HA	1.99	0.45
1:E:196:ARG:HD2	1:E:217:THR:HG23	1.98	0.45
1:F:197:LYS:CE	1:F:234:CYS:HB3	2.47	0.45
1:G:289:ARG:HD2	1:G:314:PHE:CD1	2.52	0.45
1:A:269:TRP:CZ2	1:A:288:ASN:HB2	2.51	0.45
1:F:358:ARG:HA	1:F:361:GLN:OE1	2.17	0.45
1:G:82:ILE:HG23	1:G:293:GLU:OE2	2.16	0.45
1:G:352:LYS:HG2	1:G:358:ARG:HG3	1.98	0.45
1:H:8:ASN:HB3	1:H:11:ASP:HB2	1.98	0.45
1:H:239:HIS:CD2	1:H:241:GLN:HE22	2.35	0.45
1:C:88:ALA:O	1:C:89:PRO:C	2.57	0.45
1:G:194:LYS:HZ2	1:G:196:ARG:HH21	1.64	0.45
1:G:194:LYS:HZ1	1:G:196:ARG:NH2	2.15	0.45
1:G:322:ALA:HB1	1:G:323:PRO:HD2	1.98	0.45
1:B:261:ILE:CG2	1:B:312:GLY:HA2	2.47	0.44
1:B:280:ASN:HB3	1:B:282:TYR:CE1	2.52	0.44
1:C:100:LYS:O	1:C:103:THR:CG2	2.64	0.44
1:G:97:ILE:HG21	1:G:122:TRP:O	2.18	0.44
1:B:77:ALA:HB1	1:B:287:ILE:HG12	1.99	0.44
1:D:261:ILE:CG2	1:D:312:GLY:HA2	2.43	0.44
1:E:122:TRP:NE1	1:E:165:HIS:HB2	2.32	0.44
1:G:180:ASN:HB2	1:G:212:TYR:CE2	2.52	0.44
1:H:244:MET:HA	1:H:280:ASN:OD1	2.17	0.44
1:C:382:ILE:CG2	1:D:223:GLU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ALA:HB2	1:D:163:ILE:HD12	1.99	0.44
1:E:95:GLU:O	1:E:98:TRP:HB2	2.17	0.44
1:B:91:GLU:HG2	1:B:94:ARG:HH21	1.82	0.44
1:D:84:ILE:HD11	1:D:93:GLN:HG2	1.98	0.44
1:F:18:PRO:HA	1:F:19:PRO:HD3	1.87	0.44
1:F:74:ARG:HB3	1:F:113:CYS:HA	1.99	0.44
1:F:100:LYS:HG2	1:F:104:MET:HE3	2.00	0.44
1:B:244:MET:HA	1:B:280:ASN:OD1	2.17	0.44
1:C:206:PHE:HE2	1:C:259:ALA:O	1.99	0.44
1:E:363:VAL:N	1:E:364:PRO:HD2	2.32	0.44
1:G:261:ILE:CG2	1:G:312:GLY:HA2	2.47	0.44
1:H:18:PRO:HG2	1:H:21:GLU:HB2	1.99	0.44
1:D:75:VAL:HG12	1:D:115:ILE:HB	1.99	0.44
1:G:124:MET:HB3	1:G:139:PHE:CD2	2.52	0.44
1:B:69:LYS:H	1:B:69:LYS:HG2	1.56	0.44
1:D:118:THR:OG1	1:D:165:HIS:HA	2.17	0.44
1:H:238:HIS:O	1:H:240:PRO:HD3	2.18	0.44
1:C:18:PRO:HA	1:C:19:PRO:HD3	1.84	0.44
1:D:294:GLN:HB3	1:D:310:GLU:HG2	2.00	0.44
1:B:82:ILE:CG1	1:B:83:VAL:N	2.76	0.44
1:B:208:GLU:OE2	1:B:212:TYR:OH	2.29	0.44
1:B:255:PHE:CD2	1:B:285:VAL:HB	2.52	0.44
1:C:351:VAL:HG13	1:C:355:TRP:CE3	2.51	0.44
1:D:88:ALA:O	1:D:89:PRO:C	2.60	0.44
1:D:124:MET:O	1:D:289:ARG:NH1	2.51	0.44
1:F:331:LEU:HD11	1:F:339:LEU:HB2	2.00	0.44
1:H:82:ILE:HA	1:H:97:ILE:HD11	2.00	0.44
1:D:379:LYS:HE3	1:D:379:LYS:HB2	1.70	0.43
1:C:97:ILE:HG21	1:C:122:TRP:O	2.18	0.43
1:D:269:TRP:CH2	1:D:288:ASN:HB2	2.53	0.43
1:A:215:GLY:C	1:A:216[B]:ASN:HD22	2.25	0.43
1:C:234:CYS:HA	1:C:258:SER:HB3	2.00	0.43
1:E:101:VAL:O	1:E:105:ILE:HG13	2.19	0.43
1:F:55:ILE:CD1	1:F:338:LEU:HD23	2.47	0.43
1:F:206:PHE:HE2	1:F:259:ALA:O	2.01	0.43
1:G:180:ASN:HB2	1:G:212:TYR:CZ	2.54	0.43
1:A:30:TYR:HE2	1:A:329:PRO:HA	1.84	0.43
1:A:266:GLU:N	1:A:267:PRO:HD2	2.34	0.43
1:B:58:TYR:CZ	1:B:329:PRO:HG2	2.53	0.43
1:B:104:MET:HE1	1:B:336:ASP:HB3	2.00	0.43
1:C:58:TYR:HB2	1:C:341:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:VAL:O	1:D:192:LEU:HB2	2.18	0.43
1:E:282:TYR:HA	1:E:348:CYS:SG	2.59	0.43
1:G:153:ALA:HA	1:G:185:ILE:HG21	2.00	0.43
1:H:104:MET:CE	1:H:336:ASP:HB3	2.48	0.43
1:C:87:THR:CG2	1:C:296:PRO:HG3	2.47	0.43
1:A:63:ARG:HB2	1:A:63:ARG:NH1	2.25	0.43
1:D:40:LEU:O	1:D:45:LYS:HE2	2.19	0.43
1:H:320:VAL:H	1:H:328:THR:HB	1.84	0.43
1:C:201:PRO:HB3	1:C:235:TYR:CD1	2.54	0.43
1:C:208:GLU:OE2	1:C:212:TYR:OH	2.30	0.43
1:B:134:PHE:HA	1:B:135:PRO:HA	1.87	0.43
1:C:244:MET:HE2	1:D:370:PHE:CE1	2.54	0.43
1:D:10:ASN:OD1	1:D:26:LYS:HE2	2.19	0.43
1:D:124:MET:HE1	1:D:168:LEU:HB2	2.01	0.43
1:F:219:HIS:NE2	1:F:242:ASN:OD1	2.51	0.43
1:A:379:LYS:HA	1:A:380:PRO:HD3	1.93	0.43
1:B:192:LEU:HD11	1:B:224:THR:HG22	2.01	0.43
1:D:74:ARG:HB3	1:D:113:CYS:HA	2.01	0.43
1:D:169:GLU:O	1:D:178:ILE:HA	2.19	0.43
1:D:244:MET:HA	1:D:280:ASN:OD1	2.19	0.43
1:G:263:ARG:H	1:G:263:ARG:CD	2.21	0.43
1:H:182:ALA:CB	1:H:231:VAL:HG11	2.48	0.43
1:A:18:PRO:HA	1:A:19:PRO:HD3	1.85	0.42
1:B:200:ILE:HD13	1:B:214:GLU:HA	2.01	0.42
1:B:307:ALA:N	1:C:298:GLU:OE1	2.39	0.42
1:F:63:ARG:CB	1:F:63:ARG:HH11	2.32	0.42
1:B:378:PHE:HB3	1:C:174:HIS:NE2	2.34	0.42
1:C:223:GLU:HG3	1:C:223:GLU:O	2.18	0.42
1:E:320:VAL:H	1:E:328:THR:HB	1.84	0.42
1:F:58:TYR:CD1	1:F:328:THR:HG23	2.54	0.42
1:F:201:PRO:HB3	1:F:235:TYR:CD1	2.54	0.42
1:H:232:ASN:O	1:H:256:ASN:ND2	2.45	0.42
1:B:68:ARG:HH12	1:B:349:ARG:CZ	2.32	0.42
1:C:63:ARG:HH11	1:C:63:ARG:CG	2.26	0.42
1:C:322:ALA:HB1	1:C:323:PRO:HD2	2.01	0.42
1:F:290:VAL:HG23	1:F:316:GLY:HA3	2.01	0.42
1:H:99:ASN:HA	1:H:102:LYS:HD2	2.00	0.42
1:A:361:GLN:HG2	1:B:241:GLN:HE22	1.84	0.42
1:B:71:ARG:H	1:B:346:ASN:HD21	1.66	0.42
1:F:70:ARG:HA	1:F:346:ASN:HD21	1.83	0.42
1:G:331:LEU:HD11	1:G:339:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:TYR:HE2	1:B:329:PRO:HA	1.84	0.42
1:C:352:LYS:HD3	1:C:358:ARG:HG3	2.00	0.42
1:D:80:ASN:ND2	1:D:81:SER:O	2.53	0.42
1:E:17:LEU:HA	1:E:18:PRO:HD2	1.83	0.42
1:E:171:ASP:O	1:E:176:GLU:HA	2.19	0.42
1:H:151:MET:SD	1:H:152:LEU:HD12	2.60	0.42
1:B:18:PRO:HA	1:B:19:PRO:HD3	1.88	0.42
1:D:233:ILE:HG23	1:D:257:PRO:HG2	2.02	0.42
1:B:113:CYS:O	1:B:161:MET:HE2	2.19	0.42
1:C:122:TRP:HD1	1:C:166:SER:O	2.03	0.42
1:D:82:ILE:HG12	1:D:293:GLU:HG2	2.02	0.42
1:E:263:ARG:N	1:E:263:ARG:NE	2.68	0.42
1:E:263:ARG:HA	1:F:27:ARG:HH21	1.84	0.42
1:H:168:LEU:HD23	1:H:168:LEU:HA	1.90	0.42
1:B:164:ILE:HG12	1:B:184:VAL:HG22	2.02	0.42
1:D:173:GLU:OE1	1:D:173:GLU:N	2.47	0.42
1:E:331:LEU:HD11	1:E:339:LEU:HB2	2.01	0.42
1:F:286:PRO:HD2	1:F:319:TYR:O	2.19	0.42
1:H:30:TYR:HE2	1:H:329:PRO:HA	1.85	0.42
1:A:17:LEU:HA	1:A:18:PRO:HD2	1.89	0.42
1:A:82:ILE:HG21	1:A:125:PRO:HA	2.02	0.42
1:B:90:ILE:HG13	1:B:91:GLU:N	2.35	0.42
1:D:17:LEU:HA	1:D:18:PRO:HD2	1.78	0.42
1:E:272:GLU:HA	1:F:275:ASN:HD22	1.85	0.42
1:B:62:ALA:HA	1:B:347:LEU:HD13	2.02	0.41
1:B:212:TYR:HA	1:D:359:MET:CE	2.50	0.41
1:G:169:GLU:O	1:G:178:ILE:HA	2.19	0.41
1:G:245:MET:SD	1:H:369:SER:HB3	2.60	0.41
1:H:104:MET:HE1	1:H:336:ASP:HB3	2.02	0.41
1:A:275:ASN:HB3	1:B:275:ASN:HD22	1.84	0.41
1:A:373:ALA:HA	1:A:378:PHE:CE1	2.55	0.41
1:B:120:GLU:OE1	1:B:234:CYS:HB2	2.20	0.41
1:B:351:VAL:HG13	1:B:355:TRP:CE3	2.55	0.41
1:C:155:LEU:HD22	1:C:159:TYR:CE1	2.55	0.41
1:D:30:TYR:HE2	1:D:329:PRO:HA	1.84	0.41
1:D:344:ASP:OD1	1:D:344:ASP:C	2.64	0.41
1:B:98:TRP:O	1:B:102:LYS:HB2	2.20	0.41
1:B:133:LYS:NZ	1:B:210:THR:O	2.51	0.41
1:D:11:ASP:HA	1:D:14:GLU:HG2	2.02	0.41
1:F:290:VAL:HG23	1:F:316:GLY:CA	2.51	0.41
1:A:359:MET:HG2	1:A:360:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:GLY:HA2	1:F:147:PRO:HD3	1.94	0.41
1:H:263:ARG:HG2	1:H:263:ARG:NH1	2.33	0.41
1:H:88:ALA:O	1:H:93:GLN:NE2	2.53	0.41
1:A:48:ALA:HB1	1:A:53:PHE:O	2.21	0.41
1:A:263:ARG:HD2	1:A:263:ARG:H	1.86	0.41
1:B:363:VAL:N	1:B:364:PRO:CD	2.83	0.41
1:C:67:THR:CG2	1:E:90:ILE:HD11	2.51	0.41
1:D:213:MET:HG3	1:F:359:MET:O	2.21	0.41
1:H:59:ARG:HG3	1:H:342:GLU:CG	2.50	0.41
1:C:63:ARG:HG2	1:C:63:ARG:NH1	2.30	0.41
1:E:43:SER:O	1:E:46:ASP:HB2	2.20	0.41
1:C:275:ASN:HD21	1:D:272:GLU:HA	1.82	0.41
1:C:285:VAL:HG13	1:C:320:VAL:HG22	2.03	0.41
1:G:18:PRO:HA	1:G:19:PRO:HD3	1.95	0.41
1:G:383:ILE:HD12	1:H:222:PHE:CE2	2.55	0.41
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.83	0.41
1:A:200:ILE:O	1:A:201:PRO:C	2.63	0.41
1:A:237:ARG:HG3	1:A:256:ASN:OD1	2.20	0.41
1:B:9:LEU:O	1:B:9:LEU:HG	2.20	0.41
1:C:84:ILE:HD11	1:C:93:GLN:HA	2.03	0.41
1:C:303:ASP:OD1	1:C:303:ASP:N	2.45	0.41
1:D:15:LYS:O	1:D:15:LYS:CG	2.69	0.41
1:D:300:THR:HG23	1:E:300:THR:HG23	2.03	0.41
1:G:80:ASN:C	1:G:290:VAL:HG12	2.45	0.41
1:G:115:ILE:HD13	1:G:229:LEU:HD21	2.03	0.41
1:G:182:ALA:CB	1:G:231:VAL:HG11	2.51	0.41
1:A:368:GLU:O	1:A:372:LYS:HG2	2.21	0.41
1:F:102:LYS:HG2	1:F:155:LEU:HD11	2.01	0.41
1:D:89:PRO:HG2	1:D:92:LYS:HD2	2.02	0.40
1:D:303:ASP:OD1	1:D:303:ASP:N	2.54	0.40
1:E:37:THR:HG22	1:E:38:LEU:N	2.36	0.40
1:G:84:ILE:HB	1:G:85:PRO:HD2	2.02	0.40
1:G:320:VAL:HG21	1:G:341:VAL:HG11	2.01	0.40
1:A:293:GLU:OE1	1:A:314:PHE:HE1	2.03	0.40
1:A:324:ASP:HA	1:A:355:TRP:HZ3	1.86	0.40
1:B:280:ASN:CB	1:B:282:TYR:CE1	3.04	0.40
1:C:18:PRO:HB2	1:C:21:GLU:HG3	2.02	0.40
1:C:320:VAL:H	1:C:328:THR:HG22	1.86	0.40
1:H:196:ARG:H	1:H:217:THR:HG1	1.68	0.40
1:B:239:HIS:HA	1:B:240:PRO:HD2	1.92	0.40
1:A:78:ILE:HG23	1:A:104:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:HA	1:C:185:ILE:HG21	2.04	0.40
1:F:122:TRP:HD1	1:F:166:SER:O	2.05	0.40
1:H:101:VAL:HG12	1:H:105:ILE:HD11	2.03	0.40
1:B:238:HIS:ND1	1:B:272:GLU:OE1	2.55	0.40
1:F:186:SER:OG	1:F:187:ASN:N	2.55	0.40
1:G:187:ASN:HD21	1:G:225:GLU:CD	2.28	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	341/405 (84%)	317 (93%)	24 (7%)	0	100	100
1	B	377/405 (93%)	363 (96%)	14 (4%)	0	100	100
1	C	379/405 (94%)	362 (96%)	17 (4%)	0	100	100
1	D	377/405 (93%)	362 (96%)	14 (4%)	1 (0%)	36	65
1	E	378/405 (93%)	360 (95%)	18 (5%)	0	100	100
1	F	377/405 (93%)	360 (96%)	17 (4%)	0	100	100
1	G	379/405 (94%)	362 (96%)	16 (4%)	1 (0%)	36	65
1	H	334/405 (82%)	313 (94%)	20 (6%)	1 (0%)	36	65
All	All	2942/3240 (91%)	2799 (95%)	140 (5%)	3 (0%)	48	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	234	CYS
1	D	83	VAL
1	G	83	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	297/346 (86%)	257 (86%)	40 (14%)	4	16
1	B	323/346 (93%)	281 (87%)	42 (13%)	4	17
1	C	325/346 (94%)	282 (87%)	43 (13%)	4	17
1	D	323/346 (93%)	280 (87%)	43 (13%)	4	17
1	E	324/346 (94%)	278 (86%)	46 (14%)	3	14
1	F	323/346 (93%)	286 (88%)	37 (12%)	5	21
1	G	325/346 (94%)	281 (86%)	44 (14%)	4	16
1	H	290/346 (84%)	251 (87%)	39 (13%)	4	16
All	All	2530/2768 (91%)	2196 (87%)	334 (13%)	4	17

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	LYS
1	A	22	LEU
1	A	28	ILE
1	A	32	VAL
1	A	33	GLU
1	A	34	GLU
1	A	38	LEU
1	A	56	LYS
1	A	63	ARG
1	A	68	ARG
1	A	71	ARG
1	A	73	VAL
1	A	74	ARG
1	A	75	VAL
1	A	80	ASN
1	A	90	ILE
1	A	97	ILE
1	A	119	GLN

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	166	SER
1	A	172	MET
1	A	180	ASN
1	A	212	TYR
1	A	214	GLU
1	A	223	GLU
1	A	233	ILE
1	A	260	THR
1	A	264	LEU
1	A	282	TYR
1	A	290	VAL
1	A	341	VAL
1	A	343	LEU
1	A	351	VAL
1	A	359	MET
1	A	362	ARG
1	A	363	VAL
1	A	371	LYS
1	A	382	ILE
1	A	386	THR
1	B	20	ASP
1	B	23	LYS
1	B	27	ARG
1	B	30	TYR
1	B	33	GLU
1	B	34	GLU
1	B	38	LEU
1	B	39	GLU
1	B	46	ASP
1	B	49	GLU
1	B	63	ARG
1	B	69	LYS
1	B	73	VAL
1	B	75	VAL
1	B	82	ILE
1	B	83	VAL
1	B	92	LYS
1	B	95	GLU
1	B	103	THR
1	B	123	THR
1	B	130	THR

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Mol	Chain	Res	Type
1	B	150	LYS
1	B	152	LEU
1	B	167	ILE
1	B	186	SER
1	B	200	ILE
1	B	202	ARG
1	B	207	ASN
1	B	214	GLU
1	B	237	ARG
1	B	260	THR
1	B	263	ARG
1	B	265	SER
1	B	284	THR
1	B	290	VAL
1	B	292	THR
1	B	297	ASN
1	B	310	GLU
1	B	333	ARG
1	B	341	VAL
1	B	343	LEU
1	B	386	THR
1	C	7	LYS
1	C	17	LEU
1	C	27	ARG
1	C	32	VAL
1	C	33	GLU
1	C	37	THR
1	C	38	LEU
1	C	63	ARG
1	C	64	GLU
1	C	69	LYS
1	C	74	ARG
1	C	75	VAL
1	C	78	ILE
1	C	81	SER
1	C	92	LYS
1	C	95	GLU
1	C	103	THR
1	C	123	THR
1	C	151	MET
1	C	152	LEU
1	C	157	LYS

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Mol	Chain	Res	Type
1	C	178	ILE
1	C	200	ILE
1	C	202	ARG
1	C	203	VAL
1	C	210	THR
1	C	260	THR
1	C	264	LEU
1	C	282	TYR
1	C	290	VAL
1	C	292	THR
1	C	294	GLN
1	C	297	ASN
1	C	301	SER
1	C	306	LYS
1	C	328	THR
1	C	330	SER
1	C	335	LYS
1	C	343	LEU
1	C	351	VAL
1	C	362	ARG
1	C	383	ILE
1	C	386	THR
1	D	12	CYS
1	D	17	LEU
1	D	32	VAL
1	D	33	GLU
1	D	34	GLU
1	D	38	LEU
1	D	39	GLU
1	D	49	GLU
1	D	50	GLN
1	D	61	THR
1	D	69	LYS
1	D	70	ARG
1	D	74	ARG
1	D	92	LYS
1	D	116	VAL
1	D	119	GLN
1	D	123	THR
1	D	130	THR
1	D	151	MET
1	D	152	LEU

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Mol	Chain	Res	Type
1	D	164	ILE
1	D	172	MET
1	D	178	ILE
1	D	192	LEU
1	D	202	ARG
1	D	203	VAL
1	D	210	THR
1	D	214	GLU
1	D	233	ILE
1	D	260	THR
1	D	263	ARG
1	D	282	TYR
1	D	287	ILE
1	D	289	ARG
1	D	290	VAL
1	D	292	THR
1	D	297	ASN
1	D	306	LYS
1	D	328	THR
1	D	341	VAL
1	D	343	LEU
1	D	359	MET
1	D	386	THR
1	E	27	ARG
1	E	32	VAL
1	E	33	GLU
1	E	38	LEU
1	E	42	THR
1	E	47	ILE
1	E	63	ARG
1	E	74	ARG
1	E	78	ILE
1	E	92	LYS
1	E	123	THR
1	E	130	THR
1	E	141	GLU
1	E	150	LYS
1	E	152	LEU
1	E	157	LYS
1	E	166	SER
1	E	167	ILE
1	E	168	LEU

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Mol	Chain	Res	Type
1	E	186	SER
1	E	192	LEU
1	E	200	ILE
1	E	202	ARG
1	E	203	VAL
1	E	207	ASN
1	E	221	VAL
1	E	229	LEU
1	E	231	VAL
1	E	260	THR
1	E	261	ILE
1	E	263	ARG
1	E	270	SER
1	E	282	TYR
1	E	290	VAL
1	E	292	THR
1	E	294	GLN
1	E	297	ASN
1	E	301	SER
1	E	338	LEU
1	E	341	VAL
1	E	343	LEU
1	E	355	TRP
1	E	363	VAL
1	E	368	GLU
1	E	379	LYS
1	E	386	THR
1	F	17	LEU
1	F	23	LYS
1	F	27	ARG
1	F	33	GLU
1	F	34	GLU
1	F	35	ASP
1	F	37	THR
1	F	38	LEU
1	F	39	GLU
1	F	49	GLU
1	F	63	ARG
1	F	69	LYS
1	F	74	ARG
1	F	78	ILE
1	F	82	ILE

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Mol	Chain	Res	Type
1	F	92	LYS
1	F	106	LYS
1	F	123	THR
1	F	151	MET
1	F	152	LEU
1	F	168	LEU
1	F	202	ARG
1	F	203	VAL
1	F	214	GLU
1	F	237	ARG
1	F	260	THR
1	F	261	ILE
1	F	278	ILE
1	F	282	TYR
1	F	290	VAL
1	F	292	THR
1	F	294	GLN
1	F	297	ASN
1	F	306	LYS
1	F	343	LEU
1	F	351	VAL
1	F	368	GLU
1	G	7	LYS
1	G	32	VAL
1	G	33	GLU
1	G	34	GLU
1	G	37	THR
1	G	38	LEU
1	G	39	GLU
1	G	40	LEU
1	G	42	THR
1	G	56	LYS
1	G	64	GLU
1	G	70	ARG
1	G	71	ARG
1	G	72	ILE
1	G	74	ARG
1	G	82	ILE
1	G	91	GLU
1	G	92	LYS
1	G	95	GLU
1	G	102	LYS

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Mol	Chain	Res	Type
1	G	123	THR
1	G	145	ASN
1	G	152	LEU
1	G	162	VAL
1	G	164	ILE
1	G	168	LEU
1	G	200	ILE
1	G	202	ARG
1	G	203	VAL
1	G	207	ASN
1	G	214	GLU
1	G	258	SER
1	G	260	THR
1	G	263	ARG
1	G	268	LEU
1	G	282	TYR
1	G	284	THR
1	G	285	VAL
1	G	292	THR
1	G	297	ASN
1	G	306	LYS
1	G	343	LEU
1	G	363	VAL
1	G	385	GLU
1	H	20	ASP
1	H	22	LEU
1	H	32	VAL
1	H	34	GLU
1	H	38	LEU
1	H	51	ASN
1	H	56	LYS
1	H	63	ARG
1	H	64	GLU
1	H	69	LYS
1	H	73	VAL
1	H	75	VAL
1	H	83	VAL
1	H	92	LYS
1	H	95	GLU
1	H	145	ASN
1	H	150	LYS
1	H	151	MET

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Mol	Chain	Res	Type
1	H	172	MET
1	H	214	GLU
1	H	217	THR
1	H	233	ILE
1	H	234	CYS
1	H	260	THR
1	H	263	ARG
1	H	282	TYR
1	H	284	THR
1	H	289	ARG
1	H	290	VAL
1	H	333	ARG
1	H	335	LYS
1	H	341	VAL
1	H	342	GLU
1	H	343	LEU
1	H	355	TRP
1	H	360	THR
1	H	369	SER
1	H	382	ILE
1	H	386	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	50	GLN
1	A	51	ASN
1	A	66	GLN
1	A	99	ASN
1	A	180	ASN
1	A	198	ASN
1	A	239	HIS
1	A	275	ASN
1	A	381	GLN
1	B	51	ASN
1	B	160	ASN
1	B	180	ASN
1	B	195	HIS
1	B	275	ASN
1	B	297	ASN
1	C	16	HIS

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Mol	Chain	Res	Type
1	C	66	GLN
1	C	145	ASN
1	C	160	ASN
1	C	239	HIS
1	C	275	ASN
1	D	80	ASN
1	D	239	HIS
1	D	275	ASN
1	D	308	HIS
1	D	361	GLN
1	E	50	GLN
1	E	66	GLN
1	E	239	HIS
1	E	308	HIS
1	E	361	GLN
1	F	51	ASN
1	F	114	ASN
1	F	198	ASN
1	F	308	HIS
1	F	346	ASN
1	G	180	ASN
1	G	239	HIS
1	G	256	ASN
1	G	361	GLN
1	H	8	ASN
1	H	16	HIS
1	H	51	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	348/405 (85%)	0.02	5 (1%) 73 55	18, 40, 65, 70	1 (0%)
1	B	379/405 (93%)	-0.02	0 100 100	23, 40, 62, 70	0
1	C	381/405 (94%)	0.14	3 (0%) 82 68	23, 40, 63, 70	0
1	D	379/405 (93%)	0.16	5 (1%) 75 56	23, 40, 62, 70	0
1	E	380/405 (93%)	0.19	9 (2%) 59 40	23, 40, 63, 70	0
1	F	379/405 (93%)	0.13	2 (0%) 87 76	23, 40, 62, 70	0
1	G	381/405 (94%)	0.02	1 (0%) 90 82	23, 40, 63, 70	0
1	H	342/405 (84%)	0.06	4 (1%) 76 58	23, 39, 63, 70	0
All	All	2969/3240 (91%)	0.09	29 (0%) 79 63	18, 40, 64, 70	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	MET	3.7
1	C	304	GLY	3.1
1	E	334	ASP	3.1
1	F	50	GLN	3.1
1	C	291	GLY	3.0
1	H	312	GLY	2.9
1	E	324	ASP	2.7
1	E	36	GLN	2.7
1	E	120	GLU	2.7
1	F	385	GLU	2.6
1	E	20	ASP	2.4
1	H	176	GLU	2.4
1	H	376	HIS	2.4
1	E	17	LEU	2.4
1	A	334	ASP	2.4
1	E	11	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	191	TYR	2.3
1	E	39	GLU	2.3
1	C	35	ASP	2.3
1	D	8	ASN	2.2
1	D	35	ASP	2.2
1	D	334	ASP	2.2
1	D	131	ARG	2.2
1	E	9	LEU	2.1
1	D	34	GLU	2.1
1	A	171	ASP	2.1
1	H	32	VAL	2.1
1	G	264	LEU	2.1
1	A	32	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.