



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 AM UTC

PDB ID : 5ZLI / pdb_00005zli
Title : Crystal structure of glutamine synthetase from helicobacter pylori
Authors : Joo, H.K.; Lee, J.Y.
Deposited on : 2018-03-28
Resolution : 2.80 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

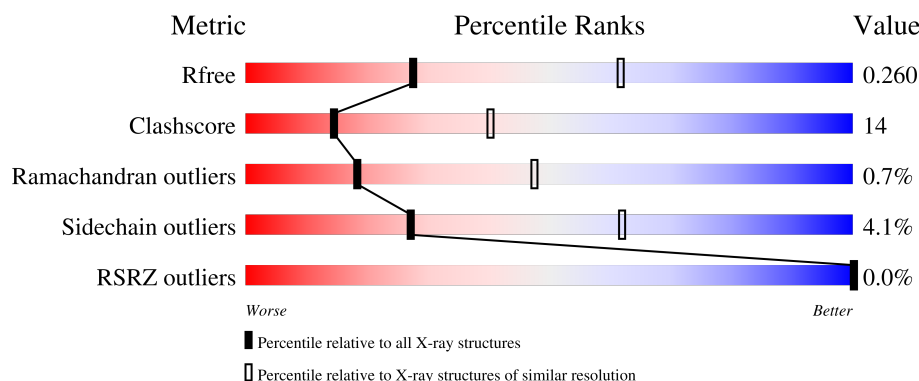
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

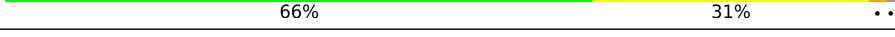
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	481	
1	B	481	
1	C	481	
1	D	481	
1	E	481	

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Mol	Chain	Length	Quality of chain
1	F	481	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 68%, a yellow segment representing 29%, and a small grey segment at the end. The text '68%' is centered under the green segment, and '29%' is centered under the yellow segment. The text '..' is at the end of the bar.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22534 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.

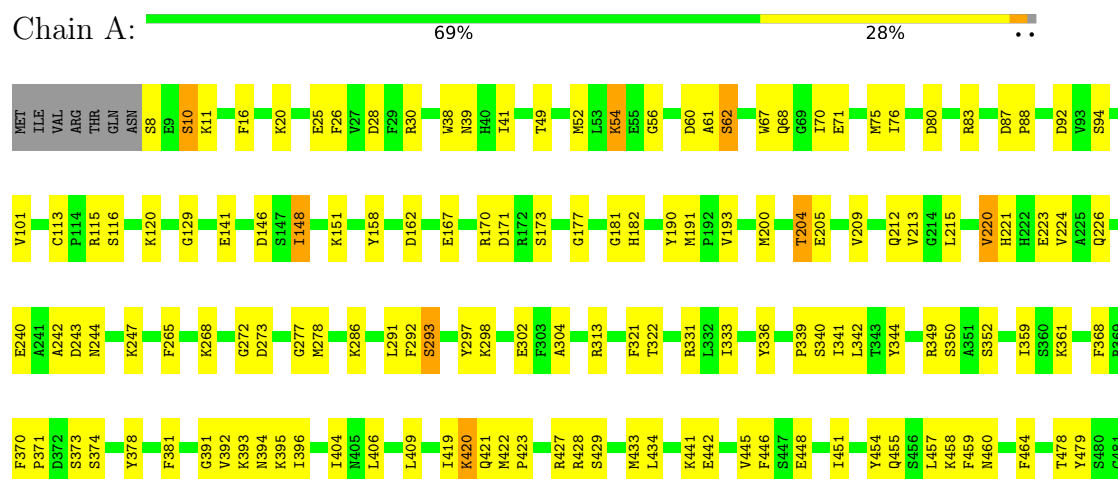
- Molecule 1 is a protein called Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3752	2404	625	705	18			
1	B	475	Total	C	N	O	S	0	0	0
			3760	2408	627	707	18			
1	C	474	Total	C	N	O	S	0	0	0
			3752	2404	625	705	18			
1	D	475	Total	C	N	O	S	0	0	0
			3760	2408	627	707	18			
1	E	474	Total	C	N	O	S	0	0	0
			3758	2407	628	705	18			
1	F	474	Total	C	N	O	S	0	0	0
			3752	2404	625	705	18			

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: Glutamine synthetase

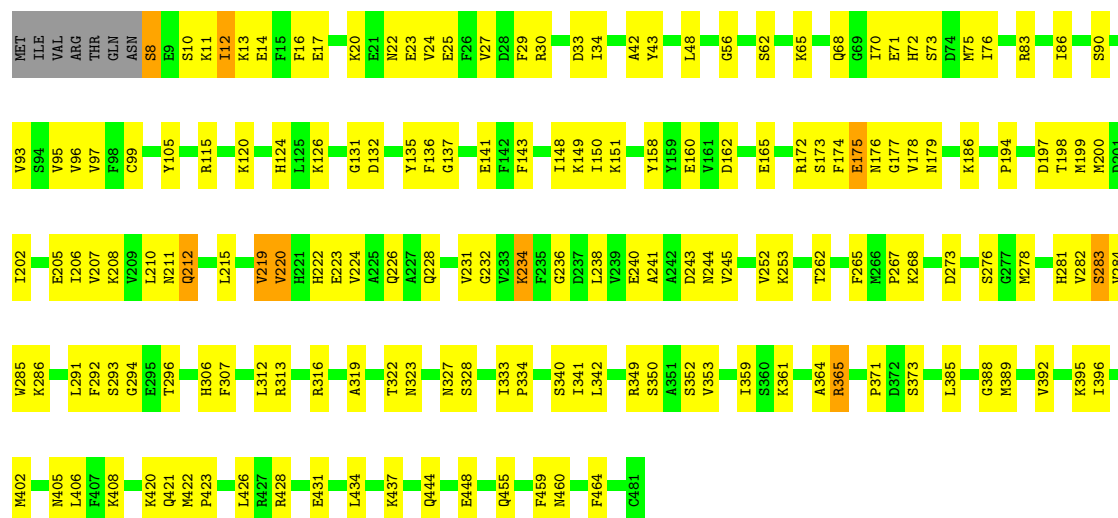


• Molecule 1: Glutamine synthetase



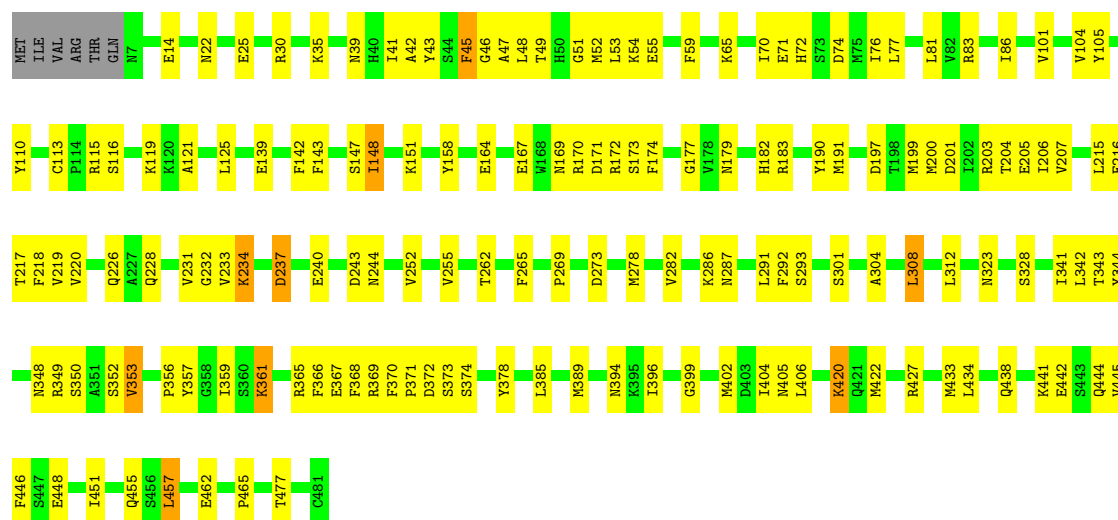
• Molecule 1: Glutamine synthetase





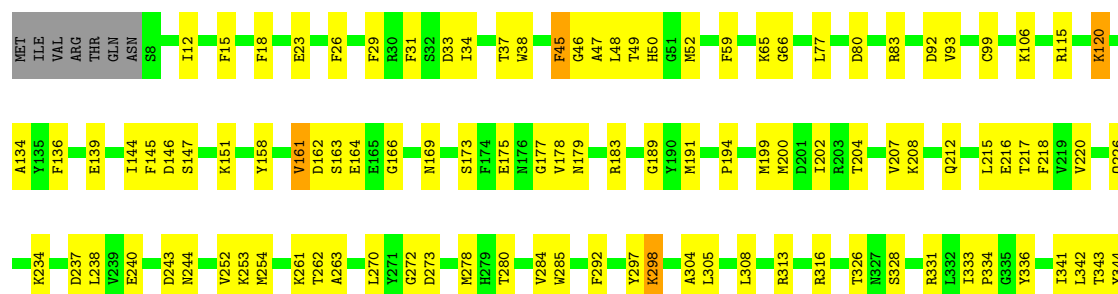
• Molecule 1: Glutamine synthetase

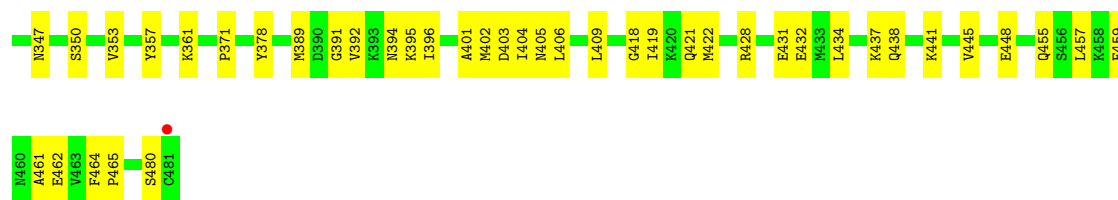
Chain D: 66% 31% ..



• Molecule 1: Glutamine synthetase

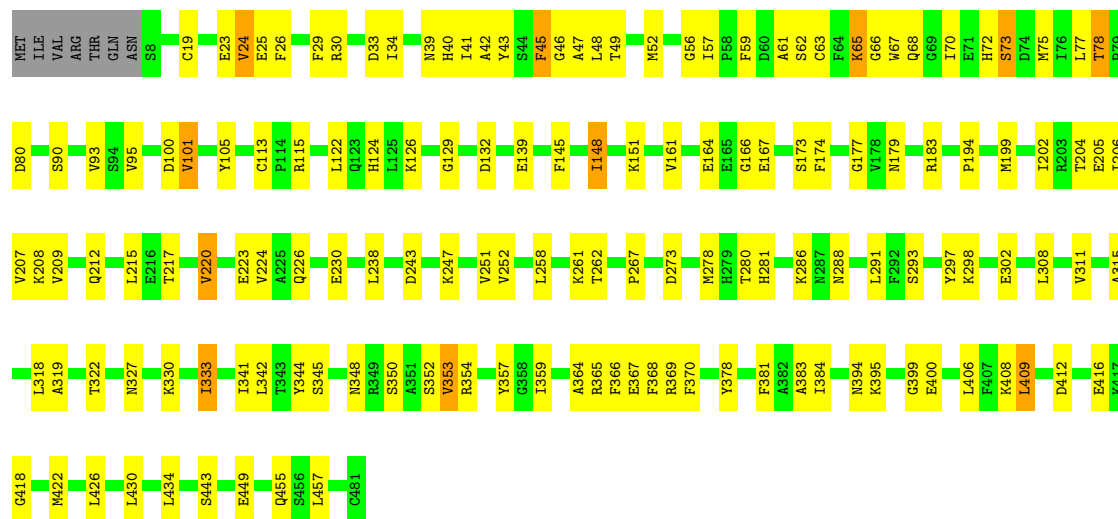
Chain E: 68% 29% ..





● Molecule 1: Glutamine synthetase

Chain F: 68% 29% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.09Å 131.46Å 131.41Å 90.00° 122.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.80) 99.3 (20.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.190 , 0.260 0.194 , 0.260	Depositor DCC
R_{free} test set	2000 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22534	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.51	0/3852	0.80	2/5207 (0.0%)
1	B	0.53	1/3860 (0.0%)	0.73	0/5218
1	C	0.53	1/3852 (0.0%)	0.76	1/5207 (0.0%)
1	D	0.46	0/3860	0.73	0/5218
1	E	0.48	0/3858	0.75	1/5214 (0.0%)
1	F	0.53	0/3852	0.79	1/5207 (0.0%)
All	All	0.51	2/23134 (0.0%)	0.76	5/31271 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	TRP	CA-C	-6.07	1.50	1.53
1	C	194	PRO	CA-C	5.77	1.55	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	VAL	CA-C-N	6.31	124.27	119.66
1	A	193	VAL	C-N-CA	6.31	124.27	119.66
1	E	194	PRO	O-C-N	6.08	124.11	121.31
1	C	283	SER	CA-CB-OG	5.35	121.80	111.10
1	F	65	LYS	CA-CB-CG	-5.05	103.99	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	174	PHE	Peptide

5.2 Too-close contacts [i](#)

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	3752	0	3580	104	0
1	B	3760	0	3586	86	0
1	C	3752	0	3580	141	0
1	D	3760	0	3586	119	0
1	E	3758	0	3591	99	0
1	F	3752	0	3580	111	0
All	All	22534	0	21503	617	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 (617) 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:293:SER:HB2	1:C:361:LYS:HD2	1.42	1.01
1:F:238:LEU:HD11	1:F:381:PHE:HB3	1.41	0.98
1:F:122:LEU:HD21	1:F:238:LEU:HB3	1.45	0.97
1:A:167:GLU:OE1	1:A:170:ARG:NH1	2.02	0.93
1:A:433:MET:HE1	1:A:451:ILE:HG23	1.50	0.91
1:E:199:MET:HE3	1:E:202:ILE:HG21	1.51	0.90
1:A:342:LEU:HD21	1:A:422:MET:HE2	1.54	0.88
1:C:283:SER:HA	1:C:365:ARG:CZ	2.04	0.87
1:C:294:GLY:O	1:C:361:LYS:NZ	2.09	0.85
1:C:83:ARG:HD3	1:C:240:GLU:HG3	1.57	0.85
1:D:441:LYS:NZ	1:D:448:GLU:OE2	2.09	0.85
1:C:342:LEU:HD21	1:C:422:MET:HE2	1.60	0.84
1:D:385:LEU:HG	1:D:389:MET:HE2	1.60	0.83
1:C:137:GLY:N	1:C:281:HIS:O	2.11	0.82
1:B:342:LEU:HD21	1:B:422:MET:HE3	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LYS:HB3	1:A:158:TYR:HB3	1.61	0.80
1:D:342:LEU:HD21	1:D:422:MET:HE2	1.63	0.80
1:C:23:GLU:O	1:C:93:VAL:HG21	1.81	0.80
1:D:293:SER:HB2	1:D:361:LYS:HD2	1.62	0.79
1:F:223:GLU:HG3	1:F:224:VAL:H	1.47	0.78
1:C:148:ILE:HD11	1:C:150:ILE:HD11	1.65	0.77
1:F:342:LEU:HD21	1:F:422:MET:HE2	1.67	0.76
1:D:215:LEU:HD11	1:D:244:ASN:HB3	1.66	0.76
1:D:434:LEU:HD11	1:D:455:GLN:HG3	1.67	0.75
1:A:80:ASP:OD2	1:A:115:ARG:NH2	2.21	0.74
1:B:49:THR:OG1	1:B:52:MET:N	2.18	0.74
1:D:70:ILE:HD12	1:E:350:SER:HB3	1.69	0.74
1:C:434:LEU:HD11	1:C:455:GLN:HG3	1.69	0.74
1:A:321:PHE:CZ	1:A:433:MET:HE3	2.22	0.74
1:C:207:VAL:HG21	1:C:220:VAL:HG21	1.69	0.73
1:F:23:GLU:O	1:F:93:VAL:HG21	1.89	0.72
1:F:344:TYR:OH	1:F:399:GLY:O	2.07	0.72
1:B:291:LEU:O	1:B:301:SER:OG	2.06	0.72
1:E:146:ASP:OD1	1:E:261:LYS:NZ	2.15	0.72
1:C:135:TYR:O	1:C:283:SER:N	2.20	0.72
1:C:282:VAL:HG23	1:C:365:ARG:HE	1.54	0.72
1:A:268:LYS:NZ	1:A:273:ASP:O	2.17	0.72
1:E:308:LEU:HD11	1:E:353:VAL:HG21	1.71	0.72
1:A:293:SER:OG	1:A:361:LYS:HD2	1.90	0.71
1:F:122:LEU:HD21	1:F:238:LEU:CB	2.19	0.71
1:D:53:LEU:HD23	1:D:81:LEU:HD11	1.71	0.71
1:E:151:LYS:HB3	1:E:158:TYR:HB3	1.72	0.71
1:C:437:LYS:NZ	1:C:448:GLU:OE2	2.24	0.71
1:A:70:ILE:HD12	1:B:350:SER:HB3	1.72	0.71
1:C:136:PHE:CE1	1:C:238:LEU:HD12	2.26	0.70
1:E:45:PHE:O	1:E:47:ALA:N	2.24	0.70
1:B:350:SER:HB2	1:B:406:LEU:HB2	1.73	0.70
1:C:206:ILE:HD13	1:C:252:VAL:HG22	1.73	0.70
1:C:282:VAL:O	1:C:365:ARG:HG3	1.92	0.70
1:C:212:GLN:N	1:C:212:GLN:OE1	2.25	0.70
1:E:341:ILE:HB	1:E:406:LEU:HD23	1.73	0.70
1:A:223:GLU:HG3	1:A:224:VAL:H	1.57	0.69
1:B:297:TYR:O	1:B:299:GLY:N	2.26	0.69
1:C:283:SER:HA	1:C:365:ARG:NE	2.07	0.69
1:E:80:ASP:OD1	1:E:115:ARG:NH2	2.26	0.69
1:B:434:LEU:HD11	1:B:455:GLN:HG3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:GLU:HB2	1:D:234:LYS:HG3	1.73	0.68
1:E:342:LEU:HD21	1:E:422:MET:HE2	1.74	0.68
1:D:206:ILE:HD13	1:D:252:VAL:HG22	1.75	0.68
1:A:349:ARG:HH11	1:F:73:SER:HB2	1.59	0.68
1:F:49:THR:CG2	1:F:52:MET:HG3	2.24	0.68
1:C:428:ARG:NH2	1:C:431:GLU:OE1	2.27	0.68
1:D:83:ARG:HD3	1:D:240:GLU:HG3	1.75	0.67
1:F:318:LEU:HD21	1:F:384:ILE:HA	1.75	0.67
1:E:115:ARG:NH1	1:E:243:ASP:OD2	2.28	0.67
1:C:283:SER:HB3	1:C:365:ARG:HG3	1.76	0.67
1:A:321:PHE:HZ	1:A:433:MET:HE3	1.60	0.67
1:F:434:LEU:HD11	1:F:455:GLN:HG3	1.77	0.66
1:E:361:LYS:H	1:E:361:LYS:HD2	1.59	0.66
1:B:83:ARG:HD3	1:B:240:GLU:HG3	1.78	0.66
1:A:49:THR:OG1	1:A:52:MET:HG3	1.94	0.66
1:B:190:TYR:CZ	1:B:191:MET:HE2	2.30	0.66
1:A:220:VAL:HG13	1:F:42:ALA:HB3	1.78	0.66
1:D:164:GLU:HG3	1:D:174:PHE:CZ	2.31	0.66
1:D:218:PHE:HD1	1:D:219:VAL:HG23	1.61	0.66
1:E:434:LEU:HD11	1:E:455:GLN:HG3	1.78	0.66
1:D:45:PHE:O	1:D:47:ALA:N	2.28	0.65
1:D:190:TYR:CZ	1:D:191:MET:HE2	2.32	0.65
1:F:25:GLU:H	1:F:93:VAL:HG23	1.61	0.65
1:E:200:MET:O	1:E:204:THR:HG23	1.96	0.65
1:D:25:GLU:OE2	1:E:208:LYS:NZ	2.30	0.65
1:E:83:ARG:HD3	1:E:240:GLU:HG3	1.78	0.65
1:A:10:SER:HB2	1:A:11:LYS:HD3	1.79	0.64
1:E:459:PHE:HB3	1:E:464:PHE:HE2	1.62	0.64
1:A:60:ASP:OD2	1:A:62:SER:OG	2.14	0.64
1:B:341:ILE:HB	1:B:406:LEU:HD23	1.78	0.64
1:D:70:ILE:HD11	1:E:405:ASN:OD1	1.97	0.64
1:A:129:GLY:O	1:A:286:LYS:HE3	1.97	0.64
1:C:284:VAL:HG23	1:C:365:ARG:HH22	1.62	0.64
1:A:70:ILE:HD11	1:B:405:ASN:OD1	1.98	0.63
1:C:148:ILE:O	1:D:179:ASN:HB3	1.98	0.63
1:C:282:VAL:HB	1:C:365:ARG:HH21	1.62	0.63
1:D:293:SER:HB2	1:D:361:LYS:CD	2.28	0.63
1:D:308:LEU:HG	1:D:312:LEU:HD13	1.80	0.63
1:A:293:SER:OG	1:A:361:LYS:HA	1.99	0.63
1:C:284:VAL:H	1:C:365:ARG:NH1	1.97	0.63
1:F:281:HIS:ND1	1:F:365:ARG:HD2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:HG23	1:F:26:PHE:CE1	2.33	0.63
1:E:316:ARG:NH2	1:E:421:GLN:O	2.31	0.63
1:F:354:ARG:NH1	1:F:367:GLU:OE2	2.31	0.63
1:D:343:THR:HG21	1:D:402:MET:HB2	1.79	0.62
1:C:278:MET:O	1:C:371:PRO:HG2	2.00	0.62
1:F:24:VAL:HG21	1:F:95:VAL:HG23	1.81	0.62
1:A:459:PHE:HB3	1:A:464:PHE:CE2	2.35	0.62
1:C:215:LEU:HD11	1:C:244:ASN:HB3	1.82	0.62
1:A:16:PHE:O	1:A:20:LYS:HG2	1.99	0.61
1:B:292:PHE:HA	1:B:304:ALA:HB2	1.82	0.61
1:B:356:PRO:HG2	1:B:365:ARG:HE	1.65	0.61
1:E:92:ASP:OD2	1:F:208:LYS:HD3	2.00	0.61
1:F:238:LEU:CD1	1:F:381:PHE:HB3	2.26	0.61
1:B:293:SER:OG	1:B:361:LYS:HD2	2.01	0.61
1:C:120:LYS:NZ	1:C:444:GLN:O	2.26	0.61
1:D:167:GLU:HG2	1:D:170:ARG:NH1	2.16	0.61
1:C:359:ILE:HD12	1:C:364:ALA:HA	1.83	0.61
1:E:326:THR:HG23	1:E:462:GLU:HB3	1.82	0.61
1:F:359:ILE:HD12	1:F:364:ALA:HA	1.82	0.61
1:D:22:ASN:HD22	1:D:86:ILE:HD11	1.65	0.61
1:E:215:LEU:HD21	1:E:244:ASN:CG	2.25	0.61
1:F:80:ASP:OD2	1:F:115:ARG:NH2	2.34	0.61
1:D:101:VAL:HG22	1:D:113:CYS:HB2	1.81	0.60
1:D:286:LYS:HE2	1:D:287:ASN:HD21	1.65	0.60
1:F:122:LEU:CD2	1:F:238:LEU:HB3	2.28	0.60
1:A:200:MET:HE3	1:F:90:SER:HB3	1.82	0.60
1:D:367:GLU:OE1	1:D:369:ARG:HG2	2.01	0.60
1:E:428:ARG:HA	1:E:431:GLU:HG2	1.82	0.60
1:A:341:ILE:O	1:A:352:SER:OG	2.14	0.60
1:B:129:GLY:O	1:B:286:LYS:HE3	2.01	0.60
1:B:422:MET:HE2	1:B:423:PRO:HD2	1.84	0.60
1:D:394:ASN:HB2	1:D:396:ILE:HG13	1.84	0.60
1:E:243:ASP:OD1	1:E:378:TYR:OH	2.16	0.60
1:C:364:ALA:O	1:C:365:ARG:HG2	2.02	0.59
1:D:101:VAL:CG2	1:D:113:CYS:HB2	2.32	0.59
1:C:136:PHE:CE2	1:C:282:VAL:HG12	2.37	0.59
1:F:145:PHE:O	1:F:261:LYS:HB3	2.02	0.59
1:D:151:LYS:HB3	1:D:158:TYR:HB3	1.83	0.59
1:C:220:VAL:HG13	1:C:231:VAL:HG22	1.85	0.59
1:E:26:PHE:CE1	1:F:204:THR:HG23	2.37	0.59
1:D:344:TYR:OH	1:D:399:GLY:O	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:TYR:OH	1:C:160:GLU:OE1	2.18	0.59
1:A:213:VAL:O	1:A:247:LYS:NZ	2.35	0.59
1:B:60:ASP:HB2	1:C:349:ARG:NH1	2.18	0.59
1:C:173:SER:HB3	1:C:177:GLY:HA2	1.83	0.59
1:D:164:GLU:HG2	1:D:183:ARG:HH21	1.68	0.59
1:C:286:LYS:HB3	1:C:291:LEU:HD11	1.84	0.58
1:C:135:TYR:HB2	1:C:283:SER:OG	2.03	0.58
1:A:441:LYS:NZ	1:A:448:GLU:HG3	2.19	0.58
1:C:143:PHE:CE2	1:C:228:GLN:HG3	2.38	0.58
1:D:101:VAL:HG23	1:D:110:TYR:CB	2.33	0.58
1:E:292:PHE:HA	1:E:304:ALA:HB2	1.85	0.58
1:B:70:ILE:HD11	1:C:405:ASN:OD1	2.03	0.58
1:E:120:LYS:NZ	1:E:445:VAL:O	2.36	0.58
1:C:70:ILE:HD12	1:D:350:SER:HB3	1.85	0.58
1:F:45:PHE:O	1:F:47:ALA:N	2.37	0.58
1:A:292:PHE:HA	1:A:304:ALA:HB2	1.86	0.58
1:A:30:ARG:HB3	1:A:38:TRP:NE1	2.19	0.57
1:A:173:SER:HB3	1:A:177:GLY:HA2	1.86	0.57
1:C:30:ARG:HG3	1:C:96:VAL:HG13	1.86	0.57
1:F:207:VAL:HG21	1:F:220:VAL:HG21	1.87	0.57
1:C:132:ASP:OD2	1:C:286:LYS:HG3	2.04	0.57
1:C:307:PHE:CE2	1:C:388:GLY:HA3	2.39	0.57
1:B:151:LYS:HB3	1:B:158:TYR:HB3	1.86	0.57
1:F:286:LYS:HB3	1:F:291:LEU:HD11	1.85	0.57
1:C:70:ILE:HD11	1:D:405:ASN:OD1	2.04	0.57
1:A:340:SER:O	1:A:421:GLN:HB2	2.04	0.57
1:C:13:LYS:HG2	1:C:17:GLU:OE2	2.04	0.57
1:E:437:LYS:NZ	1:E:448:GLU:OE1	2.34	0.57
1:A:349:ARG:NH1	1:F:73:SER:HB2	2.20	0.57
1:D:121:ALA:HB2	1:D:445:VAL:HG11	1.87	0.57
1:A:11:LYS:HD3	1:A:11:LYS:H	1.68	0.56
1:C:126:LYS:HE3	1:C:132:ASP:O	2.04	0.56
1:A:404:ILE:O	1:A:406:LEU:HD12	2.05	0.56
1:A:11:LYS:H	1:A:11:LYS:CD	2.17	0.56
1:A:92:ASP:HB2	1:B:204:THR:HG21	1.86	0.56
1:D:220:VAL:HG23	1:D:231:VAL:HG22	1.88	0.56
1:E:459:PHE:HB3	1:E:464:PHE:CE2	2.40	0.56
1:C:124:HIS:HD2	1:C:389:MET:HE1	1.69	0.56
1:F:129:GLY:O	1:F:286:LYS:HE3	2.06	0.56
1:C:312:LEU:O	1:C:420:LYS:NZ	2.23	0.56
1:E:226:GLN:HG3	1:E:273:ASP:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:ALA:HB3	1:F:75:MET:HG3	1.88	0.56
1:F:33:ASP:HA	1:F:67:TRP:CH2	2.41	0.56
1:A:25:GLU:OE1	1:A:92:ASP:HB3	2.06	0.56
1:C:172:ARG:HG2	1:C:173:SER:N	2.21	0.56
1:D:51:GLY:O	1:D:55:GLU:HG3	2.06	0.56
1:C:90:SER:HB3	1:D:200:MET:HE3	1.88	0.55
1:E:147:SER:HB2	1:F:179:ASN:H	1.71	0.55
1:A:146:ASP:N	1:A:162:ASP:O	2.35	0.55
1:D:42:ALA:HB3	1:E:220:VAL:HG13	1.88	0.55
1:D:218:PHE:CE1	1:D:232:GLY:HA3	2.41	0.55
1:D:101:VAL:HG23	1:D:110:TYR:HB3	1.89	0.55
1:F:341:ILE:HD12	1:F:406:LEU:HB3	1.88	0.55
1:B:173:SER:HB3	1:B:177:GLY:HA2	1.87	0.55
1:C:226:GLN:HG3	1:C:273:ASP:OD2	2.07	0.55
1:F:65:LYS:HD3	1:F:457:LEU:HD13	1.88	0.55
1:F:115:ARG:HG3	1:F:378:TYR:CE1	2.42	0.55
1:C:282:VAL:C	1:C:365:ARG:HE	2.14	0.54
1:B:243:ASP:OD1	1:B:378:TYR:OH	2.22	0.54
1:C:341:ILE:HD13	1:C:421:GLN:HG3	1.88	0.54
1:D:293:SER:O	1:D:301:SER:HB3	2.06	0.54
1:C:207:VAL:HG21	1:C:220:VAL:CG2	2.37	0.54
1:D:49:THR:OG1	1:D:52:MET:N	2.36	0.54
1:C:282:VAL:CB	1:C:365:ARG:HH21	2.21	0.54
1:B:194:PRO:HG2	1:B:200:MET:HE3	1.90	0.54
1:B:12:ILE:HG23	1:B:53:LEU:HD12	1.89	0.54
1:C:198:THR:OG1	1:C:199:MET:HE3	2.08	0.54
1:F:19:CYS:HB3	1:F:24:VAL:CG1	2.38	0.54
1:F:206:ILE:HD13	1:F:252:VAL:HG22	1.90	0.54
1:C:282:VAL:HG23	1:C:365:ARG:NE	2.22	0.54
1:A:393:LYS:NZ	1:A:442:GLU:OE2	2.41	0.54
1:F:139:GLU:HB3	1:F:230:GLU:OE2	2.08	0.53
1:F:173:SER:CB	1:F:177:GLY:HA2	2.39	0.53
1:F:238:LEU:HD11	1:F:381:PHE:CB	2.29	0.53
1:C:136:PHE:CD2	1:C:282:VAL:HG12	2.43	0.53
1:C:385:LEU:HG	1:C:389:MET:HE2	1.90	0.53
1:A:313:ARG:NH1	1:A:396:ILE:HG23	2.23	0.53
1:C:175:GLU:O	1:C:177:GLY:N	2.41	0.53
1:B:459:PHE:HB3	1:B:464:PHE:CE2	2.44	0.53
1:A:8:SER:HA	1:A:11:LYS:HZ1	1.74	0.53
1:C:211:ASN:HA	1:C:215:LEU:O	2.08	0.53
1:F:226:GLN:HG3	1:F:273:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:PHE:O	1:E:18:PHE:HB3	2.09	0.53
1:A:223:GLU:CG	1:A:224:VAL:H	2.23	0.52
1:A:350:SER:HB3	1:F:70:ILE:HD12	1.91	0.52
1:B:70:ILE:HD12	1:C:350:SER:HB3	1.91	0.52
1:B:152:ASP:OD1	1:B:157:GLN:NE2	2.33	0.52
1:C:16:PHE:O	1:C:20:LYS:HG2	2.09	0.52
1:D:101:VAL:HG21	1:D:110:TYR:HD2	1.74	0.52
1:E:12:ILE:HG22	1:E:50:HIS:ND1	2.24	0.52
1:A:41:ILE:HB	1:B:191:MET:SD	2.49	0.52
1:B:333:ILE:HG23	1:B:334:PRO:HD2	1.90	0.52
1:B:213:VAL:O	1:B:247:LYS:NZ	2.41	0.52
1:C:11:LYS:HA	1:C:14:GLU:HB2	1.91	0.52
1:A:278:MET:HE3	1:A:373:SER:HA	1.92	0.52
1:B:249:LYS:HE2	1:B:373:SER:HB3	1.91	0.52
1:F:49:THR:HG23	1:F:52:MET:HG3	1.90	0.52
1:F:247:LYS:O	1:F:251:VAL:HG23	2.10	0.52
1:C:115:ARG:NH1	1:C:243:ASP:OD2	2.43	0.52
1:C:323:ASN:HB3	1:C:328:SER:HB3	1.90	0.52
1:F:308:LEU:HD11	1:F:353:VAL:HG21	1.92	0.52
1:F:308:LEU:HB2	1:F:366:PHE:CZ	2.44	0.52
1:A:173:SER:CB	1:A:177:GLY:HA2	2.39	0.52
1:F:205:GLU:HA	1:F:208:LYS:HE2	1.92	0.52
1:F:173:SER:HB3	1:F:177:GLY:HA2	1.92	0.52
1:B:322:THR:HB	1:B:371:PRO:HB3	1.92	0.51
1:E:144:ILE:HB	1:E:199:MET:HE2	1.92	0.51
1:E:161:VAL:HG21	1:E:270:LEU:HD21	1.91	0.51
1:F:24:VAL:HG21	1:F:95:VAL:CG2	2.40	0.51
1:C:333:ILE:HG23	1:C:334:PRO:HD2	1.92	0.51
1:E:316:ARG:HE	1:E:432:GLU:CD	2.18	0.51
1:A:148:ILE:O	1:B:179:ASN:HB3	2.10	0.51
1:D:292:PHE:HA	1:D:304:ALA:HB2	1.93	0.51
1:C:68:GLN:CD	1:C:75:MET:HE2	2.36	0.51
1:F:19:CYS:HB3	1:F:24:VAL:HG11	1.93	0.51
1:F:311:VAL:HG11	1:F:368:PHE:CE1	2.46	0.51
1:F:62:SER:HA	1:F:68:GLN:O	2.10	0.51
1:C:223:GLU:HG3	1:C:224:VAL:H	1.75	0.51
1:D:125:LEU:HD13	1:D:389:MET:SD	2.51	0.51
1:D:357:TYR:O	1:D:359:ILE:HG12	2.10	0.51
1:A:113:CYS:HB3	1:A:116:SER:HB2	1.93	0.50
1:D:218:PHE:CZ	1:D:232:GLY:HA3	2.46	0.50
1:D:308:LEU:HB2	1:D:366:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LYS:HZ3	1:A:448:GLU:HG3	1.75	0.50
1:A:454:TYR:CE2	1:A:458:LYS:HG3	2.47	0.50
1:E:145:PHE:O	1:E:261:LYS:HB3	2.11	0.50
1:E:333:ILE:HG23	1:E:334:PRO:HD2	1.93	0.50
1:E:343:THR:HG21	1:E:402:MET:HB2	1.93	0.50
1:F:367:GLU:OE1	1:F:369:ARG:HG2	2.10	0.50
1:E:120:LYS:HZ3	1:E:445:VAL:HA	1.76	0.50
1:E:253:LYS:HA	1:E:263:ALA:HB3	1.94	0.50
1:F:30:ARG:HA	1:F:39:ASN:O	2.12	0.50
1:C:135:TYR:N	1:C:283:SER:O	2.23	0.50
1:C:149:LYS:O	1:C:150:ILE:HD13	2.12	0.50
1:D:265:PHE:HB3	1:D:373:SER:HB2	1.94	0.50
1:E:350:SER:HB2	1:E:406:LEU:HB2	1.93	0.50
1:A:226:GLN:HG3	1:A:273:ASP:OD1	2.12	0.50
1:C:24:VAL:HG21	1:C:95:VAL:HG23	1.92	0.50
1:C:70:ILE:HD11	1:D:405:ASN:CG	2.37	0.50
1:E:173:SER:HB3	1:E:177:GLY:HA2	1.93	0.50
1:A:190:TYR:CE1	1:A:191:MET:HE2	2.47	0.49
1:D:197:ASP:CG	1:D:203:ARG:HH12	2.20	0.49
1:E:272:GLY:HA2	1:E:336:TYR:OH	2.12	0.49
1:A:419:ILE:HG13	1:A:420:LYS:H	1.76	0.49
1:B:308:LEU:HD11	1:B:353:VAL:HG21	1.94	0.49
1:C:282:VAL:C	1:C:365:ARG:NE	2.70	0.49
1:D:243:ASP:OD1	1:D:378:TYR:OH	2.19	0.49
1:E:208:LYS:O	1:E:212:GLN:HG3	2.13	0.49
1:E:438:GLN:OE1	1:E:441:LYS:HE3	2.13	0.49
1:A:62:SER:HA	1:A:68:GLN:O	2.13	0.49
1:B:131:GLY:HA2	1:B:286:LYS:HB2	1.94	0.49
1:D:77:LEU:HD23	1:D:101:VAL:HG12	1.95	0.49
1:D:368:PHE:HB3	1:D:370:PHE:CE1	2.48	0.49
1:C:428:ARG:HD2	1:C:431:GLU:OE1	2.13	0.49
1:A:370:PHE:CD2	1:A:371:PRO:HD3	2.47	0.49
1:A:87:ASP:OD2	1:A:88:PRO:HD2	2.13	0.48
1:C:151:LYS:HB3	1:C:158:TYR:HB3	1.95	0.48
1:D:201:ASP:O	1:D:204:THR:HG22	2.13	0.48
1:A:427:ARG:HE	1:A:459:PHE:HE1	1.60	0.48
1:D:343:THR:HG22	1:D:344:TYR:H	1.78	0.48
1:E:297:TYR:CZ	1:E:298:LYS:HD2	2.48	0.48
1:F:24:VAL:HA	1:F:93:VAL:CG2	2.43	0.48
1:F:207:VAL:HG13	1:F:217:THR:HG21	1.94	0.48
1:B:286:LYS:O	1:B:289:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ILE:O	1:D:171:ASP:HB3	2.14	0.48
1:D:404:ILE:O	1:D:406:LEU:HD12	2.13	0.48
1:E:139:GLU:O	1:E:278:MET:HA	2.13	0.48
1:A:221:HIS:HB3	1:F:41:ILE:HG13	1.95	0.48
1:C:219:VAL:HG23	1:C:232:GLY:HA3	1.96	0.48
1:A:342:LEU:HA	1:A:352:SER:OG	2.14	0.48
1:A:434:LEU:HD11	1:A:455:GLN:HG3	1.95	0.48
1:C:72:HIS:HB3	1:C:105:TYR:CE1	2.49	0.48
1:C:282:VAL:O	1:C:365:ARG:NE	2.47	0.48
1:D:341:ILE:O	1:D:352:SER:OG	2.20	0.48
1:D:226:GLN:HG3	1:D:273:ASP:OD2	2.13	0.48
1:E:59:PHE:CD1	1:E:77:LEU:HG	2.49	0.48
1:F:29:PHE:O	1:F:40:HIS:HA	2.14	0.48
1:E:144:ILE:HB	1:E:199:MET:CE	2.43	0.48
1:B:62:SER:HA	1:B:68:GLN:O	2.14	0.47
1:B:248:LEU:O	1:B:252:VAL:HG13	2.14	0.47
1:C:22:ASN:HB3	1:C:86:ILE:HD11	1.95	0.47
1:E:404:ILE:O	1:E:406:LEU:HD12	2.13	0.47
1:A:391:GLY:HA2	1:A:396:ILE:HG13	1.96	0.47
1:B:100:ASP:OD1	1:B:115:ARG:HB3	2.14	0.47
1:E:344:TYR:CE1	1:E:401:ALA:HB2	2.49	0.47
1:F:61:ALA:CB	1:F:75:MET:HG3	2.44	0.47
1:F:319:ALA:HA	1:F:322:THR:OG1	2.14	0.47
1:F:426:LEU:O	1:F:430:LEU:HG	2.13	0.47
1:A:61:ALA:HB3	1:A:75:MET:HG3	1.95	0.47
1:C:131:GLY:HA2	1:C:286:LYS:HB2	1.96	0.47
1:D:104:VAL:HB	1:E:357:TYR:CE1	2.50	0.47
1:C:210:LEU:O	1:C:215:LEU:HB2	2.15	0.47
1:F:357:TYR:O	1:F:359:ILE:HG22	2.14	0.47
1:B:49:THR:H	1:B:52:MET:HE2	1.80	0.47
1:B:101:VAL:HG23	1:B:113:CYS:SG	2.54	0.47
1:C:8:SER:O	1:C:12:ILE:HD12	2.15	0.47
1:C:341:ILE:HB	1:C:406:LEU:HD23	1.97	0.47
1:D:45:PHE:O	1:D:48:LEU:N	2.47	0.47
1:E:136:PHE:CE1	1:E:238:LEU:HD12	2.49	0.47
1:A:8:SER:O	1:A:11:LYS:HE2	2.15	0.47
1:C:292:PHE:CG	1:C:365:ARG:NH1	2.83	0.47
1:D:142:PHE:O	1:D:228:GLN:HA	2.15	0.47
1:D:394:ASN:HB2	1:D:396:ILE:CG1	2.45	0.46
1:F:72:HIS:HB3	1:F:105:TYR:CZ	2.49	0.46
1:B:350:SER:OG	1:B:406:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:PHE:HB3	1:C:464:PHE:CZ	2.50	0.46
1:F:267:PRO:HD2	1:F:327:ASN:OD1	2.16	0.46
1:F:368:PHE:HB3	1:F:370:PHE:CE1	2.50	0.46
1:D:169:ASN:HB3	1:D:174:PHE:HZ	1.80	0.46
1:D:442:GLU:C	1:D:444:GLN:H	2.23	0.46
1:F:209:VAL:O	1:F:212:GLN:HB2	2.14	0.46
1:A:28:ASP:OD2	1:A:30:ARG:NH2	2.33	0.46
1:A:141:GLU:OE2	1:A:277:GLY:N	2.46	0.46
1:C:319:ALA:HA	1:C:322:THR:OG1	2.15	0.46
1:D:293:SER:HB2	1:D:361:LYS:HG3	1.96	0.46
1:E:199:MET:O	1:E:202:ILE:HG22	2.16	0.46
1:C:365:ARG:HD2	1:C:365:ARG:HA	1.51	0.46
1:D:49:THR:OG1	1:D:52:MET:HG3	2.16	0.46
1:F:65:LYS:HG2	1:F:66:GLY:N	2.31	0.46
1:A:67:TRP:CH2	1:A:101:VAL:HG21	2.51	0.46
1:B:292:PHE:O	1:B:300:LEU:HA	2.16	0.46
1:E:175:GLU:O	1:E:178:VAL:HG22	2.16	0.46
1:F:164:GLU:O	1:F:183:ARG:NE	2.44	0.46
1:C:71:GLU:HA	1:D:348:ASN:CG	2.41	0.46
1:E:34:ILE:HD12	1:E:66:GLY:HA3	1.97	0.46
1:F:148:ILE:HG22	1:F:262:THR:HG21	1.98	0.46
1:B:357:TYR:O	1:B:359:ILE:HG22	2.16	0.46
1:C:306:HIS:HB3	1:C:392:VAL:HA	1.97	0.46
1:C:313:ARG:NH2	1:C:396:ILE:HG23	2.31	0.46
1:E:428:ARG:HG3	1:E:431:GLU:OE2	2.16	0.46
1:F:258:LEU:HD23	1:F:258:LEU:HA	1.84	0.46
1:A:190:TYR:HA	1:A:191:MET:HG2	1.98	0.46
1:B:208:LYS:HA	1:B:208:LYS:HD3	1.74	0.46
1:B:344:TYR:CE2	1:B:401:ALA:HB2	2.51	0.46
1:D:348:ASN:OD1	1:D:350:SER:OG	2.22	0.46
1:E:313:ARG:NH2	1:E:396:ILE:HG23	2.30	0.46
1:B:15:PHE:CD2	1:B:81:LEU:HD22	2.51	0.45
1:D:30:ARG:HA	1:D:39:ASN:O	2.16	0.45
1:D:113:CYS:HB3	1:D:116:SER:HB2	1.97	0.45
1:C:71:GLU:HG3	1:C:72:HIS:ND1	2.30	0.45
1:D:143:PHE:CD2	1:D:269:PRO:HG3	2.52	0.45
1:E:120:LYS:NZ	1:E:120:LYS:HB2	2.31	0.45
1:F:315:ALA:HB3	1:F:342:LEU:HD13	1.98	0.45
1:C:33:ASP:OD1	1:C:34:ILE:N	2.47	0.45
1:D:207:VAL:HG13	1:D:217:THR:HG21	1.98	0.45
1:A:350:SER:OG	1:A:406:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:PHE:HB3	1:E:99:CYS:SG	2.57	0.45
1:D:343:THR:HG22	1:D:344:TYR:N	2.31	0.45
1:F:56:GLY:O	1:F:57:ILE:HD13	2.17	0.45
1:C:70:ILE:HA	1:C:73:SER:HB3	1.98	0.45
1:C:292:PHE:CD1	1:C:365:ARG:NH1	2.85	0.45
1:F:318:LEU:HD11	1:F:383:ALA:C	2.42	0.45
1:A:26:PHE:O	1:A:94:SER:HA	2.17	0.45
1:B:123:GLN:HG3	1:B:126:LYS:HD3	1.99	0.45
1:B:136:PHE:CE1	1:B:238:LEU:HD12	2.51	0.45
1:B:221:HIS:ND1	1:B:222:HIS:O	2.30	0.45
1:E:49:THR:HG23	1:E:52:MET:H	1.81	0.45
1:F:124:HIS:ND1	1:F:443:SER:OG	2.50	0.45
1:A:242:ALA:HB2	1:A:381:PHE:CD2	2.52	0.45
1:B:24:VAL:HG11	1:B:95:VAL:HG12	1.99	0.45
1:C:162:ASP:OD2	1:C:172:ARG:NH2	2.50	0.45
1:D:420:LYS:HD2	1:D:420:LYS:HA	1.52	0.45
1:A:115:ARG:HG3	1:A:378:TYR:CE1	2.52	0.44
1:C:175:GLU:C	1:C:177:GLY:H	2.23	0.44
1:D:462:GLU:C	1:D:465:PRO:HD2	2.42	0.44
1:A:297:TYR:HE1	1:A:344:TYR:HE2	1.65	0.44
1:B:149:LYS:O	1:B:159:TYR:HA	2.17	0.44
1:A:8:SER:HA	1:A:11:LYS:NZ	2.32	0.44
1:C:29:PHE:HB3	1:C:99:CYS:SG	2.58	0.44
1:D:72:HIS:HB3	1:D:105:TYR:CZ	2.53	0.44
1:C:165:GLU:OE2	1:C:198:THR:OG1	2.33	0.44
1:F:345:SER:HB3	1:F:348:ASN:HB3	1.99	0.44
1:A:26:PHE:CE1	1:B:204:THR:HG23	2.51	0.44
1:B:293:SER:CB	1:B:361:LYS:HD2	2.48	0.44
1:C:73:SER:OG	1:D:349:ARG:HG3	2.18	0.44
1:D:65:LYS:HD3	1:D:457:LEU:HG	1.98	0.44
1:B:226:GLN:HG3	1:B:273:ASP:OD2	2.18	0.44
1:C:282:VAL:O	1:C:365:ARG:CG	2.63	0.44
1:E:448:GLU:O	1:E:448:GLU:HG3	2.18	0.44
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.78	0.44
1:B:49:THR:HG1	1:B:52:MET:N	2.11	0.44
1:C:68:GLN:CG	1:C:75:MET:HE2	2.47	0.44
1:D:74:ASP:OD1	1:E:347:ASN:HA	2.18	0.44
1:D:205:GLU:HG2	1:D:255:VAL:HG11	2.00	0.44
1:F:164:GLU:HG2	1:F:174:PHE:CZ	2.53	0.44
1:F:350:SER:OG	1:F:406:LEU:HD13	2.17	0.44
1:A:54:LYS:HZ3	1:A:54:LYS:HG2	1.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:PHE:CD1	1:D:77:LEU:HG	2.53	0.44
1:F:78:THR:HG23	1:F:100:ASP:HB2	1.99	0.44
1:F:101:VAL:HG23	1:F:113:CYS:SG	2.58	0.44
1:A:445:VAL:HG12	1:A:446:PHE:CD1	2.51	0.44
1:B:186:LYS:O	1:B:187:GLN:HB2	2.17	0.44
1:E:164:GLU:O	1:E:183:ARG:NE	2.49	0.44
1:F:48:LEU:HD23	1:F:48:LEU:HA	1.74	0.44
1:E:146:ASP:N	1:E:162:ASP:O	2.42	0.43
1:E:216:GLU:HG3	1:E:234:LYS:HE2	2.00	0.43
1:E:328:SER:O	1:E:331:ARG:HB3	2.18	0.43
1:A:209:VAL:O	1:A:212:GLN:HB2	2.18	0.43
1:A:478:THR:O	1:A:479:TYR:C	2.61	0.43
1:B:18:PHE:O	1:B:22:ASN:ND2	2.47	0.43
1:B:360:SER:OG	1:B:361:LYS:N	2.50	0.43
1:C:205:GLU:O	1:C:208:LYS:HB2	2.17	0.43
1:C:316:ARG:HD2	1:C:421:GLN:O	2.17	0.43
1:E:207:VAL:HG13	1:E:217:THR:OG1	2.17	0.43
1:E:389:MET:HA	1:E:392:VAL:HG22	2.00	0.43
1:F:330:LYS:H	1:F:330:LYS:HG2	1.58	0.43
1:F:412:ASP:O	1:F:416:GLU:N	2.33	0.43
1:C:173:SER:CB	1:C:177:GLY:HA2	2.48	0.43
1:E:278:MET:O	1:E:371:PRO:HG2	2.18	0.43
1:D:54:LYS:HA	1:D:54:LYS:HD2	1.75	0.43
1:D:293:SER:HB2	1:D:361:LYS:CG	2.49	0.43
1:D:446:PHE:HB3	1:D:451:ILE:HD11	2.01	0.43
1:A:30:ARG:HB3	1:A:38:TRP:CE2	2.54	0.43
1:A:83:ARG:HD3	1:A:240:GLU:HG3	2.01	0.43
1:B:163:SER:O	1:B:169:ASN:ND2	2.52	0.43
1:B:343:THR:HG22	1:B:344:TYR:H	1.83	0.43
1:D:356:PRO:HG2	1:D:365:ARG:HE	1.83	0.43
1:E:45:PHE:O	1:E:48:LEU:N	2.51	0.43
1:F:115:ARG:NH1	1:F:243:ASP:OD2	2.51	0.43
1:C:22:ASN:CB	1:C:86:ILE:HD11	2.48	0.43
1:C:56:GLY:HA3	1:C:76:ILE:HG23	2.01	0.43
1:C:241:ALA:O	1:C:245:VAL:HG23	2.18	0.43
1:F:33:ASP:HA	1:F:67:TRP:CZ2	2.53	0.43
1:F:45:PHE:O	1:F:48:LEU:N	2.49	0.43
1:E:38:TRP:HD1	1:E:38:TRP:HA	1.74	0.43
1:E:297:TYR:HB3	1:E:305:LEU:HD11	2.00	0.43
1:A:11:LYS:HD3	1:A:11:LYS:N	2.33	0.43
1:D:115:ARG:O	1:D:119:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:PHE:HE1	1:D:179:ASN:ND2	2.16	0.43
1:F:62:SER:HB2	1:F:73:SER:HB3	2.01	0.43
1:F:297:TYR:CZ	1:F:298:LYS:HD2	2.54	0.43
1:A:331:ARG:O	1:A:333:ILE:N	2.44	0.43
1:B:164:GLU:HG3	1:B:174:PHE:CZ	2.54	0.43
1:C:197:ASP:OD1	1:C:222:HIS:HD2	2.01	0.43
1:E:216:GLU:HB2	1:E:234:LYS:HD3	2.01	0.43
1:A:120:LYS:HE2	1:A:445:VAL:HA	2.01	0.42
1:A:265:PHE:HB3	1:A:373:SER:HB2	2.00	0.42
1:A:322:THR:HB	1:A:371:PRO:HB3	2.00	0.42
1:B:123:GLN:N	1:B:123:GLN:OE1	2.51	0.42
1:D:48:LEU:HD23	1:D:48:LEU:HA	1.61	0.42
1:D:237:ASP:OD1	1:D:237:ASP:N	2.52	0.42
1:C:283:SER:CA	1:C:365:ARG:CZ	2.89	0.42
1:E:33:ASP:OD1	1:E:37:THR:N	2.48	0.42
1:E:52:MET:HE3	1:E:52:MET:HB2	1.68	0.42
1:B:194:PRO:HA	1:B:197:ASP:H	1.84	0.42
1:B:291:LEU:HB3	1:B:303:PHE:CD2	2.54	0.42
1:D:199:MET:O	1:D:203:ARG:HG3	2.19	0.42
1:E:462:GLU:C	1:E:465:PRO:HD2	2.44	0.42
1:F:278:MET:HE2	1:F:278:MET:HB3	1.93	0.42
1:F:342:LEU:HA	1:F:352:SER:OG	2.19	0.42
1:B:115:ARG:NH1	1:B:243:ASP:OD2	2.52	0.42
1:C:62:SER:HA	1:C:68:GLN:O	2.18	0.42
1:C:72:HIS:HB3	1:C:105:TYR:CZ	2.54	0.42
1:D:308:LEU:O	1:D:312:LEU:HD13	2.18	0.42
1:D:343:THR:HG21	1:D:402:MET:CB	2.48	0.42
1:F:43:TYR:CZ	1:F:57:ILE:HD12	2.55	0.42
1:F:166:GLY:HA2	1:F:226:GLN:OE1	2.20	0.42
1:A:272:GLY:HA2	1:A:336:TYR:OH	2.19	0.42
1:B:110:TYR:OH	1:B:112:LYS:HE3	2.19	0.42
1:A:171:ASP:OD2	1:F:151:LYS:HD3	2.19	0.42
1:B:332:LEU:C	1:B:333:ILE:HD12	2.44	0.42
1:C:27:VAL:HG21	1:C:48:LEU:HD12	2.01	0.42
1:C:267:PRO:HD2	1:C:327:ASN:OD1	2.19	0.42
1:C:283:SER:HB2	1:C:285:TRP:HE1	1.84	0.42
1:D:147:SER:HB2	1:E:179:ASN:H	1.85	0.42
1:D:370:PHE:N	1:D:371:PRO:HD2	2.34	0.42
1:A:209:VAL:HA	1:A:212:GLN:HB2	2.00	0.42
1:A:391:GLY:O	1:A:395:LYS:N	2.53	0.42
1:B:303:PHE:CE1	1:B:392:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:PHE:O	1:C:373:SER:HB2	2.19	0.42
1:E:199:MET:HB3	1:E:202:ILE:HG22	2.01	0.42
1:F:126:LYS:HE3	1:F:132:ASP:O	2.19	0.42
1:A:30:ARG:HA	1:A:39:ASN:O	2.20	0.42
1:B:165:GLU:OE2	1:B:198:THR:OG1	2.34	0.42
1:B:348:ASN:OD1	1:B:350:SER:OG	2.23	0.42
1:B:356:PRO:CB	1:B:365:ARG:HH21	2.33	0.42
1:C:8:SER:C	1:C:12:ILE:HD12	2.45	0.42
1:C:48:LEU:HA	1:C:48:LEU:HD23	1.74	0.42
1:C:268:LYS:NZ	1:C:273:ASP:O	2.38	0.42
1:C:406:LEU:C	1:C:408:LYS:H	2.27	0.42
1:E:65:LYS:HB3	1:E:457:LEU:HD13	2.01	0.42
1:E:166:GLY:HA2	1:E:226:GLN:OE1	2.19	0.42
1:E:461:ALA:O	1:E:465:PRO:HG2	2.19	0.42
1:C:459:PHE:HD1	1:C:464:PHE:CE2	2.38	0.42
1:D:203:ARG:HB3	1:D:220:VAL:HG22	2.01	0.42
1:F:308:LEU:HD22	1:F:366:PHE:CE1	2.55	0.42
1:D:172:ARG:HD3	1:D:174:PHE:CE2	2.55	0.42
1:C:234:LYS:HB2	1:C:234:LYS:HE3	1.59	0.41
1:D:164:GLU:HG2	1:D:183:ARG:NH2	2.35	0.41
1:E:163:SER:O	1:E:169:ASN:ND2	2.53	0.41
1:E:216:GLU:CB	1:E:234:LYS:HD3	2.50	0.41
1:F:62:SER:OG	1:F:70:ILE:HG23	2.20	0.41
1:F:342:LEU:HA	1:F:342:LEU:HD23	1.85	0.41
1:A:56:GLY:HA3	1:A:76:ILE:HG23	2.02	0.41
1:B:57:ILE:HB	1:B:77:LEU:HB2	2.02	0.41
1:D:148:ILE:O	1:E:179:ASN:HB3	2.20	0.41
1:D:173:SER:HB2	1:D:177:GLY:HA2	2.02	0.41
1:F:49:THR:HG22	1:F:52:MET:HG3	1.97	0.41
1:B:190:TYR:CE1	1:B:191:MET:HE2	2.54	0.41
1:E:31:PHE:CE1	1:E:77:LEU:HD11	2.56	0.41
1:E:216:GLU:HB2	1:E:234:LYS:HB2	2.02	0.41
1:F:65:LYS:HG2	1:F:66:GLY:H	1.84	0.41
1:A:243:ASP:OD1	1:A:378:TYR:OH	2.24	0.41
1:D:291:LEU:HA	1:D:291:LEU:HD23	1.78	0.41
1:E:254:MET:SD	1:F:194:PRO:HB2	2.59	0.41
1:F:223:GLU:HG3	1:F:224:VAL:N	2.24	0.41
1:F:342:LEU:HD23	1:F:352:SER:OG	2.21	0.41
1:F:408:LYS:O	1:F:409:LEU:C	2.63	0.41
1:A:181:GLY:O	1:A:182:HIS:C	2.63	0.41
1:A:215:LEU:HD21	1:A:244:ASN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:O	1:B:213:VAL:HG22	2.20	0.41
1:B:404:ILE:HD12	1:B:406:LEU:HA	2.03	0.41
1:C:83:ARG:CD	1:C:240:GLU:HG3	2.39	0.41
1:C:306:HIS:CD2	1:C:395:LYS:HD2	2.55	0.41
1:C:350:SER:OG	1:C:406:LEU:HD13	2.20	0.41
1:C:422:MET:SD	1:C:423:PRO:HD2	2.60	0.41
1:F:34:ILE:HD12	1:F:66:GLY:HA3	2.02	0.41
1:A:460:ASN:HA	1:A:464:PHE:HD2	1.85	0.41
1:D:139:GLU:O	1:D:278:MET:HA	2.20	0.41
1:D:282:VAL:HG22	1:D:368:PHE:HE2	1.86	0.41
1:B:49:THR:HG23	1:B:52:MET:CE	2.50	0.41
1:C:267:PRO:HG2	1:C:328:SER:HA	2.02	0.41
1:D:323:ASN:HB3	1:D:328:SER:HB3	2.02	0.41
1:A:297:TYR:CE1	1:A:344:TYR:HE2	2.38	0.41
1:B:90:SER:HB3	1:C:200:MET:HE2	2.01	0.41
1:B:211:ASN:HA	1:B:215:LEU:O	2.20	0.41
1:E:284:VAL:C	1:E:285:TRP:CD1	2.99	0.41
1:F:59:PHE:CD1	1:F:77:LEU:HG	2.56	0.41
1:B:148:ILE:O	1:C:179:ASN:HB3	2.20	0.41
1:B:190:TYR:HA	1:B:191:MET:HA	1.81	0.41
1:C:42:ALA:HB3	1:D:220:VAL:CG1	2.51	0.41
1:C:307:PHE:CZ	1:C:388:GLY:HA3	2.56	0.41
1:C:388:GLY:O	1:C:392:VAL:HG13	2.20	0.41
1:D:308:LEU:CD1	1:D:353:VAL:HG11	2.51	0.41
1:E:189:GLY:O	1:E:191:MET:HA	2.21	0.41
1:E:394:ASN:O	1:E:395:LYS:C	2.64	0.41
1:E:459:PHE:O	1:E:464:PHE:HD2	2.03	0.41
1:F:199:MET:HB3	1:F:202:ILE:HG22	2.03	0.41
1:A:394:ASN:O	1:A:395:LYS:C	2.64	0.41
1:B:316:ARG:HH12	1:B:428:ARG:NH1	2.19	0.41
1:C:148:ILE:HG22	1:C:262:THR:HG21	2.01	0.41
1:D:76:ILE:O	1:D:101:VAL:HA	2.20	0.41
1:D:205:GLU:HG2	1:D:255:VAL:CG1	2.51	0.41
1:E:48:LEU:HD23	1:E:52:MET:SD	2.60	0.41
1:E:391:GLY:O	1:E:395:LYS:N	2.54	0.41
1:F:208:LYS:O	1:F:212:GLN:HG3	2.21	0.41
1:F:333:ILE:HD13	1:F:333:ILE:HA	1.77	0.41
1:A:56:GLY:HA3	1:A:76:ILE:CG2	2.51	0.40
1:A:92:ASP:HB2	1:B:204:THR:CG2	2.50	0.40
1:A:286:LYS:HB3	1:A:291:LEU:HD21	2.02	0.40
1:A:368:PHE:HB3	1:A:370:PHE:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LYS:O	1:B:251:VAL:HG23	2.21	0.40
1:C:141:GLU:OE1	1:C:276:SER:HA	2.20	0.40
1:D:442:GLU:C	1:D:444:GLN:N	2.78	0.40
1:C:135:TYR:HA	1:C:236:GLY:O	2.22	0.40
1:C:361:LYS:HD3	1:C:361:LYS:HA	1.80	0.40
1:E:134:ALA:O	1:E:237:ASP:HA	2.21	0.40
1:E:403:ASP:O	1:E:404:ILE:HD13	2.21	0.40
1:F:308:LEU:HD21	1:F:344:TYR:CG	2.56	0.40
1:D:203:ARG:HB3	1:D:220:VAL:CG2	2.51	0.40
1:D:394:ASN:OD1	1:D:394:ASN:N	2.54	0.40
1:D:433:MET:SD	1:D:433:MET:C	3.04	0.40
1:E:23:GLU:O	1:E:93:VAL:HB	2.22	0.40
1:A:191:MET:SD	1:F:41:ILE:HB	2.61	0.40
1:A:339:PRO:CB	1:A:352:SER:HA	2.51	0.40
1:A:391:GLY:HA2	1:A:396:ILE:CG1	2.51	0.40
1:B:464:PHE:HB2	1:B:465:PRO:HD3	2.04	0.40
1:C:29:PHE:HD1	1:C:97:VAL:CG1	2.34	0.40
1:C:65:LYS:HE3	1:C:460:ASN:HB2	2.03	0.40
1:C:341:ILE:O	1:C:352:SER:OG	2.25	0.40
1:D:41:ILE:HB	1:E:191:MET:HE1	2.02	0.40
1:D:71:GLU:HG2	1:D:72:HIS:N	2.35	0.40
1:D:164:GLU:CG	1:D:183:ARG:HH21	2.32	0.40
1:D:323:ASN:ND2	1:D:372:ASP:OD1	2.54	0.40
1:A:423:PRO:HA	1:A:428:ARG:HH11	1.87	0.40
1:C:25:GLU:H	1:C:93:VAL:HG23	1.86	0.40
1:C:29:PHE:HE2	1:C:43:TYR:CD1	2.40	0.40
1:D:43:TYR:CE2	1:D:52:MET:HE1	2.57	0.40
1:F:394:ASN:O	1:F:395:LYS:C	2.65	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	472/481 (98%)	443 (94%)	26 (6%)	3 (1%)	21	51
1	B	473/481 (98%)	447 (94%)	23 (5%)	3 (1%)	21	51
1	C	472/481 (98%)	442 (94%)	28 (6%)	2 (0%)	30	60
1	D	473/481 (98%)	447 (94%)	23 (5%)	3 (1%)	21	51
1	E	472/481 (98%)	440 (93%)	27 (6%)	5 (1%)	11	36
1	F	472/481 (98%)	440 (93%)	27 (6%)	5 (1%)	11	36
All	All	2834/2886 (98%)	2659 (94%)	154 (5%)	21 (1%)	18	47

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	LYS
1	D	45	PHE
1	D	46	GLY
1	E	45	PHE
1	E	46	GLY
1	F	45	PHE
1	F	46	GLY
1	A	298	LYS
1	C	175	GLU
1	E	409	LEU
1	F	418	GLY
1	E	298	LYS
1	A	10	SER
1	A	409	LEU
1	B	235	PHE
1	F	167	GLU
1	F	409	LEU
1	C	176	ASN
1	D	182	HIS
1	B	418	GLY
1	E	418	GLY

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	398/415 (96%)	383 (96%)	15 (4%)	29	64
1	B	399/415 (96%)	374 (94%)	25 (6%)	16	45
1	C	398/415 (96%)	381 (96%)	17 (4%)	26	60
1	D	399/415 (96%)	383 (96%)	16 (4%)	28	63
1	E	399/415 (96%)	390 (98%)	9 (2%)	44	78
1	F	398/415 (96%)	381 (96%)	17 (4%)	26	60
All	All	2391/2490 (96%)	2292 (96%)	99 (4%)	27	62

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	62	SER
1	A	71	GLU
1	A	148	ILE
1	A	204	THR
1	A	205	GLU
1	A	220	VAL
1	A	293	SER
1	A	302	GLU
1	A	359	ILE
1	A	374	SER
1	A	392	VAL
1	A	420	LYS
1	A	429	SER
1	A	457	LEU
1	B	9	GLU
1	B	35	LYS
1	B	41	ILE
1	B	52	MET
1	B	78	THR
1	B	97	VAL
1	B	101	VAL
1	B	123	GLN
1	B	148	ILE
1	B	170	ARG
1	B	200	MET
1	B	202	ILE
1	B	207	VAL
1	B	234	LYS
1	B	252	VAL

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Mol	Chain	Res	Type
1	B	262	THR
1	B	280	THR
1	B	289	GLU
1	B	343	THR
1	B	359	ILE
1	B	365	ARG
1	B	374	SER
1	B	404	ILE
1	B	420	LYS
1	B	422	MET
1	C	8	SER
1	C	10	SER
1	C	12	ILE
1	C	178	VAL
1	C	186	LYS
1	C	202	ILE
1	C	212	GLN
1	C	219	VAL
1	C	220	VAL
1	C	234	LYS
1	C	253	LYS
1	C	296	THR
1	C	340	SER
1	C	353	VAL
1	C	365	ARG
1	C	402	MET
1	C	426	LEU
1	D	14	GLU
1	D	35	LYS
1	D	148	ILE
1	D	233	VAL
1	D	234	LYS
1	D	237	ASP
1	D	262	THR
1	D	308	LEU
1	D	353	VAL
1	D	361	LYS
1	D	374	SER
1	D	420	LYS
1	D	427	ARG
1	D	438	GLN
1	D	457	LEU

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Mol	Chain	Res	Type
1	D	477	THR
1	E	106	LYS
1	E	120	LYS
1	E	161	VAL
1	E	218	PHE
1	E	252	VAL
1	E	262	THR
1	E	280	THR
1	E	419	ILE
1	E	480	SER
1	F	24	VAL
1	F	63	CYS
1	F	73	SER
1	F	78	THR
1	F	101	VAL
1	F	148	ILE
1	F	161	VAL
1	F	215	LEU
1	F	220	VAL
1	F	280	THR
1	F	288	ASN
1	F	293	SER
1	F	302	GLU
1	F	333	ILE
1	F	353	VAL
1	F	400	GLU
1	F	449	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	124	HIS
1	A	259	ASN
1	A	279	HIS
1	B	68	GLN
1	B	347	ASN
1	D	157	GLN
1	D	287	ASN
1	D	452	GLN
1	E	421	GLN
1	F	22	ASN

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Mol	Chain	Res	Type
1	F	108	GLN
1	F	347	ASN
1	F	362	ASN
1	F	438	GLN
1	F	460	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	474/481 (98%)	-0.51	0	100	100	21, 39, 63, 99	0
1	B	475/481 (98%)	-0.47	0	100	100	22, 41, 60, 77	0
1	C	474/481 (98%)	-0.41	0	100	100	24, 43, 72, 86	0
1	D	475/481 (98%)	-0.34	0	100	100	26, 48, 72, 97	0
1	E	474/481 (98%)	-0.45	1 (0%)	91	88	24, 43, 66, 84	0
1	F	474/481 (98%)	-0.45	0	100	100	22, 39, 63, 104	0
All	All	2846/2886 (98%)	-0.44	1 (0%)	100	100	21, 42, 67, 104	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	481	CYS	2.2

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.