



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:47 AM UTC

PDB ID : 4C2D / pdb_00004c2d
Title : Crystal structure of the protease CtpB in an active state
Authors : Mastny, M.; Heuck, A.; Kurzbauer, R.; Clausen, T.
Deposited on : 2013-08-17
Resolution : 2.70 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

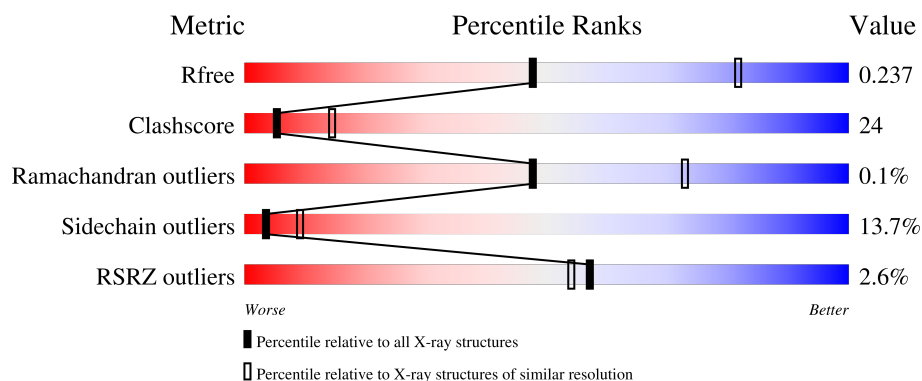
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	446	 61% 31% . .
1	B	446	 2% 61% 30% 6% .
1	C	446	 3% 45% 43% 9% . .
1	D	446	 3% 36% 35% 7% 23%
2	E	6	 67% 33%

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Mol	Chain	Length	Quality of chain
2	F	6	17% 50% 50%
2	G	6	67% 17% 17%
2	H	6	33% 17% 17% 33%
3	M	5	60% 40%
4	N	4	75% 25%
4	O	4	50% 75% 25%
4	P	4	25% 75% 50% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13353 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 CARBOXY-TERMINAL PROCESSING PROTEASE CTPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	1
			3382	2135	578	659	10			
1	B	434	Total	C	N	O	S	0	0	1
			3382	2135	578	659	10			
1	C	434	Total	C	N	O	S	0	0	1
			3382	2135	578	659	10			
1	D	344	Total	C	N	O	S	0	0	1
			2705	1709	456	533	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	initiating methionine	UNP O35002
A	481	LEU	-	expression tag	UNP O35002
A	482	GLU	-	expression tag	UNP O35002
A	483	HIS	-	expression tag	UNP O35002
A	484	HIS	-	expression tag	UNP O35002
A	485	HIS	-	expression tag	UNP O35002
A	486	HIS	-	expression tag	UNP O35002
A	487	HIS	-	expression tag	UNP O35002
A	488	HIS	-	expression tag	UNP O35002
B	43	MET	-	initiating methionine	UNP O35002
B	481	LEU	-	expression tag	UNP O35002
B	482	GLU	-	expression tag	UNP O35002
B	483	HIS	-	expression tag	UNP O35002
B	484	HIS	-	expression tag	UNP O35002
B	485	HIS	-	expression tag	UNP O35002
B	486	HIS	-	expression tag	UNP O35002
B	487	HIS	-	expression tag	UNP O35002
B	488	HIS	-	expression tag	UNP O35002
C	43	MET	-	initiating methionine	UNP O35002
C	481	LEU	-	expression tag	UNP O35002
C	482	GLU	-	expression tag	UNP O35002

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Chain	Residue	Modelled	Actual	Comment	Reference
C	483	HIS	-	expression tag	UNP O35002
C	484	HIS	-	expression tag	UNP O35002
C	485	HIS	-	expression tag	UNP O35002
C	486	HIS	-	expression tag	UNP O35002
C	487	HIS	-	expression tag	UNP O35002
C	488	HIS	-	expression tag	UNP O35002
D	43	MET	-	initiating methionine	UNP O35002
D	481	LEU	-	expression tag	UNP O35002
D	482	GLU	-	expression tag	UNP O35002
D	483	HIS	-	expression tag	UNP O35002
D	484	HIS	-	expression tag	UNP O35002
D	485	HIS	-	expression tag	UNP O35002
D	486	HIS	-	expression tag	UNP O35002
D	487	HIS	-	expression tag	UNP O35002
D	488	HIS	-	expression tag	UNP O35002

- Molecule 2 is a protein called PEPTIDE1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			35	21	6	8			
2	F	6	Total	C	N	O	0	0	0
			35	21	6	8			
2	G	6	Total	C	N	O	0	0	0
			35	21	6	8			
2	H	4	Total	C	N	O	0	0	1
			19	12	4	3			

- Molecule 3 is a protein called PEPTIDE2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	0	0	0
			32	19	6	7			

- Molecule 4 is a protein called PEPTIDE2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	4	Total	C	N	O	0	0	0
			29	17	5	7			
4	O	4	Total	C	N	O	0	0	0
			27	16	5	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	3	Total	C	N	O	0	0	0
			16	9	3	4			

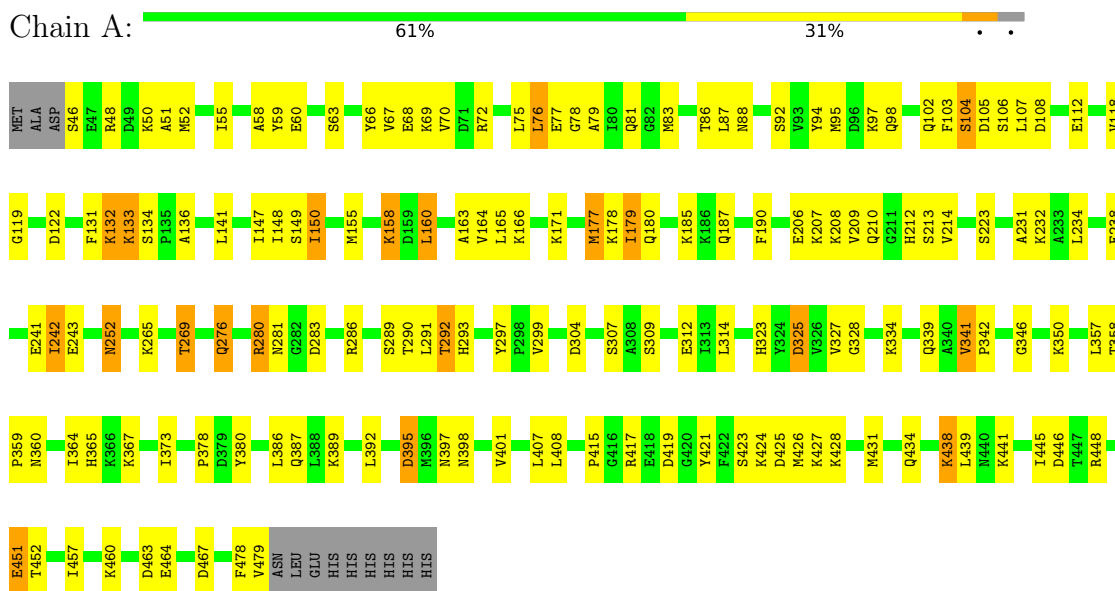
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	89	Total	O	0	0
			89	89		
5	C	37	Total	O	0	0
			37	37		
5	D	23	Total	O	0	0
			23	23		
5	E	3	Total	O	0	0
			3	3		
5	M	3	Total	O	0	0
			3	3		

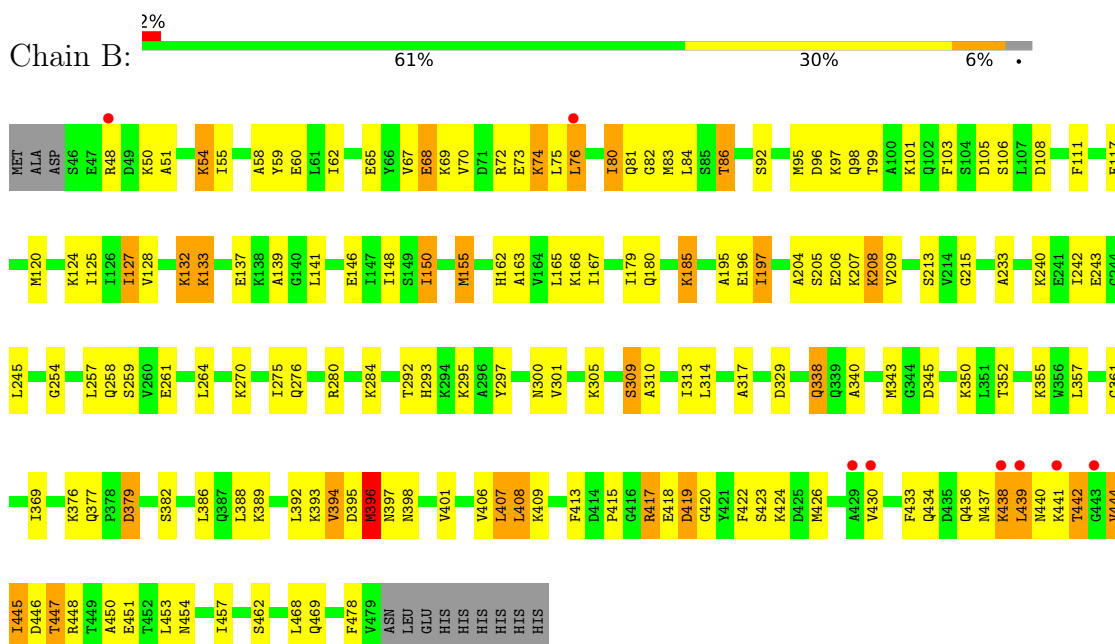
3 Residue-property plots

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: CARBOXY-TERMINAL PROCESSING PROTEASE CTPB



• Molecule 1: CARBOXY-TERMINAL PROCESSING PROTEASE CTPB

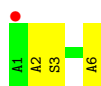


Chain E:  67% 33%



• Molecule 2: PEPTIDE1

Chain F:  17% 50% 50%



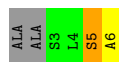
• Molecule 2: PEPTIDE1

Chain G:  67% 17% 17%



• Molecule 2: PEPTIDE1

Chain H:  33% 17% 17% 33%



• Molecule 3: PEPTIDE2

Chain M:  60% 40%



• Molecule 4: PEPTIDE2

Chain N:  75% 25%



• Molecule 4: PEPTIDE2

Chain O:  50% 75% 25%



• Molecule 4: PEPTIDE2

Chain P:  25% 75% 50% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.05Å 65.38Å 169.06Å 90.00° 95.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.70) 99.7 (20.00-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.241 0.224 , 0.237	Depositor DCC
R_{free} test set	3996 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13353	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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	0.63	1/3437 (0.0%)	0.99	3/4615 (0.1%)
1	B	0.61	1/3437 (0.0%)	0.99	2/4615 (0.0%)
1	C	0.51	2/3437 (0.1%)	0.96	14/4615 (0.3%)
1	D	0.43	1/2750 (0.0%)	0.86	2/3699 (0.1%)
2	E	0.69	0/34	1.08	1/45 (2.2%)
2	F	0.73	0/34	0.93	0/45
2	G	0.47	0/34	1.06	1/45 (2.2%)
2	H	1.73	1/18 (5.6%)	0.94	0/24
3	M	0.61	0/32	0.76	0/42
4	N	0.60	0/29	0.73	0/37
4	O	0.53	0/27	0.55	0/34
4	P	0.36	0/15	0.66	0/18
All	All	0.56	6/13284 (0.0%)	0.95	23/17834 (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	B	0	2
1	C	0	1
1	D	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	5	SER	C-N	-7.18	1.23	1.33
1	B	478	PHE	C-N	-6.90	1.23	1.33
1	C	478	PHE	C-N	-6.89	1.23	1.33
1	A	478	PHE	C-N	-6.78	1.23	1.33
1	D	478	PHE	C-N	-6.76	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	441	LYS	CA-CB	-5.40	1.46	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	431	MET	CB-CG-SD	9.00	139.71	112.70
1	C	89	ASP	CA-C-N	7.59	128.28	119.47
1	C	89	ASP	C-N-CA	7.59	128.28	119.47
1	C	441	LYS	CD-CE-NZ	-7.34	88.42	111.90
1	A	252	ASN	CA-C-N	7.26	127.42	119.87
1	A	252	ASN	C-N-CA	7.26	127.42	119.87
1	C	370	GLU	CA-C-N	6.46	126.43	120.03
1	C	370	GLU	C-N-CA	6.46	126.43	120.03
1	B	396	MET	N-CA-C	6.24	119.63	110.59
1	D	47	GLU	N-CA-C	-5.86	105.79	113.17
1	C	213	SER	N-CA-C	5.79	117.72	108.41
1	C	390	GLU	CA-C-N	5.71	126.03	119.92
1	C	390	GLU	C-N-CA	5.71	126.03	119.92
1	D	443	GLY	N-CA-C	-5.70	107.14	115.63
1	A	83	MET	N-CA-C	-5.57	104.22	111.02
1	C	47	GLU	N-CA-C	-5.50	106.34	113.16
1	C	309	SER	CB-CA-C	-5.38	109.91	117.23
1	C	142	LYS	N-CA-C	5.32	114.42	108.25
2	G	2	ALA	N-CA-C	5.25	117.80	109.50
1	C	277	ILE	N-CA-C	5.24	115.66	108.12
1	C	212	HIS	N-CA-C	5.23	118.09	109.72
1	B	355	LYS	N-CA-C	-5.11	101.94	110.17
2	E	2	ALA	N-CA-C	5.00	117.41	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	395	ASP	Peptide
1	B	417	ARG	Peptide
1	C	384	GLY	Peptide
1	D	436	GLN	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	3382	0	3433	126	1
1	B	3382	0	3433	141	1
1	C	3382	0	3433	234	2
1	D	2705	0	2709	178	2
2	E	35	0	38	1	0
2	F	35	0	38	6	0
2	G	35	0	38	3	0
2	H	19	0	14	2	0
3	M	32	0	32	3	0
4	N	29	0	27	1	0
4	O	27	0	22	1	0
4	P	16	0	8	10	0
5	A	119	0	0	23	0
5	B	89	0	0	15	0
5	C	37	0	0	4	0
5	D	23	0	0	2	0
5	E	3	0	0	1	0
5	M	3	0	0	0	0
All	All	13353	0	13225	633	4

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 24.

All (633) 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:212:HIS:CE1	1:C:243:GLU:HB3	1.77	1.20
1:D:255:GLY:N	4:P:5:ALA:OXT	1.83	1.12
1:A:95:MET:SD	5:A:2017:HOH:O	2.07	1.10
1:B:438:LYS:O	1:B:439:LEU:HG	1.52	1.06
1:A:177:MET:SD	5:A:2044:HOH:O	2.11	1.06
1:B:393:LYS:H	1:B:396:MET:HE3	0.92	1.05
1:C:249:VAL:HG11	1:C:311:SER:HB3	1.38	1.04
1:C:428:LYS:HA	1:C:431:MET:CG	1.88	1.03
1:C:431:MET:HE3	1:C:441:LYS:CE	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LYS:N	1:B:396:MET:HE3	1.77	0.97
1:D:56:GLU:O	1:D:60:GLU:HG3	1.64	0.97
1:C:417:ARG:NE	1:C:421:TYR:OH	1.98	0.95
1:C:249:VAL:CG1	1:C:311:SER:HB3	1.97	0.94
1:B:343:MET:SD	5:B:2078:HOH:O	2.25	0.93
1:B:206:GLU:OE2	1:B:208:LYS:NZ	2.04	0.91
1:B:206:GLU:OE1	1:B:240:LYS:NZ	2.04	0.90
1:A:148:ILE:HD11	1:A:180:GLN:HB2	1.51	0.90
1:C:79:ALA:HB2	1:D:83:MET:HG3	1.52	0.89
1:C:212:HIS:CE1	1:C:243:GLU:CB	2.55	0.89
1:A:479:VAL:N	5:A:2117:HOH:O	2.04	0.89
1:B:406:VAL:HA	1:B:409:LYS:HZ2	1.38	0.88
1:B:393:LYS:H	1:B:396:MET:CE	1.82	0.88
1:D:386:LEU:N	1:D:454:ASN:OD1	2.06	0.88
1:C:431:MET:HE3	1:C:441:LYS:HE3	1.56	0.88
1:C:67:VAL:HG13	1:C:68:GLU:HG2	1.54	0.87
1:C:212:HIS:HE1	1:C:243:GLU:H	1.21	0.87
1:C:48:ARG:HG3	1:C:48:ARG:HH11	1.40	0.87
1:B:436:GLN:O	1:B:437:ASN:ND2	2.07	0.86
1:A:59:TYR:HD2	1:B:83:MET:HE2	1.40	0.86
1:C:428:LYS:HA	1:C:431:MET:HG2	1.55	0.86
1:D:423:SER:O	1:D:427:LYS:NZ	2.09	0.85
1:D:295:LYS:HG3	1:D:297:TYR:CZ	2.12	0.84
1:C:212:HIS:CD2	1:C:214:VAL:HG13	2.13	0.83
1:C:428:LYS:HA	1:C:431:MET:HG3	1.56	0.83
1:C:177:MET:HE2	1:C:179:ILE:HD11	1.61	0.83
1:C:417:ARG:HH22	1:D:395:ASP:CG	1.86	0.83
1:B:357:LEU:O	5:B:2062:HOH:O	1.95	0.82
1:B:95:MET:HG2	1:B:99:THR:HG22	1.62	0.82
1:C:212:HIS:CE1	1:C:243:GLU:H	1.99	0.80
1:B:276:GLN:O	5:B:2062:HOH:O	1.98	0.80
1:A:206:GLU:OE2	1:A:208:LYS:NZ	2.15	0.80
1:A:439:LEU:O	5:A:2112:HOH:O	2.00	0.79
1:C:212:HIS:CD2	1:C:478:PHE:HZ	2.00	0.79
1:C:292:THR:HG22	1:C:293:HIS:CD2	2.17	0.79
1:D:394:VAL:CG1	1:D:427:LYS:HE3	2.12	0.79
1:B:65:GLU:OE2	5:B:2008:HOH:O	2.00	0.79
1:C:341:VAL:HG11	1:D:61:LEU:HD11	1.62	0.79
1:B:275:ILE:HG12	5:B:2062:HOH:O	1.83	0.79
1:D:273:PRO:O	1:D:359:PRO:HB3	1.82	0.79
1:C:280:ARG:NH1	1:D:64:ASN:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LYS:NZ	1:D:345:ASP:OD2	2.13	0.79
1:B:139:ALA:O	5:B:2030:HOH:O	2.01	0.78
1:C:119:GLY:HA2	1:C:160:LEU:HD21	1.66	0.78
1:C:431:MET:HE3	1:C:441:LYS:HE2	1.66	0.78
1:D:255:GLY:H	4:P:5:ALA:C	1.91	0.78
1:D:377:GLN:NE2	1:D:467:ASP:OD1	2.16	0.78
1:C:222:PHE:HB2	1:C:255:GLY:HA3	1.66	0.77
1:B:103:PHE:O	1:B:106:SER:OG	2.02	0.77
1:C:458:GLU:O	1:C:462:SER:OG	2.01	0.77
1:C:447:THR:OG1	1:C:448:ARG:N	2.14	0.77
1:B:424:LYS:NZ	5:B:2086:HOH:O	2.19	0.76
1:A:72:ARG:NH1	1:B:48:ARG:HD3	2.00	0.76
1:A:179:ILE:HD11	5:A:2044:HOH:O	1.86	0.76
1:A:231:ALA:C	5:A:2061:HOH:O	2.29	0.76
1:A:292:THR:HG1	1:A:293:HIS:HD1	0.77	0.76
1:D:393:LYS:H	1:D:396:MET:CE	1.99	0.75
1:C:431:MET:HA	1:C:441:LYS:HZ3	1.49	0.75
1:C:433:PHE:HE1	1:C:456:GLN:OE1	1.70	0.74
1:D:393:LYS:HG2	1:D:396:MET:HE2	1.70	0.74
1:C:219:ILE:O	1:C:252:ASN:ND2	2.19	0.74
1:A:323:HIS:NE2	5:A:2075:HOH:O	2.09	0.73
1:C:71:ASP:OD2	1:C:74:LYS:NZ	2.21	0.73
1:C:297:TYR:O	5:C:2028:HOH:O	2.06	0.73
1:D:406:VAL:HG12	1:D:418:GLU:HG2	1.69	0.73
1:A:397:ASN:OD1	1:B:397:ASN:ND2	2.11	0.73
1:C:212:HIS:HE1	1:C:243:GLU:N	1.86	0.73
1:C:212:HIS:CE1	1:C:213:SER:O	2.42	0.73
1:B:418:GLU:N	1:B:418:GLU:OE1	2.22	0.72
1:B:125:ILE:HD12	1:B:155:MET:HG3	1.71	0.72
1:A:122:ASP:OD2	5:A:2031:HOH:O	2.08	0.72
1:A:52:MET:HE2	1:A:55:ILE:HD12	1.71	0.72
1:B:270:LYS:NZ	1:B:292:THR:HG22	2.05	0.72
1:C:148:ILE:HD11	1:C:180:GLN:HB2	1.71	0.72
1:D:370:GLU:N	1:D:370:GLU:OE1	2.23	0.72
1:C:386:LEU:H	1:C:454:ASN:HD21	1.38	0.71
1:D:393:LYS:H	1:D:396:MET:HE3	1.54	0.71
1:B:166:LYS:NZ	5:B:2034:HOH:O	2.17	0.71
1:C:116:ALA:N	4:O:5:ALA:OXT	2.21	0.71
1:C:391:PRO:O	1:C:393:LYS:NZ	2.23	0.70
1:C:380:TYR:OH	1:C:466:ASN:ND2	2.24	0.70
1:D:309:SER:OG	4:P:5:ALA:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:N	5:A:2061:HOH:O	2.25	0.70
1:A:309:SER:HB3	1:A:334:LYS:HD3	1.74	0.70
1:A:77:GLU:HB3	5:A:2008:HOH:O	1.90	0.70
1:B:95:MET:HG2	1:B:99:THR:CG2	2.22	0.70
1:A:131:PHE:HZ	3:M:4:GLN:HG2	1.57	0.69
1:D:309:SER:HG	4:P:5:ALA:C	2.01	0.69
1:C:173:SER:OG	1:C:194:ARG:NH1	2.26	0.69
1:C:431:MET:CG	1:C:441:LYS:HZ1	2.05	0.69
1:A:148:ILE:CD1	1:A:180:GLN:HB2	2.23	0.68
1:B:409:LYS:HE2	1:B:418:GLU:CD	2.18	0.68
1:A:299:VAL:O	5:A:2089:HOH:O	2.10	0.68
1:A:463:ASP:O	5:A:2114:HOH:O	2.10	0.68
1:D:334:LYS:NZ	1:D:336:THR:O	2.26	0.68
1:A:46:SER:OG	5:A:2001:HOH:O	2.11	0.68
1:D:268:VAL:HG21	1:D:274:TYR:HB3	1.76	0.68
1:D:405:GLN:NE2	1:D:421:TYR:O	2.27	0.68
1:A:360:ASN:O	5:A:2105:HOH:O	2.12	0.68
1:A:286:ARG:HG3	5:A:2085:HOH:O	1.94	0.67
1:C:212:HIS:NE2	1:C:214:VAL:HG13	2.08	0.67
1:D:457:ILE:O	1:D:461:LYS:HG3	1.93	0.67
1:C:276:GLN:NE2	1:C:359:PRO:O	2.27	0.67
1:D:448:ARG:HA	1:D:451:GLU:OE2	1.94	0.67
1:A:339:GLN:NE2	5:A:2098:HOH:O	2.24	0.67
1:C:392:LEU:HA	1:C:396:MET:SD	2.35	0.67
1:A:389:LYS:NZ	5:A:2109:HOH:O	2.27	0.67
1:C:419:ASP:HB2	1:C:421:TYR:CZ	2.30	0.67
1:A:98:GLN:NE2	1:A:102:GLN:OE1	2.26	0.66
1:C:105:ASP:OD2	1:C:168:ARG:NH1	2.27	0.66
1:C:243:GLU:O	1:C:298:PRO:HD2	1.96	0.66
1:D:393:LYS:HG2	1:D:396:MET:CE	2.25	0.66
1:B:438:LYS:O	1:B:439:LEU:CG	2.37	0.66
1:C:370:GLU:HG3	1:C:371:PRO:HD2	1.76	0.66
1:D:371:PRO:HG2	1:D:374:ALA:HB2	1.77	0.66
1:B:83:MET:O	1:B:86:THR:HB	1.96	0.66
1:B:97:LYS:NZ	1:B:345:ASP:O	2.17	0.65
1:C:51:ALA:HB1	1:D:76:LEU:HD13	1.78	0.65
1:D:48:ARG:HH11	1:D:48:ARG:HB3	1.59	0.65
1:B:418:GLU:O	1:B:418:GLU:HG2	1.95	0.65
1:C:460:LYS:HE2	1:C:466:ASN:HD21	1.59	0.65
1:D:446:ASP:OD1	1:D:447:THR:N	2.29	0.65
1:A:323:HIS:O	5:A:2094:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:HG23	1:A:342:PRO:HD2	1.79	0.64
1:B:58:ALA:O	1:B:62:ILE:HG13	1.97	0.64
1:D:330:THR:HB	1:D:370:GLU:HA	1.77	0.64
1:C:249:VAL:HG12	1:C:249:VAL:O	1.96	0.64
1:C:393:LYS:HA	1:C:444:VAL:HG11	1.80	0.64
1:B:450:ALA:O	1:B:454:ASN:ND2	2.29	0.64
1:D:271:ASP:OD1	1:D:272:GLN:NE2	2.30	0.64
1:C:207:LYS:NZ	1:C:464:GLU:OE2	2.17	0.64
1:B:276:GLN:N	5:B:2062:HOH:O	2.14	0.64
1:D:223:SER:N	1:D:226:THR:OG1	2.23	0.64
1:C:150:ILE:HG23	1:C:155:MET:HE3	1.80	0.64
1:C:150:ILE:O	1:C:150:ILE:HG13	1.97	0.63
1:B:127:ILE:CD1	1:B:141:LEU:HD13	2.28	0.63
1:C:386:LEU:H	1:C:454:ASN:ND2	1.96	0.63
1:C:433:PHE:CE2	1:C:453:LEU:HG	2.33	0.63
1:D:442:THR:HB	1:D:444:VAL:H	1.64	0.63
1:B:101:LYS:NZ	1:B:105:ASP:OD2	2.31	0.63
1:B:398:ASN:OD1	1:B:401:VAL:N	2.30	0.63
1:A:52:MET:CE	1:A:55:ILE:HD12	2.29	0.63
1:A:212:HIS:HB3	1:A:243:GLU:OE1	1.99	0.63
1:C:427:LYS:O	1:C:431:MET:HG2	1.99	0.63
1:C:276:GLN:OE1	1:C:284:LYS:NZ	2.20	0.62
1:C:434:GLN:OE1	1:C:441:LYS:HG3	1.98	0.62
1:C:431:MET:HA	1:C:441:LYS:NZ	2.13	0.62
1:B:50:LYS:NZ	5:B:2004:HOH:O	2.31	0.62
1:B:309:SER:OG	2:F:6:ALA:C	2.42	0.62
1:B:254:GLY:HA3	5:B:2053:HOH:O	1.99	0.62
1:A:60:GLU:OE2	1:B:48:ARG:NH2	2.32	0.62
1:C:249:VAL:HG11	1:C:311:SER:CB	2.23	0.62
1:D:439:LEU:HD11	1:D:449:THR:HG23	1.82	0.62
1:C:61:LEU:HD23	1:D:349:ILE:HD12	1.81	0.61
1:C:172:GLY:HA2	1:C:193:LYS:HE3	1.82	0.61
1:C:394:VAL:O	1:C:422:PHE:HB3	2.01	0.61
1:C:399:GLU:OE1	1:C:402:LYS:NZ	2.30	0.61
1:D:403:HIS:O	1:D:406:VAL:HG22	2.01	0.61
1:A:97:LYS:HE2	1:A:346:GLY:HA3	1.82	0.61
1:C:472:THR:O	1:C:476:SER:OG	2.18	0.61
1:B:148:ILE:HD11	1:B:180:GLN:HB2	1.82	0.61
1:B:163:ALA:O	1:B:167:ILE:HG13	2.01	0.61
1:B:338:GLN:HA	1:B:352:THR:HA	1.82	0.61
1:D:375:ILE:HG12	1:D:468:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LEU:HD22	1:A:457:ILE:HG13	1.82	0.60
1:A:479:VAL:N	5:A:2116:HOH:O	2.33	0.60
1:C:149:SER:OG	1:C:178:LYS:HB2	2.00	0.60
1:D:434:GLN:OE1	1:D:443:GLY:N	2.33	0.60
1:B:438:LYS:O	1:B:438:LYS:HG3	2.01	0.60
1:C:48:ARG:HG3	1:C:48:ARG:NH1	2.14	0.60
1:C:270:LYS:NZ	1:C:292:THR:HA	2.16	0.60
1:C:433:PHE:CE1	1:C:456:GLN:OE1	2.53	0.60
1:D:426:MET:O	1:D:430:VAL:HG12	2.02	0.60
1:B:439:LEU:HD11	1:B:448:ARG:NH2	2.16	0.60
1:C:399:GLU:HA	1:C:402:LYS:HD3	1.84	0.60
1:B:394:VAL:HA	1:B:422:PHE:CD1	2.36	0.60
1:A:103:PHE:O	1:A:106:SER:OG	2.20	0.59
1:A:265:LYS:HG2	1:A:289:SER:HB2	1.82	0.59
1:D:468:LEU:C	1:D:468:LEU:HD23	2.27	0.59
1:C:264:LEU:HD13	1:C:274:TYR:HB2	1.83	0.59
1:D:208:LYS:NZ	1:D:211:GLY:O	2.32	0.59
1:A:398:ASN:HB3	1:A:401:VAL:HG23	1.84	0.59
1:B:300:ASN:OD1	1:B:300:ASN:C	2.45	0.59
1:D:407:LEU:HD22	1:D:457:ILE:HG13	1.84	0.59
1:B:388:LEU:HD22	1:B:447:THR:HA	1.84	0.59
1:C:52:MET:HE2	1:D:56:GLU:CB	2.32	0.59
1:B:444:VAL:HG23	1:B:445:ILE:N	2.17	0.59
1:D:350:LYS:HE3	4:P:4:THR:CB	2.33	0.58
1:C:212:HIS:CE1	1:C:243:GLU:N	2.67	0.58
1:D:96:ASP:HA	1:D:347:SER:HB3	1.85	0.58
1:B:442:THR:HG1	1:B:444:VAL:H	1.51	0.58
1:B:409:LYS:HE2	1:B:418:GLU:OE2	2.04	0.58
1:C:388:LEU:HD12	1:C:389:LYS:N	2.19	0.58
1:C:393:LYS:NZ	1:C:396:MET:SD	2.70	0.58
1:C:431:MET:CB	1:C:441:LYS:HZ1	2.17	0.58
1:C:431:MET:HB3	1:C:441:LYS:HE2	1.86	0.58
1:A:364:ILE:HG13	5:A:2104:HOH:O	2.04	0.58
1:D:454:ASN:HD22	1:D:454:ASN:N	2.01	0.58
1:D:107:LEU:HB3	1:D:256:TYR:CE2	2.39	0.58
1:D:451:GLU:HG2	1:D:452:THR:N	2.19	0.58
1:A:107:LEU:O	1:A:223:SER:HB3	2.04	0.58
1:C:340:ALA:HB3	2:G:2:ALA:HB1	1.86	0.58
1:D:46:SER:HB2	1:D:48:ARG:H	1.67	0.58
1:A:52:MET:HE2	1:A:52:MET:HA	1.86	0.57
1:B:150:ILE:HG21	1:B:166:LYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LEU:HD22	1:B:401:VAL:HG13	1.85	0.57
1:D:52:MET:HA	1:D:52:MET:HE2	1.85	0.57
1:A:104:SER:O	1:A:107:LEU:N	2.33	0.57
1:A:309:SER:O	1:A:312:GLU:N	2.37	0.57
1:D:276:GLN:NE2	1:D:286:ARG:HD3	2.19	0.57
1:A:95:MET:HE2	1:A:350:LYS:HB2	1.85	0.57
1:C:388:LEU:HD12	1:C:389:LYS:H	1.69	0.57
1:C:431:MET:HB3	1:C:441:LYS:CE	2.34	0.57
1:C:212:HIS:ND1	1:C:213:SER:N	2.53	0.57
1:B:329:ASP:OD1	1:B:376:LYS:HG2	2.04	0.57
1:D:448:ARG:HD2	1:D:448:ARG:O	2.05	0.56
1:A:150:ILE:HD12	1:A:155:MET:HG2	1.88	0.56
1:C:398:ASN:OD1	1:C:400:ASP:N	2.38	0.56
1:D:71:ASP:OD2	1:D:74:LYS:HG3	2.05	0.56
1:A:147:ILE:HG21	1:A:150:ILE:HD11	1.87	0.56
1:B:133:LYS:N	1:B:137:GLU:OE1	2.39	0.56
1:C:394:VAL:HA	1:C:422:PHE:CD1	2.39	0.56
1:C:431:MET:CE	1:C:441:LYS:CE	2.76	0.56
1:A:59:TYR:HD2	1:B:83:MET:CE	2.14	0.56
1:A:92:SER:HA	1:A:350:LYS:O	2.06	0.56
1:B:439:LEU:HD11	1:B:448:ARG:HH22	1.70	0.56
1:A:104:SER:OG	1:A:105:ASP:N	2.36	0.56
1:D:427:LYS:HD3	1:D:427:LYS:N	2.20	0.56
1:A:59:TYR:CD2	1:B:83:MET:HE2	2.31	0.56
1:A:451:GLU:HG2	1:A:452:THR:N	2.20	0.56
1:C:431:MET:CB	1:C:441:LYS:NZ	2.69	0.56
1:D:333:GLY:HA2	1:D:364:ILE:HD12	1.87	0.56
1:B:84:LEU:O	5:B:2013:HOH:O	2.18	0.55
1:B:419:ASP:OD1	1:B:419:ASP:N	2.34	0.55
1:B:340:ALA:HB3	2:F:2:ALA:HB1	1.88	0.55
1:C:103:PHE:O	1:C:106:SER:OG	2.25	0.55
1:A:397:ASN:ND2	1:B:419:ASP:HB2	2.21	0.55
1:C:276:GLN:HB2	1:C:357:LEU:HB2	1.89	0.55
1:C:470:LEU:HD23	1:C:471:GLN:HG2	1.89	0.55
1:D:62:ILE:HG22	1:D:70:VAL:HG21	1.88	0.55
1:D:260:VAL:O	1:D:264:LEU:HG	2.06	0.55
1:D:394:VAL:HG12	1:D:427:LYS:HE3	1.86	0.55
1:C:397:ASN:ND2	1:D:397:ASN:OD1	2.36	0.55
1:A:136:ALA:HB1	1:A:141:LEU:HD12	1.88	0.55
1:C:212:HIS:CD2	1:C:478:PHE:CZ	2.89	0.55
1:D:423:SER:CB	1:D:426:MET:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:HB3	1:A:178:LYS:HB2	1.89	0.54
1:B:309:SER:HB3	2:F:6:ALA:O	2.07	0.54
1:C:209:VAL:O	1:C:210:GLN:HG3	2.08	0.54
1:C:393:LYS:N	1:C:396:MET:SD	2.77	0.54
1:A:425:ASP:OD1	1:A:426:MET:N	2.41	0.54
1:B:338:GLN:CD	1:B:338:GLN:N	2.65	0.54
1:D:422:PHE:CD1	1:D:427:LYS:NZ	2.71	0.54
1:C:295:LYS:HD2	1:C:297:TYR:CZ	2.42	0.54
1:D:375:ILE:CG1	1:D:468:LEU:HD21	2.38	0.54
1:A:292:THR:OG1	1:A:293:HIS:ND1	1.99	0.54
1:B:386:LEU:HB3	1:B:454:ASN:HD21	1.73	0.54
1:D:223:SER:H	1:D:226:THR:HG1	1.53	0.54
1:A:163:ALA:O	1:A:166:LYS:N	2.40	0.54
1:A:378:PRO:HB2	1:A:380:TYR:CE2	2.43	0.54
1:D:338:GLN:HG3	1:D:352:THR:HA	1.88	0.54
1:C:434:GLN:HE22	1:C:443:GLY:H	1.56	0.53
1:B:436:GLN:O	1:B:437:ASN:CG	2.52	0.53
1:C:388:LEU:HD21	1:C:390:GLU:O	2.08	0.53
1:D:264:LEU:HD12	1:D:265:LYS:N	2.23	0.53
1:C:52:MET:HE2	1:D:56:GLU:HG3	1.90	0.53
1:C:397:ASN:OD1	1:D:397:ASN:ND2	2.37	0.53
1:A:281:ASN:OD1	1:A:283:ASP:HB2	2.08	0.53
1:D:398:ASN:OD1	1:D:399:GLU:N	2.42	0.53
1:C:273:PRO:HB3	1:C:286:ARG:HB3	1.91	0.53
1:D:439:LEU:HD11	1:D:449:THR:CG2	2.39	0.53
1:D:452:THR:HA	1:D:455:GLN:HG2	1.89	0.53
1:B:408:LEU:HD23	1:B:413:PHE:O	2.09	0.53
1:D:92:SER:HA	1:D:350:LYS:O	2.08	0.53
1:D:392:LEU:HD21	1:D:401:VAL:HG22	1.91	0.53
1:C:212:HIS:CE1	1:C:243:GLU:CA	2.92	0.53
1:D:276:GLN:CD	1:D:286:ARG:HD3	2.34	0.53
1:D:364:ILE:O	1:D:368:GLY:N	2.40	0.53
1:C:219:ILE:HG22	1:C:252:ASN:HD21	1.73	0.52
1:C:417:ARG:NH2	1:D:395:ASP:OD2	2.41	0.52
1:D:449:THR:O	1:D:452:THR:OG1	2.23	0.52
1:A:66:TYR:O	1:B:280:ARG:HD3	2.10	0.52
1:A:358:THR:HB	1:A:359:PRO:HD2	1.91	0.52
1:A:446:ASP:OD1	1:A:448:ARG:HB3	2.09	0.52
1:B:195:ALA:O	1:B:197:ILE:HD12	2.10	0.52
1:B:379:ASP:OD1	1:B:379:ASP:N	2.33	0.52
5:B:2055:HOH:O	2:F:3:SER:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLY:CA	4:P:5:ALA:OXT	2.57	0.52
1:D:393:LYS:O	1:D:396:MET:HE3	2.10	0.52
1:D:396:MET:SD	1:D:398:ASN:HB3	2.50	0.52
1:B:127:ILE:HD11	1:B:141:LEU:HD13	1.91	0.52
1:B:155:MET:HE1	1:B:162:HIS:ND1	2.24	0.52
1:D:230:PHE:CD1	1:D:230:PHE:C	2.87	0.52
1:A:280:ARG:HB2	1:B:67:VAL:O	2.10	0.52
1:D:46:SER:OG	1:D:48:ARG:NH1	2.41	0.52
1:D:328:GLY:O	1:D:371:PRO:HG3	2.10	0.52
1:A:119:GLY:C	1:A:160:LEU:HD11	2.35	0.52
1:C:157:GLY:N	5:C:2015:HOH:O	2.42	0.51
1:D:423:SER:OG	1:D:426:MET:HB2	2.09	0.51
1:D:427:LYS:HD3	1:D:427:LYS:H	1.75	0.51
1:A:131:PHE:CZ	3:M:4:GLN:HG2	2.43	0.51
1:D:472:THR:O	1:D:476:SER:HB3	2.10	0.51
1:A:415:PRO:O	1:A:425:ASP:CG	2.53	0.51
1:C:270:LYS:HZ2	1:C:292:THR:HA	1.75	0.51
1:C:428:LYS:CA	1:C:431:MET:HG2	2.36	0.51
1:D:393:LYS:H	1:D:396:MET:HE1	1.74	0.51
1:A:119:GLY:HA2	1:A:160:LEU:HD21	1.91	0.51
1:A:417:ARG:NH2	1:A:419:ASP:OD2	2.35	0.51
1:D:269:THR:HG22	1:D:291:LEU:HD23	1.92	0.51
1:C:212:HIS:HD2	1:C:478:PHE:HZ	1.54	0.51
1:C:249:VAL:CG1	1:C:249:VAL:O	2.59	0.50
1:C:394:VAL:HA	1:C:422:PHE:CG	2.46	0.50
1:A:72:ARG:CZ	1:B:48:ARG:HD3	2.40	0.50
1:D:412:SER:O	1:D:412:SER:OG	2.19	0.50
5:A:2082:HOH:O	1:B:69:LYS:HG2	2.10	0.50
1:B:394:VAL:O	1:B:422:PHE:HB3	2.11	0.50
1:D:355:LYS:HD3	1:D:363:TRP:CZ2	2.45	0.50
1:B:398:ASN:OD1	1:B:401:VAL:HG22	2.11	0.50
1:B:408:LEU:HD22	1:B:415:PRO:HG3	1.93	0.50
1:C:155:MET:C	1:C:158:LYS:HZ1	2.19	0.50
1:B:446:ASP:OD1	1:B:448:ARG:HB2	2.11	0.50
1:B:284:LYS:O	5:B:2064:HOH:O	2.18	0.50
1:C:299:VAL:O	1:C:324:TYR:HB3	2.11	0.50
1:C:417:ARG:NH2	1:D:395:ASP:OD1	2.41	0.50
1:A:434:GLN:OE1	1:A:441:LYS:HA	2.12	0.50
1:B:59:TYR:OH	1:B:72:ARG:HD3	2.11	0.50
1:C:248:ASP:OD2	1:C:250:ARG:NH2	2.37	0.50
1:C:417:ARG:NH2	1:D:395:ASP:CG	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:PHE:CZ	1:B:453:LEU:HD12	2.47	0.50
1:C:124:LYS:HD2	1:C:146:GLU:CD	2.37	0.50
1:C:285:LYS:HG2	1:C:287:TYR:CZ	2.46	0.50
1:C:388:LEU:HD11	1:C:390:GLU:O	2.12	0.50
1:C:423:SER:OG	1:C:424:LYS:N	2.44	0.49
1:D:478:PHE:O	5:D:2022:HOH:O	2.19	0.49
1:A:365:HIS:C	1:A:367:LYS:H	2.20	0.49
1:C:386:LEU:HB3	1:C:450:ALA:HB1	1.93	0.49
1:C:408:LEU:HD11	1:C:415:PRO:HG3	1.94	0.49
1:B:407:LEU:HD13	1:B:457:ILE:HG13	1.94	0.49
1:D:379:ASP:OD1	1:D:379:ASP:N	2.44	0.49
1:A:207:LYS:HE3	1:A:464:GLU:OE2	2.11	0.49
1:A:86:THR:HG21	1:B:74:LYS:O	2.13	0.49
1:C:246:VAL:HG23	1:C:477:LEU:HD11	1.95	0.49
1:C:452:THR:O	1:C:455:GLN:HB2	2.12	0.49
1:C:453:LEU:O	1:C:457:ILE:HG12	2.13	0.49
1:C:468:LEU:O	1:C:472:THR:HG23	2.13	0.49
1:A:327:VAL:HG12	1:A:328:GLY:N	2.28	0.49
1:C:52:MET:HG3	1:D:56:GLU:HG3	1.95	0.49
1:C:121:GLU:O	1:C:124:LYS:HB3	2.12	0.49
1:C:257:LEU:O	1:C:260:VAL:HG12	2.11	0.49
1:C:86:THR:HG21	1:D:74:LYS:O	2.13	0.49
1:C:52:MET:HE2	1:D:56:GLU:CA	2.42	0.48
1:D:380:TYR:OH	1:D:460:LYS:NZ	2.44	0.48
1:C:158:LYS:HZ3	1:C:158:LYS:CB	2.27	0.48
1:C:158:LYS:HZ3	1:C:158:LYS:N	2.11	0.48
1:C:377:GLN:HG2	1:C:469:GLN:CD	2.38	0.48
1:B:386:LEU:N	1:B:454:ASN:OD1	2.32	0.48
1:A:163:ALA:O	1:A:164:VAL:C	2.56	0.48
1:C:216:TYR:CE1	1:C:248:ASP:HB2	2.49	0.48
1:C:76:LEU:HD12	1:D:55:ILE:HG13	1.94	0.48
1:C:80:ILE:HG21	1:C:94:TYR:HD2	1.78	0.48
1:C:353:LEU:HD23	1:C:354:TYR:CZ	2.49	0.48
1:D:252:ASN:OD1	1:D:252:ASN:C	2.57	0.48
1:A:150:ILE:HD12	1:A:155:MET:CG	2.43	0.48
1:A:395:ASP:OD1	1:A:421:TYR:OH	2.19	0.48
1:B:74:LYS:HG3	5:B:2010:HOH:O	2.12	0.48
1:C:337:VAL:HB	1:C:354:TYR:HB2	1.95	0.48
1:A:269:THR:HG22	1:A:291:LEU:O	2.14	0.48
1:B:340:ALA:HB3	2:F:2:ALA:CB	2.44	0.48
1:C:59:TYR:OH	5:C:2002:HOH:O	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:H	1:A:242:ILE:HG13	1.34	0.47
1:D:201:THR:HG21	1:D:223:SER:HB2	1.95	0.47
1:A:386:LEU:HD12	1:A:387:GLN:N	2.29	0.47
1:B:401:VAL:HG21	1:B:420:GLY:O	2.15	0.47
1:D:426:MET:O	1:D:427:LYS:C	2.56	0.47
1:A:424:LYS:O	1:A:428:LYS:HG2	2.14	0.47
1:C:87:LEU:HD13	1:D:66:TYR:CE1	2.49	0.47
1:C:125:ILE:HG22	1:C:147:ILE:HB	1.96	0.47
1:A:210:GLN:O	1:A:212:HIS:ND1	2.47	0.47
1:A:423:SER:OG	1:A:424:LYS:N	2.47	0.47
1:C:96:ASP:OD1	1:C:99:THR:OG1	2.24	0.47
1:C:212:HIS:HD2	1:C:478:PHE:CZ	2.31	0.47
1:C:393:LYS:HA	1:C:444:VAL:CG1	2.42	0.47
1:C:394:VAL:HA	1:C:422:PHE:HB3	1.95	0.47
1:C:424:LYS:O	1:C:428:LYS:NZ	2.48	0.47
1:B:442:THR:OG1	1:B:444:VAL:N	2.33	0.47
1:C:441:LYS:HZ2	1:C:441:LYS:HG2	1.15	0.47
1:D:424:LYS:HD2	1:D:424:LYS:HA	1.62	0.47
1:A:460:LYS:NZ	5:A:2108:HOH:O	2.48	0.47
1:B:434:GLN:HG2	1:B:441:LYS:HG3	1.97	0.47
1:A:94:TYR:OH	1:B:54:LYS:NZ	2.48	0.47
1:A:364:ILE:HD12	1:A:364:ILE:C	2.40	0.47
1:D:320:GLU:OE1	1:D:360:ASN:HB2	2.15	0.47
1:D:401:VAL:HB	1:D:420:GLY:O	2.15	0.47
1:B:111:PHE:CZ	4:N:4:THR:HG22	2.50	0.46
1:C:417:ARG:NH1	1:D:395:ASP:OD2	2.47	0.46
1:D:72:ARG:O	1:D:75:LEU:N	2.47	0.46
1:D:446:ASP:H	1:D:449:THR:HG1	1.61	0.46
1:A:177:MET:HB2	1:A:179:ILE:CD1	2.45	0.46
1:C:394:VAL:C	1:C:422:PHE:HB3	2.41	0.46
1:D:345:ASP:OD1	1:D:347:SER:OG	2.32	0.46
1:D:394:VAL:HG11	1:D:427:LYS:HE3	1.96	0.46
1:A:252:ASN:OD1	1:A:252:ASN:C	2.58	0.46
1:C:300:ASN:ND2	1:C:473:ALA:O	2.45	0.46
1:D:379:ASP:O	1:D:382:SER:N	2.42	0.46
1:D:381:PHE:HA	1:D:461:LYS:HD2	1.97	0.46
1:C:317:ALA:O	1:C:321:ALA:HB3	2.14	0.46
1:A:392:LEU:HB2	1:A:445:ILE:HB	1.98	0.46
1:A:48:ARG:NH2	1:B:60:GLU:HG2	2.30	0.46
1:B:392:LEU:HB2	1:B:445:ILE:HG13	1.98	0.46
1:C:259:SER:O	1:C:263:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:LEU:HD11	1:D:349:ILE:HG23	1.97	0.46
1:D:89:ASP:N	5:D:2006:HOH:O	2.46	0.46
1:B:439:LEU:CD1	1:B:448:ARG:NH2	2.78	0.46
1:C:417:ARG:CZ	1:C:421:TYR:OH	2.64	0.46
1:B:132:LYS:HA	1:B:137:GLU:OE2	2.16	0.46
1:C:166:LYS:HA	1:C:166:LYS:HD3	1.46	0.46
1:A:304:ASP:O	1:A:307:SER:HB2	2.16	0.46
1:B:96:ASP:OD1	1:B:99:THR:HB	2.15	0.46
1:C:331:SER:HG	1:C:369:ILE:H	1.64	0.46
2:H:5:SER:O	4:P:5:ALA:HB3	2.16	0.46
1:C:217:ILE:HG21	1:C:230:PHE:CD2	2.51	0.45
1:C:285:LYS:HG3	1:C:286:ARG:O	2.16	0.45
1:D:84:LEU:HD11	1:D:349:ILE:CG2	2.46	0.45
1:A:232:LYS:C	5:A:2061:HOH:O	2.59	0.45
1:A:325:ASP:OD2	1:A:373:ILE:HG13	2.16	0.45
1:B:185:LYS:H	1:B:185:LYS:HG3	1.38	0.45
1:C:206:GLU:OE2	1:C:208:LYS:HD2	2.16	0.45
1:B:454:ASN:HD22	1:B:454:ASN:H	1.63	0.45
1:C:434:GLN:NE2	1:C:442:THR:H	2.14	0.45
1:A:395:ASP:CG	1:B:417:ARG:HH22	2.24	0.45
1:C:71:ASP:CG	1:C:74:LYS:HZ3	2.21	0.45
1:C:164:VAL:HG13	1:C:168:ARG:HD2	1.97	0.45
1:A:160:LEU:HD23	3:M:3:PRO:HG3	1.98	0.45
1:C:52:MET:HE1	1:D:55:ILE:HG22	1.99	0.45
1:C:203:PHE:HE2	1:C:220:SER:HB3	1.81	0.45
1:C:326:VAL:HB	1:C:371:PRO:HA	1.99	0.45
1:C:331:SER:OG	1:C:369:ILE:N	2.44	0.45
1:B:215:GLY:O	1:B:245:LEU:HD12	2.17	0.45
1:C:403:HIS:O	1:C:407:LEU:HB2	2.16	0.45
1:C:428:LYS:HB2	1:C:428:LYS:HE2	1.45	0.45
1:C:442:THR:OG1	1:C:444:VAL:O	2.33	0.45
1:B:340:ALA:O	2:F:2:ALA:HB3	2.17	0.45
1:B:424:LYS:H	1:B:424:LYS:HD2	1.82	0.45
1:C:212:HIS:CG	1:C:213:SER:N	2.82	0.45
1:D:386:LEU:HA	1:D:386:LEU:HD12	1.54	0.45
1:B:117:GLU:O	1:B:128:VAL:N	2.47	0.44
1:C:63:SER:HA	1:C:70:VAL:HG21	1.99	0.44
1:C:155:MET:C	1:C:158:LYS:NZ	2.75	0.44
1:C:213:SER:O	1:C:242:ILE:HA	2.16	0.44
1:D:370:GLU:H	1:D:370:GLU:CD	2.24	0.44
1:D:426:MET:O	1:D:429:ALA:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:LYS:HG3	1:D:288:PHE:HB3	1.99	0.44
1:B:80:ILE:O	1:B:81:GLN:C	2.58	0.44
1:C:56:GLU:HG3	1:D:52:MET:SD	2.57	0.44
1:C:80:ILE:HG21	1:C:94:TYR:CD2	2.51	0.44
1:C:341:VAL:HG11	1:D:61:LEU:CD1	2.40	0.44
1:D:286:ARG:HE	1:D:286:ARG:HB2	1.51	0.44
1:D:423:SER:O	1:D:427:LYS:HD3	2.18	0.44
1:A:68:GLU:C	1:B:280:ARG:HD2	2.43	0.44
1:B:264:LEU:HD21	1:B:314:LEU:HA	1.99	0.44
1:B:357:LEU:HD22	1:B:361:GLY:O	2.17	0.44
1:C:207:LYS:HA	1:C:207:LYS:HD3	1.60	0.44
1:A:76:LEU:HD21	1:B:54:LYS:HD2	2.00	0.44
1:A:112:GLU:CD	1:A:171:LYS:HD3	2.43	0.44
1:B:82:GLY:O	1:B:83:MET:C	2.61	0.44
1:C:158:LYS:HZ3	1:C:158:LYS:HB2	1.82	0.44
1:C:404:ALA:O	1:C:408:LEU:HD23	2.17	0.44
1:D:264:LEU:HD12	1:D:264:LEU:C	2.43	0.44
1:D:398:ASN:HD21	1:D:400:ASP:HB2	1.83	0.44
1:D:402:LYS:O	1:D:406:VAL:HG13	2.17	0.44
1:D:299:VAL:O	1:D:324:TYR:HB3	2.17	0.44
1:A:58:ALA:HB2	1:B:80:ILE:HD13	1.99	0.44
1:A:67:VAL:HG13	1:A:68:GLU:HG3	2.00	0.44
1:C:201:THR:HG22	1:C:221:THR:OG1	2.18	0.44
1:D:416:GLY:O	1:D:417:ARG:HB3	2.17	0.44
1:D:424:LYS:O	1:D:427:LYS:HB2	2.18	0.44
1:B:423:SER:O	1:B:426:MET:N	2.50	0.44
1:C:310:ALA:HA	1:C:313:ILE:HD12	1.99	0.44
1:D:278:ALA:O	1:D:354:TYR:HB3	2.18	0.44
1:D:423:SER:O	1:D:427:LYS:CE	2.66	0.44
1:D:450:ALA:O	1:D:451:GLU:C	2.61	0.44
1:A:276:GLN:HG3	1:A:357:LEU:HB2	1.99	0.43
1:A:312:GLU:OE1	1:A:334:LYS:N	2.49	0.43
1:A:439:LEU:HD21	1:A:448:ARG:HG2	2.00	0.43
1:C:450:ALA:O	1:C:454:ASN:ND2	2.51	0.43
1:D:365:HIS:C	1:D:367:LYS:H	2.25	0.43
1:D:423:SER:HB2	1:D:426:MET:H	1.83	0.43
2:H:6:ALA:N	4:P:5:ALA:HB3	2.34	0.43
1:A:132:LYS:O	1:A:133:LYS:HG2	2.18	0.43
1:A:292:THR:HG1	1:A:293:HIS:CE1	2.20	0.43
1:B:377:GLN:OE1	1:B:469:GLN:HG3	2.18	0.43
1:C:212:HIS:CE1	1:C:213:SER:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:SER:HB3	1:C:310:ALA:H	1.46	0.43
1:D:214:VAL:HG23	1:D:244:GLY:O	2.18	0.43
1:A:177:MET:HE2	1:A:177:MET:HB3	1.76	0.43
1:C:214:VAL:HG12	1:C:244:GLY:CA	2.49	0.43
1:D:245:LEU:HB3	1:D:299:VAL:HG13	1.99	0.43
1:A:423:SER:HB3	1:A:425:ASP:OD1	2.18	0.43
1:D:319:LYS:O	1:D:323:HIS:HA	2.19	0.43
1:C:52:MET:HE2	1:D:56:GLU:CG	2.48	0.43
1:C:289:SER:HB2	1:C:291:LEU:H	1.82	0.43
1:B:401:VAL:CG2	1:B:420:GLY:O	2.66	0.43
1:C:143:PRO:O	1:C:144:ASN:HB2	2.17	0.43
1:C:252:ASN:HA	1:C:253:PRO:HD2	1.86	0.43
1:C:309:SER:OG	2:G:6:ALA:C	2.61	0.43
1:C:402:LYS:HG2	1:C:403:HIS:N	2.34	0.43
1:C:469:GLN:O	1:C:470:LEU:C	2.61	0.43
1:D:223:SER:H	1:D:226:THR:CB	2.28	0.43
1:D:399:GLU:O	1:D:402:LYS:HB3	2.19	0.43
1:B:92:SER:HA	1:B:350:LYS:O	2.19	0.43
1:C:107:LEU:O	1:C:223:SER:HB3	2.19	0.43
1:B:204:ALA:CB	1:B:233:ALA:HB1	2.49	0.43
1:B:270:LYS:HZ3	1:B:292:THR:HG22	1.83	0.42
1:C:83:MET:HG3	1:D:79:ALA:HB2	2.01	0.42
5:C:2003:HOH:O	1:D:280:ARG:NH2	2.37	0.42
1:C:399:GLU:CD	1:C:402:LYS:HZ3	2.25	0.42
1:D:380:TYR:HE1	1:D:461:LYS:HG2	1.84	0.42
1:A:75:LEU:HG	1:B:83:MET:HG2	2.01	0.42
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.76	0.42
1:A:389:LYS:HE2	1:A:389:LYS:HB3	1.84	0.42
1:C:431:MET:HB3	1:C:441:LYS:NZ	2.34	0.42
1:A:51:ALA:HB1	1:B:76:LEU:HD13	2.01	0.42
1:A:76:LEU:HD13	1:B:51:ALA:HB1	2.00	0.42
1:C:94:TYR:CD1	1:C:94:TYR:C	2.97	0.42
1:C:250:ARG:HH12	1:C:467:ASP:CG	2.25	0.42
1:D:308:ALA:O	1:D:311:SER:HB2	2.19	0.42
1:D:451:GLU:CG	1:D:452:THR:N	2.81	0.42
1:C:280:ARG:H	1:C:280:ARG:HG3	1.60	0.42
1:C:301:VAL:HG13	1:C:326:VAL:HG13	2.01	0.42
1:A:133:LYS:O	1:A:133:LYS:HG3	2.19	0.42
1:C:155:MET:O	1:C:158:LYS:NZ	2.52	0.42
1:C:158:LYS:HZ3	1:C:158:LYS:H	1.67	0.42
1:C:177:MET:HE2	1:C:179:ILE:CD1	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:SER:N	1:C:312:GLU:HG3	2.35	0.42
1:C:430:VAL:HG12	1:C:434:GLN:OE1	2.20	0.42
1:D:375:ILE:HD12	1:D:376:LYS:N	2.35	0.42
1:A:87:LEU:O	1:A:88:ASN:C	2.63	0.42
1:B:257:LEU:O	1:B:261:GLU:HG3	2.19	0.42
1:D:417:ARG:NH2	1:D:421:TYR:HB3	2.34	0.42
1:D:434:GLN:HE21	1:D:449:THR:HG21	1.83	0.42
1:A:78:GLY:O	1:A:79:ALA:C	2.63	0.42
1:C:56:GLU:HG3	1:D:52:MET:CG	2.50	0.42
1:D:336:THR:OG1	1:D:338:GLN:NE2	2.53	0.42
1:D:411:LEU:O	1:D:412:SER:HB3	2.19	0.42
1:D:477:LEU:HD12	1:D:477:LEU:HA	1.80	0.42
1:A:55:ILE:O	1:A:58:ALA:HB3	2.20	0.41
1:C:249:VAL:HG13	1:C:252:ASN:CB	2.50	0.41
1:C:309:SER:O	1:C:312:GLU:N	2.53	0.41
1:C:430:VAL:HG12	1:C:434:GLN:CD	2.44	0.41
1:D:266:HIS:HB2	1:D:267:PHE:CE1	2.55	0.41
1:D:275:ILE:HG22	1:D:287:TYR:HB2	2.02	0.41
1:D:334:LYS:HE3	4:P:5:ALA:HB2	2.02	0.41
1:D:422:PHE:HD1	1:D:427:LYS:NZ	2.16	0.41
1:A:81:GLN:OE1	1:A:94:TYR:HB3	2.20	0.41
1:A:131:PHE:HB2	1:A:134:SER:HB3	2.01	0.41
1:B:264:LEU:HD22	1:B:317:ALA:HB3	2.02	0.41
1:C:69:LYS:HD2	1:C:69:LYS:HA	1.87	0.41
1:C:417:ARG:NH2	1:C:421:TYR:CE2	2.87	0.41
1:C:457:ILE:O	1:C:460:LYS:HB3	2.20	0.41
1:D:91:TYR:OH	1:D:332:PHE:HE2	2.03	0.41
1:B:70:VAL:HG11	1:B:75:LEU:HD22	2.02	0.41
1:B:124:LYS:HD2	1:B:146:GLU:OE2	2.20	0.41
1:B:447:THR:O	1:B:450:ALA:HB3	2.19	0.41
1:C:398:ASN:O	1:C:401:VAL:HG12	2.20	0.41
1:C:275:ILE:HG22	1:C:287:TYR:HB2	2.03	0.41
1:C:393:LYS:HB2	1:C:396:MET:HG3	2.03	0.41
1:C:419:ASP:HB3	1:D:397:ASN:CB	2.50	0.41
1:A:467:ASP:OD1	1:A:467:ASP:C	2.63	0.41
1:C:92:SER:HA	1:C:350:LYS:O	2.20	0.41
1:C:421:TYR:HD1	1:C:421:TYR:O	2.03	0.41
1:C:434:GLN:CD	1:C:441:LYS:HG3	2.44	0.41
1:D:89:ASP:HA	1:D:90:PRO:HD2	1.88	0.41
1:D:470:LEU:O	1:D:474:LEU:HG	2.20	0.41
1:B:258:GLN:O	1:B:259:SER:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:VAL:HA	1:B:409:LYS:NZ	2.21	0.41
1:C:212:HIS:NE2	1:C:214:VAL:CG1	2.79	0.41
1:D:309:SER:OG	4:P:5:ALA:HB1	2.20	0.41
1:A:158:LYS:HB3	1:A:158:LYS:HE2	1.78	0.41
1:C:178:LYS:HA	1:C:188:LEU:O	2.21	0.41
1:C:234:LEU:HD23	1:C:266:HIS:ND1	2.36	0.41
1:C:340:ALA:HB3	2:G:2:ALA:CB	2.49	0.41
1:D:338:GLN:HG3	1:D:352:THR:CA	2.51	0.41
1:A:59:TYR:HE1	1:B:48:ARG:HD2	1.85	0.41
1:A:150:ILE:HG21	1:A:166:LYS:HB3	2.02	0.41
1:A:177:MET:HG3	1:A:190:PHE:HB2	2.03	0.41
1:A:238:GLU:OE2	1:A:297:TYR:OH	2.25	0.41
1:B:292:THR:HG1	1:B:293:HIS:HD1	0.54	0.41
1:B:295:LYS:HE3	1:B:297:TYR:OH	2.20	0.41
1:B:313:ILE:O	1:B:314:LEU:C	2.61	0.41
1:B:409:LYS:CE	1:B:418:GLU:CD	2.91	0.41
1:C:268:VAL:O	1:C:291:LEU:HD23	2.20	0.41
1:C:300:ASN:OD1	1:C:300:ASN:N	2.54	0.41
1:C:419:ASP:HB3	1:D:397:ASN:HB2	2.03	0.41
1:D:223:SER:O	1:D:224:GLU:C	2.64	0.41
1:D:295:LYS:HG3	1:D:297:TYR:CE1	2.54	0.41
1:D:300:ASN:HB3	1:D:325:ASP:HB2	2.02	0.41
1:D:321:ALA:O	1:D:323:HIS:ND1	2.54	0.41
1:D:386:LEU:HD13	1:D:403:HIS:CG	2.55	0.41
1:D:427:LYS:O	1:D:431:MET:SD	2.79	0.41
1:D:474:LEU:O	1:D:477:LEU:HB2	2.21	0.41
1:A:408:LEU:HD23	1:A:408:LEU:HA	1.90	0.41
1:B:51:ALA:O	1:B:55:ILE:HG13	2.21	0.41
1:B:213:SER:O	1:B:243:GLU:N	2.20	0.41
1:B:309:SER:HB3	1:B:310:ALA:H	1.65	0.41
1:B:430:VAL:O	1:B:433:PHE:HB3	2.21	0.41
1:C:428:LYS:HA	1:C:431:MET:CB	2.49	0.41
1:D:427:LYS:N	1:D:427:LYS:CD	2.84	0.40
1:D:451:GLU:OE1	1:D:451:GLU:N	2.53	0.40
2:E:3:SER:HB3	5:E:2003:HOH:O	2.21	0.40
1:B:430:VAL:HG21	1:B:445:ILE:HD13	2.03	0.40
1:B:436:GLN:O	1:B:437:ASN:CB	2.68	0.40
1:C:62:ILE:HD11	1:D:84:LEU:HG	2.03	0.40
1:C:150:ILE:CG2	1:C:155:MET:HE3	2.48	0.40
1:C:378:PRO:O	1:C:381:PHE:HB2	2.21	0.40
1:C:82:GLY:O	1:C:85:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:HA	1:C:220:SER:OG	2.21	0.40
1:B:67:VAL:HG13	1:B:68:GLU:N	2.36	0.40
1:B:468:LEU:HD12	1:B:468:LEU:HA	1.72	0.40
1:D:451:GLU:HG2	1:D:452:THR:H	1.87	0.40
1:D:464:GLU:O	1:D:471:GLN:NE2	2.48	0.40
1:B:309:SER:O	1:B:310:ALA:C	2.64	0.40
1:C:417:ARG:NH2	1:C:421:TYR:CZ	2.90	0.40
1:C:434:GLN:CD	1:C:441:LYS:HA	2.46	0.40
1:C:453:LEU:O	1:C:456:GLN:N	2.53	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:SER:OG	1:D:210:GLN:OE1[2_556]	1.98	0.22
1:C:112:GLU:OE2	1:C:287:TYR:OH[2_646]	2.14	0.06
1:C:112:GLU:OE2	1:C:285:LYS:NZ[2_646]	2.15	0.05
1:A:438:LYS:NZ	1:D:280:ARG:O[2_656]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	432/446 (97%)	418 (97%)	14 (3%)	0	100	100
1	B	432/446 (97%)	415 (96%)	16 (4%)	1 (0%)	43	68
1	C	432/446 (97%)	413 (96%)	18 (4%)	1 (0%)	43	68
1	D	340/446 (76%)	311 (92%)	29 (8%)	0	100	100
2	E	4/6 (67%)	4 (100%)	0	0	100	100
2	F	4/6 (67%)	4 (100%)	0	0	100	100
2	G	4/6 (67%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	2/6 (33%)	2 (100%)	0	0	100	100
3	M	3/5 (60%)	3 (100%)	0	0	100	100
4	N	2/4 (50%)	2 (100%)	0	0	100	100
4	O	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	P	1/4 (25%)	0	1 (100%)	0	100	100
All	All	1658/1825 (91%)	1577 (95%)	79 (5%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	439	LEU
1	C	447	THR

5.3.2 Protein sidechains [i](#)

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	369/381 (97%)	333 (90%)	36 (10%)	7	19
1	B	369/381 (97%)	324 (88%)	45 (12%)	5	12
1	C	369/381 (97%)	307 (83%)	62 (17%)	2	6
1	D	295/381 (77%)	244 (83%)	51 (17%)	2	5
2	E	3/3 (100%)	3 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
2	G	3/3 (100%)	3 (100%)	0	100	100
2	H	1/3 (33%)	1 (100%)	0	100	100
3	M	2/2 (100%)	2 (100%)	0	100	100
4	N	3/3 (100%)	3 (100%)	0	100	100
4	O	2/3 (67%)	2 (100%)	0	100	100
All	All	1419/1544 (92%)	1225 (86%)	194 (14%)	3	9

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	63	SER
1	A	69	LYS
1	A	70	VAL
1	A	76	LEU
1	A	104	SER
1	A	108	ASP
1	A	118	VAL
1	A	132	LYS
1	A	133	LYS
1	A	150	ILE
1	A	158	LYS
1	A	160	LEU
1	A	165	LEU
1	A	177	MET
1	A	179	ILE
1	A	185	LYS
1	A	187	GLN
1	A	209	VAL
1	A	213	SER
1	A	214	VAL
1	A	241	GLU
1	A	242	ILE
1	A	269	THR
1	A	276	GLN
1	A	280	ARG
1	A	290	THR
1	A	292	THR
1	A	314	LEU
1	A	325	ASP
1	A	341	VAL
1	A	395	ASP
1	A	427	LYS
1	A	431	MET
1	A	438	LYS
1	A	451	GLU
1	B	54	LYS
1	B	68	GLU
1	B	73	GLU
1	B	74	LYS
1	B	76	LEU
1	B	80	ILE

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Mol	Chain	Res	Type
1	B	86	THR
1	B	98	GLN
1	B	108	ASP
1	B	120	MET
1	B	127	ILE
1	B	132	LYS
1	B	133	LYS
1	B	150	ILE
1	B	155	MET
1	B	165	LEU
1	B	179	ILE
1	B	185	LYS
1	B	196	GLU
1	B	197	ILE
1	B	205	SER
1	B	207	LYS
1	B	208	LYS
1	B	209	VAL
1	B	242	ILE
1	B	301	VAL
1	B	305	LYS
1	B	309	SER
1	B	338	GLN
1	B	369	ILE
1	B	379	ASP
1	B	382	SER
1	B	389	LYS
1	B	394	VAL
1	B	396	MET
1	B	407	LEU
1	B	408	LEU
1	B	419	ASP
1	B	438	LYS
1	B	440	ASN
1	B	442	THR
1	B	444	VAL
1	B	445	ILE
1	B	447	THR
1	B	451	GLU
1	C	47	GLU
1	C	73	GLU
1	C	76	LEU

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Mol	Chain	Res	Type
1	C	77	GLU
1	C	80	ILE
1	C	97	LYS
1	C	105	ASP
1	C	108	ASP
1	C	118	VAL
1	C	120	MET
1	C	126	ILE
1	C	127	ILE
1	C	134	SER
1	C	149	SER
1	C	150	ILE
1	C	158	LYS
1	C	164	VAL
1	C	166	LYS
1	C	179	ILE
1	C	185	LYS
1	C	207	LYS
1	C	213	SER
1	C	225	HIS
1	C	236	GLU
1	C	237	LEU
1	C	269	THR
1	C	271	ASP
1	C	279	GLU
1	C	285	LYS
1	C	289	SER
1	C	302	ILE
1	C	309	SER
1	C	311	SER
1	C	318	LEU
1	C	326	VAL
1	C	358	THR
1	C	365	HIS
1	C	375	ILE
1	C	376	LYS
1	C	386	LEU
1	C	392	LEU
1	C	393	LYS
1	C	399	GLU
1	C	406	VAL
1	C	408	LEU

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Mol	Chain	Res	Type
1	C	412	SER
1	C	421	TYR
1	C	423	SER
1	C	428	LYS
1	C	439	LEU
1	C	444	VAL
1	C	447	THR
1	C	448	ARG
1	C	457	ILE
1	C	459	LYS
1	C	462	SER
1	C	465	LYS
1	C	466	ASN
1	C	468	LEU
1	C	469	GLN
1	C	470	LEU
1	C	476	SER
1	D	48	ARG
1	D	57	LYS
1	D	63	SER
1	D	97	LYS
1	D	99	THR
1	D	104	SER
1	D	206	GLU
1	D	209	VAL
1	D	214	VAL
1	D	221	THR
1	D	224	GLU
1	D	234	LEU
1	D	235	ARG
1	D	236	GLU
1	D	240	LYS
1	D	259	SER
1	D	263	ILE
1	D	268	VAL
1	D	286	ARG
1	D	302	ILE
1	D	314	LEU
1	D	330	THR
1	D	350	LYS
1	D	354	TYR
1	D	355	LYS

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Mol	Chain	Res	Type
1	D	370	GLU
1	D	379	ASP
1	D	386	LEU
1	D	389	LYS
1	D	394	VAL
1	D	399	GLU
1	D	400	ASP
1	D	409	LYS
1	D	412	SER
1	D	417	ARG
1	D	423	SER
1	D	424	LYS
1	D	427	LYS
1	D	430	VAL
1	D	438	LYS
1	D	439	LEU
1	D	441	LYS
1	D	442	THR
1	D	448	ARG
1	D	449	THR
1	D	451	GLU
1	D	454	ASN
1	D	455	GLN
1	D	456	GLN
1	D	462	SER
1	D	476	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	225	HIS
1	A	272	GLN
1	A	360	ASN
1	A	362	ASN
1	B	225	HIS
1	B	403	HIS
1	B	466	ASN
1	C	102	GLN
1	C	210	GLN
1	C	212	HIS
1	C	293	HIS

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Mol	Chain	Res	Type
1	C	387	GLN
1	C	466	ASN
1	C	471	GLN

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

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	434/446 (97%)	-0.39	0 100 100	20, 45, 76, 95	0
1	B	434/446 (97%)	-0.27	8 (1%) 67 65	21, 41, 100, 132	0
1	C	434/446 (97%)	0.34	15 (3%) 47 43	40, 70, 129, 147	0
1	D	344/446 (77%)	0.39	14 (4%) 41 37	37, 74, 136, 153	0
2	E	6/6 (100%)	0.09	0 100 100	24, 39, 59, 61	0
2	F	6/6 (100%)	0.60	1 (16%) 4 3	27, 34, 61, 73	0
2	G	6/6 (100%)	0.22	0 100 100	50, 57, 66, 73	0
2	H	4/6 (66%)	0.64	0 100 100	59, 61, 67, 79	0
3	M	5/5 (100%)	0.94	0 100 100	68, 71, 89, 91	0
4	N	4/4 (100%)	0.03	0 100 100	44, 55, 65, 79	0
4	O	4/4 (100%)	1.60	2 (50%) 0 0	78, 87, 94, 99	0
4	P	3/4 (75%)	3.74	3 (100%) 0 0	108, 108, 118, 123	0
All	All	1684/1825 (92%)	0.01	43 (2%) 57 54	20, 59, 119, 153	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	P	4	THR	4.6
1	B	443	GLY	4.3
1	D	432	ALA	4.0
2	F	1	ALA	3.8
1	B	429	ALA	3.6
4	P	3	GLN	3.6
1	C	421	TYR	3.6
1	B	439	LEU	3.4
1	C	419	ASP	3.2
1	D	396	MET	3.2
1	D	433	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
4	P	5	ALA	3.0
1	C	123	GLY	2.9
1	D	431	MET	2.9
1	C	420	GLY	2.8
1	C	404	ALA	2.8
1	C	209	VAL	2.8
1	B	441	LYS	2.8
1	C	157	GLY	2.8
1	D	411	LEU	2.8
1	C	244	GLY	2.7
1	D	449	THR	2.7
1	D	445	ILE	2.6
1	C	212	HIS	2.5
1	D	421	TYR	2.5
1	B	438	LYS	2.4
1	C	392	LEU	2.4
4	O	4	THR	2.3
1	D	397	ASN	2.3
1	C	431	MET	2.2
1	B	48	ARG	2.2
1	B	76	LEU	2.2
1	C	449	THR	2.1
1	C	422	PHE	2.1
4	O	2	PRO	2.1
1	D	429	ALA	2.1
1	D	408	LEU	2.1
1	D	394	VAL	2.1
1	C	433	PHE	2.1
1	C	423	SER	2.1
1	D	357	LEU	2.0
1	D	439	LEU	2.0
1	B	430	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.