



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 08:05 PM JST

PDB ID : 7COP
Title : Hexameric Ring Complex of Engineered V1-ATPase: A3(De)3_empty
Authors : Kosugi, T.; Tanabe, M.; Koga, N.
Deposited on : 2020-08-05
Resolution : 2.77 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

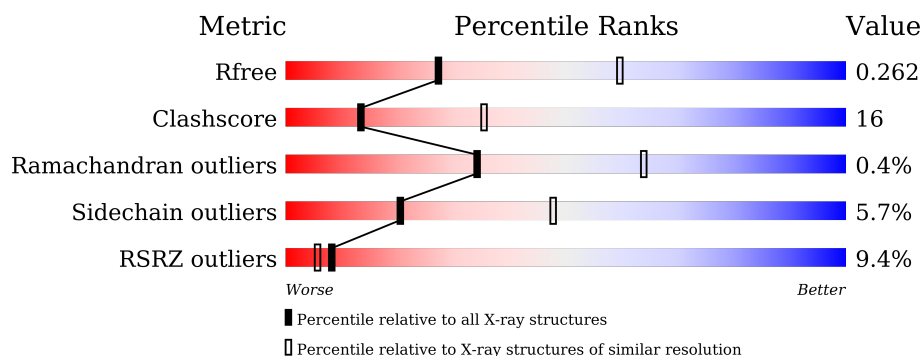
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	596	<div> <div>3%</div> <div>81% 17% ..</div> </div>
1	B	596	<div> <div>7%</div> <div>65% 31% ..</div> </div>
1	C	596	<div> <div>8%</div> <div>60% 34% ..</div> </div>
2	D	458	<div> <div>9%</div> <div>62% 29% . 6%</div> </div>
2	E	458	<div> <div>14%</div> <div>63% 29% 5% ..</div> </div>
2	F	458	<div> <div>17%</div> <div>57% 36% . .</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24314 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	1	0
			4573	2872	770	905	26			
1	B	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	C	584	Total	C	N	O	S	0	1	0
			4560	2864	768	902	26			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase designed non-catalytic subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	432	Total	C	N	O	S	0	0	0
			3369	2134	576	646	13			
2	E	449	Total	C	N	O	S	0	1	0
			3520	2230	605	671	14			
2	F	445	Total	C	N	O	S	0	0	0
			3477	2204	597	662	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLY	SER	engineered mutation	UNP Q08637
D	152	PRO	GLY	engineered mutation	UNP Q08637
D	153	PRO	SER	engineered mutation	UNP Q08637
D	155	ALA	LEU	engineered mutation	UNP Q08637
D	156	GLY	PRO	engineered mutation	UNP Q08637
D	157	LYS	HIS	engineered mutation	UNP Q08637
D	158	SER	LYS	engineered mutation	UNP Q08637
D	159	ALA	GLU	engineered mutation	UNP Q08637
D	248	GLU	THR	engineered mutation	UNP Q08637
D	339	SER	GLN	engineered mutation	UNP Q08637
E	151	GLY	SER	engineered mutation	UNP Q08637
E	152	PRO	GLY	engineered mutation	UNP Q08637
E	153	PRO	SER	engineered mutation	UNP Q08637
E	155	ALA	LEU	engineered mutation	UNP Q08637
E	156	GLY	PRO	engineered mutation	UNP Q08637
E	157	LYS	HIS	engineered mutation	UNP Q08637
E	158	SER	LYS	engineered mutation	UNP Q08637
E	159	ALA	GLU	engineered mutation	UNP Q08637
E	248	GLU	THR	engineered mutation	UNP Q08637
E	339	SER	GLN	engineered mutation	UNP Q08637
F	151	GLY	SER	engineered mutation	UNP Q08637
F	152	PRO	GLY	engineered mutation	UNP Q08637
F	153	PRO	SER	engineered mutation	UNP Q08637
F	155	ALA	LEU	engineered mutation	UNP Q08637
F	156	GLY	PRO	engineered mutation	UNP Q08637
F	157	LYS	HIS	engineered mutation	UNP Q08637
F	158	SER	LYS	engineered mutation	UNP Q08637
F	159	ALA	GLU	engineered mutation	UNP Q08637
F	248	GLU	THR	engineered mutation	UNP Q08637
F	339	SER	GLN	engineered mutation	UNP Q08637

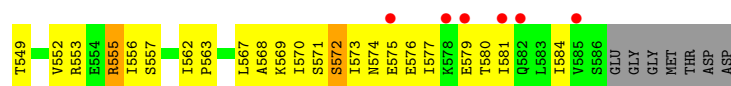
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	B	36	Total O 36 36	0	0
3	C	45	Total O 45 45	0	0
3	D	23	Total O 23 23	0	0
3	E	29	Total O 29 29	0	0

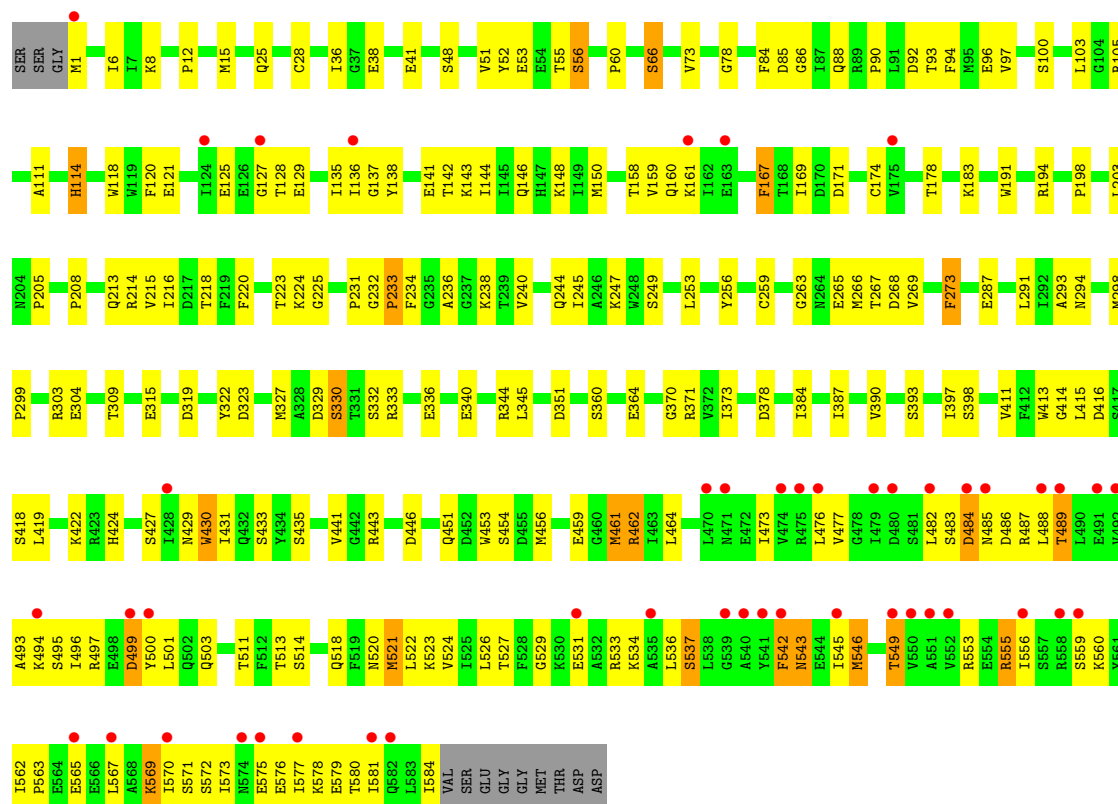
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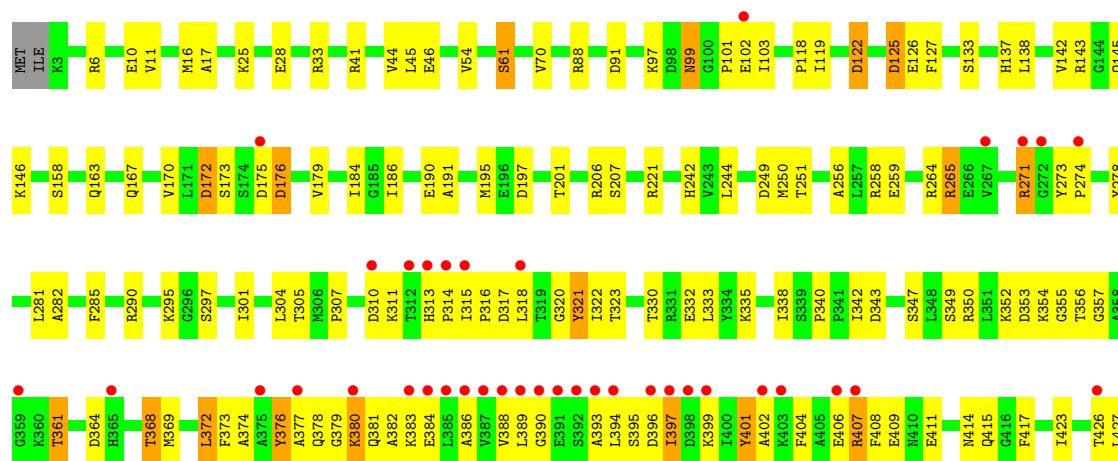
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	20	Total	O	0	0
			20	20		

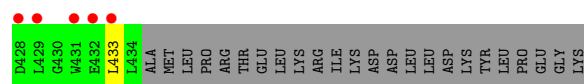


• Molecule 1: V-type sodium ATPase catalytic subunit A



• Molecule 2: V-type sodium ATPase designed non-catalytic subunit B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.45Å 122.65Å 128.70Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	44.64 – 2.77 44.64 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.64-2.77) 100.0 (44.64-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.18_3845)	Depositor
R, R_{free}	0.212 , 0.262 0.212 , 0.262	Depositor DCC
R_{free} test set	4712 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.007 for -h,-l,-k 0.000 for -l,k,h 0.000 for -k,-h,-l 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k 0.000 for l,-h,-k 0.000 for -k,-l,h 0.015 for h,-k,-l 0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24314	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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	0.30	0/4649	0.51	1/6289 (0.0%)
1	B	0.29	0/4638	0.50	0/6275
1	C	0.32	0/4636	0.54	1/6271 (0.0%)
2	D	0.37	1/3429 (0.0%)	0.60	0/4637
2	E	0.37	0/3581	0.68	6/4840 (0.1%)
2	F	0.33	0/3538	0.62	4/4782 (0.1%)
All	All	0.33	1/24471 (0.0%)	0.57	12/33094 (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
2	D	0	2
2	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	TYR	CD2-CE2	-5.27	1.31	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	318	LEU	CB-CG-CD2	-12.12	90.39	111.00
2	E	318	LEU	CB-CG-CD1	-10.82	92.61	111.00
2	E	399	LYS	CA-CB-CG	6.55	127.80	113.40
2	E	278	TYR	CA-CB-CG	6.44	125.63	113.40
2	E	363	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	A	476	LEU	CA-CB-CG	5.73	128.47	115.30
2	E	429	LEU	CA-CB-CG	5.55	128.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	398	ASP	CB-CG-OD1	5.55	123.29	118.30
2	F	398	ASP	CB-CG-OD2	-5.53	113.32	118.30
2	E	318	LEU	CB-CG-CD2	5.20	119.84	111.00
2	F	321	TYR	CA-CB-CG	5.10	123.09	113.40
1	C	85	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	176	ASP	Peptide
2	D	354	LYS	Peptide
2	F	171	LEU	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	4573	0	4540	68	0
1	B	4562	0	4528	142	0
1	C	4560	0	4526	166	0
2	D	3369	0	3377	122	0
2	E	3520	0	3549	166	0
2	F	3477	0	3507	132	0
3	A	100	0	0	5	0
3	B	36	0	0	4	0
3	C	45	0	0	2	0
3	D	23	0	0	1	0
3	E	29	0	0	2	0
3	F	20	0	0	1	0
All	All	24314	0	24027	776	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 16.

All (776) 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)
2:D:368:THR:O	2:D:372:LEU:HB2	1.52	1.08
2:E:403:LYS:HD2	2:E:436:MET:HG3	1.41	0.99
2:E:278:TYR:HB3	2:E:318:LEU:HB3	1.43	0.97
2:F:407:ARG:HA	2:F:410:ASN:HB2	1.50	0.91
2:E:258:ARG:HG2	2:E:274:PRO:HD3	1.52	0.89
2:E:271:ARG:HG2	2:E:273:TYR:HB2	1.52	0.89
2:D:395:SER:HA	2:D:399:LYS:HB2	1.55	0.89
2:E:372:LEU:HD23	2:E:404:PHE:HZ	1.38	0.88
1:B:549:THR:OG1	1:B:553:ARG:NH1	2.08	0.86
1:B:462:ARG:NH1	1:B:466:GLU:OE1	2.08	0.86
2:F:307:PRO:HG3	2:F:316:PRO:HG3	1.58	0.85
1:C:263:GLY:N	2:F:286:GLU:OE2	2.10	0.84
2:D:389:LEU:HB3	2:D:393:ALA:HB3	1.59	0.83
1:C:549:THR:HG23	1:C:553:ARG:HH21	1.42	0.83
2:E:138:LEU:HD11	2:E:373:PHE:HD1	1.43	0.82
2:E:363:GLU:OE2	2:E:363:GLU:HA	1.78	0.82
1:B:56:SER:O	1:B:105:ARG:NH2	2.13	0.80
1:C:429:ASN:O	1:C:433:SER:OG	1.99	0.79
2:E:129:GLN:HE22	2:E:422:THR:HG23	1.48	0.79
2:E:319:THR:O	2:E:323:THR:N	2.15	0.78
2:D:383:LYS:NZ	2:D:406:GLU:OE2	2.15	0.78
2:E:363:GLU:OE2	3:E:501:HOH:O	2.01	0.78
2:F:326:GLN:HE22	2:F:348:LEU:HB3	1.47	0.78
1:B:422:LYS:NZ	3:B:602:HOH:O	2.18	0.77
1:A:10:SER:HB2	2:D:46:GLU:HG3	1.67	0.77
1:C:527:THR:HG21	1:C:573:ILE:HD13	1.66	0.77
2:E:425:GLU:OE2	2:E:425:GLU:N	2.16	0.76
2:E:163:GLN:HE21	2:E:167:GLN:HE22	1.32	0.76
1:B:62:GLU:OE2	3:B:601:HOH:O	2.03	0.75
2:F:30:ILE:HD12	2:F:54:VAL:HG11	1.68	0.75
1:A:476:LEU:HD13	1:A:477:VAL:HG23	1.68	0.75
2:E:361:THR:HG21	2:E:365:HIS:ND1	2.02	0.75
2:E:249:ASP:OD1	2:E:251:THR:OG1	2.03	0.75
1:A:392:PRO:O	1:A:393:SER:OG	2.02	0.75
2:F:128:ILE:HD13	2:F:130:THR:HG23	1.69	0.74
1:B:440:GLU:OE1	1:B:443:ARG:NH1	2.20	0.74
2:D:402:ALA:O	2:D:406:GLU:HG2	1.85	0.74
2:E:278:TYR:HD1	2:E:318:LEU:HD23	1.53	0.74
2:E:293:GLY:O	2:E:295:LYS:NZ	2.21	0.74
1:B:484:ASP:HB3	1:B:542:PHE:HD2	1.52	0.73
2:E:358:ALA:HB2	2:E:363:GLU:CD	2.09	0.73
2:E:129:GLN:NE2	2:E:422:THR:HG23	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:ILE:HB	1:C:569:LYS:HE3	1.71	0.73
2:F:329:LEU:HD22	2:F:341:PRO:HD2	1.69	0.73
1:C:256:TYR:HB3	1:C:291:LEU:HD12	1.71	0.73
2:D:170:VAL:O	2:D:173:SER:OG	2.07	0.73
2:E:313:HIS:CD2	2:E:314:PRO:HD2	2.24	0.73
2:E:444:ARG:HD3	2:E:447:ASP:H	1.54	0.72
1:B:281:THR:HG23	1:B:283:GLU:H	1.53	0.71
1:C:120:PHE:HE1	1:C:137:GLY:HA3	1.56	0.71
1:C:503:GLN:NE2	3:C:601:HOH:O	2.23	0.71
1:C:298:MET:O	1:C:303:ARG:NH1	2.23	0.71
2:E:394:LEU:HB3	2:E:399:LYS:HD2	1.73	0.71
2:E:3:LYS:NZ	2:E:22:SER:O	2.25	0.70
1:C:545:ILE:O	1:C:549:THR:HG22	1.91	0.70
2:F:403:LYS:HA	2:F:406:GLU:HG3	1.74	0.70
1:B:142:THR:HG23	1:B:144:ILE:H	1.54	0.70
1:C:416:ASP:O	1:C:427:SER:OG	2.09	0.70
1:B:256:TYR:HB3	1:B:291:LEU:HD12	1.73	0.70
1:B:562:ILE:HD11	1:B:569:LYS:HB3	1.74	0.69
2:F:395:SER:HA	2:F:399:LYS:HB2	1.74	0.69
2:D:138:LEU:HA	2:D:369:MET:HG3	1.75	0.69
2:F:426:THR:HG22	2:F:427:LEU:HD23	1.74	0.69
1:B:577:ILE:O	1:B:581:ILE:HG12	1.93	0.69
2:D:133:SER:N	2:D:415:GLN:OE1	2.23	0.69
2:E:138:LEU:HD11	2:E:373:PHE:CD1	2.26	0.69
2:D:390:GLY:HA2	2:D:399:LYS:NZ	2.07	0.69
1:B:214:ARG:HH11	1:B:513:THR:HG21	1.58	0.68
1:B:573:ILE:O	1:B:577:ILE:HG13	1.94	0.68
2:D:138:LEU:HG	2:D:369:MET:HG3	1.74	0.68
1:B:491:GLU:HG3	1:B:546:MET:SD	2.34	0.67
2:F:314:PRO:O	2:F:318:LEU:HB2	1.94	0.67
1:C:86:GLY:N	1:C:294:ASN:HD21	1.92	0.67
2:E:362:ARG:HG3	2:E:362:ARG:HH11	1.57	0.67
2:F:338:ILE:HG13	2:F:409:GLU:HB3	1.77	0.67
1:A:555:ARG:NH2	1:A:572:SER:OG	2.27	0.67
2:E:326:GLN:NE2	2:E:346:PRO:O	2.28	0.67
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.76	0.67
1:C:120:PHE:CE1	1:C:137:GLY:HA3	2.29	0.67
1:C:570:ILE:HD12	1:C:570:ILE:H	1.60	0.67
1:B:41:GLU:OE1	1:B:43:ARG:NH1	2.25	0.67
1:B:207:VAL:HG13	1:B:224:LYS:HB2	1.76	0.67
2:D:25:LYS:NZ	3:D:501:HOH:O	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:ASP:O	2:D:368:THR:HG22	1.95	0.67
2:F:44:VAL:HG12	2:F:54:VAL:HG12	1.77	0.67
2:E:349:SER:O	2:E:352:LYS:HG2	1.94	0.67
1:A:517:LYS:O	1:A:521:MET:HG3	1.96	0.66
1:B:459:GLU:O	1:B:463:ILE:HG13	1.95	0.66
1:B:552:VAL:HG21	1:B:577:ILE:HG12	1.77	0.66
2:F:394:LEU:HD22	2:F:398:ASP:H	1.59	0.66
1:B:125:GLU:O	1:B:128:THR:OG1	2.13	0.66
1:C:464:LEU:HD21	1:C:496:ILE:CD1	2.26	0.66
1:B:484:ASP:HB3	1:B:542:PHE:CD2	2.31	0.66
2:F:104:LEU:HD12	2:F:105:PRO:HD2	1.78	0.66
2:D:175:ASP:N	2:D:175:ASP:OD1	2.27	0.66
1:C:430:TRP:HB2	1:C:431:ILE:HD12	1.78	0.65
1:C:473:ILE:HA	1:C:476:LEU:HD13	1.79	0.65
2:F:145:GLN:HG3	2:F:351:LEU:HD12	1.79	0.65
1:A:20:SER:OG	3:A:601:HOH:O	2.14	0.65
1:C:52:TYR:O	1:C:299:PRO:HB3	1.97	0.65
2:D:251:THR:HA	2:D:314:PRO:HG3	1.77	0.65
2:F:125:ASP:OD1	2:F:290:ARG:NH2	2.30	0.65
1:B:467:GLU:O	1:B:471:ASN:ND2	2.25	0.64
2:E:372:LEU:HD23	2:E:404:PHE:CZ	2.25	0.64
2:E:306:MET:O	2:E:308:GLU:N	2.31	0.64
2:E:434:LEU:HA	2:E:437:LEU:HD23	1.79	0.64
2:F:350:ARG:NH1	3:F:501:HOH:O	2.21	0.64
2:E:271:ARG:HH11	2:E:277:LEU:HB3	1.61	0.64
2:E:403:LYS:CD	2:E:436:MET:HG3	2.24	0.64
2:E:407:ARG:HG3	2:E:411:GLU:HB3	1.80	0.64
2:E:313:HIS:ND1	2:E:315:ILE:HG12	2.13	0.64
2:E:395:SER:O	2:E:399:LYS:N	2.24	0.64
1:C:203:LEU:HD11	1:C:373:ILE:HG13	1.81	0.63
1:C:160:GLN:OE1	1:C:161:LYS:HG3	1.99	0.63
2:D:357:GLY:H	2:D:361:THR:HG22	1.64	0.63
2:F:130:THR:HG21	2:F:135:ILE:HD11	1.79	0.63
1:A:194[A]:ARG:NH1	1:A:304:GLU:OE2	2.31	0.63
2:D:197:ASP:O	2:D:201:THR:HG22	1.98	0.63
1:B:43:ARG:HG3	2:F:10:GLU:HG3	1.81	0.62
1:C:167:PHE:HB3	1:C:171:ASP:HB2	1.81	0.62
2:E:11:VAL:HG22	2:E:16:MET:HG2	1.82	0.62
2:E:364:ASP:OD1	2:E:364:ASP:N	2.20	0.62
1:B:161:LYS:HD3	1:B:175:VAL:HB	1.81	0.62
1:C:138:TYR:CE2	1:C:146:GLN:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:LEU:O	2:E:389:LEU:HB2	1.99	0.62
2:F:371:GLN:OE1	2:F:444:ARG:NH2	2.32	0.62
2:E:403:LYS:HD2	2:E:436:MET:CG	2.26	0.62
1:C:464:LEU:HD21	1:C:496:ILE:HD11	1.79	0.62
2:F:131:GLY:O	2:F:415:GLN:NE2	2.33	0.62
1:C:514:SER:O	1:C:518:GLN:HG3	1.99	0.61
1:B:203:LEU:HD11	1:B:373:ILE:HG13	1.80	0.61
2:E:10:GLU:HB3	2:E:17:ALA:HB3	1.82	0.61
2:E:422:THR:HG22	2:E:423:ILE:H	1.65	0.61
1:A:194[B]:ARG:NH1	1:A:304:GLU:OE2	2.32	0.61
1:C:142:THR:HG21	1:C:287:GLU:O	2.00	0.61
2:D:281:LEU:HD12	2:D:318:LEU:HD22	1.81	0.61
1:C:542:PHE:HA	1:C:545:ILE:HG22	1.82	0.61
2:D:249:ASP:OD2	2:D:305:THR:OG1	2.17	0.61
2:E:278:TYR:CD1	2:E:318:LEU:HD23	2.35	0.61
1:B:562:ILE:HD13	1:B:570:ILE:HG13	1.83	0.61
1:C:327:MET:HA	1:C:387:ILE:O	2.00	0.61
1:B:231:PRO:HA	1:B:390:VAL:HG23	1.82	0.61
1:C:136:ILE:HD11	1:C:174:CYS:SG	2.41	0.61
2:E:314:PRO:O	2:E:318:LEU:HD11	2.00	0.61
2:E:422:THR:HB	2:E:425:GLU:OE2	2.01	0.61
2:F:132:ILE:HA	2:F:415:GLN:HE22	1.65	0.61
2:F:442:LEU:HD23	2:F:442:LEU:H	1.65	0.61
2:D:258:ARG:HA	2:D:274:PRO:HD3	1.82	0.60
2:D:380:LYS:HE3	2:D:383:LYS:HB3	1.83	0.60
2:E:425:GLU:H	2:E:425:GLU:CD	2.04	0.60
1:A:298:MET:O	1:A:303:ARG:NH1	2.33	0.60
2:E:93:LEU:HD12	2:E:95:ARG:NH2	2.16	0.60
2:D:172:ASP:OD1	2:D:173:SER:N	2.35	0.60
2:E:434:LEU:HD12	2:E:434:LEU:N	2.15	0.60
1:C:559:SER:HA	1:C:562:ILE:CD1	2.31	0.60
1:C:485:ASN:O	1:C:489:THR:HG23	2.02	0.60
2:D:382:ALA:HB1	2:D:394:LEU:HD11	1.82	0.60
1:C:28:CYS:HB3	1:C:66:SER:HA	1.84	0.60
1:C:573:ILE:O	1:C:576:GLU:HB3	2.02	0.60
1:B:160:GLN:HB3	1:B:161:LYS:HD2	1.83	0.59
1:B:208:PRO:HG3	1:B:441:VAL:HG22	1.84	0.59
2:D:278:TYR:HA	2:D:318:LEU:HD21	1.84	0.59
2:F:128:ILE:HG12	2:F:141:LEU:HD23	1.84	0.59
2:D:44:VAL:HG12	2:D:54:VAL:HG12	1.84	0.59
2:D:250:MET:HB2	2:D:304:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:LEU:HA	2:E:388:VAL:HG12	1.85	0.59
1:C:482:LEU:HD23	1:C:487:ARG:HE	1.68	0.59
1:B:242:GLN:HB3	1:B:327:MET:HE1	1.84	0.59
1:B:576:GLU:HA	1:B:579:GLU:HG2	1.83	0.59
2:E:270[B]:ARG:NH1	2:E:275:GLY:HA3	2.17	0.59
2:F:412:TYR:O	2:F:421:ARG:NH2	2.35	0.59
2:D:317:ASP:O	2:D:321:TYR:HB2	2.03	0.59
2:E:151:GLY:O	2:E:305:THR:HA	2.03	0.59
2:F:362:ARG:NH2	2:F:424:THR:OG1	2.35	0.59
1:C:418:SER:O	1:C:422:LYS:HG3	2.02	0.59
2:F:278:TYR:HA	2:F:318:LEU:HD23	1.84	0.58
1:B:266:MET:HE3	1:B:294:ASN:H	1.67	0.58
2:D:91:ASP:HB3	2:D:97:LYS:HD3	1.86	0.58
1:B:467:GLU:HG2	1:B:471:ASN:HD21	1.68	0.58
2:D:175:ASP:HB2	2:D:242:HIS:CD2	2.38	0.58
2:F:444:ARG:NE	2:F:444:ARG:H	2.00	0.58
1:A:477:VAL:HG12	1:A:478:GLY:N	2.17	0.58
1:C:135:ILE:HD13	1:C:148:LYS:HD3	1.86	0.58
2:E:271:ARG:NH2	2:E:275:GLY:HA2	2.19	0.58
1:C:36:ILE:HG23	1:C:52:TYR:HB2	1.84	0.58
2:F:45:LEU:HD11	2:F:55:GLN:HB2	1.86	0.58
2:F:128:ILE:CD1	2:F:130:THR:HG23	2.33	0.58
1:C:233:PRO:O	1:C:234:PHE:HD1	1.87	0.58
2:D:423:ILE:O	2:D:427:LEU:HD12	2.04	0.58
1:B:203:LEU:HB2	1:B:371:ARG:HD3	1.86	0.58
2:E:385:LEU:HA	2:E:388:VAL:CG1	2.34	0.58
2:F:343:ASP:OD2	2:F:346:PRO:HD3	2.04	0.58
2:F:179:VAL:HG22	2:F:244:LEU:HB3	1.86	0.57
2:E:315:ILE:O	2:E:318:LEU:HD12	2.04	0.57
2:F:363:GLU:CD	2:F:363:GLU:H	2.07	0.57
2:F:130:THR:O	2:F:167:GLN:HB2	2.03	0.57
2:F:157:LYS:HZ1	2:F:305:THR:HG23	1.69	0.57
1:C:556:ILE:O	1:C:559:SER:HB3	2.04	0.57
2:D:376:TYR:OH	2:D:409:GLU:OE1	2.15	0.57
2:F:319:THR:O	2:F:323:THR:HG23	2.04	0.57
2:F:389:LEU:HB3	2:F:393:ALA:CB	2.34	0.57
2:D:11:VAL:HG22	2:D:16:MET:HG2	1.86	0.57
2:D:423:ILE:O	2:D:426:THR:HB	2.04	0.57
2:E:338:ILE:O	2:E:341:PRO:HG3	2.04	0.57
2:D:390:GLY:HA2	2:D:399:LYS:HZ1	1.68	0.57
2:F:130:THR:OG1	2:F:136:ASP:OD1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:NH1	3:A:605:HOH:O	2.38	0.57
1:B:90:PRO:HB2	1:B:93:THR:HB	1.85	0.56
1:B:549:THR:HG1	1:B:553:ARG:NH1	2.01	0.56
1:C:493:ALA:O	1:C:496:ILE:HG13	2.05	0.56
2:E:163:GLN:HE21	2:E:167:GLN:NE2	2.00	0.56
1:C:129:GLU:HA	1:C:158:THR:HA	1.85	0.56
1:B:545:ILE:HD12	1:B:545:ILE:H	1.69	0.56
1:C:128:THR:O	1:C:159:VAL:HG12	2.04	0.56
1:C:146:GLN:N	1:C:146:GLN:OE1	2.36	0.56
1:C:456:MET:HG2	1:C:526:LEU:HD13	1.87	0.56
2:F:326:GLN:HE22	2:F:348:LEU:CB	2.18	0.56
1:B:97:VAL:HG11	1:B:109:LEU:HD21	1.87	0.56
1:C:127:GLY:H	1:C:159:VAL:HG13	1.71	0.56
1:B:452:ASP:O	1:B:456:MET:HG3	2.06	0.56
1:C:73:VAL:HG11	1:C:309:THR:HG23	1.88	0.56
2:D:137:HIS:CE1	2:D:368:THR:HG23	2.41	0.56
2:F:168:ALA:O	2:F:206:ARG:NH2	2.38	0.56
2:F:358:ALA:HB2	2:F:363:GLU:HG3	1.88	0.56
2:F:313:HIS:CE1	2:F:315:ILE:HG13	2.41	0.56
1:B:573:ILE:HG22	1:B:577:ILE:HG13	1.88	0.56
2:F:338:ILE:HD12	2:F:414:ASN:HB2	1.87	0.56
1:B:555:ARG:HG2	1:B:573:ILE:HG12	1.87	0.56
2:F:403:LYS:HA	2:F:406:GLU:CG	2.35	0.56
1:C:482:LEU:HB3	1:C:487:ARG:HH21	1.71	0.56
2:F:91:ASP:OD2	2:F:95:ARG:NE	2.39	0.56
1:C:555:ARG:NH1	1:C:572:SER:HB2	2.20	0.55
2:D:122:ASP:HB3	2:D:290:ARG:HB2	1.88	0.55
2:E:403:LYS:HD3	2:E:403:LYS:C	2.26	0.55
2:F:333:LEU:HA	2:F:336:SER:HB3	1.87	0.55
1:B:274:PRO:HA	1:B:286:MET:HG2	1.87	0.55
1:B:472:GLU:O	1:B:475:ARG:HG2	2.07	0.55
1:A:43:ARG:HD2	2:E:10:GLU:HG3	1.89	0.55
2:D:313:HIS:HB3	2:D:314:PRO:HD2	1.89	0.55
2:D:379:GLY:HA2	2:D:401:TYR:HB3	1.88	0.55
1:C:51:VAL:HG11	1:C:55:THR:HG23	1.88	0.55
1:C:78:GLY:N	1:C:141:GLU:OE2	2.39	0.55
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.87	0.55
1:C:553:ARG:HA	1:C:556:ILE:HG12	1.89	0.55
2:D:356:THR:OG1	2:D:361:THR:HG21	2.07	0.55
2:F:133:SER:HB3	2:F:426:THR:HG23	1.89	0.54
2:F:146:LYS:HG2	2:F:324:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:PRO:HB2	1:B:428:ILE:HD12	1.88	0.54
1:C:93:THR:O	1:C:97:VAL:HG23	2.07	0.54
1:C:208:PRO:HG3	1:C:441:VAL:HG13	1.89	0.54
2:E:315:ILE:HG13	2:E:316:PRO:HD3	1.89	0.54
1:A:144:ILE:HG21	1:A:288:ARG:HD3	1.88	0.54
1:B:96:GLU:O	1:B:99:GLN:NE2	2.40	0.54
1:C:12:PRO:HG3	1:C:344:ARG:HD3	1.88	0.54
1:C:581:ILE:HD12	1:C:584:ILE:HA	1.88	0.54
1:B:448:ILE:HG23	1:B:449:LEU:HD23	1.90	0.54
2:F:411:GLU:HA	2:F:414:ASN:HB3	1.90	0.54
1:A:323:ASP:OD1	1:A:383:SER:OG	2.21	0.54
1:C:218:THR:HG23	1:C:453:TRP:CZ2	2.43	0.54
1:C:293:ALA:C	1:C:294:ASN:HD22	2.11	0.54
2:D:343:ASP:O	2:D:347:SER:OG	2.25	0.54
2:E:133:SER:OG	2:E:426:THR:HB	2.07	0.54
2:E:360:LYS:HE3	2:E:360:LYS:HA	1.88	0.54
2:F:324:GLU:HA	2:F:350:ARG:CZ	2.38	0.54
1:B:148:LYS:NZ	1:B:322:TYR:OH	2.41	0.54
1:C:142:THR:HG22	1:C:144:ILE:H	1.72	0.54
2:D:394:LEU:HG	2:D:399:LYS:HE3	1.90	0.54
1:B:119:TRP:O	3:B:603:HOH:O	2.18	0.54
1:B:549:THR:OG1	1:B:553:ARG:HD3	2.08	0.54
2:D:163:GLN:HE21	2:D:167:GLN:NE2	2.06	0.54
2:F:382:ALA:HB1	2:F:398:ASP:O	2.08	0.54
2:E:383:LYS:HD3	2:E:402:ALA:CB	2.38	0.54
1:A:513:THR:HG23	1:A:517:LYS:HD3	1.90	0.53
1:B:399:GLU:O	1:B:403:GLN:HG2	2.09	0.53
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.90	0.53
1:C:225:GLY:O	1:C:370:GLY:HA2	2.08	0.53
1:C:231:PRO:HA	1:C:390:VAL:HG12	1.90	0.53
2:D:172:ASP:OD1	2:D:175:ASP:OD1	2.27	0.53
2:D:380:LYS:HE2	2:D:384:GLU:H	1.74	0.53
2:E:333:LEU:HB3	2:E:338:ILE:HG21	1.89	0.53
2:D:146:LYS:HD3	2:D:285:PHE:O	2.09	0.53
1:B:472:GLU:O	1:B:476:LEU:HD23	2.08	0.53
1:B:532:ALA:O	1:B:536:LEU:HB2	2.09	0.53
1:B:139:VAL:HG21	1:B:187:MET:HE3	1.90	0.53
1:B:169:ILE:O	1:B:186:THR:HG23	2.08	0.53
1:C:298:MET:HG2	1:C:299:PRO:HD2	1.91	0.53
2:D:315:ILE:HD11	2:D:318:LEU:CD1	2.38	0.53
2:E:157:LYS:NZ	2:E:305:THR:HG22	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:364:ASP:O	2:E:368:THR:OG1	2.25	0.53
2:F:381:GLN:HA	2:F:384:GLU:HG3	1.91	0.53
1:C:245:ILE:O	1:C:249:SER:OG	2.17	0.53
1:A:443:ARG:O	1:A:447:GLN:HG3	2.09	0.53
1:B:131:SER:OG	1:B:132:ALA:N	2.41	0.53
2:E:318:LEU:O	2:E:322:ILE:HG12	2.09	0.53
2:E:349:SER:O	2:E:349:SER:OG	2.25	0.53
1:B:397:ILE:HB	1:B:402:THR:HG21	1.91	0.53
1:C:397:ILE:H	1:C:397:ILE:HD12	1.74	0.53
2:F:11:VAL:HG22	2:F:16:MET:HG2	1.91	0.53
1:C:520:ASN:O	1:C:524:VAL:HG13	2.09	0.52
1:A:40:ILE:HD13	1:A:50:GLN:HG2	1.90	0.52
1:B:523:LYS:HD3	1:B:574:ASN:HD21	1.74	0.52
1:C:464:LEU:HD21	1:C:496:ILE:HG12	1.92	0.52
1:A:472:GLU:OE1	1:A:472:GLU:HA	2.09	0.52
1:B:142:THR:CG2	1:B:145:ILE:H	2.23	0.52
2:E:270[B]:ARG:HD2	2:E:271:ARG:NH2	2.24	0.52
1:A:392:PRO:HB3	1:A:399:GLU:HG2	1.90	0.52
2:D:310:ASP:OD1	2:D:310:ASP:N	2.37	0.52
1:B:298:MET:O	1:B:303:ARG:NH1	2.41	0.52
2:E:258:ARG:HD3	2:E:273:TYR:CD1	2.44	0.52
2:E:338:ILE:HG23	2:E:341:PRO:HA	1.91	0.52
2:E:362:ARG:HB3	2:E:427:LEU:HD13	1.90	0.52
2:E:383:LYS:HD2	2:E:386:ALA:HB3	1.91	0.52
1:A:95:MET:HG3	2:D:119:ILE:HD11	1.91	0.52
1:B:168:THR:HG23	1:B:170:ASP:H	1.74	0.52
1:C:484:ASP:HB3	1:C:536:LEU:HD11	1.92	0.52
2:D:16:MET:HE1	2:D:70:VAL:HG11	1.92	0.52
2:D:364:ASP:OD1	2:D:364:ASP:N	2.38	0.52
2:F:126:GLU:HG3	2:F:143:ARG:CZ	2.39	0.52
1:B:484:ASP:O	1:B:488:LEU:HB3	2.10	0.51
2:D:353:ASP:O	2:D:356:THR:HG22	2.09	0.51
2:F:340:PRO:O	2:F:342:ILE:N	2.40	0.51
2:E:317:ASP:OD1	2:E:318:LEU:N	2.42	0.51
2:F:157:LYS:HB3	2:F:329:LEU:CD1	2.40	0.51
1:B:278:ASP:HB3	1:B:281:THR:HG22	1.93	0.51
1:C:232:GLY:N	1:C:390:VAL:O	2.44	0.51
1:A:231:PRO:HA	1:A:390:VAL:O	2.11	0.51
1:C:8:LYS:HB3	1:C:15:MET:HG3	1.91	0.51
1:C:203:LEU:HD12	1:C:371:ARG:HG2	1.93	0.51
2:E:404:PHE:O	2:E:408:PHE:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLY:HA2	1:A:329:ASP:O	2.10	0.51
2:D:311:LYS:N	2:D:311:LYS:HD2	2.25	0.51
1:C:546:MET:HA	1:C:549:THR:CG2	2.40	0.51
2:D:357:GLY:H	2:D:361:THR:CG2	2.24	0.51
2:E:138:LEU:HD13	2:E:344:VAL:HG11	1.93	0.51
1:C:576:GLU:O	1:C:580:THR:HG23	2.11	0.51
1:C:543:ASN:HA	1:C:546:MET:HG2	1.92	0.51
2:D:396:ASP:O	2:D:397:ILE:HB	2.11	0.51
2:F:338:ILE:HA	2:F:414:ASN:OD1	2.11	0.51
1:B:392:PRO:HG2	1:B:397:ILE:HG22	1.92	0.51
2:F:394:LEU:HD23	2:F:396:ASP:H	1.75	0.51
1:A:336:GLU:OE1	3:A:602:HOH:O	2.19	0.50
1:B:51:VAL:HG11	1:B:55:THR:HG23	1.93	0.50
2:D:340:PRO:HB2	2:D:342:ILE:HG13	1.92	0.50
2:E:137:HIS:HE1	2:E:369:MET:HA	1.75	0.50
2:F:366:ALA:O	2:F:369:MET:HB3	2.12	0.50
1:B:28:CYS:HB3	1:B:66:SER:HA	1.93	0.50
1:C:118:TRP:CZ3	1:C:141:GLU:HA	2.46	0.50
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.76	0.50
1:C:351:ASP:OD1	2:D:258:ARG:NH2	2.39	0.50
2:D:307:PRO:HG3	2:D:313:HIS:CB	2.41	0.50
2:E:280:ASN:O	2:E:283:THR:HB	2.11	0.50
2:E:368:THR:HG22	2:E:372:LEU:HD11	1.92	0.50
2:E:405:ALA:O	2:E:408:PHE:HB3	2.11	0.50
1:B:493:ALA:O	1:B:497:ARG:HG3	2.11	0.50
1:C:125:GLU:OE2	1:C:125:GLU:HA	2.12	0.50
2:D:142:VAL:HG11	2:D:355:GLY:HA3	1.94	0.50
2:D:332:GLU:O	2:D:335:LYS:HB3	2.11	0.50
2:F:10:GLU:HB3	2:F:17:ALA:HB3	1.92	0.50
1:B:531:GLU:O	1:B:535:ALA:HB3	2.12	0.50
2:D:163:GLN:OE1	2:D:417:PHE:HA	2.12	0.50
2:E:394:LEU:CB	2:E:399:LYS:HD2	2.40	0.50
1:B:467:GLU:HG2	1:B:471:ASN:ND2	2.26	0.50
1:B:572:SER:O	1:B:576:GLU:HG2	2.12	0.50
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.93	0.50
1:A:298:MET:HE3	2:D:118:PRO:HG3	1.93	0.50
1:C:214:ARG:HD3	1:C:513:THR:HG21	1.94	0.50
2:E:152:PRO:HB2	2:E:153:PRO:HD2	1.92	0.50
1:A:517:LYS:NZ	1:A:560:LYS:O	2.42	0.50
2:E:278:TYR:CB	2:E:318:LEU:HB3	2.31	0.50
1:C:464:LEU:HD11	1:C:496:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:LEU:C	2:E:322:ILE:HG12	2.31	0.49
2:E:425:GLU:O	2:E:428:ASP:N	2.45	0.49
2:E:364:ASP:C	2:E:368:THR:HG1	2.14	0.49
2:E:367:ALA:O	2:E:371:GLN:HG2	2.13	0.49
2:F:380:LYS:HA	2:F:383:LYS:HB2	1.94	0.49
1:B:186:THR:HG22	1:B:188:MET:H	1.78	0.49
1:B:214:ARG:NH1	1:B:513:THR:HG21	2.27	0.49
1:C:459:GLU:HA	1:C:462:ARG:HB2	1.94	0.49
1:C:494:LYS:HA	1:C:497:ARG:NH2	2.27	0.49
2:E:142:VAL:HG21	2:E:351:LEU:O	2.12	0.49
2:F:122:ASP:HB3	2:F:290:ARG:HB2	1.93	0.49
2:F:428:ASP:O	2:F:432:GLU:HG3	2.11	0.49
2:E:362:ARG:HG3	2:E:362:ARG:NH1	2.27	0.49
2:E:403:LYS:NZ	2:E:407:ARG:HH22	2.09	0.49
2:E:403:LYS:HZ1	2:E:407:ARG:HH22	1.59	0.49
2:E:414:ASN:O	2:E:414:ASN:ND2	2.39	0.49
2:F:140:THR:O	2:F:349:SER:OG	2.25	0.49
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.93	0.49
2:E:157:LYS:HZ1	2:E:305:THR:HG22	1.77	0.49
2:E:356:THR:O	2:E:356:THR:OG1	2.29	0.49
2:F:315:ILE:HB	2:F:316:PRO:CD	2.43	0.49
1:C:446:ASP:OD2	1:C:454:SER:OG	2.24	0.49
2:E:148:PRO:HG3	2:E:323:THR:HG21	1.95	0.49
2:E:248:GLU:OE2	2:E:249:ASP:N	2.46	0.49
2:D:349:SER:O	2:D:352:LYS:HG2	2.12	0.49
1:B:278:ASP:N	1:B:283:GLU:O	2.40	0.49
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.94	0.49
1:C:233:PRO:CG	1:C:236:ALA:HB3	2.42	0.49
1:A:234:PHE:CE1	2:D:350:ARG:HG3	2.48	0.49
1:A:266:MET:O	1:A:270:VAL:HG13	2.12	0.49
2:E:391:GLU:O	2:E:394:LEU:HG	2.13	0.49
2:D:388:VAL:HB	2:D:389:LEU:HD12	1.95	0.49
2:F:364:ASP:O	2:F:368:THR:HG22	2.13	0.49
1:C:464:LEU:HD21	1:C:496:ILE:CG1	2.43	0.48
2:F:338:ILE:CG1	2:F:409:GLU:HB3	2.42	0.48
2:E:130:THR:OG1	2:E:136:ASP:OD1	2.19	0.48
2:E:137:HIS:CE1	2:E:369:MET:HA	2.48	0.48
2:F:176:ASP:OD1	2:F:176:ASP:N	2.45	0.48
2:F:349:SER:HB3	2:F:352:LYS:HB3	1.95	0.48
1:B:142:THR:HG22	1:B:145:ILE:H	1.78	0.48
1:C:148:LYS:NZ	3:C:607:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:PRO:HD2	1:C:413:TRP:O	2.11	0.48
1:A:273:PHE:CE1	1:A:289:THR:HG21	2.49	0.48
1:B:210:ILE:O	1:B:249:SER:HA	2.14	0.48
1:B:545:ILE:O	1:B:548:GLY:N	2.47	0.48
1:C:38:GLU:OE1	1:C:52:TYR:OH	2.27	0.48
1:C:86:GLY:H	1:C:294:ASN:HD21	1.60	0.48
2:D:271:ARG:HA	2:D:271:ARG:NE	2.27	0.48
2:F:28:GLU:H	2:F:44:VAL:HG22	1.78	0.48
2:F:389:LEU:HB3	2:F:393:ALA:HB2	1.94	0.48
1:C:205:PRO:HB2	1:C:223:THR:OG1	2.13	0.48
2:E:361:THR:HG22	2:E:362:ARG:N	2.28	0.48
2:E:407:ARG:HG3	2:E:407:ARG:O	2.13	0.48
2:F:126:GLU:OE2	2:F:126:GLU:N	2.46	0.48
2:F:226:ARG:NH2	2:F:253:TYR:OH	2.46	0.48
1:B:52:TYR:O	1:B:299:PRO:HB3	2.14	0.48
1:B:531:GLU:HG3	1:B:581:ILE:HG21	1.96	0.48
1:C:461:MET:HA	1:C:464:LEU:HB2	1.95	0.48
1:C:563:PRO:HB2	1:C:565:GLU:HG2	1.95	0.48
2:D:184:ILE:HG23	2:D:221:ARG:HG3	1.94	0.48
2:E:383:LYS:HD3	2:E:402:ALA:HB1	1.94	0.48
2:E:396:ASP:O	2:E:399:LYS:HB2	2.13	0.48
1:A:315:GLU:HA	1:A:384:ILE:HD11	1.96	0.48
1:C:142:THR:HG22	1:C:143:LYS:N	2.29	0.48
1:C:178:THR:HG21	1:C:183:LYS:HE3	1.95	0.48
2:E:376:TYR:O	2:E:379:GLY:N	2.47	0.48
1:C:546:MET:HA	1:C:549:THR:HG22	1.95	0.48
2:F:155:ALA:HB1	2:F:341:PRO:HG2	1.95	0.48
2:F:280:ASN:O	2:F:283:THR:OG1	2.28	0.48
1:B:537:SER:OG	1:B:538:LEU:N	2.47	0.48
1:C:414:GLY:H	1:C:433:SER:HB3	1.78	0.48
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.96	0.48
2:F:129:GLN:O	2:F:168:ALA:HA	2.13	0.48
1:B:142:THR:HG21	1:B:287:GLU:O	2.14	0.47
1:C:497:ARG:HA	1:C:501:LEU:HB2	1.95	0.47
2:D:244:LEU:HD11	2:D:301:ILE:HG13	1.96	0.47
2:E:313:HIS:HE1	2:E:315:ILE:HG23	1.78	0.47
2:F:233:GLU:OE1	2:F:287:ARG:NE	2.41	0.47
1:B:545:ILE:HG22	1:B:549:THR:CG2	2.44	0.47
2:D:315:ILE:HD11	2:D:318:LEU:HD13	1.96	0.47
2:E:57:PHE:CD1	2:E:219:ILE:HD12	2.49	0.47
2:E:368:THR:O	2:E:372:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:405:ALA:HB3	2:E:406:GLU:OE1	2.14	0.47
2:E:423:ILE:HA	2:E:426:THR:HG22	1.97	0.47
1:B:453:TRP:CZ3	1:B:519:PHE:HA	2.49	0.47
1:C:531:GLU:HG3	1:C:577:ILE:HG12	1.97	0.47
2:D:330:THR:OG1	2:D:333:LEU:HD12	2.14	0.47
1:A:517:LYS:HG3	1:A:567:LEU:HD21	1.96	0.47
1:C:378:ASP:OD1	1:C:378:ASP:N	2.47	0.47
2:E:138:LEU:HD13	2:E:344:VAL:CG1	2.43	0.47
1:B:33:LEU:HD12	1:B:33:LEU:H	1.79	0.47
2:F:82:SER:O	2:F:85:MET:HG3	2.15	0.47
2:F:132:ILE:HD11	2:F:163:GLN:HG2	1.96	0.47
1:B:13:LEU:HD21	1:B:345:LEU:HD21	1.96	0.47
2:D:28:GLU:H	2:D:44:VAL:HG22	1.80	0.47
2:D:386:ALA:CB	2:D:394:LEU:HD21	2.44	0.47
2:E:338:ILE:HA	2:E:414:ASN:OD1	2.15	0.47
2:F:30:ILE:HD11	2:F:70:VAL:HG13	1.97	0.47
1:A:179:GLU:HB3	1:A:180:GLN:OE1	2.15	0.47
1:B:119:TRP:O	1:B:139:VAL:HG22	2.14	0.47
1:C:567:LEU:HB2	1:C:570:ILE:HD11	1.96	0.47
2:D:278:TYR:N	2:D:318:LEU:HD11	2.30	0.47
2:D:320:GLY:HA2	2:D:323:THR:OG1	2.14	0.47
2:E:359:GLY:O	2:E:360:LYS:HD2	2.15	0.47
1:B:398:SER:O	1:B:398:SER:OG	2.28	0.47
2:D:103:ILE:HD12	2:D:103:ILE:O	2.14	0.47
2:D:378:GLN:HA	2:D:381:GLN:HB3	1.97	0.47
2:D:394:LEU:O	2:D:394:LEU:HD12	2.14	0.47
1:C:146:GLN:HG2	1:C:322:TYR:OH	2.16	0.46
1:C:220:PHE:HA	1:C:435:SER:HB3	1.98	0.46
2:E:152:PRO:CB	2:E:153:PRO:HD2	2.44	0.46
2:F:345:LEU:HB2	2:F:346:PRO:HD3	1.96	0.46
1:A:319:ASP:O	1:A:380:ARG:NH1	2.49	0.46
1:A:329:ASP:HA	1:A:330:SER:HA	1.64	0.46
1:B:156:LYS:O	1:B:178:THR:HG22	2.16	0.46
1:B:333:ARG:NH2	1:B:336:GLU:OE1	2.46	0.46
1:B:530:LYS:O	1:B:534:LYS:N	2.41	0.46
2:E:196:GLU:O	2:E:200:GLN:HG2	2.15	0.46
2:E:405:ALA:O	2:E:409:GLU:HG3	2.16	0.46
2:F:160:LEU:O	2:F:164:ILE:HG13	2.15	0.46
2:F:288:ALA:HB2	2:F:300:GLN:HG3	1.97	0.46
2:F:326:GLN:NE2	2:F:346:PRO:O	2.49	0.46
1:B:540:ALA:HB1	1:B:544:GLU:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:THR:CG2	1:C:287:GLU:HB3	2.45	0.46
2:F:314:PRO:HB3	2:F:318:LEU:HD13	1.97	0.46
1:B:263:GLY:N	2:E:286:GLU:OE2	2.42	0.46
1:C:12:PRO:HD3	1:C:344:ARG:NH1	2.30	0.46
2:D:423:ILE:HG12	2:D:427:LEU:HD11	1.98	0.46
2:E:160:LEU:O	2:E:164:ILE:HG13	2.16	0.46
2:F:394:LEU:CD2	2:F:398:ASP:H	2.28	0.46
2:F:415:GLN:HG2	2:F:416:GLY:H	1.81	0.46
1:B:124:ILE:HG22	1:B:162:ILE:HD13	1.97	0.46
1:B:456:MET:HE3	1:B:526:LEU:HD12	1.97	0.46
1:B:467:GLU:HG3	1:B:490:LEU:HD22	1.97	0.46
2:F:353:ASP:HB2	2:F:354:LYS:HZ3	1.81	0.46
2:D:390:GLY:HA2	2:D:399:LYS:HZ2	1.78	0.46
2:E:258:ARG:HD3	2:E:273:TYR:CG	2.51	0.46
2:F:352:LYS:O	2:F:356:THR:HG23	2.16	0.46
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.51	0.46
1:B:297:ASN:HB3	2:E:115:VAL:HG13	1.97	0.46
1:B:520:ASN:O	1:B:524:VAL:HG22	2.16	0.46
1:C:224:LYS:HE2	1:C:323:ASP:OD2	2.16	0.46
1:C:340:GLU:O	1:C:344:ARG:HG3	2.16	0.46
1:C:559:SER:O	1:C:569:LYS:HE2	2.16	0.46
2:D:126:GLU:HG2	2:D:143:ARG:NH2	2.31	0.46
1:C:496:ILE:HD12	1:C:496:ILE:C	2.36	0.46
2:E:415:GLN:NE2	3:E:502:HOH:O	2.49	0.46
1:B:169:ILE:HG23	1:B:188:MET:HB2	1.97	0.45
1:B:199:ILE:HG21	1:B:372:VAL:HG21	1.98	0.45
1:C:575:GLU:O	1:C:579:GLU:HG3	2.15	0.45
2:D:315:ILE:HA	2:D:316:PRO:HD3	1.76	0.45
2:E:436:MET:SD	2:E:437:LEU:HD13	2.56	0.45
2:F:166:ARG:HD3	2:F:201:THR:HG21	1.97	0.45
2:E:276:TYR:O	2:E:280:ASN:N	2.28	0.45
2:E:317:ASP:OD1	2:E:317:ASP:N	2.47	0.45
2:E:384:GLU:O	2:E:388:VAL:HG12	2.17	0.45
1:A:298:MET:HE1	2:D:118:PRO:HD3	1.98	0.45
1:B:523:LYS:HD3	1:B:574:ASN:ND2	2.30	0.45
1:B:571:SER:O	1:B:574:ASN:HB2	2.16	0.45
2:E:163:GLN:HG3	2:E:417:PHE:O	2.16	0.45
2:E:339:SER:HA	2:E:341:PRO:HD3	1.97	0.45
1:B:193:VAL:CG2	1:B:309:THR:HA	2.47	0.45
2:D:163:GLN:OE1	2:D:417:PHE:HD1	1.99	0.45
2:D:307:PRO:HG3	2:D:313:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:SER:O	2:D:395:SER:OG	2.27	0.45
2:E:372:LEU:CD2	2:E:434:LEU:HD11	2.47	0.45
1:A:462:ARG:NH1	1:A:466:GLU:OE1	2.49	0.45
1:A:549:THR:HG23	1:A:553:ARG:HH11	1.81	0.45
1:B:461:MET:HA	1:B:464:LEU:HD12	1.97	0.45
2:D:163:GLN:HG3	2:D:417:PHE:O	2.16	0.45
2:D:315:ILE:HG13	2:D:318:LEU:HB3	1.98	0.45
1:A:521:MET:O	1:A:525:ILE:HG12	2.17	0.45
1:C:529:GLY:O	1:C:533:ARG:HG3	2.17	0.45
2:E:253:TYR:OH	2:E:280:ASN:OD1	2.30	0.45
2:F:155:ALA:O	2:F:157:LYS:N	2.47	0.45
1:A:126:GLU:HG2	1:A:162:ILE:HG22	1.99	0.45
1:B:344:ARG:HG2	3:B:632:HOH:O	2.17	0.45
1:C:56:SER:O	1:C:105:ARG:NH1	2.42	0.45
1:C:523:LYS:O	1:C:527:THR:HG23	2.16	0.45
1:B:576:GLU:O	1:B:580:THR:HG22	2.17	0.45
1:C:265:GLU:O	1:C:269:VAL:HG23	2.16	0.45
1:C:487:ARG:HB3	1:C:542:PHE:CZ	2.51	0.45
1:C:495:SER:O	1:C:499:ASP:HB2	2.16	0.45
2:E:372:LEU:HD23	2:E:434:LEU:HD11	1.99	0.45
1:B:191:TRP:CZ2	1:B:198:PRO:HD3	2.51	0.45
1:B:453:TRP:HZ3	1:B:519:PHE:HA	1.81	0.45
1:C:121:GLU:OE2	1:C:138:TYR:HD1	2.00	0.45
2:E:120:ALA:O	2:E:292:ARG:HG2	2.17	0.45
2:E:315:ILE:N	2:E:316:PRO:HD2	2.32	0.45
2:D:142:VAL:HG23	2:D:145:GLN:HB2	1.98	0.45
2:F:178:ALA:HB2	2:F:241:MET:HE2	1.99	0.45
2:F:408:PHE:O	2:F:412:TYR:HB3	2.17	0.45
1:A:207:VAL:HG22	1:A:444:TYR:CE2	2.52	0.44
1:B:540:ALA:HB1	1:B:544:GLU:HB2	1.98	0.44
2:D:126:GLU:OE1	2:D:290:ARG:NH1	2.50	0.44
2:F:324:GLU:HA	2:F:350:ARG:NH2	2.31	0.44
2:F:379:GLY:HA3	2:F:405:ALA:HB2	1.99	0.44
1:B:345:LEU:O	1:B:346:GLU:HG2	2.17	0.44
1:C:51:VAL:HG12	1:C:53:GLU:O	2.17	0.44
1:C:215:VAL:HG13	1:C:216:ILE:HG23	1.98	0.44
2:F:357:GLY:N	2:F:361:THR:OG1	2.50	0.44
2:F:429:LEU:HA	2:F:432:GLU:HG3	1.99	0.44
1:A:231:PRO:HD2	1:A:413:TRP:O	2.18	0.44
1:B:144:ILE:HG21	1:B:288:ARG:HD3	2.00	0.44
1:B:470:LEU:HD21	1:B:486:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:GLU:O	1:B:579:GLU:HG2	2.18	0.44
1:C:94:PHE:CE1	1:C:103:LEU:HA	2.52	0.44
1:C:332:SER:O	1:C:336:GLU:HG3	2.17	0.44
1:C:521:MET:HE2	1:C:521:MET:HB2	1.90	0.44
2:E:129:GLN:NE2	2:E:171:LEU:HD21	2.32	0.44
2:E:137:HIS:CE1	2:E:372:LEU:HD13	2.52	0.44
2:F:149:VAL:HB	2:F:303:ILE:HG12	2.00	0.44
1:A:416:ASP:HB3	1:A:419:LEU:HB2	2.00	0.44
1:B:101:ASN:O	2:E:116:ILE:HD12	2.18	0.44
1:B:497:ARG:O	1:B:502:GLN:HG3	2.18	0.44
1:C:6:ILE:HG22	1:C:60:PRO:HA	1.99	0.44
1:C:500:TYR:OH	1:C:518:GLN:HB3	2.17	0.44
2:D:251:THR:HG23	2:D:314:PRO:HD3	2.00	0.44
1:A:261:GLU:OE1	1:A:330:SER:N	2.51	0.44
1:C:214:ARG:NH2	1:C:503:GLN:HG2	2.33	0.44
2:D:125:ASP:O	2:D:355:GLY:HA2	2.17	0.44
2:E:315:ILE:HA	2:E:318:LEU:HD11	1.99	0.44
2:E:318:LEU:O	2:E:319:THR:C	2.56	0.44
1:B:580:THR:OG1	1:B:584:ILE:HD11	2.18	0.44
1:C:267:THR:HG22	2:F:118:PRO:O	2.17	0.44
1:C:360:SER:O	1:C:364:GLU:HG3	2.17	0.44
2:F:278:TYR:CD1	2:F:278:TYR:N	2.84	0.44
1:B:562:ILE:CD1	1:B:569:LYS:HB3	2.45	0.44
2:D:11:VAL:HG22	2:D:16:MET:CG	2.48	0.44
2:F:157:LYS:HZ1	2:F:305:THR:HA	1.83	0.44
1:A:224:LYS:HE3	1:A:250:ASP:HB3	2.00	0.44
1:B:470:LEU:HD11	1:B:486:ASP:HB3	1.99	0.44
1:B:545:ILE:O	1:B:549:THR:HG23	2.18	0.44
2:D:137:HIS:NE2	2:D:368:THR:HG23	2.32	0.44
2:F:11:VAL:HG22	2:F:16:MET:CG	2.48	0.44
2:F:345:LEU:HD21	2:F:376:TYR:HD1	1.83	0.44
1:C:522:LEU:HG	1:C:526:LEU:HD12	1.99	0.44
2:E:196:GLU:CD	2:E:199:ARG:HE	2.20	0.44
2:E:422:THR:HB	2:E:425:GLU:CD	2.37	0.44
2:F:371:GLN:OE1	2:F:442:LEU:HA	2.18	0.44
2:F:396:ASP:HB3	2:F:397:ILE:H	1.67	0.43
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.99	0.43
1:B:134:ASP:O	1:B:151:VAL:HG23	2.19	0.43
1:C:191:TRP:CZ2	1:C:198:PRO:HD3	2.53	0.43
1:C:213:GLN:HA	1:C:503:GLN:HE22	1.82	0.43
2:D:142:VAL:CG1	2:D:355:GLY:HA3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:ASN:HB3	2:E:349:SER:HB3	1.99	0.43
1:A:209:MET:HG3	1:A:250:ASP:HB2	2.00	0.43
1:A:555:ARG:HH22	1:A:572:SER:HG	1.64	0.43
1:C:534:LYS:HA	1:C:537:SER:HB3	1.99	0.43
2:D:251:THR:HG23	2:D:314:PRO:CD	2.48	0.43
2:E:313:HIS:CE1	2:E:315:ILE:HG23	2.54	0.43
1:C:247:LYS:HB3	1:C:247:LYS:HE2	1.83	0.43
1:A:298:MET:CE	2:D:118:PRO:HG3	2.48	0.43
1:B:196:GLY:HA2	1:B:368:ARG:HH21	1.83	0.43
1:B:556:ILE:HD12	1:B:557:SER:N	2.32	0.43
1:B:568:ALA:O	1:B:572:SER:HB3	2.18	0.43
1:C:92:ASP:OD1	1:C:93:THR:N	2.48	0.43
2:D:45:LEU:HD22	2:D:264:ARG:NE	2.33	0.43
2:D:186:ILE:HB	2:D:190:GLU:HG3	2.01	0.43
2:E:184:ILE:HG23	2:E:221:ARG:HG3	2.01	0.43
2:E:415:GLN:H	2:E:415:GLN:HG2	1.49	0.43
2:F:179:VAL:O	2:F:207:SER:HA	2.18	0.43
1:B:205:PRO:HB2	1:B:223:THR:OG1	2.19	0.43
2:F:157:LYS:NZ	2:F:305:THR:HA	2.33	0.43
1:C:482:LEU:HD23	1:C:487:ARG:HB2	2.01	0.43
2:D:307:PRO:HB3	2:D:313:HIS:HB2	2.01	0.43
2:D:407:ARG:HG3	2:D:411:GLU:OE1	2.18	0.43
2:E:88:ARG:NH2	2:E:98:ASP:OD1	2.38	0.43
2:F:92:GLY:HA2	2:F:224:THR:HG23	2.01	0.43
1:B:297:ASN:HB2	2:E:286:GLU:HG2	1.99	0.43
1:B:486:ASP:HA	1:B:489:THR:HG1	1.84	0.43
2:D:318:LEU:O	2:D:322:ILE:HG13	2.18	0.43
2:E:330:THR:CG2	2:E:333:LEU:HD12	2.49	0.43
1:C:393:SER:HB2	2:F:321:TYR:CD1	2.54	0.43
2:F:338:ILE:HG23	2:F:414:ASN:HA	2.00	0.43
1:B:329:ASP:HA	1:B:330:SER:HA	1.59	0.43
2:E:404:PHE:HE1	2:E:433:LEU:HB3	1.84	0.43
1:C:92:ASP:O	1:C:96:GLU:HG3	2.18	0.42
1:C:125:GLU:O	1:C:128:THR:HG22	2.19	0.42
2:F:265:ARG:O	2:F:265:ARG:HG3	2.18	0.42
1:A:243:HIS:O	1:A:247:LYS:HG2	2.19	0.42
1:C:499:ASP:HA	1:C:560:LYS:NZ	2.34	0.42
2:D:88:ARG:NH2	2:D:101:PRO:O	2.47	0.42
2:E:306:MET:C	2:E:308:GLU:H	2.22	0.42
1:A:549:THR:CG2	1:A:553:ARG:HH11	2.32	0.42
1:B:237:GLY:O	1:B:241:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:MET:HA	1:B:387:ILE:O	2.19	0.42
1:B:562:ILE:HA	1:B:563:PRO:HD3	1.88	0.42
1:C:531:GLU:OE2	1:C:534:LYS:HD2	2.19	0.42
2:E:368:THR:HG22	2:E:372:LEU:CD1	2.48	0.42
2:F:190:GLU:O	2:F:193:PHE:HB3	2.19	0.42
1:C:329:ASP:HA	1:C:330:SER:HA	1.66	0.42
1:C:419:LEU:HG	1:C:424:HIS:HB3	2.01	0.42
2:D:264:ARG:O	2:D:265:ARG:HG3	2.20	0.42
2:D:290:ARG:HE	2:D:290:ARG:HB3	1.62	0.42
2:D:374:ALA:HA	2:D:377:ALA:HB3	2.01	0.42
2:F:157:LYS:HB3	2:F:329:LEU:HD11	2.02	0.42
1:A:392:PRO:HB2	1:A:396:ASP:H	1.83	0.42
1:A:515:ARG:HD2	3:A:648:HOH:O	2.19	0.42
1:A:523:LYS:HA	1:A:523:LYS:HD3	1.77	0.42
1:C:238:LYS:HB2	1:C:415:LEU:HD13	2.01	0.42
1:C:578:LYS:O	1:C:579:GLU:C	2.57	0.42
2:D:258:ARG:HH21	2:D:273:TYR:HE1	1.67	0.42
2:E:45:LEU:HD21	2:E:264:ARG:CZ	2.50	0.42
1:C:415:LEU:HA	1:C:427:SER:O	2.19	0.42
2:D:191:ALA:O	2:D:195:MET:HG3	2.18	0.42
2:E:311:LYS:NZ	2:E:312:THR:O	2.51	0.42
2:F:34:MET:SD	2:F:40:ARG:NE	2.93	0.42
2:F:340:PRO:C	2:F:342:ILE:H	2.21	0.42
1:A:549:THR:HG23	1:A:553:ARG:HD3	2.01	0.42
1:C:150:MET:HE1	1:C:319:ASP:O	2.20	0.42
1:C:244:GLN:NE2	1:C:511:THR:O	2.53	0.42
1:C:499:ASP:OD1	1:C:499:ASP:N	2.52	0.42
2:D:380:LYS:HD2	2:D:380:LYS:HA	1.57	0.42
2:E:146:LYS:HD2	2:E:285:PHE:HB3	2.02	0.42
2:E:162:ALA:O	2:E:166:ARG:HB2	2.19	0.42
2:F:137:HIS:HB3	2:F:138:LEU:HD22	2.01	0.42
1:C:208:PRO:CG	1:C:441:VAL:HG13	2.49	0.42
1:C:556:ILE:HD11	1:C:572:SER:OG	2.20	0.42
1:C:576:GLU:OE1	1:C:580:THR:HG21	2.20	0.42
2:E:288:ALA:HB2	2:E:300:GLN:HG3	2.02	0.42
2:F:188:PHE:CZ	2:F:192:GLU:HG3	2.55	0.42
1:A:562:ILE:HB	1:A:570:ILE:HD11	2.01	0.42
1:B:543:ASN:OD1	1:B:543:ASN:N	2.52	0.42
1:C:345:LEU:HD23	1:C:345:LEU:HA	1.90	0.42
1:C:411:VAL:HG23	1:C:435:SER:HB2	2.02	0.42
2:D:44:VAL:HA	2:D:54:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:403:LYS:HD3	2:E:404:PHE:N	2.34	0.42
2:F:87:GLY:HA2	2:F:204:ILE:O	2.20	0.42
1:C:114:HIS:ND1	1:C:169:ILE:HD11	2.35	0.41
1:C:543:ASN:OD1	1:C:543:ASN:N	2.52	0.41
2:D:33:ARG:HD2	2:D:33:ARG:HA	1.88	0.41
2:D:179:VAL:O	2:D:207:SER:HA	2.20	0.41
2:D:315:ILE:HG13	2:D:318:LEU:CB	2.50	0.41
1:B:5:LYS:HD3	1:B:61:GLY:HA2	2.03	0.41
1:B:327:MET:HG2	1:B:387:ILE:HB	2.02	0.41
1:C:427:SER:OG	1:C:427:SER:O	2.38	0.41
2:E:266:GLU:HG3	2:E:276:TYR:OH	2.20	0.41
2:F:239:LYS:HA	2:F:239:LYS:HD3	1.87	0.41
1:A:242:GLN:HB3	1:A:327:MET:HE1	2.03	0.41
1:B:36:ILE:HG13	1:B:108:GLN:HE21	1.84	0.41
2:D:290:ARG:NH2	2:D:295:LYS:O	2.52	0.41
2:E:148:PRO:HB2	2:E:150:PHE:HE1	1.85	0.41
1:A:144:ILE:HD12	1:A:287:GLU:HB2	2.03	0.41
1:B:188:MET:HG2	1:B:189:GLN:N	2.35	0.41
1:C:233:PRO:HG2	1:C:236:ALA:HB3	2.02	0.41
1:C:333:ARG:NH2	1:C:336:GLU:OE2	2.45	0.41
1:C:360:SER:OG	2:D:259:GLU:OE1	2.39	0.41
2:E:426:THR:HA	2:E:429:LEU:HD13	2.02	0.41
1:A:366:TYR:O	1:A:369:SER:OG	2.39	0.41
1:B:114:HIS:HB3	1:B:170:ASP:OD2	2.21	0.41
1:B:567:LEU:HD22	1:B:570:ILE:HD12	2.02	0.41
2:D:221:ARG:HD2	2:D:256:ALA:HB2	2.02	0.41
2:E:322:ILE:HD13	2:E:322:ILE:HG21	1.79	0.41
1:A:523:LYS:HD2	1:A:527:THR:HG23	2.01	0.41
1:B:410:LYS:HA	1:B:436:LEU:HD12	2.02	0.41
1:C:214:ARG:N	1:C:503:GLN:OE1	2.53	0.41
1:C:232:GLY:HA2	1:C:233:PRO:HD3	1.91	0.41
1:C:269:VAL:O	1:C:273:PHE:HB2	2.21	0.41
2:D:408:PHE:HB2	2:D:433:LEU:HD11	2.02	0.41
2:D:423:ILE:HG12	2:D:427:LEU:CD1	2.51	0.41
2:F:125:ASP:HA	2:F:354:LYS:HB3	2.02	0.41
2:F:182:ALA:O	2:F:247:MET:HA	2.20	0.41
2:F:184:ILE:O	2:F:252:ASN:ND2	2.25	0.41
1:B:429:ASN:O	1:B:433:SER:OG	2.22	0.41
1:C:483:SER:HB2	1:C:486:ASP:CG	2.41	0.41
2:E:123:TYR:O	2:E:290:ARG:NH1	2.50	0.41
2:E:422:THR:O	2:E:426:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:CG	2:E:258:ARG:HH22	2.24	0.41
1:B:77:PRO:HG2	1:B:187:MET:HE1	2.01	0.41
2:F:408:PHE:O	2:F:413:VAL:HG23	2.19	0.41
1:A:327:MET:HA	1:A:387:ILE:O	2.21	0.41
1:A:576:GLU:O	1:A:580:THR:HG23	2.20	0.41
1:C:194:ARG:NH1	1:C:304:GLU:OE1	2.53	0.41
2:E:339:SER:HB2	2:E:417:PHE:CE2	2.56	0.41
2:E:400:ILE:HG23	2:E:436:MET:CE	2.50	0.41
2:F:127:PHE:CE1	2:F:140:THR:HG23	2.56	0.41
2:F:224:THR:HB	2:F:225:PRO:HD3	2.03	0.41
1:C:28:CYS:O	1:C:36:ILE:HD12	2.20	0.41
2:F:3:LYS:O	2:F:71:ARG:HA	2.21	0.41
2:F:236:ALA:HA	2:F:241:MET:O	2.21	0.41
1:A:5:LYS:HE2	1:A:5:LYS:HB3	1.96	0.40
1:B:8:LYS:HB3	1:B:15:MET:HB2	2.02	0.40
1:B:570:ILE:O	1:B:573:ILE:HD12	2.21	0.40
2:D:338:ILE:HG23	2:D:414:ASN:HB2	2.03	0.40
2:E:87:GLY:HA2	2:E:204:ILE:O	2.20	0.40
2:F:184:ILE:HB	2:F:249:ASP:O	2.21	0.40
1:C:298:MET:CG	1:C:299:PRO:HD2	2.51	0.40
1:C:430:TRP:HE3	1:C:431:ILE:H	1.68	0.40
2:D:282:ALA:HB2	2:D:322:ILE:HD13	2.02	0.40
2:E:312:THR:O	2:E:312:THR:OG1	2.39	0.40
2:E:315:ILE:HG13	2:E:316:PRO:CD	2.50	0.40
2:F:79:LEU:HD13	2:F:227:MET:HG2	2.03	0.40
2:F:81:VAL:HG11	2:F:109:LEU:HD12	2.04	0.40
2:D:373:PHE:CD1	2:D:374:ALA:N	2.90	0.40
2:E:261:SER:O	2:E:265:ARG:N	2.55	0.40
2:F:30:ILE:HD11	2:F:70:VAL:CG1	2.51	0.40
1:A:558:ARG:NH1	3:A:617:HOH:O	2.53	0.40
1:B:148:LYS:HZ3	1:B:148:LYS:HG3	1.72	0.40
1:C:25:GLN:HG3	2:D:61:SER:HB2	2.04	0.40
1:A:91:LEU:HD13	2:D:118:PRO:HD2	2.04	0.40
1:B:415:LEU:HD23	1:B:428:ILE:HG13	2.03	0.40
1:C:315:GLU:HA	1:C:384:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

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	585/596 (98%)	569 (97%)	16 (3%)	0	100	100
1	B	584/596 (98%)	566 (97%)	18 (3%)	0	100	100
1	C	583/596 (98%)	564 (97%)	18 (3%)	1 (0%)	47	76
2	D	430/458 (94%)	406 (94%)	22 (5%)	2 (0%)	29	58
2	E	448/458 (98%)	413 (92%)	29 (6%)	6 (1%)	12	33
2	F	443/458 (97%)	410 (93%)	30 (7%)	3 (1%)	22	50
All	All	3073/3162 (97%)	2928 (95%)	133 (4%)	12 (0%)	34	64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	397	ILE
2	E	153	PRO
2	F	388	VAL
1	C	233	PRO
2	D	99	ASN
2	E	307	PRO
2	E	425	GLU
2	F	249	ASP
2	E	249	ASP
2	E	396	ASP
2	F	156	GLY
2	E	101	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	503/509 (99%)	488 (97%)	15 (3%)	41	72
1	B	502/509 (99%)	483 (96%)	19 (4%)	33	64
1	C	501/509 (98%)	467 (93%)	34 (7%)	16	39
2	D	356/380 (94%)	333 (94%)	23 (6%)	17	41
2	E	373/380 (98%)	344 (92%)	29 (8%)	12	32
2	F	368/380 (97%)	338 (92%)	30 (8%)	11	30
All	All	2603/2667 (98%)	2453 (94%)	150 (6%)	20	47

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	43	ARG
1	A	56	SER
1	A	94	PHE
1	A	95	MET
1	A	146	GLN
1	A	250	ASP
1	A	268	ASP
1	A	285	LEU
1	A	338	LEU
1	A	398	SER
1	A	403	GLN
1	A	476	LEU
1	A	479	ILE
1	A	508	ASP
1	B	20	SER
1	B	28	CYS
1	B	50	GLN
1	B	125	GLU
1	B	193	VAL
1	B	234	PHE
1	B	273	PHE
1	B	330	SER
1	B	372	VAL
1	B	398	SER
1	B	427	SER
1	B	443	ARG
1	B	472	GLU

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Mol	Chain	Res	Type
1	B	477	VAL
1	B	515	ARG
1	B	538	LEU
1	B	542	PHE
1	B	555	ARG
1	B	572	SER
1	C	1	MET
1	C	56	SER
1	C	66	SER
1	C	100	SER
1	C	114	HIS
1	C	167	PHE
1	C	240	VAL
1	C	253	LEU
1	C	259	CYS
1	C	266	MET
1	C	268	ASP
1	C	273	PHE
1	C	330	SER
1	C	398	SER
1	C	430	TRP
1	C	443[A]	ARG
1	C	443[B]	ARG
1	C	451	GLN
1	C	461	MET
1	C	462	ARG
1	C	477	VAL
1	C	484	ASP
1	C	488	LEU
1	C	489	THR
1	C	499	ASP
1	C	521	MET
1	C	537	SER
1	C	542	PHE
1	C	543	ASN
1	C	546	MET
1	C	549	THR
1	C	555	ARG
1	C	569	LYS
1	C	571	SER
2	D	6	ARG
2	D	41	ARG

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Mol	Chain	Res	Type
2	D	61	SER
2	D	99	ASN
2	D	102	GLU
2	D	122	ASP
2	D	125	ASP
2	D	127	PHE
2	D	158	SER
2	D	172	ASP
2	D	176	ASP
2	D	206	ARG
2	D	265	ARG
2	D	271	ARG
2	D	297	SER
2	D	321	TYR
2	D	361	THR
2	D	368	THR
2	D	372	LEU
2	D	376	TYR
2	D	380	LYS
2	D	404	PHE
2	D	407	ARG
2	E	6	ARG
2	E	82	SER
2	E	136	ASP
2	E	138	LEU
2	E	249	ASP
2	E	265	ARG
2	E	271	ARG
2	E	276	TYR
2	E	295	LYS
2	E	312	THR
2	E	315	ILE
2	E	318	LEU
2	E	330	THR
2	E	331	ARG
2	E	336	SER
2	E	338	ILE
2	E	349	SER
2	E	352	LYS
2	E	363	GLU
2	E	368	THR
2	E	369	MET

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Mol	Chain	Res	Type
2	E	370	ASN
2	E	381	GLN
2	E	400	ILE
2	E	401	TYR
2	E	407	ARG
2	E	414	ASN
2	E	431	TRP
2	E	447	ASP
2	F	22	SER
2	F	43	GLN
2	F	125	ASP
2	F	146	LYS
2	F	147	LEU
2	F	157	LYS
2	F	176	ASP
2	F	227	MET
2	F	248	GLU
2	F	249	ASP
2	F	276	TYR
2	F	278	TYR
2	F	279	THR
2	F	280	ASN
2	F	312	THR
2	F	313	HIS
2	F	314	PRO
2	F	318	LEU
2	F	335	LYS
2	F	349	SER
2	F	380	LYS
2	F	381	GLN
2	F	392	SER
2	F	397	ILE
2	F	407	ARG
2	F	417	PHE
2	F	437	LEU
2	F	439	ARG
2	F	442	LEU
2	F	444	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	B	242	GLN
1	B	421	GLN
1	C	242	GLN
1	C	294	ASN
2	D	167	GLN
2	D	242	HIS
2	E	137	HIS
2	E	163	GLN
2	E	381	GLN
2	F	163	GLN
2	F	167	GLN
2	F	326	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 monosaccharides 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	586/596 (98%)	0.28	17 (2%) 51 46	34, 51, 83, 125	0
1	B	586/596 (98%)	0.46	40 (6%) 17 12	41, 71, 126, 147	0
1	C	584/596 (97%)	0.51	47 (8%) 12 8	43, 74, 121, 139	0
2	D	432/458 (94%)	0.60	43 (9%) 7 5	38, 68, 136, 161	0
2	E	449/458 (98%)	0.87	65 (14%) 2 1	35, 72, 143, 160	0
2	F	445/458 (97%)	0.95	77 (17%) 1 1	41, 79, 150, 170	0
All	All	3082/3162 (97%)	0.59	289 (9%) 8 6	34, 68, 133, 170	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	393	ALA	8.9
2	F	387	VAL	8.6
2	E	272	GLY	8.1
2	F	319	THR	7.6
2	F	312	THR	7.3
2	F	437	LEU	7.2
2	D	388	VAL	7.1
2	F	397	ILE	7.0
2	E	405	ALA	7.0
2	D	385	LEU	7.0
1	C	475	ARG	6.8
2	E	397	ILE	6.7
1	B	482	LEU	6.4
2	D	392	SER	6.1
2	F	432	GLU	6.1
2	E	382	ALA	6.1
2	F	404	PHE	6.0
2	F	386	ALA	5.9
2	F	435	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
2	D	399	LYS	5.8
2	E	401	TYR	5.7
2	F	433	LEU	5.6
2	E	387	VAL	5.6
2	E	273	TYR	5.5
2	F	436	MET	5.4
2	E	392	SER	5.4
1	A	393	SER	5.3
2	D	391	GLU	5.3
2	F	174	SER	5.3
2	E	310	ASP	5.3
2	F	443	LYS	5.2
1	B	582	GLN	5.1
2	D	428	ASP	5.1
1	B	479	ILE	5.1
2	F	396	ASP	5.1
2	F	401	TYR	5.1
2	F	439	ARG	5.0
2	F	412	TYR	5.0
2	E	389	LEU	5.0
2	F	392	SER	5.0
2	F	385	LEU	4.9
2	E	434	LEU	4.8
2	F	390	GLY	4.8
2	D	393	ALA	4.8
1	B	542	PHE	4.8
2	D	272	GLY	4.8
1	B	477	VAL	4.6
2	F	400	ILE	4.6
1	B	484	ASP	4.6
1	B	541	TYR	4.6
1	A	395	GLY	4.6
2	E	436	MET	4.6
1	B	473	ILE	4.6
1	C	471	ASN	4.6
2	F	398	ASP	4.5
2	E	313	HIS	4.4
2	F	362	ARG	4.4
2	F	172	ASP	4.4
2	F	431	TRP	4.4
2	D	389	LEU	4.4
2	F	403	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	474	VAL	4.3
1	C	492	VAL	4.3
2	E	386	ALA	4.3
2	F	399	LYS	4.2
2	D	384	GLU	4.2
2	F	406	GLU	4.2
1	B	546	MET	4.2
2	E	398	ASP	4.2
2	F	173	SER	4.2
2	D	271	ARG	4.2
2	F	310	ASP	4.1
2	E	437	LEU	4.1
2	D	396	ASP	4.1
2	F	389	LEU	4.1
1	B	579	GLU	4.1
1	B	162	ILE	4.1
2	D	387	VAL	4.1
2	E	376	TYR	4.1
2	E	385	LEU	4.0
2	E	381	GLN	4.0
2	F	438	PRO	4.0
2	F	405	ALA	4.0
2	D	407	ARG	4.0
2	E	267	VAL	4.0
1	B	538	LEU	4.0
2	D	314	PRO	4.0
1	B	470	LEU	4.0
1	B	534	LYS	3.8
2	D	433	LEU	3.8
2	F	427	LEU	3.8
1	C	542	PHE	3.8
2	F	318	LEU	3.8
2	D	386	ALA	3.8
2	F	434	LEU	3.8
1	A	473	ILE	3.8
2	E	390	GLY	3.8
1	B	490	LEU	3.7
2	E	431	TRP	3.7
2	E	393	ALA	3.7
2	F	175	ASP	3.7
1	C	582	GLN	3.7
1	B	585	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	432	GLU	3.7
1	B	478	GLY	3.7
1	B	540	ALA	3.6
2	E	321	TYR	3.6
2	F	423	ILE	3.6
2	F	363	GLU	3.6
1	B	474	VAL	3.6
2	E	440	THR	3.5
2	E	312	THR	3.5
2	E	309	ASP	3.5
2	F	270	ARG	3.5
1	B	581	ILE	3.5
1	C	574	ASN	3.5
2	D	390	GLY	3.5
2	F	374	ALA	3.4
1	C	175	VAL	3.4
1	B	476	LEU	3.4
2	F	378	GLN	3.4
2	D	315	ILE	3.4
2	F	379	GLY	3.4
2	E	274	PRO	3.4
2	E	399	LYS	3.4
2	F	440	THR	3.3
2	F	375	ALA	3.3
2	F	388	VAL	3.3
2	D	175	ASP	3.3
2	F	339	SER	3.3
2	E	361	THR	3.3
1	C	480	ASP	3.3
1	C	540	ALA	3.3
1	C	488	LEU	3.3
2	D	394	LEU	3.3
1	A	479	ILE	3.2
2	F	382	ALA	3.2
1	A	549	THR	3.2
2	E	374	ALA	3.2
2	F	376	TYR	3.2
2	F	429	LEU	3.2
2	E	396	ASP	3.1
1	A	541	TYR	3.1
2	F	268	PRO	3.1
1	C	575	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	444	ARG	3.1
1	C	549	THR	3.1
2	F	428	ASP	3.1
2	E	359	GLY	3.1
2	E	395	SER	3.1
2	E	391	GLU	3.1
2	F	391	GLU	3.0
1	B	519	PHE	3.0
2	F	402	ALA	3.0
1	B	1	MET	3.0
1	C	489	THR	3.0
2	F	321	TYR	3.0
2	F	424	THR	3.0
2	D	380	LYS	2.9
2	D	312	THR	2.9
1	C	551	ALA	2.9
2	F	103	ILE	2.9
1	C	558	ARG	2.9
2	E	269	GLY	2.9
2	E	404	PHE	2.9
2	F	267	VAL	2.9
2	E	435	ALA	2.9
2	F	360	LYS	2.9
1	B	539	GLY	2.9
2	D	397	ILE	2.9
2	D	318	LEU	2.9
2	E	314	PRO	2.9
2	D	431	TRP	2.8
1	C	541	TYR	2.8
2	D	402	ALA	2.8
2	E	388	VAL	2.8
1	C	499	ASP	2.8
2	D	310	ASP	2.8
1	A	477	VAL	2.8
2	D	383	LYS	2.8
2	D	406	GLU	2.8
1	C	124	ILE	2.8
2	E	271	ARG	2.7
2	D	274	PRO	2.7
2	F	384	GLU	2.7
1	C	581	ILE	2.7
2	E	311	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	577	ILE	2.7
1	B	161	LYS	2.7
2	D	377	ALA	2.7
2	F	444	ARG	2.7
1	C	535	ALA	2.6
2	F	442	LEU	2.6
2	F	327	ILE	2.6
1	C	476	LEU	2.6
1	B	475	ARG	2.6
2	E	380	LYS	2.6
2	E	429	LEU	2.6
2	D	398	ASP	2.6
2	E	315	ILE	2.6
2	E	102	GLU	2.6
1	B	124	ILE	2.5
1	C	484	ASP	2.5
2	F	373	PHE	2.5
1	B	575	GLU	2.5
1	C	545	ILE	2.5
2	F	315	ILE	2.5
1	C	470	LEU	2.5
1	A	475	ARG	2.5
2	E	270[A]	ARG	2.5
1	B	535	ALA	2.5
2	D	429	LEU	2.5
1	A	528	PHE	2.5
2	F	408	PHE	2.5
1	A	480	ASP	2.5
2	F	131	GLY	2.5
1	A	476	LEU	2.5
2	F	342	ILE	2.5
2	F	410	ASN	2.5
2	E	449	LEU	2.4
1	A	474	VAL	2.4
1	A	551	ALA	2.4
2	E	423	ILE	2.4
2	F	345	LEU	2.4
1	A	296	SER	2.4
1	C	550	VAL	2.4
2	D	267	VAL	2.4
2	E	101	PRO	2.4
2	E	137	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	2.4
1	B	528	PHE	2.4
1	B	174	CYS	2.4
1	B	527	THR	2.4
2	E	400	ILE	2.4
2	E	430	GLY	2.4
2	F	128	ILE	2.3
1	B	531	GLU	2.3
1	C	127	GLY	2.3
2	E	394	LEU	2.3
1	C	136	ILE	2.3
1	B	524	VAL	2.3
1	C	539	GLY	2.3
2	D	102	GLU	2.3
2	D	426	THR	2.3
2	E	377	ALA	2.3
1	C	485	ASN	2.3
2	E	276	TYR	2.3
2	E	278	TYR	2.2
2	E	307	PRO	2.2
2	F	307	PRO	2.2
1	C	1	MET	2.2
2	F	445	ILE	2.2
1	C	428	ILE	2.2
2	E	174	SER	2.2
1	B	547	GLU	2.2
1	C	494	LYS	2.1
1	B	516	GLU	2.1
2	F	371	GLN	2.1
2	E	373	PHE	2.1
1	B	448	ILE	2.1
1	C	556	ILE	2.1
2	E	378	GLN	2.1
1	C	482	LEU	2.1
2	D	403	LYS	2.1
1	C	163	GLU	2.1
1	C	559	SER	2.1
1	A	552	VAL	2.1
2	D	365	HIS	2.1
2	D	375	ALA	2.1
1	A	259	CYS	2.1
1	C	479	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	570	ILE	2.1
1	C	565	GLU	2.1
1	C	552	VAL	2.1
1	C	500	TYR	2.1
2	D	313	HIS	2.1
2	D	359	GLY	2.1
2	F	441	GLU	2.1
1	A	390	VAL	2.1
1	C	491	GLU	2.1
2	E	442	LEU	2.0
2	E	268	PRO	2.0
1	B	393	SER	2.0
1	C	531	GLU	2.0
1	B	578	LYS	2.0
1	C	161	LYS	2.0
2	F	314	PRO	2.0
2	E	445	ILE	2.0
1	C	567	LEU	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 monosaccharides 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.