Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 11:34 PM EST

PDB ID : 1JLE
Title : CRYSTAL STRUCTURE OF Y188C MUTANT HIV-1 REVERSE TRAN-
SCRIPTASE
Authors : Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart,
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Deposited on : 2001-07-16
Resolution : 2.80 Å(reported)

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

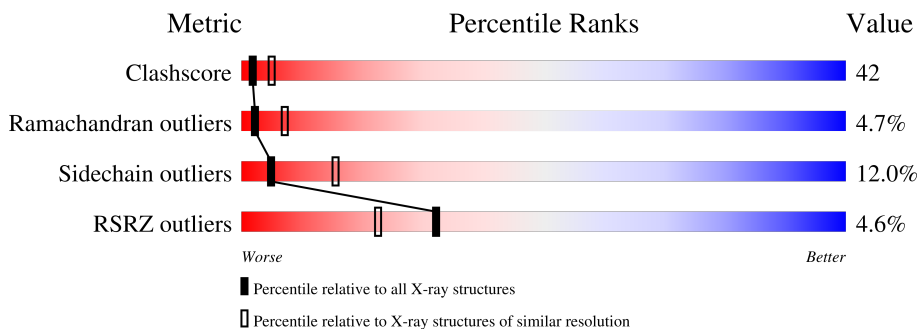|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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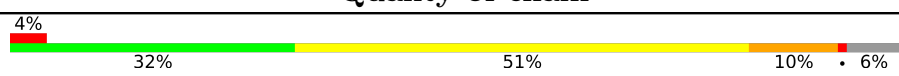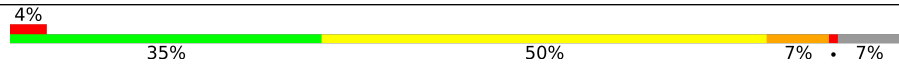*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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

Metric	Percentile Ranks	Value
Clashscore		42
Ramachandran outliers		4.7%
Sidechain outliers		12.0%
RSRZ outliers		4.6%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	560	4% 32% 51% 10% · 6%
2	B	440	4% 35% 50% 7% · 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7679 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 HIV-1 RT, A-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total 4289	C 2770	N 712	O 798	S 9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	CSD	TYR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

- Molecule 2 is a protein called HIV-1 RT, B-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	408	Total 3366	C 2186	N 561	O 611	S 8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	188	CYS	TYR	engineered mutation	UNP P04585

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total 13	O 13	0	0
3	B	11	Total 11	O 11	0	0

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: HIV-1 RT, A-CHAIN
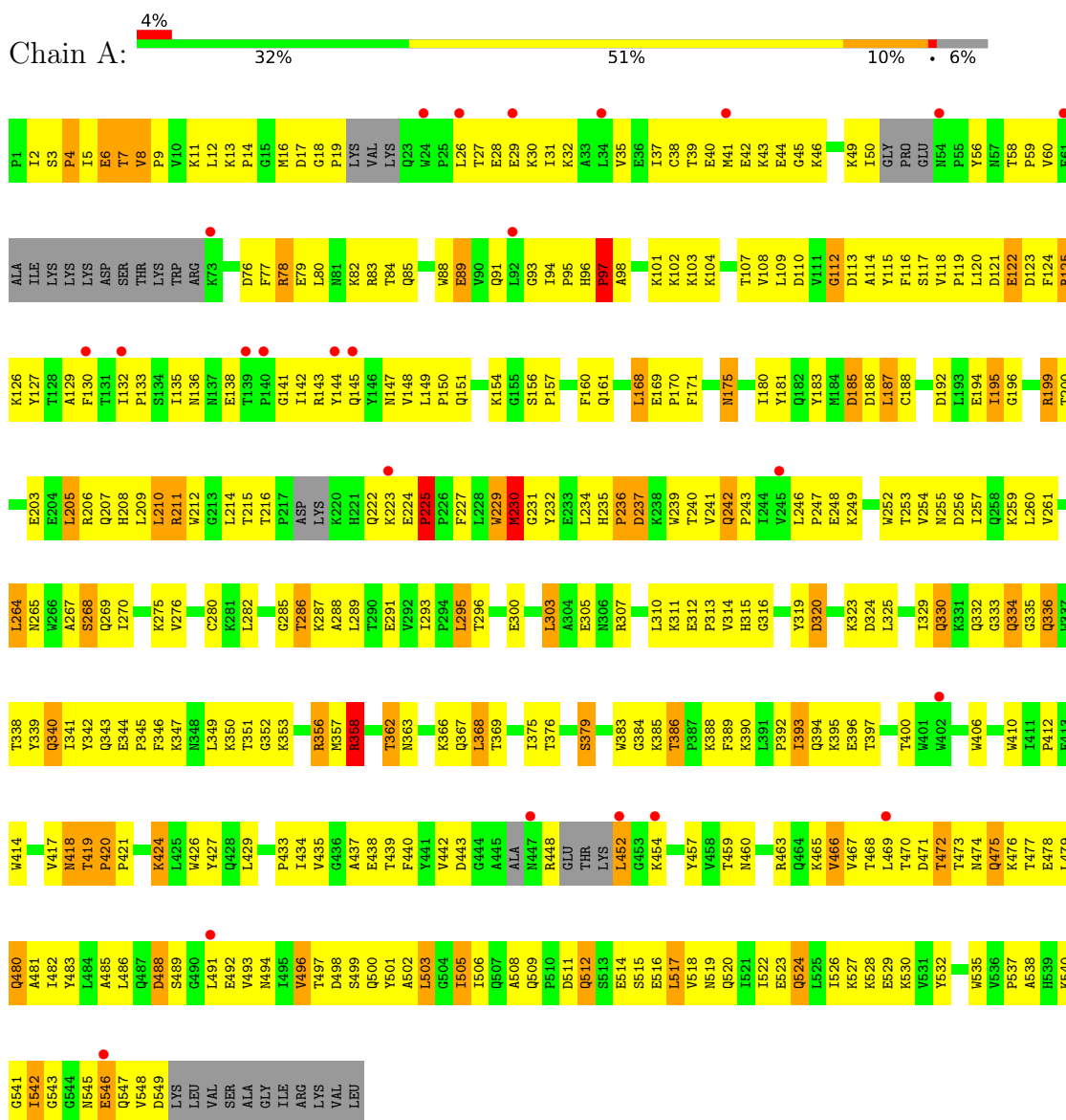
• Molecule 2: HIV-1 RT, B-CHAIN
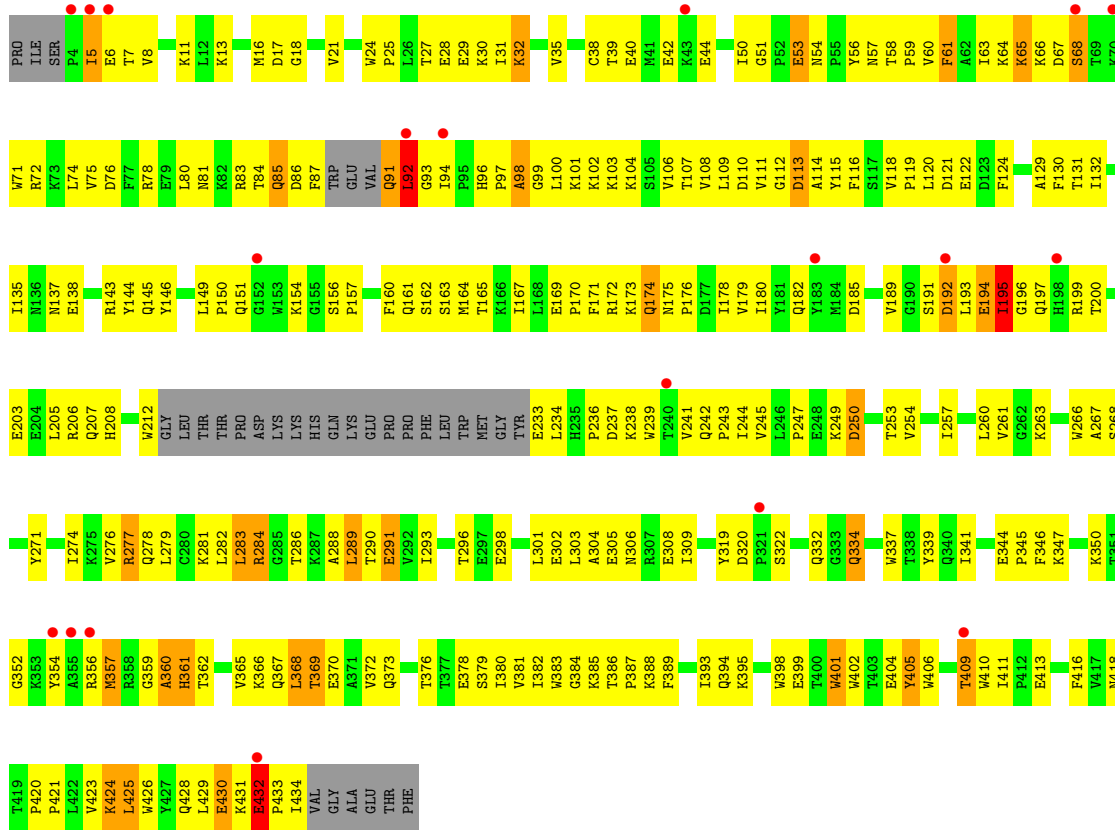
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.80Å 109.50Å 72.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.80 29.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.63-2.80) 93.4 (29.63-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.337 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	69.8	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 108.2	EDS
L-test for twinning[1]	$< |L| > = 0.41, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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

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	0.58	0/4380	0.79	0/5949
2	B	0.56	0/3458	0.78	2/4694 (0.0%)
All	All	0.57	0/7838	0.79	2/10643 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	432	GLU	N-CA-C	-9.21	86.14	111.00
2	B	401	TRP	N-CA-C	5.04	124.60	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4289	0	4304	384	0
2	B	3366	0	3410	281	0
3	A	13	0	0	1	0
3	B	11	0	0	1	0
All	All	7679	0	7714	651	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 42.

All (651) 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:A:235:HIS:HB3	1:A:236:PRO:HD2	1.28	1.09
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.29	1.09
1:A:465:LYS:HG3	1:A:466:VAL:H	1.23	1.02
2:B:241:VAL:HG12	2:B:350:LYS:HG3	1.40	1.01
1:A:320:ASP:H	1:A:343:GLN:HE22	0.99	0.97
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.31	0.95
1:A:478:GLU:O	1:A:481:ALA:HB3	1.69	0.93
2:B:431:LYS:O	2:B:433:PRO:HD3	1.70	0.92
1:A:119:PRO:HA	1:A:148:VAL:HG12	1.51	0.91
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.51	0.91
2:B:72:ARG:HH21	2:B:151:GLN:HE22	1.11	0.91
1:A:443:ASP:HB3	1:A:548:VAL:HB	1.50	0.90
1:A:491:LEU:HD22	1:A:529:GLU:HG3	1.54	0.90
2:B:263:LYS:HD3	2:B:429:LEU:HD21	1.53	0.89
1:A:362:THR:HG22	1:A:363:ASN:H	1.39	0.87
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.57	0.87
1:A:330:GLN:HG2	1:A:338:THR:OG1	1.74	0.86
1:A:196:GLY:HA2	1:A:199:ARG:HE	1.40	0.86
1:A:224:GLU:HG3	1:A:225:PRO:HD2	1.56	0.86
1:A:452:LEU:HD13	1:A:471:ASP:H	1.40	0.86
1:A:240:THR:HG22	1:A:315:HIS:ND1	1.91	0.86
1:A:358:ARG:O	1:A:358:ARG:HG3	1.73	0.85
1:A:248:GLU:HA	1:A:307:ARG:HH22	1.39	0.85
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.12	0.85
1:A:358:ARG:NH2	1:A:514:GLU:HA	1.90	0.84
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.60	0.84
1:A:210:LEU:HD11	1:A:215:THR:HG22	1.59	0.84
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.08	0.83
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.14	0.83
1:A:235:HIS:CB	1:A:236:PRO:HD2	2.09	0.82
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.61	0.82
1:A:472:THR:HG22	1:A:476:LYS:HB2	1.61	0.82
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.60	0.81
2:B:87:PHE:O	2:B:91:GLN:HG2	1.81	0.81
2:B:72:ARG:HH21	2:B:151:GLN:NE2	1.79	0.81
1:A:241:VAL:O	1:A:243:PRO:HD3	1.81	0.80
1:A:320:ASP:N	1:A:343:GLN:HE22	1.79	0.79
1:A:229:TRP:HB2	1:A:234:LEU:CD1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.15	0.79
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.65	0.79
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.18	0.78
1:A:142:ILE:N	1:A:142:ILE:HD12	1.98	0.78
2:B:87:PHE:C	2:B:91:GLN:HG2	2.03	0.78
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.66	0.78
2:B:51:GLY:HA3	2:B:53:GLU:OE2	1.85	0.77
1:A:358:ARG:CZ	1:A:514:GLU:HA	2.13	0.77
2:B:344:GLU:HB3	2:B:347:LYS:HE2	1.65	0.77
1:A:320:ASP:H	1:A:343:GLN:NE2	1.81	0.77
2:B:379:SER:CB	2:B:387:PRO:HD3	2.13	0.77
2:B:376:THR:CG2	2:B:386:THR:HG22	2.15	0.77
2:B:61:PHE:N	2:B:61:PHE:CD2	2.53	0.77
1:A:516:GLU:O	1:A:519:ASN:HB2	1.85	0.76
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.01	0.76
1:A:170:PRO:HG2	1:A:171:PHE:H	1.49	0.76
2:B:421:PRO:O	2:B:425:LEU:HD22	1.86	0.76
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.50	0.76
2:B:428:GLN:O	2:B:432:GLU:HG3	1.84	0.76
1:A:112:GLY:HA2	1:A:185:ASP:HB3	1.68	0.75
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.67	0.75
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.22	0.75
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.01	0.75
2:B:434:ILE:O	2:B:434:ILE:HG13	1.85	0.75
1:A:366:LYS:O	1:A:369:THR:HB	1.86	0.75
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.69	0.75
1:A:194:GLU:OE2	1:A:195:ILE:HG12	1.86	0.74
1:A:206:ARG:HH11	1:A:216:THR:HB	1.52	0.74
1:A:344:GLU:O	1:A:347:LYS:HB2	1.87	0.74
1:A:39:THR:O	1:A:43:LYS:HG3	1.87	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.88	0.73
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.69	0.73
1:A:465:LYS:HG3	1:A:466:VAL:N	2.01	0.73
1:A:229:TRP:HA	1:A:229:TRP:HE3	1.53	0.73
1:A:203:GLU:OE2	1:A:203:GLU:HA	1.89	0.73
1:A:253:THR:HB	1:A:256:ASP:OD2	1.87	0.73
1:A:257:ILE:O	1:A:261:VAL:HG23	1.88	0.72
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.71	0.72
1:A:91:GLN:HE21	1:A:93:GLY:HA3	1.53	0.72
2:B:78:ARG:HH11	2:B:411:ILE:HG21	1.55	0.72
1:A:224:GLU:CG	1:A:225:PRO:HD2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.71	0.72
2:B:92:LEU:HD13	2:B:161:GLN:HB3	1.72	0.71
1:A:229:TRP:O	1:A:230:MET:C	2.28	0.71
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.25	0.71
1:A:229:TRP:HB2	1:A:234:LEU:HD13	1.72	0.71
1:A:257:ILE:HD13	1:A:282:LEU:HD13	1.71	0.71
1:A:242:GLN:O	1:A:242:GLN:HG3	1.90	0.71
2:B:40:GLU:HG2	2:B:44:GLU:OE2	1.90	0.71
1:A:210:LEU:CD2	1:A:215:THR:HA	2.20	0.71
2:B:163:SER:O	2:B:167:ILE:HG13	1.91	0.71
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.73	0.70
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.20	0.70
2:B:431:LYS:O	2:B:433:PRO:CD	2.39	0.70
2:B:120:LEU:HD21	2:B:124:PHE:HB3	1.74	0.70
1:A:95:PRO:HG3	2:B:137:ASN:HB2	1.74	0.70
1:A:231:GLY:O	1:A:242:GLN:HG2	1.91	0.70
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.39	0.70
1:A:452:LEU:HD12	1:A:470:THR:HA	1.74	0.70
1:A:118:VAL:O	1:A:148:VAL:HB	1.93	0.69
2:B:72:ARG:NH2	2:B:151:GLN:HE22	1.88	0.69
1:A:452:LEU:HD13	1:A:471:ASP:N	2.06	0.69
1:A:229:TRP:O	1:A:232:TYR:N	2.24	0.69
1:A:91:GLN:HE21	1:A:93:GLY:CA	2.05	0.69
1:A:248:GLU:HB2	1:A:307:ARG:CZ	2.21	0.69
1:A:291:GLU:OE2	1:A:293:ILE:HD11	1.92	0.69
1:A:452:LEU:CD1	1:A:470:THR:HA	2.23	0.69
1:A:475:GLN:NE2	1:A:479:LEU:HD11	2.07	0.69
2:B:368:LEU:O	2:B:372:VAL:HG23	1.93	0.68
2:B:5:ILE:HG13	2:B:6:GLU:N	2.07	0.68
1:A:5:ILE:HD12	1:A:5:ILE:O	1.93	0.68
2:B:369:THR:O	2:B:373:GLN:HG3	1.93	0.68
1:A:474:ASN:O	1:A:477:THR:OG1	2.10	0.68
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.75	0.67
2:B:174:GLN:O	2:B:176:PRO:HD3	1.93	0.67
1:A:254:VAL:HG21	1:A:288:ALA:O	1.95	0.66
1:A:384:GLY:CA	2:B:135:ILE:HD12	2.25	0.66
1:A:435:VAL:HA	2:B:290:THR:HG21	1.77	0.66
2:B:169:GLU:HG2	2:B:170:PRO:CD	2.16	0.66
2:B:404:GLU:HB2	2:B:405:TYR:CE1	2.32	0.65
2:B:65:LYS:N	2:B:68:SER:HB2	2.11	0.65
2:B:278:GLN:HB2	2:B:302:GLU:OE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:THR:O	2:B:380:ILE:HG13	1.96	0.65
1:A:516:GLU:O	1:A:520:GLN:HG2	1.97	0.65
1:A:427:TYR:OH	1:A:509:GLN:HA	1.96	0.65
1:A:17:ASP:O	1:A:83:ARG:HD3	1.97	0.65
1:A:210:LEU:CD1	1:A:215:THR:HG22	2.25	0.65
2:B:278:GLN:HE21	2:B:298:GLU:CB	2.09	0.65
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.78	0.65
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.79	0.65
1:A:253:THR:HG23	1:A:289:LEU:O	1.96	0.65
1:A:516:GLU:HA	1:A:516:GLU:OE2	1.97	0.64
1:A:522:ILE:O	1:A:526:ILE:HG13	1.97	0.64
1:A:11:LYS:O	1:A:85:GLN:HB3	1.97	0.64
1:A:27:THR:HB	1:A:30:LYS:HG3	1.79	0.64
1:A:323:LYS:HD2	1:A:344:GLU:OE1	1.98	0.64
2:B:169:GLU:HA	2:B:172:ARG:HB2	1.79	0.64
1:A:470:THR:O	1:A:471:ASP:HB3	1.98	0.64
2:B:78:ARG:HH11	2:B:411:ILE:CG2	2.09	0.64
2:B:115:TYR:OH	2:B:157:PRO:HB3	1.98	0.64
2:B:135:ILE:O	2:B:138:GLU:HG3	1.98	0.64
1:A:210:LEU:HD21	1:A:215:THR:HA	1.79	0.63
1:A:252:TRP:CD1	1:A:295:LEU:HD21	2.33	0.63
2:B:288:ALA:O	2:B:291:GLU:HB3	1.98	0.63
2:B:101:LYS:O	2:B:236:PRO:HB2	1.97	0.63
1:A:12:LEU:HD22	1:A:83:ARG:O	1.99	0.63
1:A:78:ARG:HG3	1:A:79:GLU:N	2.13	0.63
1:A:492:GLU:HA	1:A:530:LYS:O	1.99	0.63
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.64	0.63
1:A:332:GLN:NE2	1:A:353:LYS:NZ	2.47	0.62
2:B:254:VAL:HB	2:B:289:LEU:HA	1.81	0.62
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.12	0.62
1:A:255:ASN:HB3	1:A:259:LYS:HE2	1.81	0.62
2:B:97:PRO:O	2:B:99:GLY:N	2.28	0.62
1:A:210:LEU:HD22	1:A:214:LEU:O	1.98	0.62
1:A:26:LEU:HD12	1:A:133:PRO:HD2	1.80	0.62
1:A:340:GLN:CB	1:A:351:THR:HG22	2.28	0.62
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.28	0.62
1:A:254:VAL:HB	1:A:289:LEU:O	1.99	0.62
2:B:24:TRP:HZ2	2:B:61:PHE:CE2	2.18	0.62
2:B:379:SER:HB3	2:B:387:PRO:HD3	1.82	0.62
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.80	0.62
1:A:498:ASP:OD2	1:A:538:ALA:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.82	0.62
2:B:31:ILE:O	2:B:35:VAL:HG23	1.99	0.62
1:A:517:LEU:O	1:A:520:GLN:HB2	2.00	0.61
1:A:91:GLN:NE2	1:A:93:GLY:HA3	2.14	0.61
2:B:250:ASP:OD2	2:B:250:ASP:N	2.27	0.61
2:B:178:ILE:HG12	2:B:191:SER:CB	2.30	0.61
2:B:29:GLU:HG3	2:B:30:LYS:N	2.15	0.61
2:B:169:GLU:CG	2:B:170:PRO:HD3	2.18	0.61
1:A:229:TRP:HB2	1:A:234:LEU:HD11	1.80	0.61
2:B:5:ILE:HG13	2:B:6:GLU:H	1.65	0.61
2:B:365:VAL:O	2:B:369:THR:OG1	2.17	0.61
2:B:50:ILE:HG13	2:B:143:ARG:HG3	1.82	0.60
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.35	0.60
1:A:91:GLN:HE21	1:A:93:GLY:N	1.99	0.60
1:A:19:PRO:O	1:A:56:TYR:HD1	1.84	0.60
2:B:426:TRP:O	2:B:429:LEU:HB2	2.01	0.60
1:A:506:ILE:O	1:A:509:GLN:N	2.33	0.60
1:A:323:LYS:O	1:A:343:GLN:OE1	2.19	0.60
1:A:101:LYS:O	1:A:103:LYS:HG2	2.01	0.60
1:A:224:GLU:HG3	1:A:225:PRO:CD	2.29	0.60
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.36	0.60
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.84	0.60
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.84	0.60
1:A:542:ILE:O	1:A:545:ASN:HB3	2.01	0.59
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.32	0.59
1:A:418:ASN:HD22	1:A:420:PRO:HD3	1.68	0.59
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.18	0.59
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.83	0.59
1:A:320:ASP:OD2	1:A:323:LYS:HE2	2.03	0.59
2:B:78:ARG:NH1	2:B:411:ILE:HG21	2.18	0.59
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.64	0.58
1:A:7:THR:HG21	1:A:121:ASP:HA	1.85	0.58
2:B:29:GLU:HG3	2:B:30:LYS:H	1.68	0.58
2:B:319:TYR:CD1	2:B:383:TRP:HD1	2.21	0.58
2:B:366:LYS:O	2:B:370:GLU:HG3	2.03	0.58
1:A:114:ALA:O	1:A:117:SER:HB2	2.04	0.58
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.37	0.58
1:A:358:ARG:NH2	1:A:514:GLU:CA	2.66	0.58
1:A:168:LEU:C	1:A:170:PRO:HD2	2.24	0.58
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.22	0.58
2:B:28:GLU:O	2:B:31:ILE:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ASP:OD2	2:B:113:ASP:N	2.33	0.58
1:A:210:LEU:HD22	1:A:215:THR:HA	1.86	0.58
2:B:31:ILE:HD12	2:B:135:ILE:HD11	1.86	0.58
2:B:54:ASN:HD22	2:B:143:ARG:HH21	1.51	0.57
2:B:131:THR:OG1	2:B:143:ARG:NH1	2.36	0.57
2:B:169:GLU:O	2:B:173:LYS:HB2	2.04	0.57
2:B:78:ARG:HD2	2:B:411:ILE:O	2.04	0.57
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.87	0.57
1:A:89:GLU:HG2	1:A:91:GLN:H	1.68	0.57
1:A:478:GLU:O	1:A:481:ALA:CB	2.48	0.57
2:B:17:ASP:OD1	2:B:18:GLY:N	2.37	0.57
2:B:101:LYS:HG3	2:B:102:LYS:HG3	1.85	0.57
2:B:203:GLU:OE1	2:B:203:GLU:HA	2.04	0.57
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.84	0.57
1:A:466:VAL:O	1:A:467:VAL:HG23	2.05	0.57
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.40	0.57
1:A:420:PRO:HA	1:A:421:PRO:C	2.25	0.57
2:B:271:TYR:HB2	2:B:274:ILE:HG12	1.85	0.57
1:A:27:THR:O	1:A:31:ILE:HG13	2.05	0.56
2:B:118:VAL:HB	2:B:149:LEU:HG	1.87	0.56
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.39	0.56
1:A:334:GLN:HG3	1:A:334:GLN:O	2.03	0.56
1:A:454:LYS:HA	1:A:467:VAL:O	2.05	0.56
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.88	0.56
1:A:472:THR:HG22	1:A:476:LYS:CB	2.34	0.56
2:B:380:ILE:O	2:B:384:GLY:N	2.38	0.56
1:A:200:THR:O	1:A:203:GLU:HB3	2.06	0.56
1:A:282:LEU:HD22	1:A:293:ILE:HG22	1.87	0.56
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.39	0.56
2:B:341:ILE:N	2:B:341:ILE:HD12	2.21	0.56
2:B:425:LEU:O	2:B:429:LEU:HD13	2.06	0.56
1:A:253:THR:O	1:A:257:ILE:HG13	2.06	0.56
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.70	0.56
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.88	0.56
1:A:420:PRO:HB3	1:A:421:PRO:HA	1.88	0.56
1:A:253:THR:CG2	1:A:254:VAL:N	2.68	0.56
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.87	0.56
2:B:169:GLU:O	2:B:173:LYS:N	2.38	0.56
2:B:242:GLN:HA	2:B:242:GLN:NE2	2.21	0.56
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.05	0.56
1:A:142:ILE:N	1:A:142:ILE:CD1	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:HA2	1:A:199:ARG:NE	2.14	0.56
1:A:475:GLN:HE21	1:A:479:LEU:HD11	1.70	0.56
2:B:242:GLN:HA	2:B:242:GLN:HE21	1.71	0.55
1:A:27:THR:HG22	1:A:29:GLU:H	1.70	0.55
1:A:475:GLN:HE21	1:A:501:TYR:HE2	1.54	0.55
2:B:11:LYS:HB2	2:B:85:GLN:HE22	1.71	0.55
2:B:398:TRP:O	2:B:402:TRP:HD1	1.88	0.55
1:A:180:ILE:O	1:A:181:TYR:HD2	1.90	0.55
1:A:229:TRP:HB3	1:A:232:TYR:HB2	1.87	0.55
2:B:241:VAL:CG1	2:B:350:LYS:HG3	2.27	0.55
2:B:320:ASP:OD1	2:B:322:SER:HB2	2.07	0.55
1:A:114:ALA:HB1	1:A:214:LEU:HD12	1.88	0.55
1:A:520:GLN:O	1:A:523:GLU:HB2	2.07	0.55
1:A:496:VAL:HG11	2:B:289:LEU:HD11	1.88	0.55
1:A:475:GLN:HG3	1:A:501:TYR:CE2	2.42	0.55
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.36	0.55
2:B:395:LYS:O	2:B:399:GLU:HG3	2.07	0.55
2:B:108:VAL:O	2:B:109:LEU:HD12	2.07	0.55
2:B:61:PHE:CE1	2:B:74:LEU:HG	2.42	0.54
1:A:499:SER:HB3	1:A:502:ALA:HB3	1.89	0.54
2:B:120:LEU:HD23	2:B:121:ASP:N	2.22	0.54
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.90	0.54
1:A:307:ARG:O	1:A:311:LYS:HG3	2.08	0.54
1:A:3:SER:HB3	1:A:5:ILE:HG23	1.90	0.54
2:B:106:VAL:HB	2:B:234:LEU:HB2	1.90	0.54
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.90	0.54
1:A:119:PRO:CA	1:A:148:VAL:HG12	2.31	0.54
1:A:454:LYS:HE2	1:A:468:THR:HG22	1.90	0.54
1:A:170:PRO:CG	1:A:171:PHE:H	2.21	0.54
2:B:193:LEU:HB3	2:B:197:GLN:HB2	1.90	0.54
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.43	0.54
1:A:329:ILE:HG22	1:A:330:GLN:H	1.72	0.53
1:A:295:LEU:HD23	1:A:295:LEU:N	2.22	0.53
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.96	0.53
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.44	0.53
1:A:543:GLY:HA3	2:B:283:LEU:O	2.08	0.53
2:B:118:VAL:HG21	2:B:160:PHE:HD2	1.74	0.53
1:A:418:ASN:HD22	1:A:418:ASN:C	2.11	0.53
2:B:84:THR:HB	2:B:154:LYS:HE2	1.91	0.53
1:A:475:GLN:NE2	1:A:501:TYR:HE2	2.05	0.53
1:A:538:ALA:C	1:A:540:LYS:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:ARG:N	2:B:302:GLU:OE1	2.42	0.53
1:A:291:GLU:HG2	1:A:293:ILE:CD1	2.39	0.53
1:A:332:GLN:NE2	1:A:353:LYS:HZ3	2.06	0.53
1:A:43:LYS:O	1:A:45:GLY:N	2.42	0.53
1:A:246:LEU:O	1:A:307:ARG:NH1	2.36	0.53
2:B:194:GLU:OE1	2:B:195:ILE:HG23	2.08	0.53
2:B:393:ILE:HG12	2:B:394:GLN:N	2.24	0.53
1:A:252:TRP:CG	1:A:295:LEU:HD21	2.44	0.52
2:B:60:VAL:C	2:B:61:PHE:HD2	2.12	0.52
2:B:405:TYR:CD1	2:B:405:TYR:N	2.76	0.52
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.50	0.52
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.91	0.52
2:B:376:THR:HG23	2:B:387:PRO:HD2	1.90	0.52
1:A:207:GLN:O	1:A:211:ARG:N	2.41	0.52
1:A:424:LYS:HE3	1:A:426:TRP:CD1	2.45	0.52
1:A:465:LYS:CG	1:A:466:VAL:H	2.06	0.52
2:B:237:ASP:OD2	2:B:238:LYS:N	2.42	0.52
2:B:39:THR:O	2:B:42:GLU:HB3	2.09	0.52
2:B:245:VAL:O	2:B:245:VAL:HG23	2.10	0.52
1:A:171:PHE:O	1:A:175:ASN:ND2	2.43	0.52
1:A:196:GLY:CA	1:A:199:ARG:HH21	2.23	0.52
2:B:78:ARG:NH1	2:B:411:ILE:CG2	2.73	0.52
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.45	0.52
1:A:443:ASP:HB2	1:A:548:VAL:HG21	1.92	0.52
2:B:247:PRO:HD2	2:B:260:LEU:HD13	1.90	0.52
2:B:268:SER:HA	2:B:271:TYR:O	2.11	0.52
1:A:195:ILE:HD13	1:A:195:ILE:N	2.24	0.51
2:B:203:GLU:OE1	2:B:206:ARG:HD3	2.10	0.51
1:A:160:PHE:CD1	1:A:160:PHE:C	2.82	0.51
1:A:5:ILE:HD12	1:A:5:ILE:C	2.30	0.51
1:A:329:ILE:HG22	1:A:330:GLN:N	2.25	0.51
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.45	0.51
2:B:61:PHE:CZ	2:B:76:ASP:HB2	2.46	0.51
1:A:78:ARG:O	1:A:82:LYS:HG3	2.11	0.51
2:B:56:TYR:O	2:B:143:ARG:NH2	2.44	0.51
2:B:63:ILE:CD1	2:B:74:LEU:HD22	2.38	0.51
1:A:260:LEU:HG	1:A:264:LEU:CD2	2.41	0.51
2:B:60:VAL:HG21	2:B:130:PHE:HD1	1.75	0.51
2:B:434:ILE:O	2:B:434:ILE:CG1	2.57	0.51
1:A:49:LYS:O	1:A:50:ILE:HG23	2.10	0.51
2:B:161:GLN:HE21	2:B:161:GLN:CA	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:C	1:A:249:LYS:HG2	2.31	0.51
1:A:452:LEU:N	1:A:452:LEU:HD22	2.26	0.51
2:B:60:VAL:C	2:B:61:PHE:CD2	2.85	0.51
2:B:72:ARG:HH22	2:B:409:THR:CG2	2.23	0.51
2:B:99:GLY:O	2:B:102:LYS:N	2.42	0.51
2:B:195:ILE:CD1	2:B:199:ARG:CZ	2.89	0.51
1:A:84:THR:HG22	1:A:85:GLN:N	2.25	0.50
1:A:248:GLU:HB2	1:A:307:ARG:NH1	2.26	0.50
1:A:37:ILE:O	1:A:40:GLU:HB3	2.11	0.50
2:B:80:LEU:O	2:B:83:ARG:N	2.38	0.50
1:A:110:ASP:HB2	1:A:223:LYS:HE3	1.92	0.50
1:A:8:VAL:O	1:A:121:ASP:HB2	2.11	0.50
2:B:242:GLN:HB2	2:B:430:GLU:OE1	2.12	0.50
1:A:124:PHE:O	1:A:127:TYR:CD2	2.65	0.50
1:A:241:VAL:O	1:A:243:PRO:CD	2.57	0.50
1:A:253:THR:HB	1:A:256:ASP:CG	2.32	0.50
1:A:253:THR:HG22	1:A:255:ASN:N	2.26	0.50
2:B:191:SER:HB2	2:B:193:LEU:HD23	1.93	0.50
2:B:281:LYS:HA	2:B:284:ARG:NH2	2.26	0.50
1:A:346:PHE:N	1:A:346:PHE:CD2	2.77	0.50
2:B:24:TRP:CB	2:B:25:PRO:HD2	2.38	0.50
1:A:28:GLU:CD	1:A:32:LYS:HE3	2.33	0.50
1:A:135:ILE:HD12	1:A:135:ILE:N	2.26	0.50
1:A:120:LEU:N	1:A:148:VAL:HA	2.27	0.49
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.11	0.49
1:A:362:THR:CG2	1:A:363:ASN:H	2.12	0.49
1:A:511:ASP:O	1:A:512:GLN:HB3	2.11	0.49
2:B:98:ALA:O	2:B:101:LYS:HE2	2.12	0.49
2:B:106:VAL:O	2:B:233:GLU:HB3	2.12	0.49
1:A:26:LEU:HG	1:A:133:PRO:HG2	1.93	0.49
1:A:333:GLY:N	1:A:336:GLN:HE21	2.10	0.49
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.42	0.49
2:B:284:ARG:HB2	2:B:284:ARG:CZ	2.41	0.49
2:B:94:ILE:CD1	2:B:182:GLN:H	2.25	0.49
2:B:104:LYS:CB	2:B:192:ASP:HA	2.36	0.49
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.95	0.49
1:A:114:ALA:HB3	1:A:160:PHE:HE2	1.78	0.49
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.47	0.49
1:A:339:TYR:CE2	1:A:352:GLY:HA3	2.47	0.49
1:A:473:THR:CG2	1:A:474:ASN:N	2.75	0.49
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:O	1:A:32:LYS:HG3	2.13	0.49
1:A:287:LYS:HG2	1:A:291:GLU:OE1	2.13	0.49
1:A:8:VAL:HG12	1:A:9:PRO:HD2	1.95	0.48
2:B:319:TYR:CD1	2:B:383:TRP:CD1	3.00	0.48
1:A:418:ASN:ND2	1:A:420:PRO:HD3	2.28	0.48
1:A:491:LEU:O	1:A:528:LYS:HB3	2.12	0.48
2:B:257:ILE:HG21	2:B:283:LEU:HD13	1.95	0.48
1:A:43:LYS:C	1:A:45:GLY:N	2.66	0.48
1:A:50:ILE:HD12	1:A:50:ILE:C	2.34	0.48
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.95	0.48
2:B:354:TYR:OH	2:B:370:GLU:CB	2.61	0.48
1:A:255:ASN:OD1	1:A:289:LEU:HB3	2.13	0.48
1:A:356:ARG:NH2	1:A:367:GLN:O	2.46	0.48
1:A:443:ASP:HB3	1:A:548:VAL:CB	2.35	0.48
1:A:443:ASP:CB	1:A:548:VAL:HB	2.34	0.48
1:A:454:LYS:HG2	1:A:468:THR:HA	1.95	0.48
1:A:470:THR:O	1:A:471:ASP:CB	2.62	0.48
2:B:281:LYS:C	2:B:283:LEU:H	2.17	0.48
1:A:43:LYS:C	1:A:45:GLY:H	2.16	0.48
1:A:357:MET:O	1:A:358:ARG:CB	2.62	0.48
2:B:60:VAL:CG2	2:B:130:PHE:HB2	2.43	0.48
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.48	0.48
2:B:171:PHE:CE2	2:B:205:LEU:HD12	2.48	0.48
1:A:253:THR:HG22	1:A:254:VAL:N	2.29	0.48
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.96	0.48
1:A:255:ASN:O	1:A:259:LYS:HG3	2.14	0.48
1:A:358:ARG:O	1:A:358:ARG:CG	2.54	0.48
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.14	0.48
1:A:319:TYR:CD1	1:A:383:TRP:HD1	2.31	0.47
1:A:519:ASN:O	1:A:523:GLU:HG2	2.13	0.47
2:B:58:THR:HG23	2:B:76:ASP:O	2.14	0.47
1:A:129:ALA:HA	1:A:144:TYR:O	2.14	0.47
2:B:17:ASP:OD1	2:B:56:TYR:HE1	1.97	0.47
2:B:57:ASN:HA	2:B:129:ALA:O	2.14	0.47
2:B:376:THR:HG22	2:B:386:THR:HG22	1.95	0.47
1:A:115:TYR:HA	1:A:160:PHE:HD2	1.78	0.47
1:A:122:GLU:H	1:A:122:GLU:CD	2.18	0.47
1:A:214:LEU:N	1:A:214:LEU:HD22	2.30	0.47
1:A:356:ARG:NE	1:A:367:GLN:HE21	2.12	0.47
2:B:194:GLU:CD	2:B:195:ILE:HG23	2.34	0.47
1:A:488:ASP:OD2	1:A:488:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.50	0.47
1:A:482:ILE:O	1:A:486:LEU:HD12	2.15	0.47
2:B:50:ILE:HD12	2:B:54:ASN:HB3	1.97	0.47
1:A:56:TYR:O	1:A:143:ARG:NH2	2.41	0.47
1:A:104:LYS:HD2	1:A:192:ASP:O	2.14	0.47
1:A:305:GLU:HG2	1:A:305:GLU:O	2.15	0.47
1:A:332:GLN:NE2	1:A:353:LYS:HZ1	2.12	0.47
1:A:466:VAL:HG22	1:A:467:VAL:N	2.30	0.47
2:B:179:VAL:C	2:B:180:ILE:HD12	2.34	0.47
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.02	0.47
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.50	0.47
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.96	0.47
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.96	0.47
2:B:11:LYS:H	2:B:85:GLN:CD	2.19	0.47
2:B:72:ARG:NH2	2:B:409:THR:CG2	2.78	0.47
2:B:334:GLN:OE1	2:B:334:GLN:HA	2.14	0.47
2:B:320:ASP:OD1	2:B:322:SER:N	2.46	0.47
2:B:332:GLN:OE1	2:B:428:GLN:HB2	2.15	0.47
1:A:121:ASP:OD1	1:A:123:ASP:HB2	2.15	0.46
1:A:180:ILE:C	1:A:181:TYR:HD2	2.18	0.46
2:B:11:LYS:H	2:B:85:GLN:NE2	2.13	0.46
1:A:356:ARG:HE	1:A:367:GLN:HE21	1.63	0.46
2:B:51:GLY:CA	2:B:53:GLU:OE2	2.60	0.46
1:A:460:ASN:HA	2:B:286:THR:O	2.15	0.46
2:B:96:HIS:CE1	2:B:100:LEU:HD21	2.50	0.46
2:B:196:GLY:O	2:B:200:THR:HG23	2.14	0.46
2:B:244:ILE:HA	2:B:430:GLU:HA	1.97	0.46
1:A:118:VAL:O	1:A:148:VAL:CB	2.63	0.46
1:A:124:PHE:O	1:A:126:LYS:N	2.48	0.46
1:A:340:GLN:HA	1:A:351:THR:HG22	1.96	0.46
2:B:170:PRO:O	2:B:174:GLN:HB2	2.16	0.46
2:B:278:GLN:HG3	2:B:298:GLU:CB	2.45	0.46
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.98	0.46
1:A:537:PRO:HG2	1:A:542:ILE:HD11	1.98	0.46
2:B:424:LYS:HE3	2:B:425:LEU:HD13	1.96	0.46
1:A:253:THR:CG2	1:A:289:LEU:O	2.64	0.46
1:A:524:GLN:O	1:A:527:LYS:HB2	2.15	0.46
1:A:13:LYS:NZ	1:A:154:LYS:NZ	2.63	0.46
1:A:114:ALA:HB3	1:A:160:PHE:CE2	2.51	0.46
1:A:121:ASP:O	1:A:122:GLU:C	2.54	0.46
1:A:358:ARG:HH21	1:A:514:GLU:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.97	0.46
1:A:515:SER:CB	1:A:518:VAL:HG23	2.45	0.46
2:B:431:LYS:C	2:B:433:PRO:N	2.66	0.46
1:A:237:ASP:OD1	1:A:237:ASP:N	2.49	0.46
1:A:248:GLU:HB2	1:A:307:ARG:NH2	2.30	0.46
1:A:168:LEU:O	1:A:170:PRO:CD	2.64	0.45
1:A:235:HIS:CB	1:A:236:PRO:CD	2.83	0.45
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.98	0.45
2:B:106:VAL:HG12	2:B:107:THR:N	2.30	0.45
2:B:160:PHE:O	2:B:160:PHE:CD1	2.69	0.45
1:A:497:THR:O	1:A:535:TRP:HA	2.16	0.45
2:B:205:LEU:HD23	2:B:205:LEU:O	2.16	0.45
2:B:234:LEU:N	2:B:234:LEU:HD12	2.30	0.45
1:A:46:LYS:O	1:A:147:ASN:ND2	2.49	0.45
1:A:343:GLN:HG3	1:A:349:LEU:HD21	1.98	0.45
1:A:486:LEU:O	1:A:528:LYS:NZ	2.44	0.45
1:A:511:ASP:HA	1:A:522:ILE:HG21	1.98	0.45
2:B:30:LYS:NZ	2:B:404:GLU:OE2	2.42	0.45
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.99	0.45
2:B:276:VAL:HG22	2:B:276:VAL:O	2.16	0.45
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.51	0.45
1:A:368:LEU:HD11	1:A:393:ILE:HD11	1.99	0.45
1:A:376:THR:HG21	2:B:401:TRP:CZ2	2.52	0.45
1:A:246:LEU:O	1:A:248:GLU:N	2.50	0.45
1:A:267:ALA:O	1:A:269:GLN:N	2.50	0.45
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.17	0.45
1:A:275:LYS:HD3	3:A:1010:HOH:O	2.17	0.45
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.52	0.45
1:A:335:GLY:O	1:A:356:ARG:HB2	2.16	0.45
1:A:141:GLY:C	1:A:142:ILE:HD12	2.38	0.44
1:A:345:PRO:O	1:A:346:PHE:HB2	2.17	0.44
2:B:194:GLU:HG3	2:B:197:GLN:HG3	1.99	0.44
1:A:265:ASN:O	1:A:268:SER:OG	2.29	0.44
1:A:282:LEU:HD22	1:A:293:ILE:CG2	2.47	0.44
2:B:80:LEU:O	2:B:81:ASN:C	2.56	0.44
1:A:479:LEU:HB2	1:A:517:LEU:HD13	1.99	0.44
1:A:332:GLN:C	1:A:336:GLN:HE21	2.21	0.44
1:A:390:LYS:HA	1:A:390:LYS:HD3	1.80	0.44
1:A:410:TRP:CD1	2:B:362:THR:O	2.70	0.44
1:A:541:GLY:O	1:A:542:ILE:C	2.55	0.44
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:LYS:C	2:B:283:LEU:N	2.70	0.44
1:A:28:GLU:OE1	1:A:32:LYS:HE3	2.17	0.44
1:A:39:THR:O	1:A:42:GLU:HB3	2.18	0.44
1:A:108:VAL:HG22	1:A:188:CSD:HA	2.00	0.44
1:A:115:TYR:CE1	1:A:151:GLN:HB2	2.53	0.44
1:A:124:PHE:O	1:A:125:ARG:C	2.56	0.44
1:A:323:LYS:HB2	1:A:323:LYS:HE3	1.73	0.44
1:A:518:VAL:O	1:A:522:ILE:HG13	2.17	0.44
2:B:253:THR:O	2:B:257:ILE:HG12	2.17	0.44
1:A:303:LEU:O	1:A:303:LEU:HD22	2.17	0.44
1:A:330:GLN:OE1	1:A:340:GLN:OE1	2.35	0.44
1:A:181:TYR:CE2	2:B:138:GLU:HB3	2.52	0.44
1:A:505:ILE:HG22	1:A:506:ILE:N	2.33	0.44
2:B:242:GLN:OE1	2:B:431:LYS:HD2	2.17	0.44
2:B:303:LEU:O	2:B:304:ALA:C	2.55	0.44
1:A:96:HIS:O	1:A:97:PRO:C	2.56	0.44
2:B:337:TRP:CZ3	2:B:368:LEU:HG	2.53	0.44
2:B:362:THR:O	2:B:362:THR:HG22	2.17	0.44
1:A:473:THR:HG22	1:A:474:ASN:N	2.32	0.44
2:B:120:LEU:CD2	2:B:124:PHE:HB3	2.46	0.44
1:A:291:GLU:HG2	1:A:293:ILE:HD11	1.99	0.43
2:B:239:TRP:HH2	2:B:381:VAL:HG21	1.83	0.43
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.53	0.43
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.83	0.43
1:A:149:LEU:HD13	1:A:156:SER:HA	2.00	0.43
1:A:180:ILE:CG2	1:A:187:LEU:HD12	2.48	0.43
1:A:241:VAL:CG2	1:A:314:VAL:HG23	2.48	0.43
1:A:345:PRO:O	1:A:346:PHE:CB	2.65	0.43
2:B:72:ARG:HH22	2:B:409:THR:HG22	1.83	0.43
2:B:393:ILE:O	2:B:416:PHE:HB3	2.18	0.43
2:B:430:GLU:HB3	2:B:431:LYS:H	1.38	0.43
1:A:60:VAL:O	1:A:60:VAL:HG13	2.18	0.43
1:A:115:TYR:HE1	1:A:151:GLN:HB2	1.83	0.43
1:A:194:GLU:O	1:A:195:ILE:C	2.57	0.43
1:A:205:LEU:CD2	1:A:209:LEU:HG	2.49	0.43
2:B:301:LEU:O	2:B:304:ALA:HB3	2.18	0.43
1:A:114:ALA:CB	1:A:160:PHE:HE2	2.31	0.43
1:A:122:GLU:CD	1:A:122:GLU:N	2.71	0.43
1:A:477:THR:O	1:A:478:GLU:C	2.57	0.43
1:A:543:GLY:HA2	2:B:284:ARG:HG3	2.00	0.43
1:A:545:ASN:O	1:A:549:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASP:O	2:B:83:ARG:HD3	2.18	0.43
2:B:345:PRO:O	2:B:346:PHE:HB2	2.19	0.43
2:B:388:LYS:HD2	2:B:413:GLU:HB3	2.00	0.43
1:A:439:THR:O	1:A:459:THR:HA	2.18	0.43
2:B:54:ASN:ND2	2:B:129:ALA:CB	2.81	0.43
1:A:385:LYS:HG2	1:A:386:THR:N	2.33	0.43
1:A:501:TYR:OH	1:A:505:ILE:HD11	2.19	0.43
1:A:516:GLU:CA	1:A:519:ASN:HD22	2.26	0.43
2:B:54:ASN:HD21	2:B:129:ALA:CB	2.31	0.43
1:A:168:LEU:O	1:A:170:PRO:HD2	2.19	0.43
1:A:209:LEU:HB3	1:A:214:LEU:HB2	2.01	0.43
2:B:29:GLU:O	2:B:32:LYS:HB2	2.18	0.43
2:B:91:GLN:HB2	2:B:92:LEU:H	1.63	0.43
2:B:92:LEU:O	2:B:161:GLN:HG2	2.19	0.43
2:B:278:GLN:OE1	2:B:278:GLN:HA	2.19	0.43
2:B:406:TRP:CZ2	2:B:410:TRP:O	2.71	0.43
2:B:87:PHE:CE1	2:B:154:LYS:HE3	2.54	0.43
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.54	0.43
1:A:248:GLU:CA	1:A:307:ARG:HH22	2.19	0.43
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.53	0.43
2:B:112:GLY:HA2	2:B:115:TYR:CE2	2.54	0.43
2:B:195:ILE:O	2:B:199:ARG:HG3	2.19	0.43
1:A:5:ILE:CG1	1:A:119:PRO:HD2	2.49	0.42
1:A:465:LYS:CG	1:A:466:VAL:N	2.71	0.42
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.54	0.42
2:B:61:PHE:HZ	2:B:76:ASP:HB2	1.84	0.42
1:A:180:ILE:HG22	1:A:181:TYR:N	2.34	0.42
1:A:375:ILE:O	1:A:379:SER:OG	2.37	0.42
1:A:483:TYR:CE1	1:A:524:GLN:HG3	2.54	0.42
2:B:173:LYS:HD2	2:B:173:LYS:HA	1.73	0.42
1:A:5:ILE:HD11	1:A:119:PRO:CG	2.49	0.42
1:A:506:ILE:C	1:A:508:ALA:N	2.73	0.42
1:A:156:SER:CB	1:A:157:PRO:HD3	2.37	0.42
1:A:452:LEU:HD13	1:A:470:THR:HA	1.98	0.42
1:A:291:GLU:HG2	1:A:293:ILE:HD13	2.00	0.42
2:B:7:THR:CG2	2:B:119:PRO:HG2	2.49	0.42
1:A:41:MET:O	1:A:46:LYS:HB2	2.19	0.42
1:A:58:THR:CG2	1:A:76:ASP:O	2.68	0.42
2:B:54:ASN:ND2	2:B:129:ALA:HB2	2.35	0.42
2:B:85:GLN:O	2:B:85:GLN:HG2	2.19	0.42
1:A:83:ARG:NH1	1:A:83:ARG:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:NE2	1:A:93:GLY:N	2.67	0.42
1:A:332:GLN:C	1:A:336:GLN:NE2	2.73	0.42
1:A:505:ILE:O	1:A:508:ALA:HB3	2.20	0.42
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.60	0.42
2:B:359:GLY:O	2:B:361:HIS:N	2.53	0.42
1:A:4:PRO:HD2	1:A:212:TRP:O	2.19	0.42
1:A:207:GLN:O	1:A:208:HIS:C	2.57	0.42
1:A:209:LEU:O	1:A:214:LEU:HB2	2.20	0.42
1:A:330:GLN:HE21	1:A:330:GLN:HB3	1.67	0.42
2:B:91:GLN:C	2:B:93:GLY:H	2.22	0.42
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.50	0.42
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.55	0.42
2:B:180:ILE:HG13	2:B:189:VAL:HG22	2.01	0.42
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.19	0.42
1:A:524:GLN:HA	1:A:524:GLN:HE21	1.85	0.41
1:A:546:GLU:HG2	1:A:547:GLN:NE2	2.35	0.41
2:B:282:LEU:HD21	2:B:296:THR:HG23	2.01	0.41
1:A:84:THR:CG2	1:A:85:GLN:N	2.83	0.41
1:A:506:ILE:C	1:A:508:ALA:H	2.24	0.41
1:A:234:LEU:HD12	1:A:234:LEU:N	2.36	0.41
2:B:30:LYS:NZ	3:B:1013:HOH:O	2.52	0.41
2:B:162:SER:O	2:B:165:THR:OG1	2.37	0.41
2:B:261:VAL:HG22	2:B:276:VAL:CG2	2.51	0.41
2:B:424:LYS:HD2	2:B:424:LYS:O	2.20	0.41
1:A:248:GLU:CA	1:A:307:ARG:NH2	2.81	0.41
2:B:94:ILE:HD13	2:B:182:GLN:O	2.21	0.41
2:B:305:GLU:O	2:B:309:ILE:HG13	2.20	0.41
1:A:480:GLN:O	1:A:483:TYR:HB3	2.20	0.41
2:B:376:THR:HG21	2:B:386:THR:HG22	2.00	0.41
2:B:424:LYS:HD2	2:B:424:LYS:C	2.41	0.41
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.87	0.41
1:A:180:ILE:CG2	1:A:187:LEU:CD1	2.99	0.41
1:A:248:GLU:CB	1:A:307:ARG:NH2	2.84	0.41
2:B:146:TYR:CE2	2:B:150:PRO:HB3	2.55	0.41
2:B:156:SER:HB2	2:B:157:PRO:CD	2.50	0.41
2:B:254:VAL:HG21	2:B:288:ALA:O	2.20	0.41
2:B:382:ILE:HG22	2:B:383:TRP:CE2	2.56	0.41
1:A:483:TYR:HE1	1:A:524:GLN:HG3	1.84	0.41
2:B:267:ALA:CB	2:B:426:TRP:CH2	2.96	0.41
1:A:375:ILE:HG21	1:A:389:PHE:CE2	2.56	0.41
1:A:438:GLU:OE1	1:A:459:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ILE:CG1	2:B:6:GLU:H	2.30	0.41
2:B:27:THR:O	2:B:31:ILE:HG13	2.21	0.41
1:A:7:THR:CG2	1:A:121:ASP:HA	2.48	0.41
1:A:97:PRO:HD3	1:A:229:TRP:CD1	2.56	0.41
1:A:107:THR:HG22	1:A:108:VAL:N	2.36	0.41
1:A:156:SER:HB2	1:A:157:PRO:CD	2.43	0.41
1:A:171:PHE:HD1	1:A:208:HIS:HD2	1.68	0.41
1:A:239:TRP:O	1:A:239:TRP:CE3	2.74	0.41
1:A:324:ASP:OD1	1:A:388:LYS:HE2	2.21	0.41
1:A:366:LYS:HA	1:A:366:LYS:HD2	1.95	0.41
1:A:429:LEU:N	1:A:509:GLN:OE1	2.51	0.41
1:A:493:VAL:HG12	1:A:494:ASN:N	2.36	0.41
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.02	0.41
2:B:86:ASP:OD2	2:B:154:LYS:NZ	2.51	0.41
2:B:174:GLN:CD	2:B:174:GLN:C	2.80	0.41
2:B:401:TRP:O	2:B:404:GLU:HB2	2.20	0.41
1:A:285:GLY:O	1:A:286:THR:C	2.60	0.41
1:A:418:ASN:C	1:A:418:ASN:ND2	2.75	0.41
1:A:499:SER:HB3	1:A:502:ALA:CB	2.51	0.41
2:B:75:VAL:HG12	2:B:76:ASP:N	2.35	0.41
2:B:357:MET:HB2	2:B:370:GLU:OE2	2.21	0.41
1:A:5:ILE:HD11	1:A:119:PRO:HD2	2.02	0.40
1:A:18:GLY:HA3	1:A:127:TYR:HD1	1.85	0.40
2:B:63:ILE:HD13	2:B:74:LEU:CD2	2.41	0.40
2:B:359:GLY:C	2:B:361:HIS:H	2.25	0.40
1:A:434:ILE:HB	1:A:437:ALA:HB3	2.03	0.40
2:B:303:LEU:O	2:B:306:ASN:N	2.54	0.40
1:A:80:LEU:O	1:A:80:LEU:HD12	2.21	0.40
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.57	0.40
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.21	0.40
2:B:24:TRP:CZ2	2:B:61:PHE:CE2	3.04	0.40
2:B:360:ALA:CB	2:B:366:LYS:HD3	2.51	0.40
2:B:380:ILE:O	2:B:381:VAL:C	2.58	0.40
2:B:65:LYS:NZ	2:B:110:ASP:OD1	2.54	0.40
2:B:111:VAL:HG22	2:B:185:ASP:O	2.21	0.40
2:B:112:GLY:O	2:B:113:ASP:C	2.59	0.40
1:A:96:HIS:CD2	1:A:98:ALA:H	2.40	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.86	0.40
1:A:384:GLY:HA3	2:B:135:ILE:CD1	2.42	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	510/560 (91%)	405 (79%)	75 (15%)	30 (6%)	1	4
2	B	402/440 (91%)	344 (86%)	45 (11%)	13 (3%)	4	13
All	All	912/1000 (91%)	749 (82%)	120 (13%)	43 (5%)	2	7

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	A	169	GLU
1	A	195	ILE
1	A	225	PRO
2	B	5	ILE
2	B	98	ALA
2	B	430	GLU
1	A	6	GLU
1	A	125	ARG
1	A	230	MET
1	A	420	PRO
1	A	466	VAL
1	A	542	ILE
2	B	66	LYS
2	B	360	ALA
1	A	122	GLU
1	A	247	PRO
1	A	268	SER
1	A	475	GLN
2	B	68	SER
2	B	92	LEU
2	B	361	HIS
2	B	432	GLU
1	A	44	GLU
1	A	183	TYR

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Mol	Chain	Res	Type
1	A	358	ARG
1	A	412	PRO
1	A	463	ARG
1	A	512	GLN
2	B	65	LYS
1	A	113	ASP
1	A	161	GLN
1	A	236	PRO
1	A	286	THR
1	A	503	LEU
2	B	32	LYS
2	B	195	ILE
2	B	334	GLN
1	A	242	GLN
1	A	505	ILE
1	A	14	PRO
1	A	392	PRO
1	A	97	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	469/498 (94%)	404 (86%)	65 (14%)	3	11
2	B	372/400 (93%)	336 (90%)	36 (10%)	8	24
All	All	841/898 (94%)	740 (88%)	101 (12%)	5	15

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	PRO
1	A	6	GLU
1	A	7	THR
1	A	8	VAL

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Mol	Chain	Res	Type
1	A	16	MET
1	A	78	ARG
1	A	89	GLU
1	A	97	PRO
1	A	102	LYS
1	A	116	PHE
1	A	136	ASN
1	A	138	GLU
1	A	145	GLN
1	A	168	LEU
1	A	175	ASN
1	A	185	ASP
1	A	186	ASP
1	A	187	LEU
1	A	199	ARG
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	222	GLN
1	A	225	PRO
1	A	229	TRP
1	A	230	MET
1	A	237	ASP
1	A	264	LEU
1	A	270	ILE
1	A	276	VAL
1	A	295	LEU
1	A	296	THR
1	A	303	LEU
1	A	310	LEU
1	A	312	GLU
1	A	313	PRO
1	A	320	ASP
1	A	330	GLN
1	A	334	GLN
1	A	336	GLN
1	A	340	GLN
1	A	356	ARG
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	379	SER

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Mol	Chain	Res	Type
1	A	386	THR
1	A	393	ILE
1	A	396	GLU
1	A	400	THR
1	A	418	ASN
1	A	419	THR
1	A	424	LYS
1	A	448	ARG
1	A	452	LEU
1	A	472	THR
1	A	480	GLN
1	A	488	ASP
1	A	496	VAL
1	A	500	GLN
1	A	503	LEU
1	A	517	LEU
1	A	524	GLN
1	A	546	GLU
2	B	8	VAL
2	B	53	GLU
2	B	61	PHE
2	B	67	ASP
2	B	85	GLN
2	B	91	GLN
2	B	92	LEU
2	B	113	ASP
2	B	116	PHE
2	B	122	GLU
2	B	164	MET
2	B	174	GLN
2	B	175	ASN
2	B	192	ASP
2	B	194	GLU
2	B	195	ILE
2	B	207	GLN
2	B	208	HIS
2	B	212	TRP
2	B	243	PRO
2	B	249	LYS
2	B	250	ASP
2	B	277	ARG
2	B	283	LEU

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Mol	Chain	Res	Type
2	B	284	ARG
2	B	289	LEU
2	B	291	GLU
2	B	308	GLU
2	B	357	MET
2	B	368	LEU
2	B	369	THR
2	B	405	TYR
2	B	409	THR
2	B	424	LYS
2	B	425	LEU
2	B	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	96	HIS
1	A	136	ASN
1	A	145	GLN
1	A	151	GLN
1	A	174	GLN
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	278	GLN
1	A	306	ASN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	343	GLN
1	A	418	ASN
1	A	475	GLN
1	A	487	GLN
1	A	507	GLN
1	A	519	ASN
1	A	524	GLN
1	A	545	ASN
1	A	547	GLN
2	B	54	ASN
2	B	57	ASN
2	B	85	GLN

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Mol	Chain	Res	Type
2	B	91	GLN
2	B	96	HIS
2	B	145	GLN
2	B	151	GLN
2	B	161	GLN
2	B	182	GLN
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	CSD	A	188	1	3,7,8	1.30	0	1,8,10	1.05	0
1	CSD	A	280	1	3,7,8	0.97	0	1,8,10	8.03	1 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	188	1	-	2/2/6/8	-
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	8.03	120.83	105.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	188	CSD	N-CA-CB-SG
1	A	188	CSD	CA-CB-SG-OD1
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	188	CSD	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	524/560 (93%)	0.03	24 (4%)	32	22	23, 92, 135, 150	0
2	B	408/440 (92%)	0.03	19 (4%)	31	22	40, 82, 136, 150	0
All	All	932/1000 (93%)	0.03	43 (4%)	32	22	23, 88, 135, 150	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	PRO	5.8
1	A	245	VAL	5.6
1	A	61	PHE	4.6
2	B	94	ILE	4.6
2	B	4	PRO	4.5
2	B	240	THR	4.0
1	A	26	LEU	3.6
1	A	144	TYR	3.5
1	A	139	THR	3.4
1	A	145	GLN	3.4
1	A	92	LEU	3.0
2	B	183	TYR	3.0
1	A	34	LEU	2.9
2	B	70	LYS	2.9
1	A	29	GLU	2.9
1	A	452	LEU	2.9
2	B	355	ALA	2.9
1	A	132	ILE	2.8
1	A	24	TRP	2.8
2	B	354	TYR	2.8
2	B	152	GLY	2.8
2	B	198	HIS	2.7
1	A	130	PHE	2.7
1	A	223	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	356	ARG	2.5
1	A	402	TRP	2.5
2	B	409	THR	2.5
2	B	5	ILE	2.4
1	A	54	ASN	2.4
1	A	491	LEU	2.4
1	A	447	ASN	2.4
2	B	6	GLU	2.3
2	B	432	GLU	2.3
1	A	73	LYS	2.2
1	A	546	GLU	2.1
2	B	92	LEU	2.1
2	B	192	ASP	2.1
2	B	43	LYS	2.1
1	A	454	LYS	2.1
2	B	68	SER	2.0
1	A	41	MET	2.0
1	A	469	LEU	2.0
2	B	321	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	CSD	A	188	8/9	0.94	0.18	49,65,70,75	0
1	CSD	A	280	8/9	0.94	0.14	78,91,96,104	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.